



Graduate School Yearbook 2024

Graduate School Yearbook 2024

PhD students solving present and future challenges

I am proud to present the DTU Chemical Engineering Graduate School Yearbook 2024 that highlights the important work of our PhD students.

At DTU Chemical Engineering, we host just over 100 PhD students from all over the world every year. They create a valuable international environment at the department and play a key role in shaping our ambitious future in an international research environment.

In this year's edition of the yearbook, you will gain an insight into the numerous and varied research areas covered at DTU Chemical Engineering. Some of the PhD students have just initiated their work, whereas others have nearly finished their thesis.

Common to them all is a focus on sustainability supporting the Danish and UN climate and sustainability goals. Hence, the PhD students have selected the most relevant goals for their project.

We want to highlight the importance of technological development to support future sustainable growth. For this purpose, we need to have a very wide and strong focus on sustainability – and we believe that many of the environmental challenges we face today, can be solved by using science and technology.

Consequently, at DTU Chemical Engineering we develop and utilize knowledge, methods, technologies, and sustainable solutions within:

- Chemical and biochemical process engineering and production
- Design of chemical and biochemical products and processes
- Energy and environment

Sustainable growth asks for lasting solutions and requires the ability to think big and innovative – and for that, we believe in our PhD students. Their work is of utmost importance and contributes to shaping future development not only in Denmark, but around the world.

Kim Dam-Johansen

Professor, Head of Department

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Accurate determination of dehydroxylation reaction kinetics from thermogravimetric measurements

(March 2023 – February 2026)

13 CLIMATE ACTION



Contribution to the UN Sustainable Development Goals

This project is aligned with the 13th UN SDG for a climate action. The knowledge obtained during this PhD Project will give insights towards the design and optimization of clay calcination plants. The use of an increased amount of calcined clay in cementitious materials will reduce the CO₂ emissions from one of the biggest greenhouse gas emitters: the cement industry. This project deals with the development of a particle model of clay calcination that is relevant for the design of clay calciners.



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Abstract

Amongst the scientific efforts towards the production of environmentally friendly construction materials, calcined clay cements are convenient alternatives. To study the flash calcination of raw clay models that can predict the conversion of clay particles at high temperatures and short residence times are wanted. In such model, knowledge of the kinetics of the raw clay dehydroxylation is of paramount importance. In this work, we apply several methods of determining the kinetic model for kaolinite dehydroxylation and its parameters based on TGA measuring data.

Introduction

Ordinary Portland Cement (OPC) may be responsible for 10-15% of CO₂ emissions by the year 2050 if CO₂ reduction measures are not implemented [1]. Calcined clays are an adequate alternative for CO₂ reduction on cement production, as cement that includes up to 50% calcined clays show similar strength development than OPC without the additional CO₂ release from limestone calcination during clinker production [2]. For calcined clay synthesis, the material can be calcined on a kiln for relatively long times over moderate temperatures to minimize the recrystallization of the active pozzolanic material into inert crystalline phases (soak method) or it can be exposed to higher temperature sources over short periods of time and subsequently quenched to avoid recrystallization (flash method). Modelling either of these processes for its design requires a kinetic model that describes the evolution of the raw clay conversion over time accurately for different heating rate conditions, as soak and flash calcination heat the material at low and high heating rate respectively. For even the most widely studied clay such as kaolinite, the kinetic mechanism is still debated.

Objectives

The application of different kinetic determination techniques based on Thermogravimetric (TG)

data is used to both obtain a reliable and accurate kinetic model to be applied for process modeling of clay calcination.

Experimental procedure

Pure kaolinite sourced from Sigma-Aldrich is used for TG measurements at five different heating rates to cover a low-medium heating speed range: 5, 10, 20, 50 and 100 K/min. Samples of 5 mg were calcined inside an alumina crucible under a nitrogen gas flow of 100 mL/min. The samples were initially dried at 105 °C for 1 hour to release all moisture. The conversion curve $\alpha(t)$ was directly derived from the measurements using equation 1:

$$\alpha(t) = \frac{m_0 - m(t)}{m_0 - m_f} \quad (1)$$

Where m_0 , m_f and $m(t)$ correspond to the initial, final and the mass at time t respectively.

Modelling strategy

The procedure to determine the kinetic model is based on the ICTAC recommendations [3]. First, we use the isoconversional method of Vyazovkin [3] to obtain the dependence of the activation energy E_a on conversion. The method consists of minimizing the objective function Φ with respect to E_a for every α :

$$\Phi(E_a(\alpha)) = \sum_{i=1}^{N_{HR}} \sum_{j \neq i}^{N_{HR}} \frac{I(E_a(\alpha), T_i(\alpha)) \beta_j}{I(E_a(\alpha), T_j(\alpha)) \beta_i} \quad (2)$$

$$I(E_a, T) = \int_0^T \exp\left(-\frac{E_a}{RT}\right) dT \quad (3)$$

If the activation energy remains constant over the conversion range, usual conversion methods like model fitting can be used. We apply a direct model fitting with a least squares function:

$$OF(A, E_a) = \sum_{i=1}^{N_{HR}} \sum_{j=1}^{N_p} (\alpha_{ij}^{exptl} - \alpha_{ij}^{model})^2 \quad (4)$$

Where α_{ij} is the conversion at time point j on a heating rate experiment j .

Results and Discussion

The activation energy seen in Figure 1 shows an almost constant activation energy at a conversion range [0.05,0.95]. The extremal intervals of the conversion are discarded from the analysis, as the experimental temperature for each conversion becomes ill-defined and noise becomes relevant. However, we can still state that for kaolinite dehydroxylation E_a remains constant with conversion.

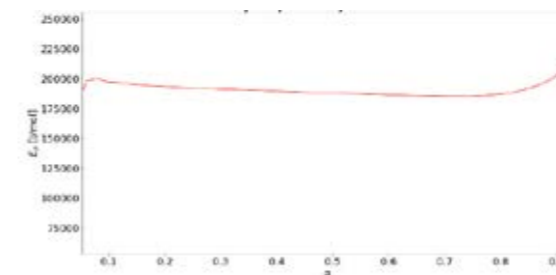


Figure 1: Evolution of activation energy with conversion obtained with Vyazovkin's isoconversional method.

Then using Equation 4 we fit 13 different kinetic models. The best fit was obtained by a third order reaction (F3), with preexponential factor, activation energy and R^2 of $3.70 \times 10^{10} s^{-1}$, 189.2 kJ/mole and 0.9986 respectively. The comparison of the model fit with the experimental data on Figure 1 shows that with the fitted model and model parameters the dehydroxylation of kaolinite is described accurately at all heating rates. Additionally, The model and magnituded of the parameters are consistent with previous studies [4].

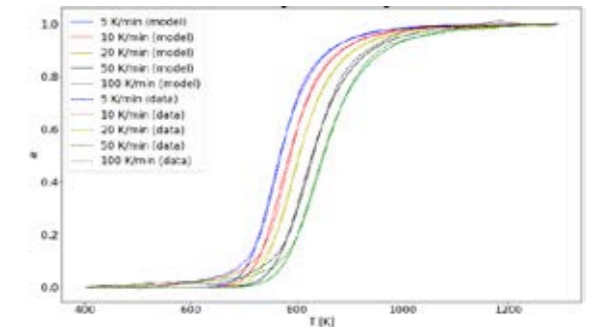


Figure 2: Comparison of experimental conversion of kaolinite with the best model obtained from the fitting method at different heating rates.

From Figure 2 we can also observe that the initial rise in conversion cannot be captured quite accurately by the model. However, this was confirmed to happen as well for similar models.

Conclusions

An exhaustive kinetic analysis has been performed for the reaction of kaolinite dehydroxylation using thermogravimetric data. The isoconversional method demonstrates that the reaction was determined to be a single step with constant activation energy. The model fitting procedure proved that the best model is a third order reaction, which can be used to model the reaction at low and medium heating rate conditions relevant for the clay calcination process.

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Cleanable Cargo Hold Coatings

(April 2023 – March 2026)



Contribution to the UN Sustainable Development Goals

By improving cargo hold coatings for the shipping industry, this project aligns with the United Nations Sustainable Development Goal 7: Affordable and Clean Energy. It promotes sustainability by reducing the need for frequent and energy-intensive cleaning processes and the use of chemicals, and lowering maintenance costs, contributing to more affordable and clean energy solutions in the industry.



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Abstract

This project focuses on enhancing the performance and sustainability of cargo hold coatings, which is vital for protecting vessels in harsh marine environments. Frequent cleaning with strong chemicals risks damaging coatings and increasing dirt buildup. By mapping surface properties, particularly roughness, we aim to improve coating durability. Comparing epoxy-based coatings and acrylic panels exposed to coal highlights the need for coatings with superior cleaning properties. Future research will focus on minimizing roughness changes post-coal exposure to optimize performance and longevity of cargo hold coatings.

Introduction

Cargo holds are vital components of cargo ships, designed to store and transport a wide range of goods across the oceans. These spaces must handle various types of cargo, like coal and grain to packaged goods and machinery. Cargo holds face mechanical impacts during loading and unloading, causing abrasion and scratches on coating surfaces. This wear and tear can reduce the effectiveness and lifespan of protective coatings, increasing maintenance needs and risking the vessel's structural integrity. Damaged coatings are harder to clean, trapping residues, which makes cleaning more labor-intensive and time-consuming [1], [2].

Specialized coatings are essential for protecting cargo holds from these harsh conditions. These coatings act as barriers against mechanical abrasion, preserving the structural integrity of the holds. The effectiveness of these coatings is closely linked to their ease of cleaning. The choice of coating materials and application methods can significantly impact durability, protection, and maintenance efficiency [3].

To enhance the cleaning surface properties of coatings, an investigation was conducted to observe and characterize specific surface properties of plastic materials, with the aim of mapping out the ideal characteristics for optimal cargo hold coatings. This study focuses on evaluating two key features of these materials:

cleaning performance, assessed using a test designed for cargo hold coatings, and alterations in surface roughness, measured with a 3D profilometer.

Experimental

The experimental setup was designed to replicate real-world cargo hold conditions and assess the coatings' resistance to mechanical stress and coal particle retention. The Hempel-designed test apparatus, shown in Figure 1, was used to simulate these conditions.

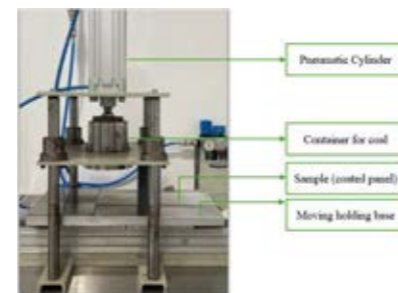


Figure 1: Side view of the Hempel-designed coal cargo test apparatus.

The experiment involved applying 300 kPa of pressure using a pneumatic cylinder, which dragged coal particles across the coating surface at a speed of 1.3 mm/s. This setup aimed to mimic the mechanical stresses experienced during the loading and unloading of cargo and to evaluate the coatings' susceptibility to coal accumulation.

Before-and-after images of the coatings were captured to visually assess the extent of damage and the accumulation of coal particles. Surface roughness measurements were taken using 3D profilometry (KEYENCE VR-3000), both before and after the test. These measurements facilitated a quantitative evaluation of changes in surface topography caused by dirt accumulation and mechanical wear. The data obtained from the 3D profilometry helped establish a direct correlation between surface roughness and the extent of coal particle adhesion.

Visual assessment and 3D profilometry offered detailed insights into coatings' response to dirt and mechanical stress, with immediate performance feedback and microscopic analysis of coal-coating interactions

Results

The epoxy-based coating, as shown in Figure 2, exhibited substantial surface changes after the coal test. Initially, the coating appeared uniform, but post-test images revealed visible coal residue and linear scratches across the surface. This indicates that the coal particles not only deposited on the surface but also caused deeper abrasions. The presence of coal suggests significant dirt pickup during the test, demonstrating the coating's vulnerability to coal accumulation and mechanical damage.

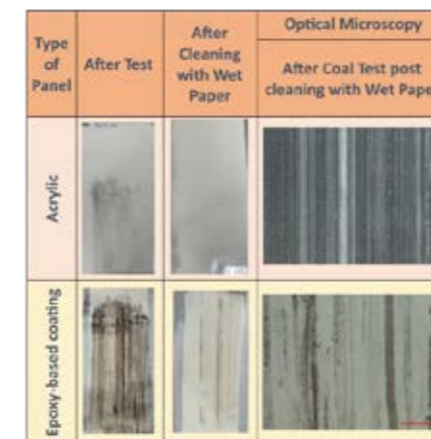


Figure 2: Images of Acrylic panel and an epoxy-based coating after the coal cargo test, followed by cleaning with wet paper, and optical microscopy images of the panels post-cleaning

In contrast, the acrylic panel displayed no visible coal residues after the test, maintaining a clean surface, which highlights its superior cleaning performance compared to the epoxy-based coating. Figure 3 provides a comparison of

roughness measurements before and after the rough test for both materials. The epoxy-based coating experienced a significant increase in roughness, with its average roughness (Ra) increasing fivefold compared to the acrylic panel. This substantial roughness alteration underscores the acrylic panel's resilience to coal-induced surface damage.

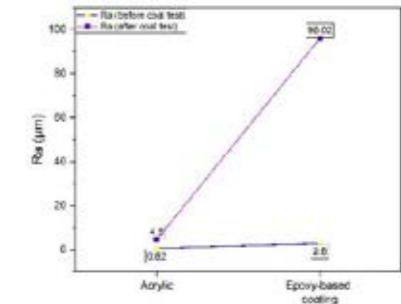


Figure 3: Roughness measurement before and after coal cargo test

Although both materials showed an increase in roughness after exposure to coal, the extent and mechanisms of this change differed. The acrylic panel's superior surface and mechanical properties significantly reduced the impact of coal on the coating, limiting surface alterations. These findings suggest that optimizing surface mechanical properties is crucial for minimizing surface damage and ensuring better cleaning performance in cargo hold coatings.

Conclusion

In conclusion, this study demonstrates the superior performance of acrylic panels over epoxy-based coatings in resisting coal accumulation and surface damage in cargo hold environments. Acrylic showed minimal surface alterations and better cleaning properties, while the epoxy-based coating experienced significant roughness increase. These findings highlight the need for coatings with enhanced cleaning performance to reduce dirt accumulation and improve durability. Future studies will focus on minimizing roughness changes to further optimize cargo hold coating performance.

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Redispersible Powder Coatings

(December 2021 – November 2024)

13 CLIMATE ACTION



Contribution to the UN Sustainable Development Goals

The majority of coatings are currently transported and stored in liquid form. This project aims to investigate the specifics of transforming polymer dispersions and liquid paints into powder form. In this way, significantly higher amount of products can be transported and stored in powder form compared to liquid form. Consequently, the efficient transportation and storage of products has a great potential to reduce the emissions. Furthermore, removing the water from the paint bucket eliminates the need for biocides throughout the supply chain.



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Abstract

Redispersible powder coatings (RPCs) present an eco-friendly alternative for lightweight transportation and biocide-free storage of architectural coatings by eliminating the need for water in storage. Despite their potential, challenges in spray drying, and film formation have limited their adoption compared to traditional waterborne coatings. This study focuses on optimizing the spray drying process for vinyl acetate-ethylene (VAE) polymer dispersions and exploring the film formation mechanisms of redispersible polymer powders (RPPs) in water. The findings reveal that the wet scrub resistance (WSR) of coatings varies significantly with the type of VAE polymer used. Coatings formulated with low T_g emulsifier- and PVA-stabilized VAE (EP-VAE) demonstrated superior film formation and higher WSR. In contrast, high T_g EP-VAE resulted in lower WSR. Additionally, PVA-stabilized VAE (P-VAE) powders failed to form coherent films and degraded after 200 WSR cycles, although their performance improved with the addition of a solid plasticizer. These insights could pave the way for more reliable and sustainable RPCs, enhancing their viability as an alternative to traditional coatings.

Introduction

In the architectural coatings industry, solventborne coatings have largely been supplanted by waterborne alternatives. Water offers numerous benefits, including being non-toxic and odorless [1]. However, completely removing water from coatings could offer even greater benefits. Powder coatings can significantly reduce transportation fuel usage and associated CO₂ emissions, eliminate the need for in-can biocides and volatile residual monomers, and enhance freeze-thaw resistance and shelf-life. Additionally, using paper packaging for powder storage and transportation, instead of plastic, makes packaging more cost-effective and environmentally friendly [2–5].

To meet these needs, RPPs are promising candidates. These versatile materials are primarily used in the construction industry to enhance the properties of mortar and other building materials. RPPs are produced by spray-drying polymer dispersions, resulting in a powder that can be easily redispersed in water [6,7]. This technological approach presents certain challenges, the most significant being the energy-

intensive nature of spray drying required to produce the powders with a high process yield [8].

Due to the wide range of parameters influencing the product formation, the drying process is highly complex and requires extensive optimization. In this study, we examined the effects of various feed characteristics, including the addition and quantity of protective colloids, types of drying agents, T_g of polymer, spray drying inlet temperature, solid feed concentration, and polymer stabilization methods.

The results were analyzed for particle size and process yield. Prepared RPPs were mixed with deionized water for film formation analysis using SEM. We compared the film formation ability and WSR of the original P-VAE and EP-VAE dispersions (without spray drying) with reconstituted dispersions to understand the changes after spray drying.

Results

Spray drying of polymer dispersions indicated that the stabilization type affects the morphology of the RPPs. PVA stabilization provides raspberry structure, which leads to redispersion of individual particles while combined emulsifier – PVA

stabilization provided larger spherical particles due to the lack of protection against the particle growth (Figure1).

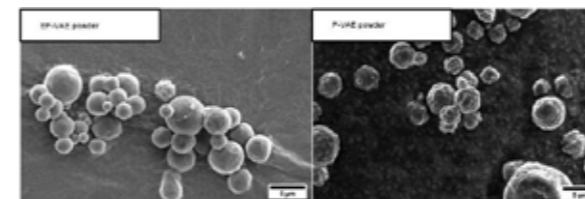


Figure 1. SEM view of P-VAE and EP-VAE-1 powders after spray drying.

Film formation of EP-VAE-1 dispersions were better than P-VAE-1 dispersions both in original form and reconstituted form. This was due to the diminishing effect of PVA on film formation. For EP-VAE dispersions, emulsifiers were probably disrupting the shell and allowing a better film formation (See Fig 2).

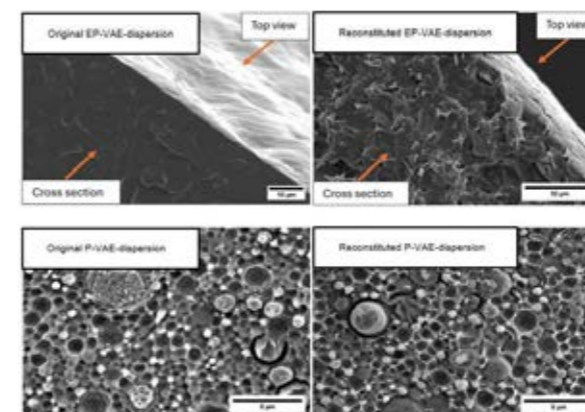


Figure 2. SEM view of P-VAE and EP-VAE-1 coating films before and after spray drying.

Coatings made with P-VAEs exhibited less favorable WSR compared to EP-VAEs. This was due to the diminishing effect of PVA stabilization, which led to incomplete film formation (Table 1). In contrast, EP-VAEs showed better film formation because the PVA did not fully cover the EP-VAE particle surface.

Table 1. WSR results of coating formulations

WSR test results	EP-VAE	EP-VAE powder	P-VAE	P-VAE powder
Thickness loss, μm	5.9 \pm 0.25	34.4 \pm 4.3	15.5 \pm 2.7	57.7 \pm 13.4

Conclusions

Results indicated that the type of stabilization significantly impacts the particle size and yield of spray-dried powders. Even with reduced amounts

of protective colloids, smaller particle sizes and higher yields were achieved with P-VAE dispersions. However, the WSR of coatings made with P-VAEs was less favorable compared to those made with EP-VAEs. This was due to the reduced effectiveness of protection layer, which leads to incomplete film formation. In contrast, EP-VAEs demonstrated more successful film formation because the PVA did not fully cover the EP-VAE particle surfaces.

It was also observed that the type of stabilization influences the morphology of the RPPs. PVA stabilization results in a raspberry-like structure, promoting the redispersion of individual particles. In contrast, combined emulsifier-PVA stabilization leads to the formation of larger spherical particles due to insufficient protection against particle growth.

Acknowledgements

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Novel intumescent coatings for passive fire protection

(April 2022 – April 2025)

9 INDUSTRY, INNOVATION AND INFRASTRUCTURE



Contribution to the UN Sustainable Development Goals

Next generation intumescent coatings for steel protection with an improved health and sustainability profile can provide an innovative solution to the passive fire protection industry. Moreover, replacing toxic components and the release thereof are expected to aid the applications within commercial, high-rise buildings. A more inorganic nature of intumescent coatings may provide sustainable and cheap protection of steel structures to ultimately preserve property and life in the event of fire.



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Abstract

The next breakthrough in passive fire protective (PFP) thin film coatings require a more sustainable profile. Improvements in terms of replacing toxic components or providing more stable systems heavily rely on understanding the working mechanisms of intumescent systems. Applying dedicated techniques such as hot stage microscopy (HSM) to in-situ investigate their behavior at high temperatures can aid the mapping of chemical reactions and intumescence mechanisms of existing and alternative coatings.

Introduction

Passive fire protection of load-bearing steel structures can be pursued by means of intumescent coatings. These appear as decorative paint under ambient conditions, while they undergo several temperature-activated chemical reactions during fire to form an expanded, thermal insulating char. Currently, intumescent coatings are predominantly organic based with major drawbacks including exothermic decomposition, toxic ingredient incorporation, toxic gas release, and low mechanical strength [1]. Therefore, alternative systems are needed to overcome the limitations and provide better PFP solutions. Alternative systems such as silicate- and silicone-based intumescent coatings have gained increased interest in recent years due to their inorganic nature that overcomes most of the aforementioned challenges [2], [3].

Moreover, the chemical and physical behavior of intumescent coatings at high temperatures are not comprehensively understood. Currently, various heat tests followed by post-mortem characterization techniques are commonly applied to examine the reaction mechanisms [4]. Hot stage microscopy (HSM) is an in-situ method to combine thermal analysis with microscopy to reveal morphological changes at high temperatures. Figure 1 shows a dedicated heating

stage for HSM. This relatively unexplored technique is expected to contribute with novel findings in the research of intumescent coatings.

Specific Objectives

The focus of the project is on the development of novel intumescent coatings in the aspects of formulation, testing, and characterization. The research formulations are to investigate inorganic silicate- and silicone-based coatings together with hybrid systems. Fire protection performances will be assessed under hydrocarbon fire conditions in lab-scale setups. Ultimately, dedicated characterization methods are applied to understand and improve the coating performance and sustainability profile.

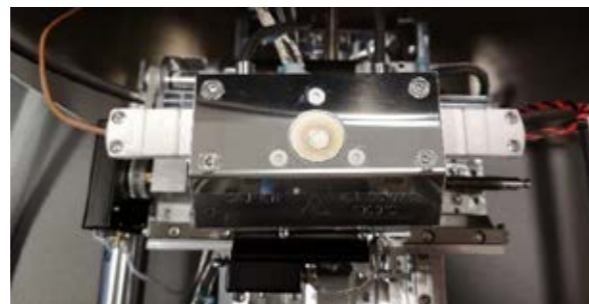
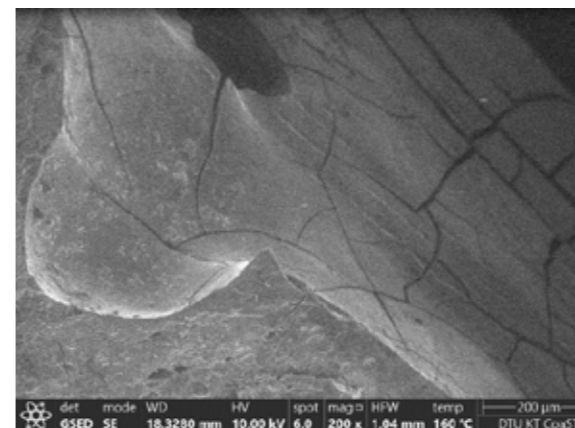


Figure 1: Hot stage for environmental scanning electron microscope (HS-ESEM) applications.

160 °C



500 °C

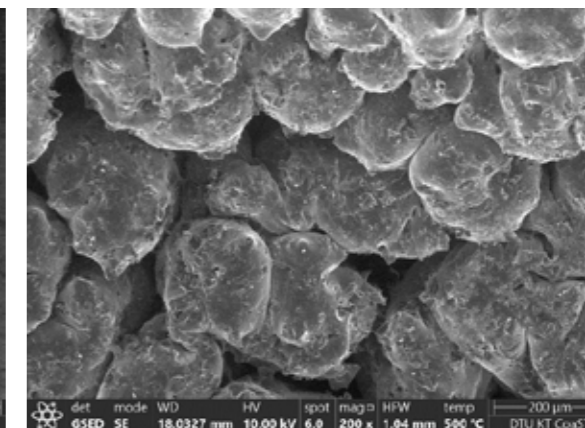


Figure 2: HT-ESEM characterization of cured potassium silicate with calcium carbonate and magnesium carbonate at 160 and 500 °C.

Results and Discussion

An alternative to conventional organic intumescent coatings can be found in alkali silicates. Previous work has mapped their fire protection performance and suggested their working mechanisms [3]. Herein, it is evident that the solid-bound water in alkali silicates provides the driving force for intumescence. Furthermore, the types of bound water are physical, ionic, and in the form of OH-groups. They are all expected to contribute to the intumescence process. However, the expansion potential is not only dependent on the water quantity but also the timing of viscoelastic melt formation of the alkali silicates [4].

To our knowledge, microscopy techniques have been limited to microstructure characterization of already burned intumescent coatings. Hence, Figure 2 provides new insights into the dynamic changes of a potassium silicate-based intumescent system during heating. Although pure alkali silicates have a softening point from about 140 °C that allow the simultaneous water release to provide expansion, the investigated sample revealed late viscoelastic melt formation. For this reason, the misbalance in water evolution and viscosity is assumed to result in crack initiation as the ionically bound water escapes the system. The late expansion at higher temperatures is most likely due to the release of strongly bonded water as the sample starts to soften from.

The structural changes of intumescent coatings can be observed by HSM. When combined with other techniques such as thermogravimetric analysis (TGA) and rheometer, it is possible to elucidate the complete working mechanism including viscoelastic melt formation, gas release, solidification and melting. Furthermore, test parameters such as atmosphere, flow, and

heating rate can be adjusted to a large degree, which have a great influence on the working mechanisms of intumescent coatings [4].

Conclusions

The study clarifies the capabilities of HSM, herein, its use within intumescent coatings research. The learning is to enhance the understanding of current intumescent systems and provide the next generation PFP coatings solutions.

Acknowledgements

The project was carried out as part of CoaST, The Hempel Foundation Coating Science and Technology Centre. Financial support from the Hempel Foundation is highly appreciated.

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Benchmark of thermodynamic models for prediction of derivative properties

(Jan 2024 – Jan 2026)



Contribution to the UN Sustainable Development Goals

This research analyzes the accuracy of thermodynamic models by evaluating second-order properties like heat capacities, speed of sound, and the Joule-Thomson coefficient. These improvements are vital for optimizing industrial processes such as chemical manufacturing and refrigeration, reducing energy consumption and operational costs. By supporting innovation and infrastructure development, the work helps industries design safer and more efficient systems. Accurate models also improve predictions of key variables, ensuring greater safety and resilience in industrial operations.



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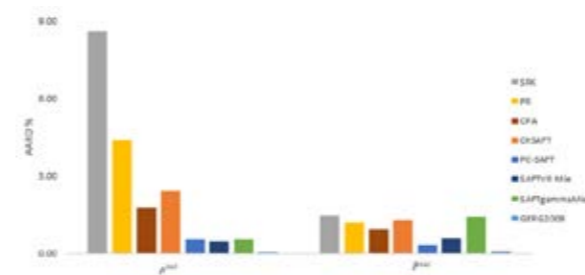


Figure 1. The average AARD% of vapor pressure and saturation liquid density of alkanes for SRK, PR, CPA, CK-SAFT, PC-SAFT, SAFT- γ Mie, SAFT-VR Mie, and GERG2008 models at reduced temperature ranges (0.5 - 0.9).

models in predicting second-order properties in most cases. Notably, PC-SAFT provides the most accurate prediction for isobaric heat capacity, as indicated by the lowest AARD% among all models. While the accuracy of results for isochoric heat capacity is not reliable.

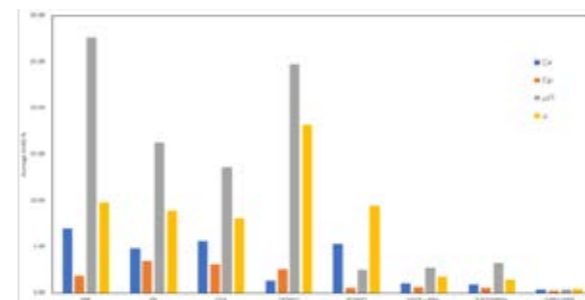


Figure 2. Average AARD% of second-derivative properties of alkanes for SRK, PR, CPA, CK-SAFT, PC-SAFT, SAFT- γ Mie, SAFT-VR Mie, and GERG-2008 models at $T_r = 0.7$ and 2-100 (MPa) pressure. Blue, orange, gray, and yellow are used for isochoric heat capacity, isobaric heat capacity, Joule Thomson coefficient, and speed of sound, respectively.

Figure 3 shows the dP/dT and dP/dV results of selected alkanes with SRK, CPA, PC-SAFT, and SAFT- γ Mie models, while the AARD% of for all models can be found in Figure 10 for a more comprehensive comparison. The PC-SAFT, CPA, and SRK models provide dP/dV and dP/dT derivative predictions that are in fair agreement with the NIST data [1]. However, these models show greater accuracy at lower pressures in predicting dP/dV , but the deviation becomes more pronounced as the pressure increases.

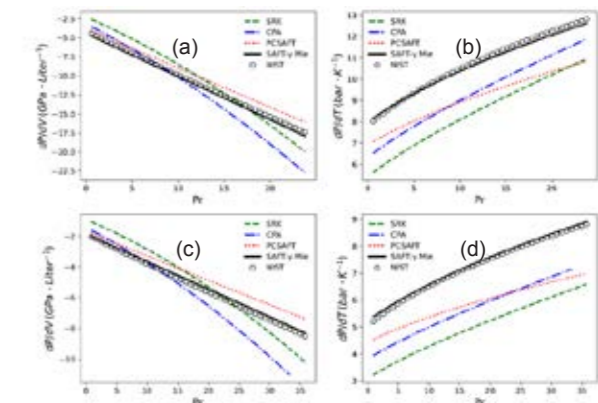


Figure 3. Pressure-Volume derivative (dP/dV) and pressure-temperature (dP/dT) in the liquid region at $T_r=0.7$ temperature. (a), (b) propane, (c), (d) heptane. The dashed line (SRK), dashed-dotted line (CPA), dotted line (PC-SAFT), and solid line (SAFT- γ Mie), and the Points represent NIST data [1].

Conclusions

This study highlights the superior performance of the PC-SAFT, SAFT- γ Mie, and SAFT-VR Mie models over conventional cubic equations of state in predicting second-order thermodynamic properties for n-alkanes. While still some challenges exist for low temperature and high-pressure ranges.

Acknowledgements

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List of Publications

This work has been submitted for publication in the journal of Fluid Phase Equilibria.

Abstract

Thermodynamic models have been developed for many decades, but identifying the most effective model for a given system is a pervasive challenge. In this study, a wide range of thermodynamic models have been analyzed at different pressure and temperature ranges to analyze the first and second-order derivatives properties, including saturation liquid density, saturation pressure, isobaric and isochoric heat capacity, speed of sound, and Joule-Thomson Coefficient. Both the SAFT-VR Mie and SAFT- γ Mie models provide satisfactory results in estimating these properties.

Introduction

Equations of State (EOS) are essential tools in the field of chemical engineering, playing a crucial role in the analysis of fluid and fluid mixture phase equilibria. Initially, they were used for pure substances and later expanded to nonpolar and slightly polar mixtures. Nowadays, EOSs are capable of accurately determining phase equilibria for both nonpolar and polar mixtures. Their adaptability enables their application across a broad spectrum of temperatures and pressures, and they can manage a variety of mixtures, from light gases to dense liquids, for vapor-liquid, liquid-liquid, and supercritical fluid-phase equilibria.

Specific Objectives

To gain a deeper understanding, we divided the comparison procedure into three steps: (i) comparison of derivative properties, (ii) evaluation of the model's capability in predicting dP/dV and dP/dT derivatives, and (iii) analysis of contributions of each term of residual Helmholtz energy to the derivatives such as $(\partial^2 A^{res} / \partial V^2)_{T,n}$, $(\partial^2 A^{res} / \partial T \partial V)_n$ and $(\partial^2 A^{res} / \partial T^2)_{P,n}$.

Results and Discussion

Historically, the primary objective of thermodynamic models has been to provide satisfactory results for phase equilibria and VLE properties, including saturation density and vapor pressure. Figure 1 presents a comparative Average Absolute Relative Deviation (AARD%) analysis for the two key thermodynamic properties (Saturation liquid density, vapor pressure) across various thermodynamic models. The traditional cubic models (PR, SRK) show limitations in accurately describing the saturation liquid density of alkanes. Advanced models such as PC-SAFT, SAFT-VR Mie, and SAFT- γ Mie generally outperform simpler cubic models because they provide a more sophisticated treatment of molecular interactions when calculating VLE properties.

Figure 2 presents the absolute average relative deviation percentage (AARD%) between the second-order derivative properties of n-alkanes estimated by various thermodynamic models and the reference data provided by NIST [1]. As can be seen, it is evident PC-SAFT, SAFT- γ Mie, and SAFT-VR Mie generally outperform the cubic

High temperature synthesis of functional pigment

(November 2022 – November 2025)



Contribution to the UN Sustainable Development Goals

The project aims to synthesize a new pigment that could improve the performance of anticorrosion coatings. An improved performance of anticorrosion coating will contribute to a longer lifetime of it, which reduces the materials and energy consumption in the production process, and thereby lowering the CO₂ emission. Also, we are exploring to use no solvent one step production process that can potentially contribute to a lower release of volatile organic compounds and CO₂ emissions, resulting in fewer negative impacts on the environment and human health.

Abstract

The most conventional coatings that have been used for anti-corrosion application are zinc-rich epoxy coatings. It is commonly acknowledged that the minimum amount of zinc in a zinc-rich coating should be 80 wt.% in dry film so that a conductive pathway among zinc pigments as well as zinc and the substrate can be formed. Although more than 80 wt.% zinc is used in zinc-rich coatings formulation, only 30% of it will participate in cathodic protection of the substrate due to the inhibition of conductive network caused by insulating corrosion product forms around zinc particles. The aim of this project is to synthesize, evaluate, and optimize a high-performance pigment containing zinc and carbon materials using high temperature process to improve the utilization rate of zinc particles and an extension of the protection period.

Introduction

Zinc-rich primers are extensively utilized in aggressive environments such as offshore and industrial settings due to their distinctive ability to protect the metal. When formulating a zinc-rich primer, the zinc content should be more than 80% by weight. This is because the sacrificial action of zinc only begins when there is continuous contact between the zinc particles, forming what is known as a percolation path [1]. However, the oxidation of zinc particles creates non-conductive zinc oxides that hinder the galvanic effect, making the unreacted zinc dust inactive. Consequently, they only act as a barrier to protect the substrate against invasive elements. To address this, carbonaceous and polymer conductive additives such as carbon black (CB), conductive graphite (CG), multiwalled carbon nanotubes (MWCNT), and polyaniline (PANI) have been introduced to partially replace zinc dust in these primers [2].

Lv et al. [2] explored how four different conductive additives (Carbon black, MWCNT, conductive graphite, and PANI) influenced the corrosion resistance of a coating. They suggested that these additives acted as a bridge between zinc particles, thereby enhancing electron pathways. This enhancement would improve galvanic protection and make the zinc

more active. The results of salt spray and electrochemical impedance spectroscopy (EIS) tests indicated that the carbon black coating outperformed the others. This was due to the presence of nanosized spherical carbon black, which provided more electron pathways and had a better interaction with the epoxy matrix, resulting in a more durable coating. When it came to conductive graphite, it offered a superior barrier effect compared to an unmodified coating but still did not match up to carbon black. Furthermore, conductive graphite displayed weak chemical bonding with epoxy. Multi-wall carbon nanotubes, on the other hand, yielded the least favorable results among the samples. This was attributed to their high oil absorption, which led to increased clumping and excessive conductivity within the coating. Therefore, this accelerated the corrosion of zinc, even when it was not directly in contact with the substrate, as illustrated in Figure 1.

Marchebois et al. [3] investigated the effect of addition of carbon black on corrosion behavior of zinc-rich powder coating. They compared two coatings, one containing 2.1% carbon black by weight and the other containing 5%, alongside their zinc content, with a coating consisting of 50% zinc alone. Higher CB content leads to a higher porosity, but it also leads to a better



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percolation between pigments. Therefore, while the electrolyte reaches the substrate more rapidly, a greater amount of zinc is exposed to the electrolyte and in contact with the substrate that can act as sacrificial pigment and provide enhanced protection to the substrate. So, they suggested this addition is not beneficial whatever the carbon content is.

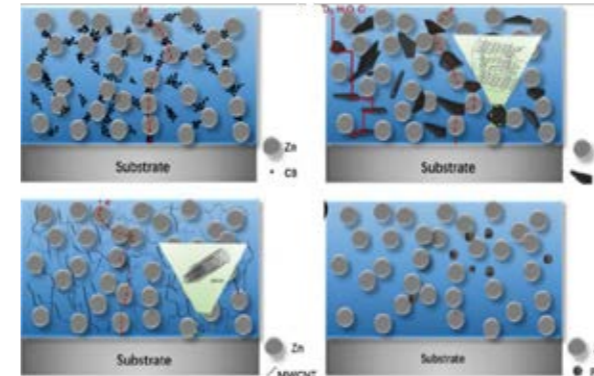


Figure 1: Schematic representation of anti-corrosion mechanism in conductive additive modified zinc rich epoxy coatings [2].

The existing literature has explored the incorporation of conductive additives with zinc-rich primers, both as an addition to zinc dust and as a potential substitute for a portion of the zinc content. It is well-established that achieving a percolation network with conductive additives like carbon black is crucial to establish a conductive pathway connecting the zinc dust and the substrate. However, there remains a gap in the literature regarding the optimal amount of zinc required in such formulations. It is conceivable that utilizing a lower zinc content might still yield the desired performance, since there is only 30% of zinc content participate in corrosion protection by sacrificing themselves [4]. Additionally, there has been limited exploration of the simultaneous production of zinc and carbon particles and their application, as well as their overall performance within the coating system. This aspect presents an opportunity for further research and investigation.

Specific objectives

This project aims to a systematic evaluation of the effect of mass percentage of zinc and carbon black and their properties on the anticorrosion coating performance. In addition, an innovative pigment that can serve as either a full or partial substitute for zinc dust in anti-corrosion coatings will be developed using a high temperature process.

Experiment

An epoxy coating with CB content above its percolation threshold with different ratios of zinc will be formulated, characterized, and compared with conventional zinc rich coatings.

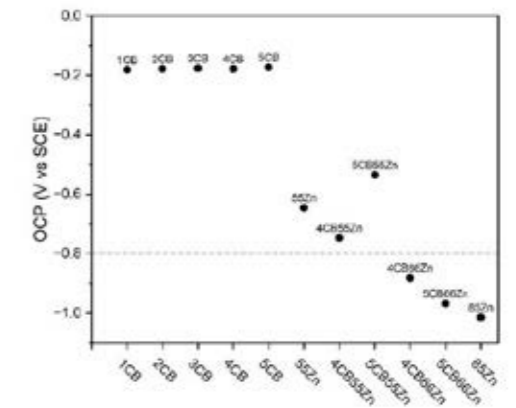


Figure 2: Open Circuit Potential (OCP) after 24 hours of immersion (numbers before CB and Zn show the wt.% of each component in the formulation).

As can be seen from Figure 2, for both coatings with 4 and 5 wt.% carbon black and 66 wt.% zinc, the mixed potentials are moved to a more negative value, which shows the conductive network of carbon black can connect more zinc with each other so that more zinc can contribute to the mix potential of the system.

Pigment synthesis

For the development of innovative pigments, a mixture of carbon black and zinc will be gone under a high temperature process, above melting and boiling point of zinc. Subsequently, the generated pigment will be characterized. Following characterization, we will incorporate this new pigment into a coating formulation. The anti-corrosion performance of this innovative coating will then be evaluated and compared against that of traditional coatings.

Acknowledgements

The financial support from the Hemple Foundation is gratefully acknowledged.

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Decoupled Bioprocess of Recombinant *Pseudomonas putida* KT2440 as a Whole-Cell Biocatalyst for *trans*-Cinnamic Acid Production

(July 2022 – June 2025)



Contribution to the UN Sustainable Development Goals

The goals of industry, innovation and infrastructure are to build resilient infrastructure, promote inclusive and sustainable industrialization and foster innovation. One of the challenges is to enhance scientific research and upgrade the technological capabilities of industrial sectors in all countries. Focusing on industrial technologies, the application of fermentation-based process improvement allows for understanding and improving the performance metrics of the biomanufacturing industry and it can be used for the transition from traditional industry to Industry 4.0



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Abstract

Increasing concern about global greenhouse gas emissions and a general desire for environmentally friendly processes have driven interest in developing new bioprocess routes using whole-cell biocatalysts to produce sustainable *trans*-cinnamic acid. In this study, a decoupled bioprocess was conducted to improve *t*CA production metrics (titer, rate, and yield) using recombinant *P. putida* KT2440 expressing RmXAL. Moreover, mathematical models were developed to predict cells and *t*CA behavior, resulting in a titer of 29.88 g L⁻¹, rate of 5.99 g L⁻¹ h⁻¹, and yield on glucose of 0.27 g *t*CA g glucose⁻¹.

Introduction

trans-Cinnamic acid (*t*CA) is an aromatic compound that is used in a broad range of industries, such as food and beverages, cosmetics, etc. [1]. Conventional *t*CA synthesis is accomplished through either a chemical process using the condensation of benzaldehyde and acetic anhydride in the presence of sodium acetate at high temperatures (180°C) or alternatively extraction from plants [2]. However, these production processes are not sustainable and use toxic chemicals that negatively impact human health and the environment. The alternative route is the biological method using the phenylalanine ammonia-lyase (PAL) enzyme, which deaminates L-phenylalanine (L-phe) to *t*CA. However, one of the biggest challenges to compete with conventional chemical processes or petroleum-based synthesis is that the production metrics, including titer, rate and yield (TRY), need to be substantially improved because they directly impact economic and industrial feasibility. Notably, the inherent trade-off between cell production (the biocatalyst converting substrate to product) and product yield means that the rate and

yield cannot be optimized independently. To break this trade-off, decoupling growth and production using a decoupled operating strategy can be used to improve the crucial performance metrics. Therefore, this work aims to develop a decoupled bioprocess (Figure 1) for *t*CA production to enhance the production metrics and to develop mathematical models for predicting cells and *t*CA production behavior, which would apply to larger-scale production.

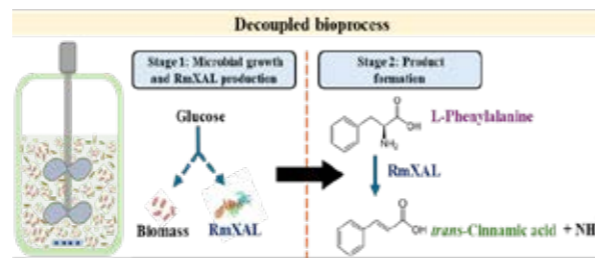


Figure 1: A schematic diagram of decoupled bioprocess for *t*CA production where stage 1 is cell growth and RmXAL production and stage 2 is whole-cell biotransformation.

Material and methods

The fermentation of recombinant *P. putida* KT2440 expressing RmXAL was cultured in a 0.5 L stirred-tank bioreactor. The fermentation started with batch fermentation by inoculating the starter to a modified M9 medium (initial OD₆₀₀ ~ 1.0) and cultivating it under optimum conditions [3]. After the glucose was completely consumed, fed-batch fermentation was performed. The feeding medium (500 g L⁻¹ glucose and 2.5 mM rhamnose) was fed into a bioreactor to increase the biocatalyst concentration of 10-50 g_{DCW} L⁻¹. The process was switched to *t*CA production phase by adding 35 g_{L-phe} L⁻¹ of L-phe and raising the pH to 8.5 and temperature to 37°C. A model of cell growth and *t*CA production was determined to interpret the fermentation profiles. In this research, the logistic-based equation was applied to explain the rate of cell growth ($\frac{dX}{dt}$), as shown in Eq. 1 and 2.

$$\text{Growth phase } \frac{dX}{dt} = \mu_{max}X \left(1 - \frac{X}{X_m}\right) \quad (1)$$

$$\text{Production phase } \frac{dX}{dt} = \left[\frac{X_m}{1 + \left(\frac{X_m - X}{X}\right)e^{-k_d(t-t_0)}} \right] \quad (2)$$

The *t*CA formation rate ($\frac{dP}{dt}$) in the second stage was described using the Michaelis-Menten-based model with competitive inhibition (Eq. 3).

$$\frac{dP}{dt} = \left[\left(\frac{V_{max}S_{L-phe}}{K_m(1 + (e^{-kt}/K_i) + S_{L-phe})} \right) \cdot X \right] \quad (3)$$

Results and Discussion

Increasing whole-cell biocatalysts markedly promoted *t*CA production. Therefore, a whole-cell biocatalyst of 50 g_{DCW} L⁻¹ provided the highest *t*CA titer and *t*CA production rate over the biotransformation time (Q_p). Nevertheless, *t*CA yield on glucose ($Y_{p/s}$), specific *t*CA production rate (q_p), and *t*CA production rate over the total time (overall Q_p) were observed in the culture using 10 g_{DCW} L⁻¹ of biocatalyst. The inverse relationship between cell concentration and biocatalyst efficiency indicates a potential trade-off. These findings make 30 g_{DCW} L⁻¹ a favorable condition for *t*CA production, balancing overall production and process efficiency (Table 1).

Table 1: *t*CA production parameters at different biocatalyst concentrations.

Parameters	Whole-cell biocatalyst (g _{DCW} L ⁻¹)				
	10	20	30	40	50
Titer (g L ⁻¹)	20.11±0.52 ^d	26.78±0.40 ^c	29.88±0.23 ^b	31.02±0.12 ^a	31.70±0.25 ^a
$Y_{p/x}$ (g g ⁻¹)	1.83±0.01 ^a	1.28±0.02 ^b	1.04±0.01 ^c	0.79±0.02 ^d	0.64±0.00 ^e
Q_p (g L ⁻¹ h ⁻¹)	4.02±0.00 ^e	5.36±0.00 ^d	5.99±0.03 ^c	6.20±0.05 ^b	6.34±0.04 ^a

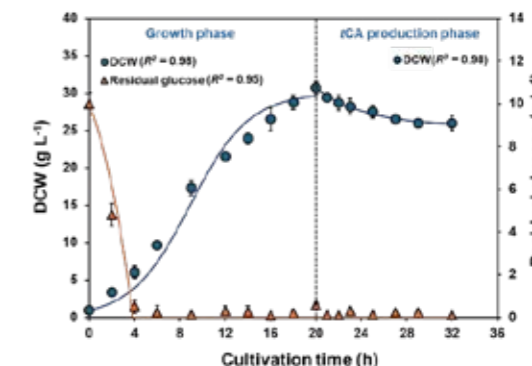


Figure 2: Comparison of the experimental data (symbols) and model predictions (lines) of whole-cell concentrations.

The kinetic models describing cell growth and *t*CA production were constructed to predict the behavior of a production process using a whole-cell biocatalyst. The estimated kinetic parameters aligned well with the measured experimental values, as indicated by determination coefficient (R^2) values > 0.94 (Figure 2). However, kinetic models of *t*CA production showed product inhibition (Figure 3), giving the inhibition constant (K_i) of 7 mg L⁻¹.

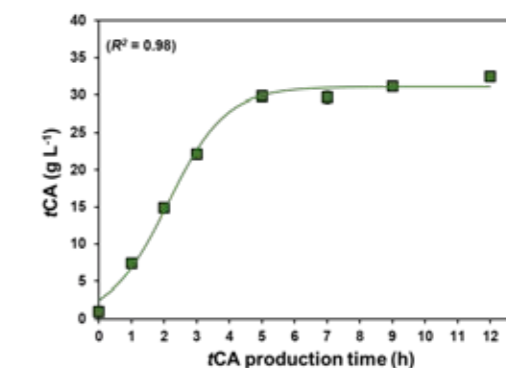


Figure 3: *t*CA production from experimental data (symbols) and model predictions (lines).

Conclusion

A whole-cell biocatalyst concentration of 30 g_{DCW} L⁻¹ was the optimal value to switch from the growth phase to the production phase. The integration of experimental data and mathematical models was successfully used to describe the impact of cell growth and *t*CA formation.

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Understanding the film formation of waterborne coating systems for high and extreme corrosivity

(April 2023 – March 2026)



Contribution to the UN Sustainable Development Goals

This project aligns with several UN Sustainable Development Goals (SDGs). By reducing the use of volatile organic compounds (VOCs) during coating application and developing sustainable protective coatings, this project mainly contributes to the sustainable production and consumption patterns in industries that rely on protective coatings. Traditional solvent-based coatings often involve VOCs that contribute to air pollution and environmental degradation. In contrast, waterborne (WB) coatings, with their low or zero VOC content, reduce harmful emissions and minimize environmental impact during manufacturing and application.

Abstract

Despite the wide range of environmental benefits of WB coatings, the conventional solvent-based coatings still offer superior performance, especially in higher corrosivity categories (defined in ISO 12944-2). WB systems are much more sensitive towards the coating application conditions compared to their respective solvent-based counterparts. The first goal of the project is to understand film formation/coalescence in WB systems and its sensitivity towards the coating application conditions. Having better film formation under a broader range of environmental factors (e.g., low temperatures and high humidities) and applications conditions (e.g., various types of substrates), and ability to understand key parameters driving coalescence in film formations will ensure the integrity and performance of futuristic WB coatings.

Introduction

The importance of anti-corrosive coatings cannot be overstated, as they play a vital role in safeguarding assets and infrastructure across various industries. Within this context, the emergence of waterborne (WB) coatings stands out for their paramount significance, offering a sustainable alternative to traditional solvent-based (SB) coatings and addressing pressing environmental concerns [1]. WB anti-corrosive coatings are commonly used in various industries to enhance the longevity and durability of metal components, thereby contributing to sustainability by reducing VOC emissions and promoting environmentally friendly practices.

Despite their eco-friendliness, the complexity of their film formation mechanism and the lack of understanding present challenges in enhancing the performance of waterborne coatings for corrosion protection [2]. These coatings are created by dispersing polymers in water, which then form a protective film on a substrate. The process involves stages like water evaporation, particle packing, and polymer interdiffusion, often leading to films with defects and inferior protection against extremely corrosive environments compared to SB coatings [3]. WB coating systems

applied and cured in controlled lab conditions tend to perform on par with solvent-based coating system alternatives. However, necessary application and drying conditions for WB coatings are very narrow and are difficult to replicate in real life industrial conditions, especially in areas with harsh environments.

To address the current challenges in the field, the interplay of factors affecting film formation in application, including coalescing agents, environmental factors, and application conditions are being studied in this project. To achieve this goal, different experimental methods accompanied by computational tools have been developed to simultaneously achieve new understandings and solutions.

Specific objectives

- Effect of substrate properties on the film formation behavior of WB coatings
- Effect of environmental conditions on the film formation behavior.
- Trying new innovative methods to study the film formation behavior in-situ.



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Methodology

- Comprehensive literature review to obtain a proper perspective before taking any steps forward.
- Investigating the effects of substrate properties on the film formation behavior, as illustrated in Figure 1.
- Investigating the effects of environmental factors on the film formation behavior, by letting the films dry and cure in the climate chamber while monitoring the water-loss using an innovative sensor.
- Modeling the film formation mechanism, in such a way illustrated in Figure 2.

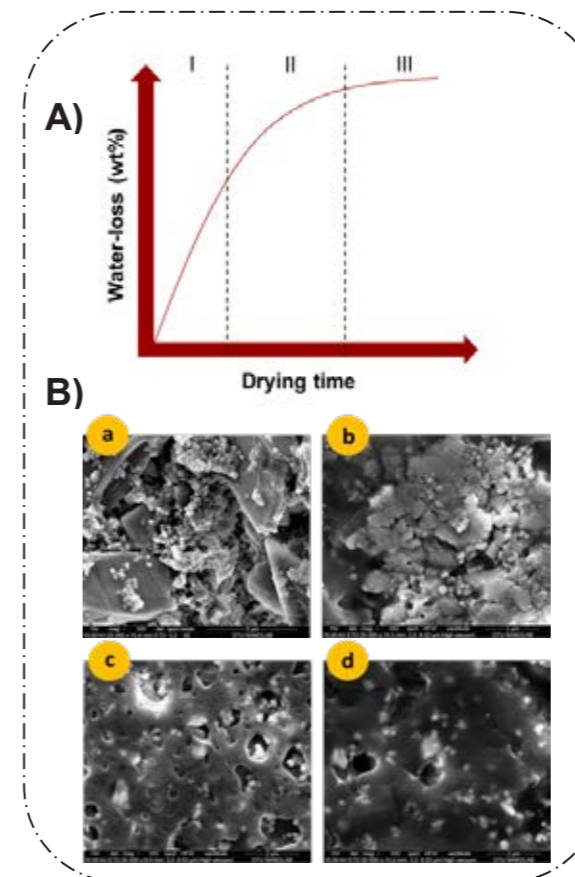


Figure 1. (A) Water-loss profiles can represent the effects of substrate properties on the film formation behavior; obtainable through gravimetric and FTIR methods, (B) Film formation during the drying phase using the freeze-drying technique and SEM imaging, going from the freshly applied film (a) to the completely dried film (d).

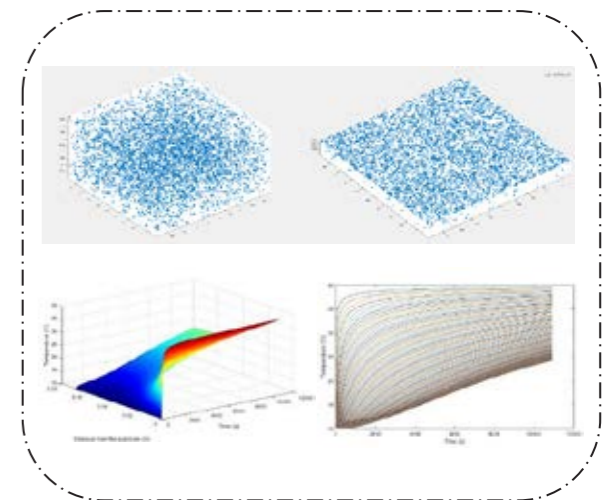


Figure 2. Simplified summary of film formation modeling results based on heat transfer coefficients and Brownian motion equations.

Acknowledgement

Financial support from the Hempel Foundation to CoaST (The Hempel Foundation Coatings Science & Technology Centre) is gratefully acknowledged.

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Scale-up, design, and cost estimation of technologies under development

(October 2023 – September 2026)

9 INDUSTRY, INNOVATION AND INFRASTRUCTURE



Contribution to the UN Sustainable Development Goals

MiEI [1] research and training project directly contributes to SDG 9 (Industry, Innovation, and Infrastructure) by developing novel electrosynthesis technology that combines the advantages of electrochemistry, micro-process engineering, and flow chemistry. The project supports sustainable industrialization by enabling reliable, flexible, safe, and environmentally friendly synthetic routes for the chemical industry.

Abstract

This research develops a comprehensive framework for evaluating the feasibility of novel electrochemical synthesis technologies in early-stage design. The framework includes advanced simulation-based optimization techniques to solve complex optimization problems allowing for rigorous exploration of the engineering design space. The work aims to support the scaling up of innovative electrosynthesis technologies from the laboratory to industrial-scale applications, contributing to more sustainable and cost-effective manufacturing methods.

Introduction

The traditional manufacturing methods used in the pharmaceutical and fine chemical industries have significant environmental impacts, including high greenhouse gas emissions and the generation of hazardous by-products. Evolving towards environmentally friendly synthesis methods that reduce waste, energy consumption, and reliance on toxic solvents is crucial for these industries. As the demand for greener and more sustainable processes grows, electrochemical synthesis has emerged as a promising alternative. It offers several environmental benefits, such as atom-efficient reactions, lower energy requirements, and the ability to use electricity from renewable sources as a clean and flexible power supply.

Electrochemical methods were considered expensive due to the high costs associated with electricity and electrochemical reactors which prevented the adoption of this technology. However, recent advancements in renewable energy technologies have drastically reduced the cost of electricity, making electrochemical synthesis more affordable and increasingly viable for industrial applications.

The MiEI project [1] focuses on combining the advantages of electrochemistry, micro process engineering, and flow chemistry to develop novel electrosynthesis technology that meets industrial demands while reducing costs. The research

objective is to develop scalable electrosynthesis routes that are both technically feasible and economically viable for industrial applications, particularly in the pharmaceutical and fine chemical industries.

To ensure that the developed electrosynthesis routes are applicable to the industry, they need to be scalable, safe, efficient, sustainable, and cost-effective. For these purposes, performing early-stage design of scaled-up processes is crucial. Early-stage design is important to prevent the risks, costs, and potential problems that might cause the termination of the scaled-up processes in the later phases. The early-stage design allows engineers to find the optimal process conditions and minimize the unpredictability of outcomes. By focusing on early-stage design, this research aims to minimize risks, reduce development costs, and increase the likelihood of success in later stages of technology deployment.

Specific Objectives

This research aims to model and evaluate the new integrated electrochemical synthesis technologies during early-stage design using a generic methodology. For this purpose, a highly scalable, innovative simulation-based optimization framework will be developed for rapid techno-economic evaluation and provide insights into the cost, scalability and performance of novel



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electrosynthesis processes. A superstructure will be introduced to the framework including the library of models and database of capital expenditures (CAPEX) and operational expenditures (OPEX). This database is essential for accurately estimating the costs associated with scaling up new technologies. For robust decision-making and optimizing under uncertainty for the scaled-up models, sensitivity analysis and uncertainty analysis will be made using global sensitivity analysis methods and Monte Carlo simulations.

The potential of each electrosynthesis route will be monitored considering the target economic metrics, specific upscaling, and parallelizing potential. The work will be applied to novel electrosynthesis processes in pharmaceutical/fine chemicals production. Thus, the promising potential in the industrial applications will be identified and the business opportunities will be defined accordingly.

Results and Discussion

Initial work has focused on developing flexible and robust methodology for early-stage design, optimization, and techno-economic analysis. The framework has been tested on preliminary case study from pharmaceutical industry. The case study results highlight the ability of the simulation-based optimization framework to assess both technical and economic performance under various process conditions. It is seen that considering uncertainties is crucial for obtaining more reliable and robust results in optimizing pharmaceutical processes. The simulation-based optimization approach coupled with Monte Carlo simulations proved valuable for addressing uncertainties and enhancing the robustness of the optimization process.

The framework will be further developed and validated through case studies using developed electrosynthesis processes for pharmaceuticals and fine chemicals. These case studies will demonstrate the practical applications of the framework and provide valuable insights into the economic feasibility of new technologies. This will support decision-making in early-stage design and help identify promising industrial applications.

Conclusions

The initial phase of the project has successfully established a robust methodology for early-stage design and techno-economic analysis. Future work will involve applying this methodology to specific case studies, refining the framework, and validating the results through practical applications in the pharmaceutical and fine chemical industries.

Acknowledgements

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Doctoral network for microprocess engineering for electrosynthesis

List of Publications

T. Asrav, M. Alvarado-Morales, G. Sin, Optimization with Uncertainty for Pharmaceutical Process Design -Ibuprofen Synthesis as case study, Computer Aided Process Engineering, 2024

Transparent Antifouling Coating

(August 2024 – July 2027)

9 INDUSTRY, INNOVATION AND INFRASTRUCTURE



Contribution to the UN Sustainable Development Goals

This project supports **UN Sustainable Development Goal 9: Industry, Innovation, and Infrastructure** by developing innovative transparent antifouling coatings tailored for underwater optical devices, such as solar-powered autonomous underwater vehicles (AUVs), sensors, and cameras. Biofouling on these devices not only obstacles their operational efficiency but also reduces energy generation in underwater photovoltaic systems, increasing maintenance costs and lowering sustainability. The project combines antifouling efficiency with optical clarity, reducing energy loss and maintenance. By enhancing the performance durability and transparency of underwater devices, the project champions innovative approaches to sustainable solutions.

Abstract

The development of transparent antifouling coatings seeks to address the challenge of biofouling on underwater equipments, where optical clarity is a pre-requisite. This PhD project focuses on optimizing a self-sustaining binder system and utilization of nanoparticles to achieve antifouling efficiency and yet maintaining transparency for a minimum of three months. The results of this research present promising solutions for applications, particularly in solar-powered underwater vehicles and their accompanying devices, such as cameras and sensors.

Introduction

Biofouling, the accumulation of marine organisms like algae, bacteria, and barnacles on submerged surfaces, has become a growing concern due to its widespread negative impacts on the marine ecosystem, underwater equipment, and infrastructure [1]. The accumulation of marine organisms on submerged surfaces can significantly increase the weight of ships and cause greater water maneuvering resistance, resulting in higher fuel consumption, increased maintenance costs, and elevated greenhouse gas emissions. Similarly, marine biofouling presents a significant challenge for underwater equipment such as sensors, cameras, and solar panels, particularly in long-duration deployments like Unmanned Underwater Vehicles (UUVs) and solar-powered Autonomous Underwater Vehicles (AUVs). These vehicles rely on solar panels for power, and biofouling dramatically reduces the optical efficiency of these panels by obstructing light transmission, which is essential for energy generation [2]. Moreover, the accumulation of marine organisms on these surfaces affects the hydrodynamic performance and maneuverability of vehicles. As a result, ensuring the long-term transparency and anti-fouling effectiveness of such devices in harsh marine conditions has

become a critical focus for researchers and engineers.

To address the biofouling challenge, antifouling coatings have been widely applied to submerged surfaces to prevent the settlement and growth of marine organisms. These coatings act as a barrier, reducing the attachment of fouling species and maintaining surface cleanliness.

Among the various antifouling approaches, self-polishing coatings represent a highly effective solution to combating marine biofouling by utilizing controlled erosion when exposed to seawater [3]. These coatings are engineered to gradually degrade, thus continually exposing fresh surface material while facilitating the release of biocides, such as antimicrobial nano pigments, into the surrounding environment. The underlying mechanism involves a leaching process, wherein a thin layer of the coating dissolves upon contact with seawater, resulting in a smooth surface that minimizes the adhesion of fouling organisms, including algae and bacteria. The pigment front, consisting of antimicrobial particles, provides an initial defense against biofouling, and as the coating wears away, these particles are released, further enhancing the antifouling efficacy. Additionally, the use of organic booster biocides amplifies the protection against a broader spectrum of marine organisms. This dynamic



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renewal of the coating surface, coupled with the continuous release of biocides, effectively reduces the need for frequent maintenance interventions, thereby providing significant advantages for underwater applications that demand high durability and optimal functionality.

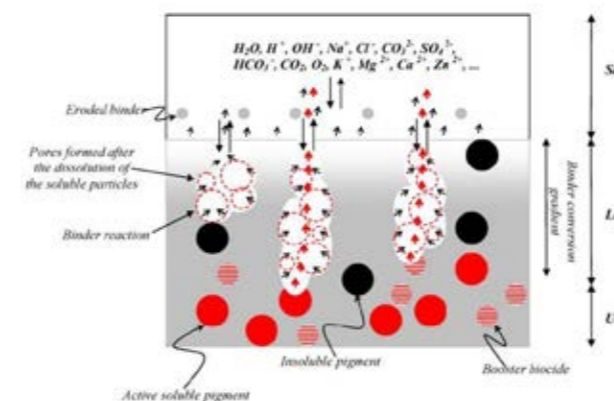


Figure 1. Schematic illustration of the behavior of a biocide-based antifouling system exposed to sea water [1].

However, traditional antifouling coatings often face a critical limitation: their lack of transparency, which significantly reduces their utility for applications where optical clarity is essential. This research seeks to overcome that limitation by developing advanced coatings that not only provide robust antifouling protection but also maintain the transparency required for underwater optical devices. The core innovation of this project is the design and development of self-sustaining coatings to achieve prolonged antifouling efficacy without compromising transparency. At the heart of this innovation is the incorporation of seawater-soluble nano pigments with potent antimicrobial and antifouling properties, embedded within a self-polishing binder system. This strategic combination allows the coating to continuously renew its surface, ensuring prolonged effectiveness over extended periods. By minimizing the need for frequent maintenance or mechanical cleaning, which can be both costly and disruptive, these coatings provide a highly efficient, durable solution for applications that demand both transparency and robust antifouling performance.

The potential applications of these transparent antifouling coatings are ideally suited for underwater devices that depend on optical clarity, including solar-powered autonomous underwater vehicles (AUVs), underwater sensors, and monitoring equipment. By ensuring both superior antifouling performance and exceptional transparency, these coatings significantly enhance the operational efficiency of such

devices, paving the way for more reliable and effective marine technology solutions.

Specific Objectives

The initial development of transparent antifouling coatings have shown promising antifouling performance; however, exposure to seawater resulted in haziness, compromising optical clarity [4]. This research aims to investigate the causes of this haziness and optimize the coatings to maintain transparency for at least three months under static seawater conditions. Central to this effort is the optimization of self-polishing binder systems and the incorporation of seawater-soluble nanoparticles, specifically nano-Cu₂O and nano-ZnO, which are known to enhance both antifouling efficacy and optical properties. By strategically combining these elements, the aim is to create coatings that deliver superior performance and long-lasting protection without sacrificing clarity.

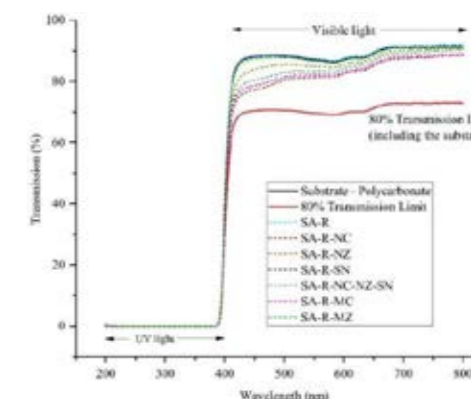


Figure 2. UV-Vis spectroscopy measurements show that the initial transparent antifouling coatings, formulated with the silyl acrylate-rosin (SA-R) binder system, achieve over 80% transmission, indicating high transparency alongside promising antifouling performance [4].

Acknowledgements

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Digitalization and automation of the CoaST Maritime Test Centre

(November 2022 – November 2025)



Contribution to the UN Sustainable Development Goals

Digitalization and automation are emerging trends in the industry aimed at enhancing efficiency and performance. In the field of anticorrosive and antifouling coatings development, numerous onsite experiments and regular evaluations are crucial. Automated and digitalized experiments and data management assist the researchers by improving infrastructure, reducing researchers' time consumption, and increasing accuracy.



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Abstract

CoaST, the Hempel Foundation Coatings Science and Technology Centre, is leading a digital revolution in coating research. Since 2017, it has focused on developing innovative and sustainable coating solutions, especially in anticorrosion and antifouling. CoaST is currently working on implementation of digitalization and automation technologies, transforming experimental processes. The Maritime Test Centre in Hundested Harbour, Denmark, serves as a testing ground for these advancements, enabling researchers to conduct and monitor experiments remotely. This approach enhances efficiency and precision in coating research. Additionally, sample and experiment details, including results and images, are recorded in a structured database, simplifying data management for researchers and making the data accessible for future analysis and data science.

Introduction

Coatings significantly enhance surface properties, with a primary focus on corrosion protection. The Hempel Foundation Coatings Science and Technology Centre (CoaST) specializes in anticorrosion, antifouling, and intumescent coatings. On-site experiments at the CoaST Maritime Test Centre (CMTC) [1] in Denmark provide valuable real-world insights. By integrating digitalization and automation, especially in remote locations, research efficiency is greatly improved.

Coatings

Coatings are surface applications designed to enhance appearance and properties, with a primary focus on protection, especially for metal surfaces to prevent corrosion [2]. They typically consist of three layers: primer, intermediate coats, and topcoat. The primer prevents corrosion, the intermediate coats add thickness and protect the primer, and the topcoat provides the desired appearance and shields against environmental conditions. The topcoat of marine surfaces prevents the surface from biofouling [3].

Protective coatings are made from various materials such as pigments, fillers, rheology agents etc, chosen based on the application and surface. For example, epoxy coatings are known for their durability and chemical resistance, while polyurethane coatings are noted for their abrasion resistance and UV stability. Powder and ceramic coatings are also widely used for their specific properties.

Coatings have evolved significantly from natural substances to synthetic chemicals and polymers, with recent advancements in nanotechnology introducing unique properties like super hydrophobicity. Ongoing research aims to improve adhesion, durability, scratch resistance, and UV protection, broadening the applications of coatings across various industries.

CoaST

The Hempel Foundation Coatings Science and Technology Centre (CoaST) has been actively conducting research on coatings since 2017, focusing on developing innovative and sustainable solutions for the coatings industry. The centre's research efforts primarily target three main areas:

anticorrosion coatings, antifouling coatings, and intumescent coatings.

One of the key aspects of CoaST's research is its emphasis on both laboratory and on-site experiments. This approach allows researchers to study the performance of coatings in various real-world environments and conditions. For instance, the centre is currently conducting on-site experiments on antifouling and anticorrosion coatings at the Maritime Test Centre in Hundested Harbour, Denmark. This unique testing environment enables researchers to evaluate the performance of coatings in a marine setting, where fouling and corrosion are significant issues.

Digital data handling in research

Researchers often take extensive notes during lab experiments. When these notes are recorded traditionally with pen and paper, searching through them and sharing can be challenging. Therefore, converting these notes into digital form is necessary. A modern solution to this is using electronic lab notebooks (ELNs) [4]. ELNs are software applications that run on cloud servers and can be accessed from computers or mobile devices, allowing researchers to record experimental data directly during the experiment. This study aims to develop a data management system for CMTC that can be used onsite to record and manage data efficiently.

Digitalization of CMTC

To facilitate its research efforts, CoaST is also exploring the use of digitalisation and automation technologies. These technologies enable researchers to conduct experiments more efficiently and effectively while also providing remote access to the experiments. This is particularly important for the Maritime Test Centre, which is located in a remote location [5].

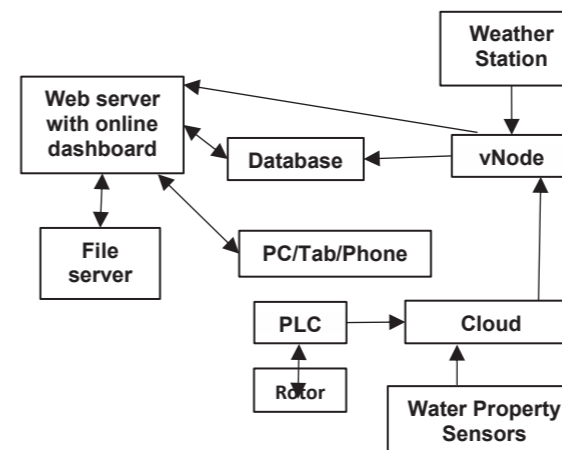


Figure 1: Architecture of the remote access system

Weather data is crucial for analysing results during onsite coating tests. This data is captured by an onsite weather station and recorded in a database. Similarly, water data is collected using sensors, which is essential for evaluating antifouling coatings and conducting onsite

immersion tests of anticorrosion coatings. Samples with antifouling coatings are mounted on rotors to assess their performance under dynamic exposure conditions. The system tracks the rotors and records their speed in the database. Users can take pictures of the samples and upload them to a file server via a web-based dashboard. The system links the samples to the pictures, making it easy for users to organize them. Consequently, all data related to each sample is stored in a structured database, as shown in **Figure 2**. This helps the researchers to query data of samples faster without manual searching through all the records and search for the samples with specific properties such as the samples that are exposed onsite for more than a month.

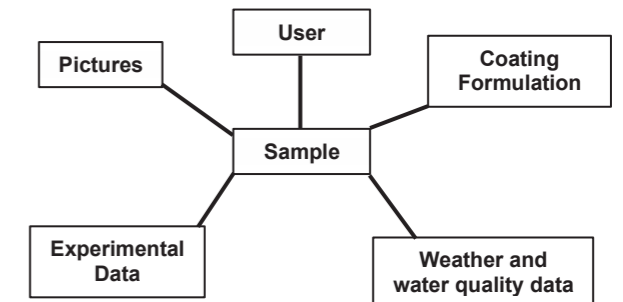


Figure 2: Structure of the database

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Pyrolysis of waste and wood to synthetic fuels on cement plants

(December 2021 – March 2025)



Contribution to the UN Sustainable Development Goals

8% of global anthropogenic CO₂ emissions is caused by the cement manufacturing industry. Switching the role of fossil fuels with synthetic fuels is essential to reduce the CO₂ footprint of the cement industry. Pyrolysis is one way to convert various feedstocks into a combination of solids, gas and liquid products that can be used as fuels. In this project, a pyrolysis process integrated with a cement plant is investigated. The char and gas will be applied to supply energy for cement processes, while liquid fuel can be sold to external customers.



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Abstract

As a result of rapid urbanization and economic development across the world, cement production has increased thirtyfold since 1950 resulting in a significant amount of CO₂ emission. A newly developed FLSmidth fuel treatment reactor, the FUELFLEX reactor, can treat waste fuels such that no fossil fuel is needed on the cement plant calciner and thereby cement plant CO₂ footprint is reduced. This PhD project collaborates with FLSmidth on a further development of the FUELFLEX technology such that it can be further developed to produce pyrolysis oils. At DTU is constructed an electrically heated pyrolysis reactor that can simulate the conditions in a modified FUELFLEX reactor. Different operation conditions and feedstocks are being tested in the DTU pyrolysis reactor to study the influence on oil yield and oil properties. From pyrolysis measurements, the use of cement raw meal (CRM) as a fluid bed material did not show a large change in the physicochemical oil properties while the use of waste as a feedstock created a large change compared to biomass in the liquid oil quality. whereby a pyrolysis oil with low water and oxygen content was obtained.

Introduction

Cement production is a major contributor to climate change. The global production of cement reached 4.2 billion tons in 2023, and the industry stands as a very energy-intensive manufacturing process, comprising 7% of the industrial energy use [1], [2], and generated around 2 billion tons of CO₂ in 2023 [3]. Two sources in the cement production process result in 85 – 90% of the CO₂ emissions: calcination (i.e., decomposition) of limestone, and the combustion of fossil fuels generating the energy needed for the calcination of the raw materials and to produce the clinker. Typically, 30 – 40% of direct CO₂ emissions originate from the combustion of the fossil fuels and, 60 – 70% originate from the calcination process [1], [2].

The cement industry has already replaced a part of its fossil fuel use with waste or biomass, which leads to a reduction of CO₂ emissions [1]. However, the integration of waste-derived fuels into the cement manufacturing process is demanding because these fuels have different physical and chemical properties compared to typical fossil fuels. Particularly, larger particle size and higher water content are parameters that

make it challenging to achieve a complete burnout within the short residence time in the calciner [2].

To support the development of a process for production of pyrolysis oil in a cement plant, pyrolysis experiments were conducted on a small-scale pyrolysis set up at DTU and on a pilot plant pyrolysis unit at FLSmidth Cement. The following objectives was set up for this study:

- To provide a comparison of the properties of waste and wood-based pyrolysis oils.
- To investigate the influence of using raw meal compared to sand as bed material in the fluid bed pyrolysis process.

To compare the pyrolysis oils properties of waste-based oils produced from a laboratory and pilot plant process.

Materials and Methods

Beech wood (< 1 mm) and RDF waste were used as feedstocks. The RDF waste material was provided by Geminor, Norway. To obtain a well-mixed feed material dense enough for continuous screw feeding the RDF1 was first cryo-milled and then pelletized. For the DTU fraction, 10 wt.% water and lignosulfate mixture was added before

pelletization. FLS Cement used the RDF2 pellets directly, while DTU grinded RDF1 to 1.4 – 4.75 mm particle size. The ultimate and proximate characterization of beech wood and RDF waste materials are shown in Table 1. It can be seen that the RDF2 fuel has a high biomass fraction as it has an oxygen content of 21%, while the RDF1 fuel has a higher fraction of plastics materials.

Table 1. Ultimate and proximate analysis of applied feedstocks.

Parameter	Unit	Results		
		as received		
		Beech wood	RDF1	RDF2
HHV	MJ/kg	18.2	33.4	23.4
LHV	MJ/kg	16.9	31.7	21.7
Water	%	7.1	1.1	3.7
Ash	%	0.5	7.7	16.3
Sulfur (S)	%	0.011	0.15	<0.02
Chlorine (Cl)	%	0.002	1.3	0.4
Carbon (C)	%	45.7	70.2	51.0
Hydrogen (H)	%	5.6	8.2	7.5
Nitrogen (N)	%	0.1	0.4	0.36
Oxygen (O)	%	48.1	12.3	21.2

Results and Discussion

Physicochemical properties of pyrolysis oils produced from the experiments conducted at DTU and FLSmidth Cement are summarized in Table 2. Overall, two beech wood-derived oils pyrolyzed with sand and CRM as fluid bed materials (BS and BC) demonstrated notably similar characteristics. Both oils exhibited the same amount of water content of 31 wt.% while it was significantly low (1.5 and 0.64 wt.%) for the waste-based oils. The BS oil had a slightly lower oxygen content of 38 wt.% (db) than BC oil (41 wt.%, db), which showed a higher reduction compared to the feedstock (44 wt.% O, db). RDF1-based pyrolysis oil (WS) had a significantly higher oxygen content and TAN compared to the FLS waste oil together with a higher sulfur content (0.043 wt.%) which agrees with the ~10-fold higher S concentration in the feedstock (see Table 1). The densities of BS and BC oils were close to each other and in agreement with the densities of biomass-derived pyrolysis oils reported in the literature as 1.0 – 1.2 g/cc [4]. However, the WS oil had a higher density value of 1.214 g/cc while FLS's density exhibited very low value (0.819 g/cc). The WS oil appeared as wax at room temperature and its viscosity measured at 40 °C (45.5 cSt) demonstrated higher values than the beech wood oils (10 – 12 cSt). Higher hydrocarbon content and fewer oxygenated species is present in the waste-derived pyrolysis oil (WS) reflected as higher heating value of 37.3 MJ/kg (db), while HHV values of wood oils were lower for both BS and BC, (23 MJ/kg and 21.7 MJ/kg, respectively). It is interesting, that even the RDF2 waste used in the FLS experiments have a relatively high oxygen content of 21%, then the oxygen content of the FLS oil is much lower than that of the WS oil. This indicates that the pyrolysis conditions in the FLS

experiment may have been reasonably harsh with high temperature and some oxygen ingress. Those conditions probably destroy a large fraction of the biomass derived oils and then leave a larger fraction of plastic derived components in the collected pyrolysis oil.

Table 2. Comparison of physical and chemical properties of DTU oils and FLSmidth Cement oil (BS: beech wood + sand, BC: beech wood + CRM, WS: RDF1 + sand, FLS: RDF2 + CRM).

Sample	BS	BC	WS	FLS
Water, wt.%	31	31	1.5	0.64
Density 40 °C, g/cc	1.135	1.143	1.214	-
Viscosity 40 °C, cSt	11.1	10.4	45.5	-
SG 60/60	1.1625	1.1569	0.8644	0.8596
CAN, mgKOH/g	130	140	65	-
PhAN, mgKOH/g	86	60	< 20	-
TAN, mgKOH/g	216	200	65-85	5.48
C, wt.%	38	36	76	84.4
H, wt.%	7.9	8	9.8	12.1
N, wt.%	< 0.5	< 0.5	< 0.5	0.93
S, wt.%	0.006	0.005	0.043	0.022
O, wt.%	54	56	14	3
O (db), wt.%	38	40.8	13.5	2.44
Cl, mg/kg	77	47	900	51.9
HHV (db), MJ/kg	23	21.7	37.3	43.1
LHV (db), MJ/kg	20.7	19.6	34.6	40.8
Pour point, °C	-26	-29	> 51	> 51
Flash point, °C	67.8	69	45.3	40.5

Conclusion

The pyrolysis experiments provided repetitive results and reasonably yields of 51 – 63 wt.% for the biomass experiments and 60 wt.% yield for the DTU waste pyrolysis. In the present study, BS and BC showed very similar physicochemical characteristics which indicated that the use of raw meal as feed material do not lead to large changes in oil properties. Moreover, WS and FLS exhibited significantly improved qualities compared to wood-based oils in terms of water, oxygen, TAN contents and heating values. The difference in the waste-based oils WS (DTU experiments) and the FLS (FLS experiments) are probably caused by differences in the local operation conditions. Research is ongoing with studies on how waste properties and operation conditions influence pyrolysis oils properties.

Acknowledgement

The Innovation Fund Denmark is gratefully acknowledged for funding this research through the project: "CircFuel". Contract no. 0224-00079A.

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Corrosion mitigation of steel monopiles for the offshore wind industry by coatings

(December 2022 – November 2025)



Contribution to the UN Sustainable Development Goals

The development of an effective and feasible corrosion mitigation method for the offshore wind turbines will lead to an increase in their life expectancy. As a result, the required materials for production, installation and corrosion protection for the offshore wind turbines will be reduced. The simultaneous decrease in the use of fossil fuels for their production, installation, and transportation, will contribute to a more sustainable consumption and production, while reducing CO₂ emissions.



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Abstract

Severe corrosion conditions at offshore locations threaten the longevity and safety of steel monopiles of the offshore wind industry. The rising installations number establishes the necessity of structural integrity protection improvement against the harsh corrosive environment. Integrating organic coatings with cathodic protection offers a promising measure against corrosion. The project aims to experimentally study the environmental factors associated with monopile corrosion and assess the cathodic protection and organic coatings impact on corrosion mitigation, while highlighting the major offshore corrosion factors and developing a novel corrosion mitigation method, by simulating and performing experiments under real-field conditions, for the integrated coating-cathodic protection approach evaluation.

Introduction

Wind power is a clean, cost-effective, renewable energy source, driving the green transition, with steel monopiles as the preferred foundation type, due to their simple design, lower cost and suitability for waters up to 30 m [1]. Offshore wind turbines face severe corrosion due to the harsh marine environment, including high salinity exposure, wet-dry cycles, dissolved oxygen level, pH and temperature variations, threatening their structural integrity and challenging their 25-year designed service life [2]. Corrosion mitigation efficiency optimization is required for higher monopile lifespan and reduced maintenance costs [3]. Internal monopile corrosion challenges, include near-stagnant, anaerobic and acidic developed conditions, tidal movement, and oxygen ingress, leading to higher corrosion rates [2], [4]. These conditions have made essential the coatings and cathodic protection incorporation in future designs, for internal corrosion mitigation, as internal use is optional under current standards [5]. Anode selection optimization is essential for internal cathodic protection to prevent acidification and ensure the calcareous layer formation [6]. For

both internal and external monopile durability, compatibility between the two systems is required [7], [8].

Specific Objectives

This study aims to examine the marine environment's impact on offshore wind monopile corrosion and offer a comprehensive solution to the challenges encountered by the offshore wind industry, enhancing the monopile's lifespan. The main focus lies on understanding the factors impacting internal corrosion and the calcareous layer formation, enhancing the monopile's corrosion resistance with the integration of coatings and Impressed Current Cathodic Protection (ICCP). Coating systems performance will be assessed regarding their effectiveness, limitations and characteristics under ICCP, with both lab and field tests. A comparative analysis of the results obtained will be performed.

Materials and methods

Different organic coatings will be evaluated under combined use with ICCP on steel panels both in lab and field conditions. Lab-scale experiments will be conducted, utilizing a developed setup that simulates internal monopile conditions, regarding water chemistry and chemical attacks, under implementation of coating and ICCP. The panels are exposed under various conditions, with post-exposure analysis taking place with several characterization techniques, to evaluate the method performance. In addition, real-field testing will be performed, with an experimental setup installed at the CoaST Maritime Test Center (CMTC) at Hundested harbor for the system performance assessment under real field conditions and provide a comparative analysis between lab and field conditions. A PC is used for ICCP control and data logging for both setups.

Results

The post-exposure analysis results include calcareous layer formation data under various conditions. The layer's adherence and thickness exhibited the same pattern on the reference bare steel panels. The developed calcareous layer on bare steel under polarization conditions for 24h at -1.15V under immersion in artificial seawater is presented with Figures 1 a), b). Figure 1 a) refers to the layer at the top part of the panel, when exposed vertically, while Figure 1 b) to the middle part. The thickness profile of the developed layer exhibit similarities for the two locations, as presented with Figures 2 a) and b), regarding the layer's 3D obtained profile, representing the top and middle part of the panel. Lower thickness locations can also be identified. Further research will be conducted on coating protective properties and the ICCP efficiency through electrochemical and characterization techniques.

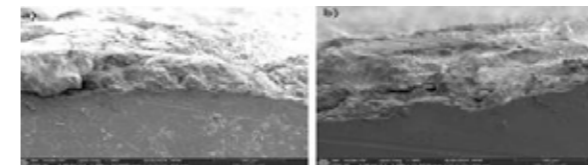


Figure 1: Bare steel sample cross-sectional SEM, 24h exposure: a) top, b) middle part.

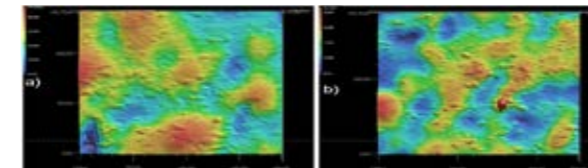


Figure 2: Post-exposure bare steel panel surface topography: a) top part, b) middle part.

Conclusions

Offshore wind monopiles encounter major challenges from the harsh marine environment, accelerating corrosion, reducing the structure's lifespan and increasing the maintenance cost.

This study highlights the corrosion mitigation efficiency significance to safeguard the monopile's service-life. The integrated utilization of coatings-ICCP provides several advantages, with its overall performance requiring further investigation, regarding the internal monopile water chemistry, and chemical attacks. The expected result is the design, implementation, and testing of a coating-ICCP based method, while understanding the internal monopile corrosion challenges.

Acknowledgements

Financial support from the Hempel Foundation to CoaST (The Hempel Foundation Coatings

Science and Technology Centre) is greatly acknowledged.

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Microplastics from fouling control coatings

(February 2023 – January 2026)



Contribution to the UN Sustainable Development Goals

Plastic pollution in the world's oceans has been a known and growing problem for marine wildlife. Particularly, microplastics have received a lot of concern from both society and the scientific community. Amongst other sources, fouling control coatings on ships have been found to generate microplastics. How these microplastics are formed and how much of the coating gets released as microplastics is currently not fully understood. By gaining more knowledge on these microplastics, the groundwork will be laid for future solutions to reduce or mitigate their release into the environment.



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Abstract

Microplastics are a persistent and ubiquitous contaminant in the marine environment. There are various sources of microplastics, amongst which are fouling control coatings. These coatings are used to combat biofouling on the hull of a ship or other submerged structures by employing biocides and self-polishing polymer matrices. While these matrices are expected to polish away over a coating's lifetime, the processes of releasing microplastics are not fully understood. This project aims to gather information on release rates and gain a better understanding of the release mechanisms and properties of microplastics from fouling control coatings. This will be done by performing controlled laboratory experiments, simulating ship hulls with different types of ship coatings and analyzing the generated particles.

Introduction

Submerged artificial structures experience the attachment of a wide variety of organisms to their surfaces. This is called biofouling and causes a variety of problems, for ships this is primarily the increase of drag and accelerated deterioration of the ship hull. To compensate for the increased drag resistance, a ship needs to use more fossil fuel to maintain the same speed, resulting in more harmful emissions. Modern ships make use of fouling control coatings on the hull to combat biofouling [1].

Fouling control coatings can be classified based on the mechanism used to combat biofouling. The main categories are antifouling coatings, employing biocides to deter organisms, and foul release coatings, using surface hydrophobicity to prevent the attachment of organisms. Antifouling coatings contain biocides (often Cu- or Zn-based) which react and dissolve in seawater to form heavy metal ions, which are toxic to biofouling organisms [2]. The release of these biocides is limited by mass-transport through the porous outer layer left behind from the dissolution of the biocides. As this porous layer grows, biocide release decreases. To counteract this, most polymer matrices are designed to erode on the

coating surface. This erosion is in turn controlled by several components of the paint. The polymeric binder is essential here and can be classified based on their polishing control mechanisms. Controlled depletion polymers are water soluble polymers, such as rosin, which slowly dissolves as the coating is submerged in seawater. Self-polishing coatings use acrylic copolymers which are initially water insoluble, however through hydrolysis of hydrophobic functional groups they become hydrophilic and eventually water soluble [3].

It has thus far been assumed that self-polishing and controlled depletion coatings dissolve and pose little further harm to non-target organisms, aside from the emitted biocides. However, in recent oceanic microplastic surveys, microplastics likely originating from these antifouling coatings have been found, seemingly challenging this assumption [4].

Microplastics are microscopic insoluble solid anthropogenic polymer particles and are a ubiquitous contaminant in nearly every natural environment. In the marine environment they pose a great threat due to their potential toxicity to marine life and continual poorly reversible

accumulation [5]. While microplastic surveys have been ongoing since their rise in popularity 20 years ago, only recently have paint particles been found to make up a significant part of the total microplastic count. They have not been detected much before due to their high metal and pigment content compared to other plastic products. This causes the particles to be significantly smaller and have a higher density, resulting in unintended omission from microplastic surveys as size exclusion and density separation are some of the main principles used for collection and separation of microplastics [6].

As with many other types of microplastics found in the marine environment, the exact mechanisms of the formation of these microplastics are unknown. Through controlled laboratory experiments and specialized analysis techniques, a more comprehensive understanding of the generation and nature of fouling control coating microplastics can be found.

Specific Objectives

The specific objectives of this project are:

1. Develop a robust testing methodology for microplastic release from fouling control coatings.
2. Quantify microplastic release from fouling control coatings and compare different coatings.
3. Understand and compare the properties and release mechanisms of fouling control microplastics.

Experimental Setup

The experimental setup used for studying microplastic release consists of a simulation of a ship hull coating. Here, the coating is exposed to similar seawater conditions and sailing speeds as a ship would be exposed to. From this, particles are extracted and can be analyzed through various techniques.

In this project, SEM/EDX is used to study microplastics which provides the advantage of allowing even the smallest size fraction of microplastic to be studied.

This technique has been successfully applied to study microplastic release rates and will continue to be used for a systematic study of several different coatings and exposure conditions.

An example of microplastics extracted from the setup can be seen in Figure 1.



Figure 1: Light microscope image of some microplastics from antifouling coatings released during controlled exposure.

Acknowledgements

Financial support from the Hempel Foundation to CoaST (The Hempel Foundation Coatings Science and Technology Centre).

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Real-time Monitoring for Sustainable Process Development

(March 2023 – February 2026)

9 INDUSTRY, INNOVATION AND INFRASTRUCTURE



Contribution to the UN Sustainable Development Goals

Challenges in efficient process monitoring and maintaining product quality can reduce efficiency and increase energy consumption and CO₂ emissions. This project focuses on industrial digitalization in the biomanufacturing and food industry, developing a real-time monitoring framework and an open-source simulator. The use of these tools has demonstrated improvements in production capacity and supports sustainable process development, contributing to UN Sustainable Development Goal 9: Industry, Innovation, and Infrastructure.



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Abstract

Feed quality variability, high production capacity, and harsh conditions pose significant challenges in process monitoring, control and operation. This study explores different approaches to enhance monitoring capabilities in the biochemical and food industries. The first phase involves the development of open-source software for continuous biomanufacturing simulation. A comprehensive dynamic model, named KTB1, was introduced to cover both upstream and downstream components, providing an integrated view of the production process. It has been demonstrated that this simulator can be used for process monitoring, optimization, and educational purposes. The second part of the project presents a framework that enhances the application of soft (virtual) sensors in complex industrial environments. This approach utilizes machine learning and process insights to improve monitoring through a plant-wide control system. A soft sensor was developed to predict Brix values as a Quality Indicator Variable (QIV) in batch crystallization. Applied to sugar manufacturing, the soft sensor reduced the mean residence time of crystallization by 2.12%, leading to lower energy consumption, reduced CO₂ emissions, and improved production efficiency.

Introduction

In industrial processes, improving operations is driven by the need for safety, efficiency, cost-effectiveness, and quality. Soft sensors have become practical for monitoring QIVs that are challenging to measure in real-time. These sensors aim to capture dynamic, nonlinear relationships between key and easily measurable variables. Traditionally, model-driven approaches were used, relying on physical and chemical principles, but these methods often require assumptions that limit their accuracy in complex, dynamic settings. This has led to increased interest in data-driven and hybrid approaches in both industry and academia.

Data-driven models, or black-box models, use historical data for rapid development without needing deep process knowledge. Advances in data management have made these models attractive, as they can identify complex patterns and adapt to changing environments. However,

they also face issues like high data costs, limited interpretability, and noise sensitivity. Conversely, knowledge-driven methods offer clarity but lack adaptability. Recently, hybrid models combining data-driven techniques with domain knowledge have gained traction, enhancing process monitoring by integrating the strengths of both approaches.

Specific Objectives

The main objective of this project is to develop a hybrid modeling approach to enhance process monitoring capabilities in the biochemical and food industries. The novelty and contributions of this project are summarized as follows:

1. Develop a benchmark model for continuous biomanufacturing monitoring and control.
2. Create a framework for industrial virtual sensor development.

3. Implement the framework to promote sustainable development in the biochemical and food industries.
4. Utilize artificial intelligence and process knowledge to address challenges in monitoring.

Results and Discussion

Considering the objective of the project, the following research and product have been developed in this project:

- 1- KTB1: a dynamic simulation model for continuous biomanufacturing as an open-source software [1, 2]
- 2- A framework for smart monitoring of bio and food industrial processes [3]

As the project's first output, the KTB1 model was developed as an open-source benchmark for biomanufacturing. This benchmark holds considerable potential for a range of applications, including process monitoring, optimization, control, education, pre-feasibility studies, and sensitivity and uncertainty analysis. Figure 1 shows the upstream overview of the developed model.

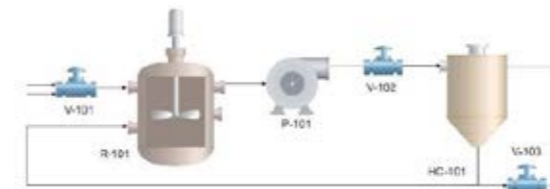


Figure 1: An overview of the upstream of the KTB1 model including valves (V), reactor (R), Hydro-cyclone (HC), and pump (P) [1]

The second part of the project developed a framework for designing virtual sensors tailored to industrial processes, emphasizing sustainable development. Using batch sugar crystallization data as a case study, the framework was tested with machine learning and deep learning techniques, achieving accurate predictions of the QIV. The soft sensor, which monitors Brix as the QIV, reduced mean batch residence time by 2.12%, leading to lower energy use, reduced CO₂ emissions, and increased production efficiency. Since sugar is widely used in biomanufacturing, this advancement is expected to benefit sustainability across the sector. Figure 2 highlights the framework's role in supporting sustainable practices in food and biomanufacturing.



Figure 2: Overview of soft sensor effect on industrial sustainable development

Conclusions

Challenges in process monitoring can lead to out-of-specification products, resulting in increased energy consumption and reduced process sustainability. This project addressed monitoring challenges in the food and biomanufacturing industries by developing innovative software and frameworks. The findings demonstrated that these solutions could significantly enhance sustainable process supervision, benefiting both production efficiency and environmental sustainability.

Acknowledgments

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Catalytic upgrading of pyrolysis oils from beech wood with calcium-based catalysts

(May 2022 – November 2024)



Contribution to the UN Sustainable Development Goals

Ensuring access to sustainable energy and modern fuels for all requires substituting fossil fuels by other greener alternatives. Residual biomass as well as plastic waste can be one such alternative. Using catalytic fast pyrolysis, fuels and chemicals can be produced from these solid feedstocks. However, the initial quality of the pyrolysis oils is poor due to a high water and oxygen content and therefore the oils must be upgraded. Understanding and improving the catalytic upgrading process of pyrolysis oils will help pave the way for a sustainable use of wastes as resources and decrease consumption of fossil-based fuels.



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Abstract

Waste streams are currently an underutilized energy source and are believed to have high potential in being a sustainable source of carbon in a fossil-free future in the form of liquid fuels [1; 2]. Being part of the project CircFuel, this work aims to stabilize the pyrolysis vapors from a catalytic fast pyrolysis unit and transform them into a fuel for ship engines using multi-stage catalytic upgrading.

Calcined cement raw meal showed significant activity in stabilizing fast pyrolysis oil vapors from beech biomass in a fixed bed reactor with a degree of deoxygenation of 46% at 500° C without additional hydrogen while the carbonated raw meal did not show any catalytic activity. At the same time the combined organics yield decreased from initially 37 wt% to 26 wt% and the gas yield increased from 26 wt% to 35 wt%. It is proposed that decarboxylation occurred on the basic sites of the calcined cement raw meal catalyst leading to increased formation of carbon dioxide and improved oil characteristics. Further investigations of the product oil will be performed and an application as marine fuel investigated.

Introduction

Fast pyrolysis of biomass waste can produce a crude bio-oil with a high water and oxygen content, leading to high acidity, low storage stability and energy density [3, 4]. Further, the utilization of plastics leads to a waxy product with long chain hydrocarbons.

Vapors are cleaned using cyclones and hot gas filters before being converted in a fixed bed catalytic upgrading unit, afterwards the oil is condensed and the gas analyzed by using an online GC-MS.

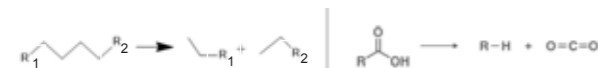


Figure 3: Cracking of higher hydrocarbons and decarboxylation reaction occurring on basic sites of CaO-containing catalysts.

Calcium-based solids from the cement industry like cement raw meal (CRM) and calcined cement raw meal (cCRM) with high amounts of CaCO₃ and CaO respectively, following the mechanism in Figure 1 can be used as low-cost catalytic materials in both cracking and deoxygenation reactions.

Methods

A fluidized bed pyrolysis unit with sand and nitrogen as fluidizing agents and beech wood as feed is used for the pyrolysis experiments.

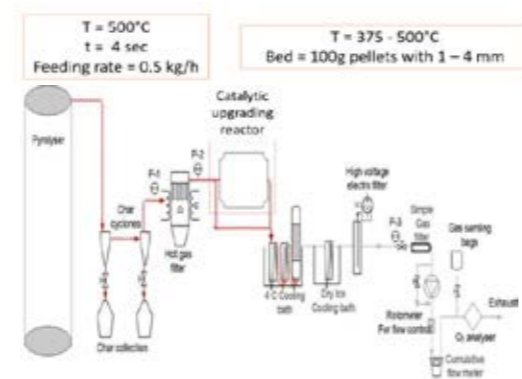


Figure 2: Schematic process diagram of flash pyrolysis with fixed bed catalytic upgrading reactor and subsequent condensation units.

Results

The products of the process are solid char found in the fluid bed and captured in the cyclones, gas leaving after the condensation steps, the pyrolysis

oil which mostly splits up into a light and a heavy phase and deposit of CO₂ as carbonate in the catalyst as well as coking. The amount of organic phase in both light and heavy phase and the amount of water can be calculated.

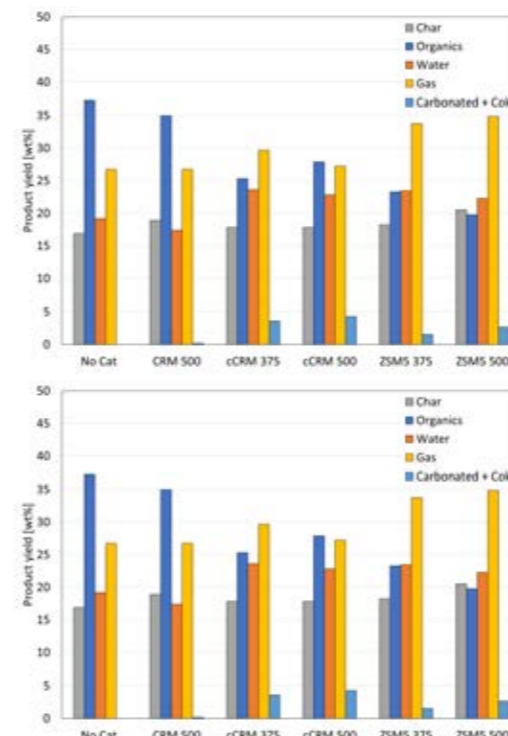


Figure 3: Product yield, pyrolysis with different materials (CRM-Cement raw meal; cCRM-calcined cement raw meal; ZSM5-H-ZSM-5 zeolite) at temperatures 375 or 500 °C in the upgrading reactor. Base case without catalytic upgrading.

Figure 3 shows a reduction of the organics yield with increasing activity of the catalyst and reaction temperature and more gas phase being formed. Around 4 wt% carbonate and coke can be found in experiments with cCRM. No significant influence of CRM is visible.

Table 1: Properties relevant for an application as shipping fuel. Density, sulfur and nitrogen content.

Condition	Density [g/cm ³]	Nitrogen [ppm]	Sulfur [ppm]
Base case	1,11	844	72
CRM 500	1,09	890	44
cCRM 375	1,11	1650	114
cCRM 500	1,10	2022	152
ZSM5 375	1,12	1393	122
ZSM 5 500	1,10	807	134

Nitrogen and sulfur content of the oils (see Table 1: Properties relevant for an application as shipping fuel. Density, sulfur and nitrogen content. are higher for cases with active upgrading agents, highest in the case of cCRM and 500° C. Further, elemental composition of the heavy fraction shows a decrease of the oxygen content leading to a DOD of 44 - 46% with cCRM and a simultaneous increase of carbon content. Results for the heavy oil phase between experiments with cCRM and ZSM-5 zeolite exhibit similar results

with a slightly higher oil yield and carbon content at the same reaction temperature in the upgrading reactor. The formation of carbonate in cCRM experiments indicates further a fast deactivation of the active phase, which can be addressed with taking fresh catalyst from the cement factory and returning the spent material into the calciner cyclones.

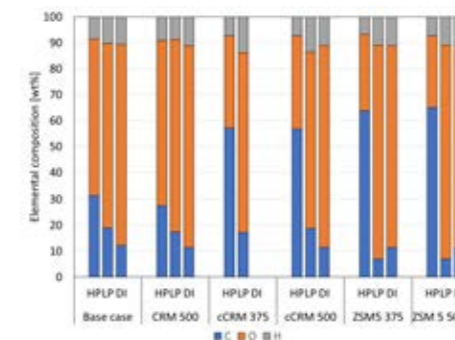


Figure 4: Elemental composition of the liquid products (HP=heavy phase; LP= light phase; DI=dry ice).

Conclusion

Ex situ catalytic upgrading of beech pyrolysis vapors using cement raw meal based materials showed that calcined forms with high amounts of CaO has strong activity in converting oxygenated species leading to an upgraded bio oil. The organic phase yield decreased, and the gas yield increased with higher temperature in the reactor and stronger basicity/acidity of the catalyst. Calcined raw meal deactivated through coking and especially recarbonation.

The sulphur and nitrogen content in the heavy oil increased through upgrading showing that these elements were selectively retained in the oil. The density was mostly unaffected and in a suitable range for marine application. The elemental composition of heavy phase strongly shifted towards more carbon and less oxygen content with catalytic treatment.

Overall calcined cement raw meal showed a similar performance as the benchmark H-ZSM5 catalyst and is therefore a promising candidate for a low-cost catalyst in stabilization of pyrolysis oils.

Acknowledgements

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Unveiling the water-energy nexus for water utilities wastewater reuse for district heating applications

(March 2023 – February 2026)



Contribution to the UN Sustainable Development Goals

Wastewater treatment plants (WWTP) significantly impact energy, climate, and water, making these facilities a major contributor to environmental challenges and climate change. This project aims to transform WWTPs into resource recovery facilities by converting wastewater into an energy resource and contribute to Denmark's goal of achieving carbon neutrality by 2050, assessing the potential to reuse wastewater for energy purposes.



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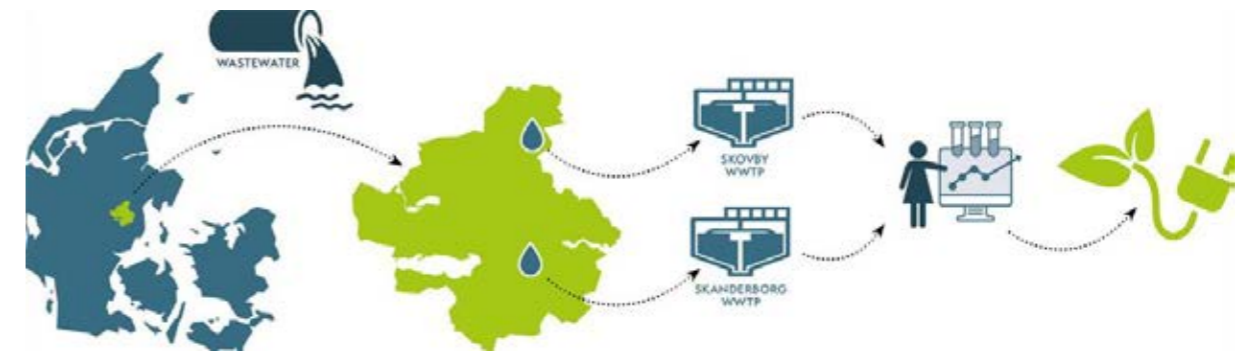


Figure 1: Conceptual schematic of the project

Data collection and model development

Mathematical models (influent generator, WWTP, and catchment) have been developed to capture the heat transfer dynamics in the two WWTPs studied (Skovby and Skanderborg), considering different system configurations and wastewater sources. The models are being used for system design, optimization, and addressing different scenarios [2,3,4].

The influent generator model presented has been used to capture the variation of the inlet water and how this can affect the heat recovery locations in the catchment or within the WWTP.

The WWTP performance model was utilized to analyze the behavior and performance of the WWTP. This model can also predict the quality of the effluent and evaluate the economic benefits and operating costs of the WWTPs.

The models consider different system configurations and wastewater sources, allowing for precise system design and optimizations. The optimization process considers factors such as heat exchanger sizing, heat pump efficiency, heat transfer rates, and different experimental outcomes. In the experimental set-up, the water will undergo filtration before being directed to the heat exchanger, allowing for investigations into the effects of temperature and seasonal changes.

In addition to optimization, the developed tools serve a wider purpose in addressing decisive questions. These include exploring the effects of centralization on system performance, assessing the impact of temperature reduction on the nitrification process, determining reactor capacity adjustments, and evaluating infrastructure resilience under uncertain climate scenarios. The scenario analysis helps in understanding the potential challenges and opportunities associated with the implementation of WWHR systems in different contexts.

Conclusions

The project has demonstrated significant environmental benefits through reduced emissions and energy savings. Key focus areas for optimizing heat recovery processes include:

- Optimization of heat recovery processes crucial for operational efficiency and sustainability.
- Developing models to assess heat recovery locations is essential for maximizing energy efficiency.
- Calculating KPIs and conducting assessments key to achieving optimal heat recovery outcomes.
- Focus on heat recovery optimization enhances resource efficiency, environmental sustainability, and operational performance.

Acknowledgments

The author gratefully acknowledges the financial support from Innovation Fund Denmark Grant Number 2108-00003B.

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Abstract

This PhD project focuses on developing and evaluating wastewater heat recovery (WWHR) systems for district heating purposes in Scandinavia. By harnessing thermal energy from wastewater, these systems improve energy efficiency and reduce greenhouse gas emissions. The research involves data collection, mathematical modeling, and optimization to assess system performance and achieve sustainability goals.

Introduction

A WWTP plays a significant role in the water industry's greenhouse gas emissions, accounting for approximately 3% of the global energy demand [1]. This makes them a substantial contributor to environmental challenges and climate change, particularly due to their high energy consumption compared to other sectors. Considering the interconnections between energy, climate, and water, the efficient management of WWTPs becomes crucial for sustainable development and mitigating environmental impacts.

Wastewater, whether originating from households, industrial processes, or businesses, carries a valuable and often overlooked resource: thermal energy. This thermal energy is a by-product of various factors such as heating, cooling, and chemical reactions. By harnessing the thermal energy present in wastewater, we could not only reduce energy consumption but also effectively mitigate greenhouse gas emissions.

Advanced wastewater heat recovery (WWHR) systems, such as heat exchangers and heat pumps, can effectively capture and utilize thermal energy from wastewater. These technologies not only offer energy efficiency and cost savings but also have applications in various sectors, including residential, commercial, industrial, and district heating networks. By adopting these

innovative solutions, we can transform wastewater from being considered waste into a valuable resource, contributing to a more sustainable future.

Objectives of the project

The primary objective of this project collaboration between Skanderborg Forsyning, DTU, and VIA University College, is to develop and evaluate the feasibility and effectiveness of wastewater heat recovery (WWHR) systems. The research focuses on developing and testing mathematical models in two distinct locations: Skovby (a small WWTP belonging to Skanderborg Forsyning) and Døjsøvej (the main WWTP in Skanderborg), bridging engineering and mathematical models with the obtained data set and assessing potential heat recovery model options using process simulations/scenarios.

Gas cleaning of H₂O feed for Solid Oxide Electrolysis Cell Stacks

(March 2023 – March 2026)

13 CLIMATE ACTION



Contribution to the UN Sustainable Development Goals

This research project has direct impact on Climate Action Objective, which is a crucial element of the United Nations' Sustainable Development Goals. It is specifically focused on the development of solid oxide electrolysis cells (SOEC) by Topsoe. Recently, Topsoe is close to finalizing the construction of a specialized manufacturing facility in Denmark dedicated to SOEC production. The facility is expected to have an annual capacity of 500 MW for electrolysis modules. Consequently, the project plays a direct role in advancing the transition towards sustainable and environmentally friendly fuels. The primary objective of the project is to enhance the durability and lifetime of these systems, thereby making them more competitive for large-scale applications.



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Abstract

My research activities are carried out in the Power-to-X department at Topsoe, a company being a global leader in carbon emission reduction technologies. Their strategy is centered on the development of energy-efficient solutions that can generate fuels like ammonia, methanol, and hydrogen in a sustainable way. This project will have its main impact on Topsoe's solid oxide electrolysis cell (SOEC) development, in turn affecting the green hydrogen production. The project aims to understand the detrimental effect of different impurities in the SOEC system, as this is one of the well-known reasons for degradation and limiting the lifetime of SOECs. This understanding of the role of impurities and their reaction with the cell is going to be used to mitigate these problems and improve the lifetime of the SOEC.

Introduction

This PhD project is an industrial PhD based on the collaboration between DTU Chemical Engineering and the Power-to-X department at Topsoe.

The project's overall goal is to contribute to the change from fossil fuels to sustainable fuels, thereby reducing the total emission of greenhouse gases (GHG). This is because these fuels are produced using GHG effectively removing as much GHG as the fuels emit. The combustion of fossil fuels in 2021 resulted in the emission exceeding 34000 MtCO₂eq [1], highlighting the significant impact that the shift to sustainable fuels would have.

Topsoe is a global leader in carbon emission reduction technologies. To achieve this, a range of different energy-efficient solutions are being developed, to produce sustainable transportation fuels such as ammonia, methanol, and hydrogen. To develop these solutions Topsoe is using its eight decades of experience in heterogeneous catalysis and its industrial chemical application.

An important technology for this shift to a sustainable solution is the solid oxide electrolysis

cell (SOEC) technology, which is acknowledged as the most energy-efficient among the electrolysis solutions. SOECs work at an elevated temperature of 600-850 °C, which is one of the reasons for it to have a higher energy-efficiency due to thermodynamics. Because of the high temperature operation point, it can be integrated with a synthesis loop making the overall efficiency higher. [2]

This is the area where Topsoe's expertise in heterogeneous catalysis plays a crucial role in ensuring the downstream catalytic conversion of SOEC products such as H₂ and/or CO into sustainable fuels and chemicals.

To tackle climate change at the necessary pace, it is a requirement to establish industrial application of the SOEC in a large-scale.

Topsoe is close to finalizing the construction of a large-scale SOEC manufacturing facility in Herning, Denmark. This facility will be able to produce electrolysis modules with the capacity of 500 MW per year. The facility is planned to be in operation in 2025[3].

This PhD is a part of this large development that Topsoe is having in the field of SOEC technology. The project is investigating the different impurities that affect the lifetime of the system. One of the failure mechanisms of the SOEC is in fact the cell degradation, which is heavily influenced by the adsorption of impurities on the active sites of the electrode, a mechanism also called cell poisoning.

The operation of SOEC can involve various reactant gases, which would lead to different impurities. However, this project primarily focus on water as reactant gas. From the literature as well as from internal tests at Topsoe, have identified several possible impurities such as Si, Cr, Al, Na, K, Ca among others [4,5]. These impurities can potentially affect the cell performance and consequently its lifetime, by binding itself to the cell's active site.

These impurities will be the focus of the project with the aim of understanding how to mitigate their negative effect.

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Digital quality by design with model-based design of experiments

(January 2024 – January 2027)



Contribution to the UN Sustainable Development Goals

Through the implementation of model-based design of experiments (MBD_{oE}), fewer experiments are required to obtain critical bioprocess parameters, such as the volumetric mass transfer coefficient ($k_{L,a}$). A reduction in experimental redundancy leads to lower material usage, waste production and energy consumption. This project aims to optimize experimental design thus contributing to more sustainable manufacturing practices.



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Abstract

This project demonstrates the application of model-based design of experiments (MBD_{oE}) for the determination of the volumetric mass transfer coefficient ($k_{L,a}$) in lab-scale stirred tank reactors. $k_{L,a}$ is a critical bioprocess parameter and is quantified with minimal experimental effort. The MBD_{oE} framework iteratively updates a mathematical model with real time experimental data collection and re-fitting of the model with new data. This approach can reduce the required number of experiments while maintaining the model accuracy.

Introduction

The pharmaceutical industry, a sector that is heavily regulated by entities such as the FDA and the EMEA, has undergone a substantial shift in the quality control guidelines and regulations. In the early 2000s, these shifted from end-product quality control to control strategies employed during the manufacturing processes. Process Analytical Technology (PAT) and Quality by Design (QbD) are thus two concepts comprehending guidelines on how to properly design, control and test the processes within pharmaceutical production [1].

To develop a QbD framework, it is essential to understand the process in question. This includes input/output interplay and technological, physical, chemical, and biological validity domains. The relationship between all these domains is what composes the design space, also defined within the QbD guidelines as "the multidimensional combination and interaction of input variables and process parameters that have been demonstrated to provide assurance of quality" [2]. A cornerstone of the QbD strategy is the Design of Experiments (DoE) methodology.

Design of Experiments (DoE) is a statistical method that explores a design space by providing a detailed statistical perspective that helps identify

optimal operating conditions and ranges. However, a DoE is of very limited information if the selected levels and factors were not appropriate, leading to repetition of several experimental points.

Model-based design of experiments (MBD_{oE}) approaches were developed [3] to train a model along the way and plan new most informative experiments. These approaches begin with an *in silico* exploration of a mathematical prototype model, built on preliminary data, expert knowledge and initial hypotheses. Dynamic experiments are designed which aim to maximize information gain. Along with the experiments there is a constant and iterative retrofitting of the model with new data, which ensures minimal experimental redundancy and inclusion of information gathered throughout the process [4]. This means that only the minimal number of experiments is needed because all the information gathered along the way is included to plan the next most informative action.

Specific Objectives

To demonstrate how MBD_{oE} can significantly reduce the effort of reactor characterization, the determination of the volumetric mass transfer

coefficient ($k_{L,a}$) in lab scale was chosen as the first experimental platform. This choice is motivated by the critical role of oxygen supply in aerobic biological processes, which can directly influence the productivity and efficiency of the system. The quantification of the efficiency of oxygen transfer from the gas phase into the liquid phase, given by the $k_{L,a}$, is therefore a key parameter in the design and operation of bioreactors.

Results and Discussion

The MBD_{oE} algorithm and workflow applied to determine $k_{L,a}$ in a stirred tank reactor is represented in Figure 1. This workflow starts with a first experiment, which is user defined. For real-time data acquisition and automatic execution of experiments a bidirectional communication between the MBD_{oE} implementation and the physical reactor system was established. The algorithm then proceeds to solve the ODE representative of the oxygen transfer rate and calculates $k_{L,a}$. Following that, the model parameters are estimated by fitting the data to the Van't Riet relation [5]. To redesign a new experiment, an *in silico* analysis based on this model is performed by randomly sampling experiments across the design space and using a genetic algorithm. The new experimental setpoint which lead to highest information gain (D- or E-optimality of the Fisher Information Matrix) are thereafter sent to the stirred tank, where a new experiment is performed. The data is collected in real time and added back to the data pool. The workflow then enters an iterative flow with re-fitting of the model and redesign of experiments until a stop criterion based on parameter identifiability, is reached.

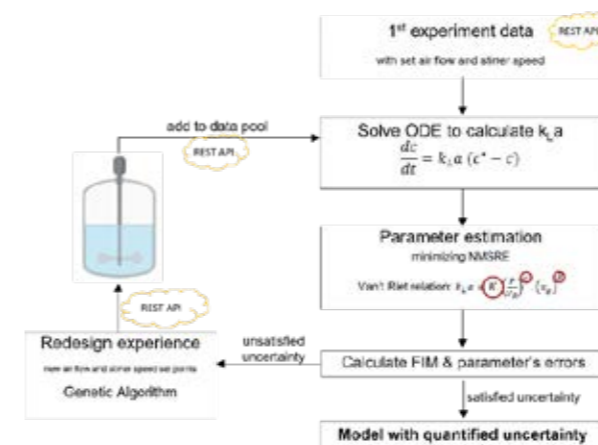


Figure 14: Overview of the automated process of MBD_{oE} for $k_{L,a}$ determination.

The MBD_{oE} can find the next experimental setpoints which provide the most information gain. The algorithm is able to estimate the Van't Riet model parameters and quantify $k_{L,a}$ across

the design space, with a limited set number of experiments.

Conclusions

Model-based design of experiments (MBD_{oE}) is a valuable tool for bioprocess development, where due to high costs and time investments only a limited number of experiments can be done for strain and process characterization. As compared to other DoE approaches, MBD_{oE} can reach a similar information gain with a lower number of experiments. This approach reaches relatively low model uncertainties with few experiments, and it is most valuable when the purpose is to perform the lowest number of experiments.

Acknowledgements

The authors acknowledge the financial support provided by the Novo Nordisk Foundation Start Package grant for Bioprocess Control and Digitalization (NNF220C0081250).

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Continuous hydrogenation of pharmaceutical intermediates

(June 2023 – June 2026)

9 INDUSTRY, INNOVATION AND INFRASTRUCTURE



Contribution to the UN Sustainable Development Goals

Hydrogenation is one of the most important processes in the pharmaceutical industry. With batch reactors dominating the hydrogenation of pharmaceutical intermediates, continuous reactors such as jet loop reactors are promising in terms of improving energy efficiency and raw material utilization, decreasing operation time, and promoting flexibility in reactor operation. By optimizing the hydrogenation process of pharmaceutical intermediates, this project aligns with the UN's sustainable development goals which advocate for innovation, and efficient use of energy and materials.

Abstract

Conventional batch reactors are widely used in the pharmaceutical industry for the hydrogenation of intermediates. Due to the increased sustainable energy requirements, and the requirement for flexibility of the operation, continuous reactor technologies such as jet loop reactors (JLRs) offer promising alternatives. JLRs offer enhanced mass and heat transfer in reduced reaction run times compared to traditional batch reactors. This project focuses on testing and improving a JLR system that can be used for different pharmaceutical intermediates at Lundbeck A/S.

Introduction

Heterogeneous catalysis has a huge role in the treatment of intermediates in the pharmaceutical industry. Since many intermediates have complex chemical structures, the reaction conditions, catalyst design, and reactor designs are critical in terms of achieving high conversion and selectivity. Batch reactors are widely adopted in the pharmaceutical industry due to their easy operation and maintenance. However, batch reactors are hard to scale up and in terms of operational flexibility, their capability is limited due to capacity consideration, downtime, and long reaction times. As an alternative to batch reactors, continuous-type reactors offer more flexibility with decreased reaction run times, easily adjusted reaction conditions during reaction, and more consistent product quality. These contribute to the shift towards continuous reactors in the pharmaceutical industry. Research on continuous reactors in the pharmaceutical industry has been gaining attention in recent years.[1]

The limiting factors for scale-up of batch reactors are primarily mass and heat transfer limitations. Fixed bed reactors with trickle or continuous flow are being tested for hydrogenation reactions in the pharmaceutical industry, but the mass transfer limitations in the catalyst bed and the amount of catalyst remain challenges for these systems.[2]



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Alternative to fixed bed reactors, JLRs are continuous-type reactors that promote enhanced mass and heat transfer due to a circulating loop and a jet ejector. The reaction volume constantly circulates in JLR through a high-powered pump, and the jet created by the jet ejector enhances the mass transfer. The JLR system used in this project is shown in Figure 1.

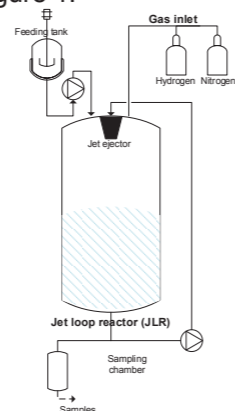


Figure 1. General PID diagram of JLR setup.

Specific objectives

- Testing a model compound for hydrogenation in a JLR and a small batch reactor to compare the mass transfer efficiency.
- Improving the design of the JLR by focusing on the jet ejector and process conditions.
- Scaling up the existing JLR to have a system that can handle multiple chemistries in Lundbeck A/S facilities.

Experimental

Batch reactor experiments are conducted in a 300 mL autoclave. Acetophenone (AP) is chosen as the model compound with 5 wt.% Pd/C as the catalyst and 2-propanol as the solvent. With the Pd catalyst, the target is the carbonyl group hence the reaction has two steps: the first step is the hydrogenation of AP to 1-phenylethanol (EP) and the second step is EP hydrogenation to ethylbenzene (EB). The possible ring hydrogenation products are 1-cyclohexyl ethanol (CHE) and ethyl cyclohexane (ECH). For the initial experiments, three temperatures with three different reaction times were used to explore the kinetics of the model compound. The products are quantified with GC-FID.

CFD simulations for different jet ejector designs were run in Ansys Fluent with 3D models meshed to > 500,000 cells. To illustrate mass transfer, water, and air are used as primary and secondary fluids in steady-state mode.

Results and Discussion

The results for batch reactor experiments are given in Figure 2. The increase in the temperature increases the conversion of AP, and as the reaction time increases the amount of EB produced increases. Based on these results, it can be concluded that the conversion of AP is faster than PE to EB conversion.

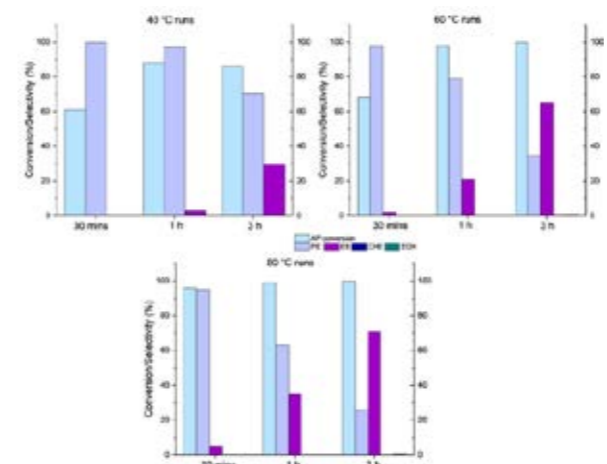


Figure 2. GC-FID results of AP hydrogenation experiments in the batch reactor.

CFD simulations were run with Eulerian-Eulerian multiphase and k-epsilon turbulence models. Firstly, cold flow experiments were done to estimate $k_L a$ values for each jet ejector design, and then two-phase flow was simulated to observe mixing behavior within the ejector. The air volume fraction contours are given in Figure 3. For the flow of two fluids, a clear phase separation can be seen for all designs. This might lead to insufficient mixing in the ejectors; hence the designs of the ejectors are to be improved as the next step.

The scalability of the JLR system depends on the high circulation rates and the mixing capacity of the jet ejectors. To have an improved mixing within ejectors, the mass transfer area should be increased which is directly related to the formation of fine bubbles from the entrained phase.

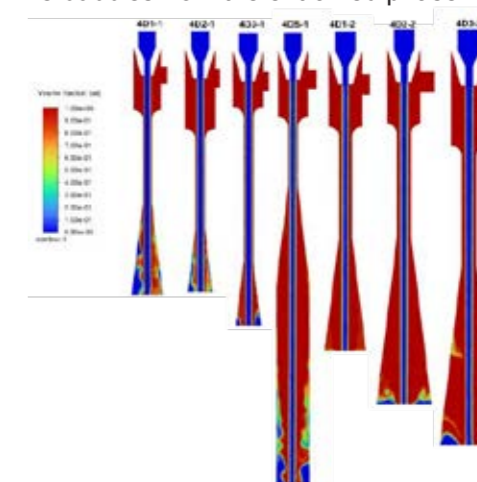


Figure 5. The air volume fraction contours simulated in Fluent for different jet ejector designs.

Conclusions The initial experiments done in the batch reactor with AP hydrogenation show that the kinetics of the reaction increase considerably above 60 °C and the first hydrogenation step is faster than the second step. The CFD simulations of the investigated jet ejector designs showed clear phase separation between the two fluids, which will be the focus point of future improvements.

Acknowledgements

The authors thank DTU Chemical Engineering and Lundbeck A/S for funding this project.

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Catalytic Reduction of N₂O by NH₃+NO over Fe-CHA, Fe-BEA and Fe-FER Catalysts

(December 2021 – November 2024)



Contribution to the UN Sustainable Development Goals

With a steep increase in world population and the resulting industrial boom, global warming has been a matter of serious concern in the recent years. In the wake of increased energy demand, there has been a worldwide push to do away with conventional carbon-based fossil fuels and instead utilize carbon-free alternative fuels. This would result in lower CO₂ emissions and address the issues of global warming and atmospheric pollution. The current Ph.D. project is an important component of one such endeavor to decarbonize the shipping industry by using sustainably produced NH₃ as fuel and thus, contributes to the 13th UN Sustainable Development Goal.



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Abstract

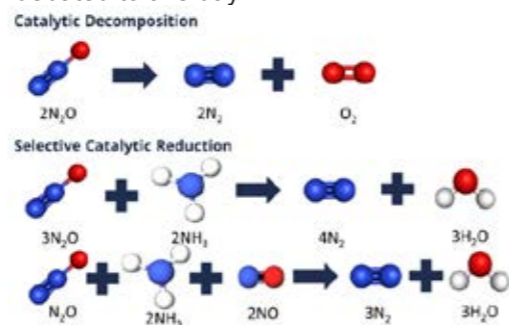
According to the International Maritime Organization (IMO), present shipping activities are responsible for ~2.5% of global GHG emissions and this contribution is expected to increase in the coming years due to increasing global trade. To decarbonize the shipping sector, it is imperative that we come up with an alternative, carbon-free fuel. Ammonia (NH₃) is one such promising candidate for fueling ship engines, but it leads to enhanced flue gas concentrations of NO_x, N₂O and unburnt NH₃, which need to be managed by using a dedicated Exhaust Aftertreatment System (EATS). Among the flue gas species, N₂O has a concerning potential for global warming and its removal via novel catalytic technologies is the primary objective of the present Ph.D. work.

Introduction

With a steep increase in world population and the resulting industrial boom, global warming has been a matter of serious concern in recent years. Of all the different anthropogenic sources accountable for greenhouse gases (especially CO₂) in the atmosphere, shipping activities constitute an industry that is often overlooked. Therefore, the IMO has come to an agreement to work towards certain ambitious targets such as reducing GHG emissions from international shipping by at least 50% by 2050, decreasing carbon intensity by at least 40% (compared to a benchmark set in 2008) by 2030 and achieving complete decarbonization of the shipping sector by the end of the 21st century (1).

Although it is feasible to use ammonia as the main fuel in a dual-fuel compression-ignition (CI) engine (2), it could lead to enhanced emission of N₂O (nitrous oxide), which is known to be ~300 times more potent to cause global warming than CO₂ on a per mass basis (3). In addition, N₂O can react with oxygen in the atmosphere to form nitric oxide, which is one of the contributors of ozone layer depletion (3, 4). Anthropogenic sources are

responsible for ~35% of N₂O emissions and the N₂O concentration in the atmosphere has increased at an alarming rate of ~0.2–0.3%/year in the last century (4). N₂O emissions can be countered by either direct catalytic decomposition into N₂ and O₂ or selective catalytic reduction (SCR) into N₂ and H₂O/CO₂ depending on type of reductant (3). Fe-zeolite catalysts have been predominantly studied in the literature and used in practice to catalyze the reduction of N₂O using NH₃. However, the nature of active sites and the effects of zeolite topologies in such catalysts are still debated to this day.



Materials and Methods

Three Fe-zeolite catalysts (~1 wt.% Fe) – Fe-CHA, Fe-BEA, and Fe-FER – were synthesized via ion-exchange method and their catalytic activities for N₂O reduction were tested in a quartz U-tube reactor in the range of 150–450 °C. 250–750 mL/min of gas mixture was passed through a bed of 50 mg of catalyst having particles in the size range of 150–300 μm. In addition, 2 and 4 wt.% Fe/BEA, Fe/CHA and Fe/FER catalysts were synthesized via incipient wetness impregnation for testing in the future.



Figure 1. Representative synthesis process (ion-exchange) for fabricating Fe-zeolite catalyst.

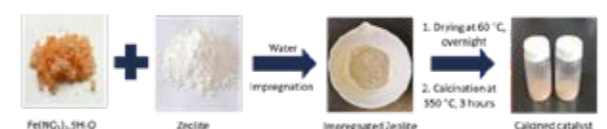


Figure 2. Representative synthesis process (incipient wetness impregnation) for fabricating Fe/zeolite catalyst.

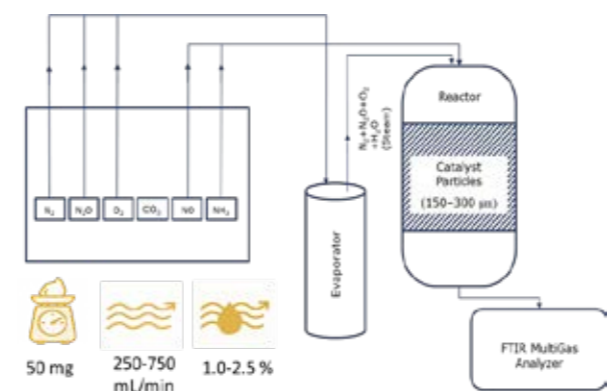


Figure 3. Schematic representation of experimental setup for N₂O removal.

Results and Discussion

Light-off curves were obtained in the presence of 5% O₂, 2.5% H₂O and either NH₃ ([N₂O]:[NH₃] = 1:1) or NH₃+NO ([N₂O]:[NH₃]:[NO] = 1:2:2) as the reductant. Both in the presence and absence of NO, the Fe-BEA catalyst resulted in the highest N₂O conversion, followed by Fe-CHA and Fe-FER catalysts. This confirms why Fe-BEA catalysts are the preferred choice in the industry at present.

Then, steady-state kinetic data ([N₂O]:[NH₃]:[NO] = 2:1:1, 1% H₂O, 10% O₂) were also collected for all the catalysts at 350 °C. The reactions carried

out in the absence of O₂ yielded conversions for all the nitrogenous species in the differential regime, and hence the data obtained thereof were used for comparing the rate of N₂O reduction over the three catalysts. Fe-CHA and Fe-BEA catalysts yielded very similar reaction rates, suggesting similar Fe ion active sites in these materials. In contrast, the rate over Fe-FER catalyst was about 4 times lower, suggesting that there are either fewer active Fe ionic species, or that the Fe ions have lower intrinsic reactivity.

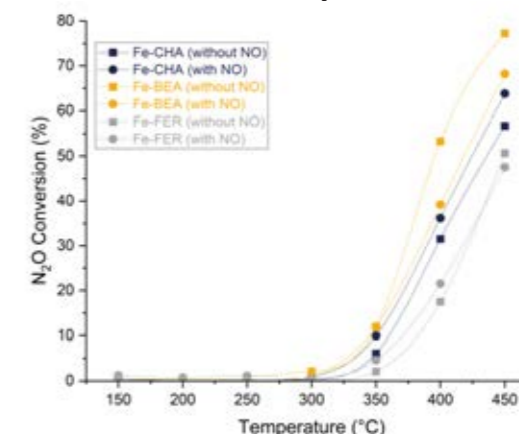


Figure 4. N₂O conversions using 1 wt.% Fe-zeolite catalysts, in the presence and absence of NO. N₂O: 250 ppm, NH₃, NO: [250, 0] or [500, 500] ppm, O₂: 5%, H₂O: 2.5%, flow: 250 mL/min

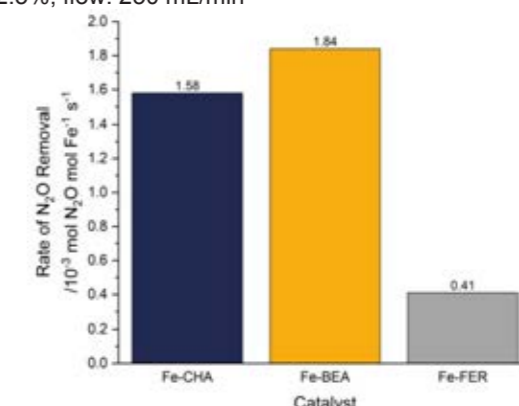


Figure 5. N₂O reaction rates using 1 wt.% Fe-zeolite catalysts at 350 °C. N₂O: 600 ppm, NH₃, NO: 300 ppm, H₂O: 1%, CO₂: 7%, flow: 750 mL/min

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Recyclable Silicone Elastomers from Natural Phenols

(August 2023 – August 2026)

12 RESPONSIBLE CONSUMPTION AND PRODUCTION



Contribution to the UN Sustainable Development Goals

This project supports UN Sustainable Development Goal 12 by developing recyclable silicone elastomers through innovative crosslinking chemistry. By incorporating dynamic hydrogen bonds, we enable easier recycling, reducing both the need for new raw materials and the energy consumption of conventional silicone production. By promoting recyclability and contributing to a circular economy, this initiative encourages responsible consumption, enhances resource efficiency, and fosters sustainable manufacturing practices, contributing to a more sustainable future.

Abstract

In this study, novel strategies to improve the recyclability and sustainability of silicone elastomers were investigated. Non-covalent bonds were incorporated into silicone elastomer networks using phenolic compounds as cross-linkers for aminopropyl-terminated polydimethylsiloxane (PDMS). The system was analyzed through Fourier Transformed Infrared spectroscopy (FTIR) analysis, which indicated the newly formed chemical bonds. Furthermore, rheological analyses confirmed the successful cross-linking, as the storage modulus (G') became greater than the loss modulus (G'') over time, indicating the formation of a stable network. These findings contribute to developing a simple and efficient recycling methodology for sustainable silicone elastomer products, offering a significant advancement in reducing industrial silicone waste.

Introduction

Polysiloxanes, also known as silicones, are an important class of polymers due to their outstanding thermal and oxidative stability, low glass transition temperature, and biocompatibility [1]. Owing to these properties, they are widely used in diverse applications, including biomedical devices, automotive, and construction industries.

A significant quantity of silicones is sold as resins or elastomers that are challenging to recycle due to their crosslinked nature [2].

Due to the energy-intensive process of producing silicon from quartz sand, silicone elastomers are not easily regarded as sustainable materials [3]. Utilizing non-covalent bonding such as hydrogen bonds, π - π associations, ionic linkages, or dynamic bonding interactions within the structure of silicone elastomers makes these materials thermally processable, enabling reuse, repurposing, and ultimately recycling [2].

In this project, we aim to create dynamic bonds between hydroxyl- and amino-groups of phenol and aminopropyl-terminated silicone to create non-covalently bonded elastomers. Before investigating the reaction between naturally derived, complex phenolics and aminopropyl-terminated PDMS, model phenols having simpler

structures are reacted with aminopropyl-terminated PDMS to gain information about the system. The structure of the expected reaction product between hydroquinone and amino-PDMS is shown in Figure 1.

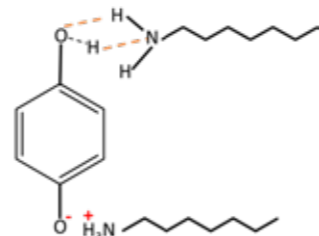


Figure 1. The expected chemical structure of the reaction product between aminopropyl-terminated PDMS and hydroquinone. Both hydrogen bonding and ionic bonding can possibly form.

Specific Objectives

The specific objectives for the projects include:

- Establishing a green chemistry approach using natural phenols to produce recyclable silicone elastomers.
- To develop a recycling process for the synthesized phenol-silicone elastomers.



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Results and Discussion

Fourier Transform Infrared (FTIR) spectroscopy analyses were conducted to gain information about the bonding between the amino and hydroxyl groups. The spectra of the synthesized elastomer and the starting materials are shown in Figure 2. In the elastomer spectrum, the disappearance of the hydroxyl band at around 3000 cm^{-1} indicates that the hydroxyl groups in hydroquinone reacted. Furthermore, a new band at 1571 cm^{-1} in the elastomer spectrum may be attributed to the formation of a new bond through the amino groups of PDMS (N-H bending vibrations).

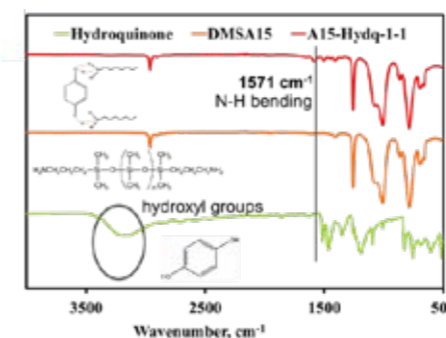


Figure 2. FTIR spectra of a synthesized elastomer (A15-Hydq-1-1) and the starting materials, hydroquinone and amino-PDMS (DMSA15).

The viscoelastic behavior of the hydroquinone with amino-PDMS pre-elastomer liquid mixture was characterized by monitoring the storage modulus (G') and loss modulus (G'') over time at 60°C to investigate the crosslinking process and the formation of a stable elastomeric network, as shown in Figure 3. The temperature was 60°C to represent the curing temperature. After nearly 42 hours, the crossover point was reached, and beyond that point, G' became greater than G'' , indicating that the material exhibited a predominantly solid-like response [4]. When using hydroquinone, a phenolic compound containing two hydroxyl groups, a solid, crosslinked network was achieved. This demonstrates that even with minimal crosslinking points, a solid structure can be obtained, pointing to multiple system reaction mechanisms (i.e., hydrogen bonding and ionic clustering). Increasing the number of reactive groups is expected to further enhance the network's stability and crosslink density.

The investigation of the interaction types within the network is still ongoing. In addition to hydrogen bonds, there is potential for ionic interactions and clustering between the functional groups of the hydroquinone and aminopropyl-PDMS. In future work, these ionic bonding mechanisms will be explored in greater detail to better understand their contributions to the overall network structure and properties.

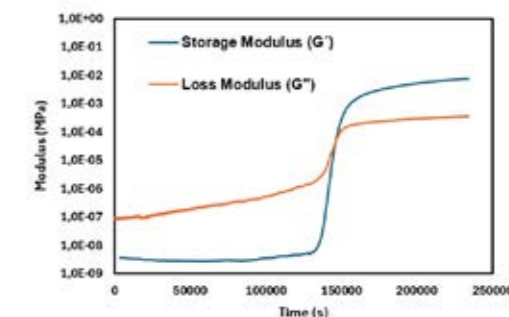


Figure 3. Curing profile: Storage modulus (G') and loss modulus (G'') as a function of time for an elastomer prepared with hydroquinone and telechelic amino-functional PDMS at 60°C .

Conclusion

In conclusion, this study focuses on developing sustainable silicone elastomers by incorporating dynamic bonds into their network structure by means of phenolic compounds, thereby enhancing their recyclability. The appearance of new bands and the disappearance of hydroxyl group bands in the FTIR spectra indicate successful bond formation between the amino groups of PDMS and the hydroxyl groups of hydroquinone. Additionally, rheological analysis confirmed the formation of a solid network between hydroquinone and aminopropyl-terminated PDMS.

Acknowledgements

This project is funded by the Independent Research Fund Denmark.

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Development of novel silicone materials for soft wearables

(March 2023 – February 2026)



Contribution to the UN Sustainable Development Goals

The project aims to develop soft, high-energy-density elastomers for use in exoskeletons and haptic devices. Current exoskeletons often feature rigid joints and are limited to a narrow range of movements, making them impractical for everyday use. By introducing lightweight, high-force wearable exoskeletons, a significant enhancement in the quality of life and an acceleration of recovery for disabled and older individuals can be achieved.



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Abstract

Due to their unique properties, dielectric elastomer actuators are widely used in soft robotics and biomedical fields. Silicone elastomers are noted for their exceptional elasticity and biocompatibility. However, their permittivity requires the use of high voltages for effective actuation. To overcome this limitation, this study investigates the incorporation of gelatin, a collagen-derived protein, into silicone elastomers. The results indicate that blending silicone with 2 % wt. gelatin enhances the dielectric permittivity from 3,6 to 4,5, thereby improving the performance of the elastomer.

Introduction

Dielectric elastomer actuators (DEAs) are promising candidates for artificial muscles due to their notable properties, including large deformation, high energy density, rapid response, and lightweight nature [1]. Among the various soft elastomers used in DEAs, silicone elastomers stand out with their exceptional elasticity [2], durability, and biocompatibility. However, their low dielectric constant ($\epsilon_r < 3$) requires the application of high voltages (> 500 V), which may pose safety concerns in wearable devices [3].

Gelatin, a collagen-derived protein fragment, contains structural dipoles that can improve dielectric properties. Additionally, gelatin is cost-effective, has an upper critical solution temperature of approximately 30–35 °C, and forms a hydrogel at temperatures $< 30^\circ\text{C}$ [4]. This research aims to incorporate gelatin into silicone elastomers. The silicone is crosslinked using aldehydes, that can react even in the presence of water.

Specific objectives

The specific objectives of the project are:

1. Incorporation of proteins into silicone elastomers.

2. Exploring various strategies that enable silicone cross-linking in the presence of proteins and water.

Methods

A gelatin hydrogel was prepared by dissolving gelatin (5 wt. %) in deionized water. The mixture was heated at 40 °C until the gelatin completely dissolved, then cooled at 4 °C to obtain a solid hydrogel.

Aminopropyl-terminated polydimethylsiloxane was mixed with the gelatin hydrogel using a dual asymmetric centrifuge SpeedMixer DAC 150 FVZ-K (Germany) to form an emulsion.

The emulsion was subsequently cross-linked using a solution of 1,3,5-triformylbenzen dissolved in DMSO. The molar ratio between the $[\text{C}=\text{O}]$ groups and the $[\text{NH}_2]$ groups was 2:1. The mixture was allowed to react for 24 hours, followed by drying at 65 °C for 24 hours to allow for the evaporation of DMSO and water.

A Leica DM LB optical microscope was used to investigate the morphology of silicone-gelatin mixtures. Broadband dielectric spectroscopy (BDS) was performed on a Novocontrol Alpha-a high-performance frequency analyzer

(Novocontrol Technologies GmbH & Co. KG, Germany) operating in the 10^{-1} – 10^6 Hz frequency range.

Results and discussion

Incorporation of the gelatin hydrogel

In order to incorporate the gelatin hydrogel in the silicone, the two phases were mixed using high shear. This method was previously used by Mazurek et. al who reported a similar emulsion [5], in which silicone was mixed with glycerol, resulting in stable glycerol droplets within the silicone matrix.

At high mixing shears, the gelatin hydrogel formed small droplets with an average droplet size of 4.6 μm , as seen in Figure 1. The emulsion remained stable over time due to the hydrogen bonds formed between the peptide chains.

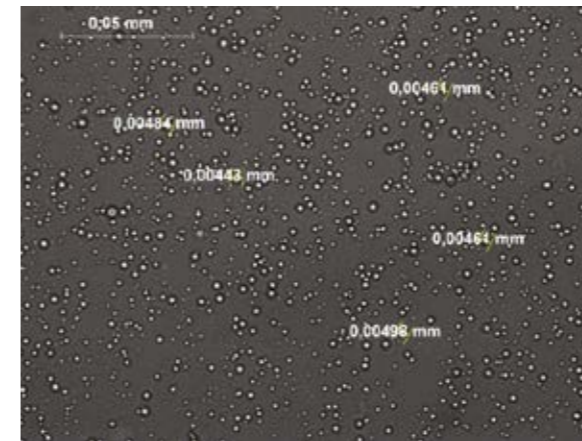


Figure 1: Microscopy image of a gelatin hydrogel dispersed in APDMS.

Dielectric properties of silicone-gelatin hydrogel

The silicone-protein mixture was cured using aromatic aldehydes resulting in silicone-gelatin composites. Incorporating protein into the silicone elastomer enhanced the dielectric permittivity from 3,6 to 4,5 at 1 Hz, which represents an increase of 25 %. The increase in permittivity was attributed to the presence of dipoles within the gelatin structure (Figure 2). At the same time, a slight increase in dielectric loss was observed.

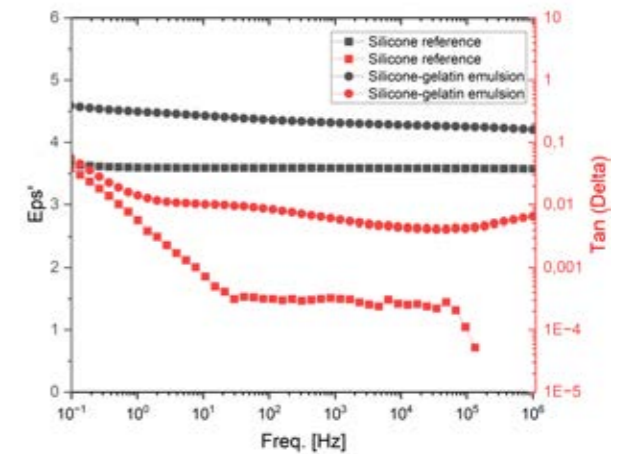


Figure 2: Dielectric permittivity (ϵ_s') and loss tangent ($\tan(\Delta)$) of a pure silicone elastomer reference and the silicone-gelatin composite elastomer.

Conclusion

The gelatin hydrogel was successfully incorporated into the silicone despite the difference in the water affinity between the two phases.

Silicone-gelatin elastomers were fabricated by cross-linking the silicone polymer with aldehydes. The addition of gelatin to the silicone elastomer resulted in increased dielectric permittivity.

Future studies aim to explore how varying protein concentrations influence the silicone matrix and examine the effects of different proteins, such as collagen and fibroin, on the dielectric properties.

Acknowledgments

The author expresses their sincere gratitude for the funding provided by the Novo Nordisk Foundation through the Challenge Program, grant no. NNF22OC0071130.

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Catalytic Upgrading in Slurry Reactor of Biomass Pyrolysis Oil to Fuels for Heavy Transport and Aviation

(January 2024 – December 2026)

7 AFFORDABLE AND CLEAN ENERGY



Contribution to the UN Sustainable Development Goals

With the eminent energy shift that the world needs to perform to achieve the UN sustainable development goals regarding greenhouse gas emissions, major efforts are necessary to find new processes that can provide energy sources that are not only clean, but also affordable and reliable. This project belongs to this field, as it aims to study and optimize a pilot-scale unit in continuous operation for the production of a liquid fuel from biomass, which can be used in heavy transport and aviation.



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Abstract

The liquid bio-oil that can be obtained from the pyrolysis of biomass has the potential to replace fossil fuel sources. However, to overcome its negative properties, the catalytic upgrading of this liquid is necessary. To avoid the coking behaviour of bio-oil, the process can start with a lower temperature step, to stabilize the reactive molecules. Initial experiments in a slurry reactor set-up with a model compound mixture showed that guaiacol can be totally converted even at 120 °C, with the main products being cyclohexanol and 2-methoxycyclohexanol. Temperatures higher than 200 °C led to formation of dimers. Regarding octanol, which was used as a solvent for guaiacol, was also converted above 200 °C, and led to the production of considerable amounts of methane.

Introduction

Fossil fuels are known to be limited and impact the environment, therefore new alternatives have to be found. While electric vehicles look like a promising alternative to cars running on fossil fuels, other alternatives are needed for long distance transportation and aviation.

Bio-oil is a liquid that can be obtained through the pyrolysis of biomass. To improve some of its negative properties, such as high reactivity and acidity and a lower heating value, its upgrading is necessary [1]. This process employs a specific catalyst that promotes the reaction at high temperatures between the bio-oil and hydrogen, which is used at high pressures [2]. Due to the tendency of converting bio-oil to coke at high temperatures, which may deactivate the catalyst and plug the reactor, the upgrading process can be performed in two steps, with the first one at lower temperatures (between 150 and 200 °C), with the single goal of stabilizing the bio-oil, and the second one at the usual higher temperatures (250 to 450 °C) to further upgrade the oil [3].

Fixed bed reactors are the usual benchmark in the upgrading process. However, these are

associated with plugging and coking of the catalyst. A slurry reactor set-up can be an alternative to this, since it allows the catalyst to be well dispersed and mixed with the oil, meaning that it contacts with partly converted and only low concentrations of fresh bio-oil [4]. This is expected to prevent the fast deactivation of the catalyst and the plugging of the reactor, therefore, allowing for longer running times in continuous operation.

Specific Objectives

With the project still being in its early stages, the first experiments aimed at getting familiar with the set-up and optimizing operating parameters that were crucial for continuous operation. These included the size of the outlet dip tube, the response of the PID temperature controller, among others. Once a stable continuous operation was established, the experiments focused on processing a model compound mixture containing guaiacol (10 wt%) and octanol (90 wt%) at temperatures in the range from 120 to 250 °C.

The results are presented and discussed in this contribution.

Results and Discussion

The experiment was performed in a 0.5 L reactor from Parr, which operated continuously for more than 90 hours. Four temperatures were studied, with each being in place for around 1 day. The liquid flow was 0.5 mL/min with an expected residence time of 2.5 hours, the hydrogen flow was 300 mL/min and the hydrogen pressure inside the reactor was 100 bar. The mass of catalyst was 5 grams, and the stirring speed was set to the maximum, which was around 730 rpm.

The main results are presented in figures 1 to 3. Figure 1 shows that at lower temperatures, guaiacol was successfully upgraded while octanol was not, which was the goal, as it mainly works as a solvent. However, as the temperature increased, guaiacol started producing some dimers and octanol started being converted mainly to heptane and some dimers, which is not desirable. This also led to the production of methane, as shown in Figure 1. Nevertheless, the yield of gas species remained low.

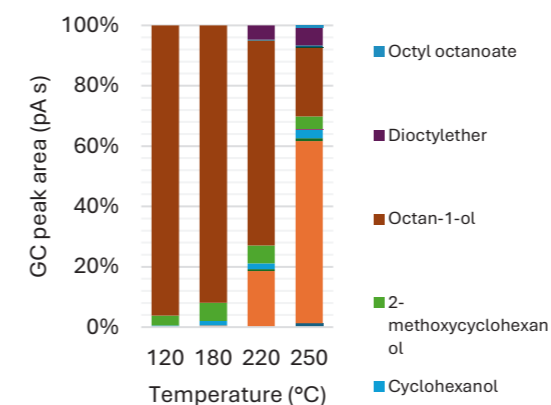


Figure 1: Liquid composition at different temperatures; Liquid analysis by GC-MS-FID.

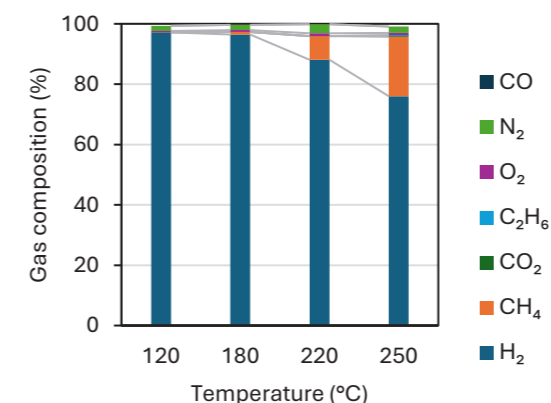


Figure 2: Gas composition at different temperatures; Gas analysis by GC-TCD-FID.

Throughout the experiment, it was visible that the liquid samples had a black powder suspended in them. This resulted from an extensive crushing of

the catalyst, as shown in Figure 2, where only fine powder is left from the original extrudates.



Figure 3: Sample of the crushed catalyst pellets after processing for 90+ hours.

Conclusions

The set-up was successful at converting a model compound mixture for over 90 hours. However, two distinct challenges were identified. Firstly, the catalyst was crushed down to a size smaller than the one of the dip tube filter leading to catalyst being present in most liquid samples taken. Secondly, a leak in the top of the outlet dip tube allowed the gas to escape through the top of the reactor, leading to a variation of the liquid level inside of the reactor. Regarding the products, guaiacol was successfully converted, even at 120 °C, and octanol was only converted at higher temperatures, 220 to 250 °C, leading mostly to the production of heptane and methane. At these higher temperatures where octanol was converted, dimers, higher molecular weight compounds and phase separation were also identified in the liquid.

Acknowledgements

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Advanced simulation of large-scale Bioreactors

(December 2021 – March 2025)

9 INDUSTRY, INNOVATION AND INFRASTRUCTURE



Contribution to the UN Sustainable Development Goals

This research aims at improving the operation and design of large-scale fermentation processes, based on state-of-the-art monitoring and modeling. The development of advanced monitoring and control systems is critical for bioprocesses to become more efficient in terms of resources and energy consumption, but also to compete against the traditional chemical industry. As the utilization of bioprocess is expected to further increase over the next decades, innovations in the area have the potential to highly impact the industry.



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Abstract

This research project, carried out in collaboration with UNIBIO A/S, aims at improving the design and operation of large-scale bioreactors. The basis of this research is that at larger scales, material transport limitations start having an impact on the process dynamics and it needs to be considered for accurate modeling of the system, as well as in the development of digital twins. To achieve this, one must include the two main phenomena involved in material transport in bioreactors: liquid phase mixing and interfacial mass transfer. The objective of the project is therefore to include these two phenomena in real-time bioreactor models. The models can be used for optimizing the design and operation of bioreactors.

Introduction

Fermentation has become an increasingly important chemical process in a wide range of applications, from pharmaceutical to bulk chemical and biofuel productions [1]. Despite its increasing use in industry, many fermentation processes are run as batch operations at low technological level, lacking measurement-based control [2]. With the scope of up-scaling bioprocesses, to allow economies of scale and competitiveness against traditional chemical processes, automation and optimization of bioprocesses is essential. Operating industrial scale fermentations comes with its own set of challenges, mainly related to the inhomogeneous mixing conditions and the mass transfer limitations, both related to the fluid dynamics of the system. Thus, understanding and accurately modeling the fluid dynamic behavior of the system is a key element for predicting the overall behavior of the fermentation process. The main challenge with modeling fluid behavior in large-scale equipment originates from the complex and chaotic nature of turbulent flow, which limits the accuracy of deterministic models in macroscopic simulations.

Computational fluid dynamics (CFD) has improved the understanding of turbulence by

modeling equipment at a very high resolution and has become a useful tool for investigating hydrodynamic conditions in multiphase systems. This numerical study of gas-liquid hydrodynamics is carried out in collaboration with UNIBIO A/S, specializing in the production of Single Cell Protein using methane gas as carbon source. Being an aerobic fermentation, and using a gaseous substrate, mass transfer between the phases is of crucial importance to the process, and a thorough understanding of the multiphase mixing is essential. To this purpose, the company has developed an alternative bioreactor design, the so-called “U-loop” design, which greatly improves volumetric mass transfer due to differences in the hydrodynamics and pressure profiles. However, the contribution of each phenomena to the enhanced mass transfer has not yet been identified.

Modeling

One aspect of this research project is to include fluid dynamics in the modeling of fermentation processes, to account for material transport dynamics. The typical approach is to use

Computational Fluid Dynamics (CFD), coupled with biokinetic models to calculate the resulting concentration profiles over space and time. The geometry of a typical U-loop reactor is shown in figure 1.

However, for a model to be used in real time applications, it should be solvable in real time. This limits the use of complex CFD models to develop Digital Twins. Therefore, computationally lighter models need to be developed, that contain the material transport dynamics, as well as the reaction kinetics. The approach taken in this project is to use the information from the CFD models to build simplified mixing models, e.g. CFD based compartment models.

Finally, the models are to be implemented as Digital Twins on an industrial scale U-loop bioreactor at the DTU Pilot Plant. Here, the objective is to continuously update the model parameters based on process measurements and assess the prediction capabilities and control performances of the different models.

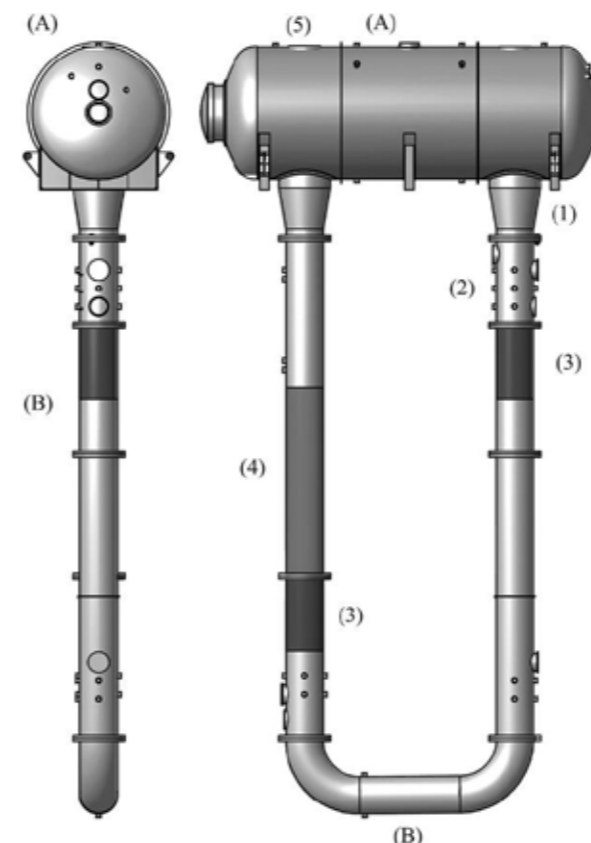


Figure 1: Illustration of a U-loop bioreactor (A) Degassing unit, (B) U-shaped section, (1) circulation pump, (2) inlets, (3) static mixers, (4) heat exchanger, (5) gas outlet.

Process Monitoring

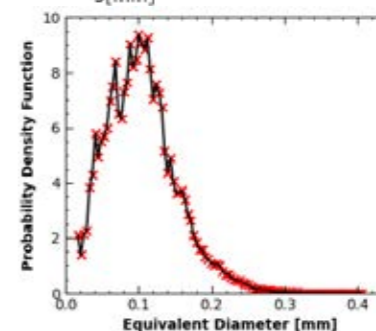
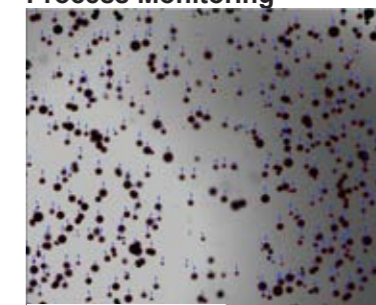


Figure 2: (Left) Shadowgraphic image of bubbles rising in water, with contour lines and velocity vectors of the bubbles (Right) Resulting bubble size distribution based on the image data.

Accurate monitoring of the process is essential for the development of digital twins: for model validation and for real time model update. For model validation, fluid dynamic measurements of the liquid phase (Laser Particle Image Velocimetry) and the multiphase structures (Shadowgraphy) are performed on the modelled process.

Moreover, in-line monitoring of the process is used to update the model parameters, for the model to be aligned with the process.

Acknowledgements

I would like to thank PROSYS, DTU Chemical Engineering and UNIBIO A/S for co-financing this research project.

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Conversion of plastic waste to synthesis gas

(March 2023 – February 2026)

12 RESPONSIBLE CONSUMPTION AND PRODUCTION



Contribution to the UN Sustainable Development Goals

This research could significantly contribute to the achievement of more sustainable consumption and production patterns, aligning with the SDG 12. The overall objective of this project is to develop a carbon-neutral technology for converting plastic waste to methanol. The technology is designed to accept the plastic waste which cannot currently be recycled. Its implementation will reduce the amount of plastic waste sent to landfills and incineration plants, and lead to a decline in traditional carbon-based methanol production.



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Abstract

With the growing problem of plastic waste, there is an urgent need to find sustainable solutions for its disposal. This research project, in collaboration with SemperCycle, focuses on converting plastic waste into methanol with minimal CO₂ emissions. The technology is based on a two-step process: fluidized bed gasification and partial oxidation (POX) for removing the tars. The key focus has been on addressing issues with the tar collection system, feeder reliability, and conducting a CFD simulation for designing a partial oxidation (POX) reactor. Currently, we are upgrading the auxiliary system and installing the newly commissioned POX reactor.

Introduction

The pressing issue of plastic solid waste (PSW) demands immediate attention, as its problem continues to escalate. One approach is chemical recycling, which converts plastic waste into valuable resources through processes such as pyrolysis and gasification [1]. Gasification provides a remarkable degree of flexibility compared to pyrolysis, as it allows for the valorisation of plastics with different compositions or mixtures. Waste plastics possess specific traits, such as low thermal conductivity, sticky behavior when heated, high volatile content, and significant tar formation, which make it difficult to treat them using conventional gasification technologies, posing a considerable challenge to the implementation of the process [2]. The PhD project is part of a collaborative effort with the company SemperCycle, aimed at developing and demonstrating a sustainable process for converting waste plastic to methanol using renewable electricity with minimal carbon dioxide emissions. The scope of work includes experimental studies in a fluidized bed reactor, partial oxidation of tar-containing gases, and detailed analysis of operational parameters to optimize syngas production.

Troubleshooting the system

Combustion tests were performed to obtain: hot testing of the reactor and its subsystems, choose the system configuration, identify the cause of fluctuations in the composition of the gases at the outlet (exhaust or syngas), and find a stable operating point of the system by minimizing the plastic feeding gas flow.

In early tests, we noticed large fluctuations in gas composition at the reactor outlet, which were traced to instability in the fuel feeding rate. The feeder was initially operated in gravimetric mode, where load cells monitored the fuel weight. However, the readings were inconsistent, leading to variations in fuel flow. To resolve this, we switched to volumetric control, using a constant auger rotation speed. This change reduced the amplitude of oscillations in gas composition and improved overall system stability. Additionally, the geometry of the auger was modified using a twin concave fine auger with a smaller pitch, which resulted in a more uniform and consistent fuel feeding, particularly for high-density materials such as polyethylene (PE). Simultaneously, the effect of feeding gas velocity was analysed. The diameter of the fuel inlet pipe was reduced from 21.6 mm to approximately 10.2 mm. This

adjustment enabled the reduction of the feeding gas flow rate while achieving stable fuel loading.

Gasification tests

In the case of gasification tests, we are primarily interested in knowing the yield and composition of the syngas and the tar content. Gas sampling was conducted at a height of 50 cm above the distributor using a gas probe, while the air probe, used for syngas combustion, was positioned at 70 cm above the distributor. Mass balance closure during gasification was approximately 85-95% (Figure 1). During the initial series of tests with steam (GSB01 and GSPE01), a malfunction of the collection system prevented the sampling of the condensates and solids entrained by the syngas. This is also evident from the hydrogen and oxygen balances. In the subsequent tests (GSPE02-05), with a higher feed rate, a low carbon balance closure became evident, reaching a maximum of 60%. The main cause was identified as the syngas sampling system. The use of gas bags resulted in a loss of hydrocarbons, which increased significantly with the number of carbon atoms. This suggests that condensation occurred on the surface of the gas bags. To verify this hypothesis and assess the impact, the air-steam gasification tests were repeated using both gas bags and by directly connecting the syngas to the gas chromatograph (GC). This resulted in an improvement in the carbon balance closure from 60% to 80% (Figure 1, GPE01 and GPE01(2)).

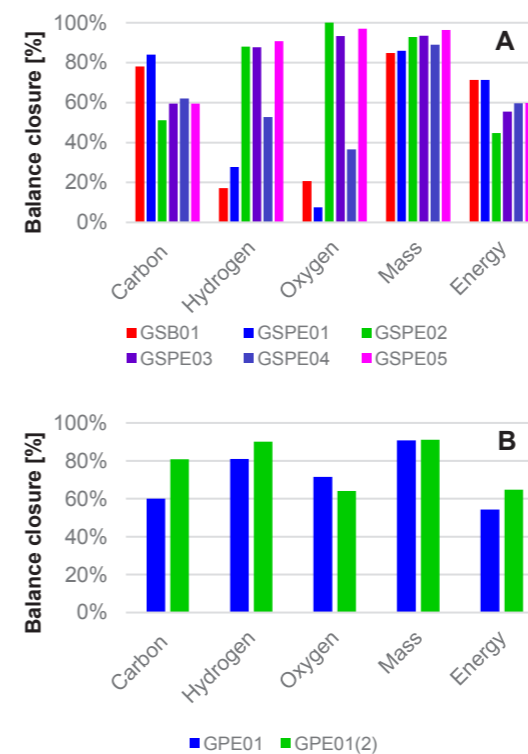


Figure 1: Heat and mass balances of steam (A) and air-steam (B) gasification tests.

POX reactor design

The partial oxidation of tar-containing producer gas involves intricate interplay among diffusion, turbulent mixing, and chemical reactions. Computational fluid dynamics (CFD) allowed us to evaluate the mixing efficiency, and temperature profiles within the reactor under various operating conditions; and thereby support the design process of the POX reactor. For the POX reactor, we considered two cases: slow and fast mixing. The slow mixing case is intended to provide insight into how the reactor would behave in the event of a mixing problem, due to incorrect sizing or failure. Figure 2 shows the streamlines and the velocity field for the fast mixing case.

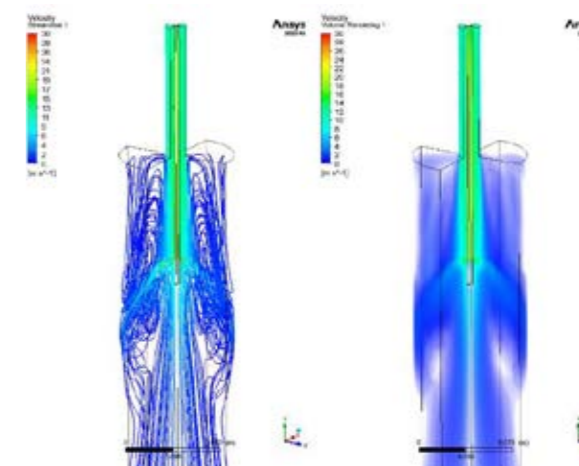


Figure 2: Streamlines and velocity field for the fast mixing case.

In addition, the assessment of the maximum temperature was used for material selection.

The reactor has been constructed and awaits commissioning. We are currently renovating the auxiliary systems and in the next months, the POX reactor will be installed.

Acknowledgements

This work is supported by the EUDP funded project: Conversion of plastic waste to methanol.

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Advanced configurations for carbon capture and flue gas cleaning

(January 2024 – December 2026)



Contribution to the UN Sustainable Development Goals

Carbon dioxide is emitted in large quantities from hard-to-abate sectors and must be effectively captured to mitigate climate change. Developing advanced configurations for flue gas treatment, this research aims to optimize process designs to lower the energy demands of CO₂ capture. Combining data analysis from industrial campaigns with precise modeling of CO₂ capture processes, the work aims to create a validated thermodynamic model to simulate and optimize these configurations. Such innovations promote more sustainable, energy-efficient carbon capture solutions, supporting efforts to reduce global greenhouse gas emissions.

Abstract

Carbon capture from hard-to-abate industrial sectors is essential for reducing global greenhouse gas emissions. This research investigates advanced configurations for CO₂ capture using amine-based innovative solvent blends to improve process efficiency. Focusing on the CESAR1 solvent (27 wt% aminomethyl propanol mixed with 13 wt% piperazine in water), the study analyzes steady-state data from pilot-scale industrial campaigns to evaluate the effects of various configurations on specific reboiler duty—a critical factor in reducing the energy consumption of thermal-driven carbon capture. A robust thermodynamic model has been developed based on the CESAR1 solvent's thermodynamic, kinetic, and physicochemical properties. This model will then be used to simulate steady-state points from real pilot plant campaigns, providing insights into process optimization for energy-efficient CO₂ capture. The findings support scalable, sustainable carbon capture practices aligned with global climate change mitigation efforts.

Introduction

Since the Industrial Revolution, greenhouse gas (GHG) emissions—especially carbon dioxide (CO₂), methane (CH₄), and nitrous oxide (N₂O)—have caused global temperatures to rise by 1 °C above pre-industrial levels [1]. Among these gases, CO₂ has drawn particular concern because it remains in the atmosphere for up to 1,000 years, contributing significantly to global warming [2]. The Paris Agreement seeks to limit global warming to well below 2 °C, with an ideal target of 1.5 °C, by reducing GHG emissions [3]. Achieving this requires substantial reductions from major CO₂ sources, including hard-to-abate sectors like power generation and large-scale industry, which continue to drive GHG accumulation.

To address these emissions, carbon capture, utilization, and storage (CCUS) technologies are considered essential by the Intergovernmental Panel on Climate Change (IPCC) [4]. Among various methods, post-combustion CO₂ capture using aqueous amine solutions has proven to be the most mature and widely implemented technology at large scales [4]. Advanced process

configurations such as lean vapor compression (LVC), intercooled absorber (ICA), and cold solvent split (CSS) can further reduce energy requirements, with reported reductions in reboiler duty of up to 40% [5]. Additionally, novel amine blends, such as the CESAR1 solvent—a combination of aminomethyl propanol (AMP) and piperazine (PZ)—have shown promise in reducing regeneration energy and improving CO₂ capture efficiency compared to traditional amines like monoethanolamine (MEA).

Modeling and simulation play a crucial role in optimizing advanced configurations and novel solvents, providing a foundation for scaling up CO₂ capture processes with higher accuracy and efficiency. By developing a functional thermodynamic model for the CESAR1 solvent, which combines aminomethyl propanol (AMP) and piperazine (PZ), this project aims to capture the complex thermodynamic, kinetic, and physicochemical properties of this solvent blend. This comprehensive approach helps to evaluate and predict performance metrics, particularly focusing on minimizing the specific reboiler duty, which is a critical factor for lowering the energy intensity and operational costs of CO₂ capture



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systems. The model will incorporate pilot plant data from ongoing research to ensure reliable parameterization and validation, thus enabling simulation-based optimization and contributing valuable insights toward the design of large-scale, energy-efficient CO₂ capture technologies tailored for industrial applications. By bridging experimental data with process modeling, this study seeks to support the development of scalable solutions that align with energy reduction targets and provide actionable insights for the wider implementation of carbon capture in hard-to-abate sectors.

Methodology

To achieve our research objectives, we will employ a multi-faceted approach. Firstly, we will develop a rigorous thermodynamic model for the CESAR1 solvent, incorporating relevant physical and chemical properties such as vapor-liquid equilibria, enthalpy, and heat capacity. This model will be validated against experimental data from literature and pilot-scale studies.

Secondly, we will utilize a commercial process simulator like Aspen Plus to model various CO₂ capture process configurations, including baseline, LVC, ICA, and CSS. The developed thermodynamic model for the CESAR1 solvent will be integrated into the simulator to enable accurate simulations of steady-state operating conditions.

Finally, we will analyze the simulated results to evaluate the impact of different process configurations on key performance indicators like specific reboiler duty, energy consumption, and CO₂ capture efficiency. By identifying optimal operating conditions and configurations, we aim to minimize energy consumption and enhance the overall efficiency of the CO₂ capture process. Sensitivity analyses will be conducted to assess the impact of uncertainties in model parameters and operating conditions on process performance.

Future Work

In the coming year, we will focus on several key areas to further advance our research. First, we will conduct experimental studies to validate the developed thermodynamic model and to investigate the impact of operating conditions on solvent degradation and regeneration.

Second, we will develop dynamic models to analyze the transient behavior and control strategies for CO₂ capture processes. This will enable us to optimize the operation of these processes and improve their overall performance.

Third, we will perform detailed economic assessments to evaluate the cost-effectiveness of various process configurations and solvent blends. This will help identify the most

economically viable options for large-scale CO₂ capture deployment.

Finally, we will explore the potential for integrating CO₂ capture with other technologies, such as carbon utilization and storage, to enhance the overall sustainability of the process. By combining CO₂ capture with carbon utilization and storage, we can create a more circular economy and reduce greenhouse gas emissions even further.

Conclusion

This research aims to advance the understanding of amine-based CO₂ capture processes by developing a robust thermodynamic model for the CESAR1 solvent and optimizing process configurations for energy efficiency. By leveraging rigorous modeling and simulation techniques, we seek to provide valuable insights for the design and operation of large-scale CO₂ capture plants. Ultimately, this research contributes to the development of sustainable and cost-effective solutions for mitigating climate change.

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Influence of acid wash on gas purification in post-combustion capture

(February 2023 - January 2026)

13 CLIMATE ACTION



Contribution to the UN Sustainable Development Goals

Global warming is linked to the increasing concentration of CO₂ in the atmosphere. Amine-based carbon capture processes are the most developed technology to mitigate the carbon emissions being released. A challenge of using amines as a capture solvent is the oxidative and thermal degradation byproducts, which are formed due to the presence of oxygen or the high operation temperatures. These components are highly volatile and can cause damage to human health and the environment. This project contributes to mitigate the emission of amine degradation byproducts by utilizing a packed-bed acid scrubbing column.



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Abstract

Amine-based chemical absorption is the most developed state-of-the-art technology, currently being tested in high TRL post-combustion capture pilot plants. However, amine solutions are susceptible to degradation and are corrosive to metal surfaces¹. The byproducts of amine degradation are highly volatile and are emitted with the CO₂ lean gas to the atmosphere². Several methods have been developed to treat post-combustion CO₂ lean gases, such as catalytic combustion, membrane separation, activated carbon filtration, among others. One of the more promising developing methods is the packed-bed acid scrubbing method, reaching impurity removal efficiencies up to 90%³, which is studied in this Ph.D. project.

Introduction

In recent years, there has been a strong interest in carbon capture technologies with the aim of mitigating climate change and reaching climate neutrality in the next decades. Amine-based carbon capture processes are considered to be the most developed state-of-the-art technologies for CO₂ capture. However, it is widely known that amines degrade through oxidative and thermal pathways.

Most of the byproducts produced from the degradation of amines are very harmful to the environment and human health. Due to their high volatility, they escape the system mainly with the CO₂ lean stream. In recent years, there has been an increase interest in the development of technologies to treat these components before they escape into the atmosphere, with the most promising one being the installation of an acid wash scrubbing column.



Figure 1: The mobile capture plant being commissioned at Aalborg Portland.

This study investigates the effect of pH on amine byproduct capture efficiency and aims to determine the effects on the operation of the carbon capture unit (seen in Figure 1), from a set of parametric changes in the operation of the acid wash.

Experimental work

The experiments were carried out using DTU's carbon capture plant, located in Aalborg Portland cement plant, Denmark. The flow diagram of the pilot plant is illustrated in Figure 2. The amine-based CO₂ capture pilot plant is equipped with an acid wash tower, following the absorption column, through which the treated flue gas passes. The solvent blend used for CO₂ absorption was an aqueous solution of 2-amino-2-methyl-1-propanol (AMP), promoted with piperazine (PZ). AMP/PZ is a promising absorption liquid alternative to monoethanolamine (MEA), having lower energy requirements for solvent regeneration, less corrosion and less amount of degradation compared to MEA⁴.

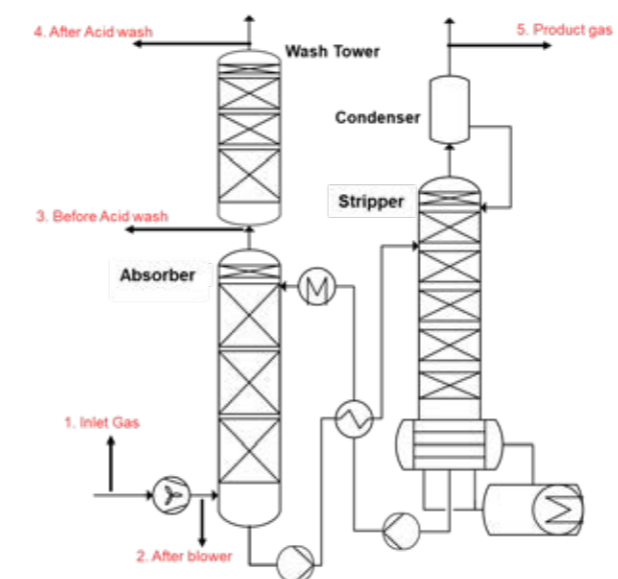


Figure 2: Process flow diagram for an absorption-desorption capture unit with an acid tower. The efficiency of a packed-bed acid scrubbing tower in reducing the amine-based contents in the treated gas stream of a post-combustion carbon capture pilot plant was evaluated. We use a high-resolution multi-component Fourier transform infrared (FTIR) gas analyzer to determine the amount of degradation products. The pH levels of the acid wash varied, and tests were performed while changing the operating parameters of the pilot plant.

The FTIR gas analyzer is connected to the pilot plant through four sampling positions. As shown in Figure 1, samples from five different gas streams

were analyzed: 1) the inlet gas, 2) after the blower, 3) before the acid wash tower, 4) after the acid wash tower (CO₂ lean gas stream) and 5) Product gas (CO₂ rich gas stream).

Conclusion

The current work concludes that the acid wash successfully reduces amines and solvent degradation compounds. The performance of the wash section is influenced by the change of acid concentration, the different flow rates and operation parameters of the thermal driven carbon capture plan.

Acknowledgements

We would like to thank the European Research Council (ERC) for funding this project under the Horizon2020 Research Program "Formate for Renewable Energy Storage (FRESH)" (Grant Agreement No. 101069605).

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Experimental and Computational Evaluation of Solvation Phenomena in Electrolyte Solutions

(May 2022 – May 2025)

9 INDUSTRY, INNOVATION AND INFRASTRUCTURE



Contribution to the UN Sustainable Development Goals

Solvation constitutes a major topic of research in electrolyte solutions, with applications in electrical power storage, water processing, protein engineering and more. Despite the development of many models and the computational assessment of solvent-solute interactions, the current description of more complex systems is limited in terms of accuracy. This project aims to gather and develop experimental methodologies in IR spectroscopy for the estimation of useful properties in solvation modelling.



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Abstract

The water-ethanol binary system has a strong presence in many industrial, biotechnology and food applications. As evidenced from its thermodynamic properties, its physical picture on the molecular level is incredibly complex as well as the topic of several scientific works focusing on hydrogen bonding, the defining feature of hydroxyl-containing solvents. In order to obtain a deeper understanding of hydrogen bonding on the binary system, a combined study that utilizes IR spectroscopy on water/deuterated ethanol and quantum mechanics calculations is carried out that provides an estimate of the ethanol donor hydrogen bond strength profile dependent on the system composition.

Introduction

The water-ethanol binary system exhibits unique intricacies in its macroscopic thermodynamic properties that reflect its complex molecular interactions manifesting primarily as hydrogen bonding. A very notable excess property profile is the excess entropy solution, which seems to be irregular when the comparison to other lower alcohols is made. Given that entropy is tightly connected to structure, there have been systematic efforts on the investigation of several solvation regimes that arise at different compositions, suggesting that the water-ethanol system is microheterogeneous in the liquid phase [1].

From a spectroscopic point of view, a simple but invaluable tool for the extraction of meaningful information on hydrogen-bonding systems is the Badger-Bauer rule [2]. Originating from the early days of infrared spectroscopy in the 1930s, the rule describes the linear correlation between hydrogen bonding enthalpy and the peak redshift of -X-H stretching bands of hydrogen bonding compounds.

Specific Objectives

- Determination of the ethanol donor hydrogen bond (HB) profile over the entire composition range of the binary system at room conditions.
- Estimation of implicit solvation model effects on intermolecular interactions.

Results and Discussion

The density and ref. index values at room conditions are measured for the entire composition range of water/deuterated ethanol-OD solutions. The mid-infrared spectra of the OH and OD stretching bands are subsequently measured (Figure 1) using the Attenuated Total Reflectance (ATR) sampling method in order to mitigate the band saturation issue that is known to appear in hydroxyl-containing substances. The deuteration of ethanol's hydroxyl group allows the isolation of its corresponding, rendering the recording of its peak shift possible. From the interpretation derived from the Badger-Bauer rule, it is deduced that the ethanol donor hydrogen bond is weakening as ethanol-OD is diluted with

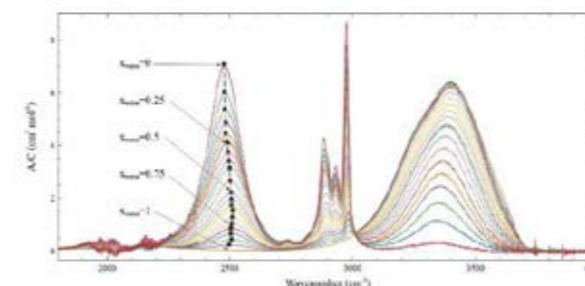


Figure 1: ATR-IR spectra of water/ethanol-OD solutions in room conditions.

water, with this behavior inverting after ethanol-OD is further diluted past the 3:1 water:ethanol-OD ratio. For the quantification of the hydrogen bonding strength change, DFT calculations on water/ethanol clusters are conducted. Two clusters are considered, reflecting pure ethanol and ethanol at infinite dilution. The IEFPCM solvation model is applied in order to render the quantum calculation results relevant to the condensed phase. The B3LYP functional paired with Grimme's D3 dispersion correction term [3] was found to be aligned with higher-level method results. Energetic values can be calculated by designating fragments and then recording their individual interaction energy arising from their dissociation. Following the same procedure for interaction enthalpies that are obtained from room temperature frequency calculations, the ethanol donor hydrogen bond energies are determined (Table 1).

Table 1: Ethanol donor hydrogen bond energetic values (B3LYP-D3/aug-cc-pVDZ, in kcal/mol).

Cluster	Electronic energy	Enthalpy
Pure ethanol	-13.04	-6.97
Ethanol at infinite dilution	-8.98	-6.26

Judging from the two extreme cases, it can be observed that the addition of water in ethanol leads to the weakening of the ethanol donor hydrogen bond. By employing the linear correlation between peak shifts and hydrogen bond enthalpies, the combination of the quantum calculation estimations and the experimentally observed peak shifts is feasible. Figure 2 depicts the ethanol donor hydrogen bond profile as a function of the solution composition. A maximum appears at $x_w = 0.74$, indicating that the ethanol donor HB is weakest at this specific composition. This feature coincides with the minimum in the excess entropy profile, hinting at unique structural

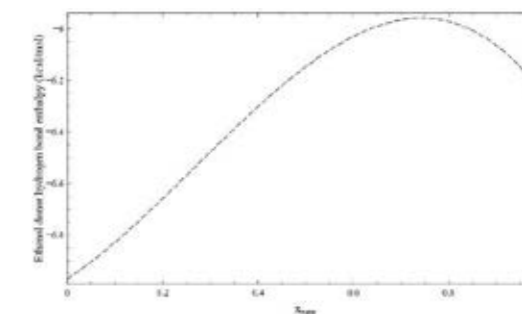


Figure 2: Ethanol donor hydrogen bond enthalpy as a function of water mole fraction.

phenomena. The application of the IEFPCM model to connect the quantum calculation results to the condensed phase has direct effect on the lowest-energy cluster geometry, although a variation of the implicit solvent properties revealed had no effect on the hydrogen bonding strength, suggesting that the primary environmental driver is HB cooperativity.

Conclusions

A maximum has been observed in the composition-dependent ethanol hydrogen bond enthalpy profile. Quantum calculations have been conducted in order to provide a quantitative estimation of the hydrogen bonding interaction enthalpy. A sweep on the implicit solvent properties revealed the HB independence of the HB strength from long-range interactions, highlighting the cooperative nature of hydrogen bonding systems.

Acknowledgements

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List of Publications

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Scaling-up Trickle Bed Bioreactors for high-rate gas fermentation

(January 2022 – January 2025)

7 AFFORDABLE AND CLEAN ENERGY



Contribution to the UN Sustainable Development Goals

Surge in the consumption of natural gas due to exponential increase of energy demand and incineration or degradation of organic waste leading to release of CO and CO₂ into the atmosphere have driven researchers to venture the production of alternative renewable energy source. Syngas fermentation technology aims to create a biobased circular economy for conversion of 2nd generation lignocellulosic biomass and other recalcitrant organic wastes to biofuels such as biomethane which can be directly supplied to the natural gas grid and reduce greenhouse gas emissions derived from usage of fossil fuels.

Abstract

Syngas fermentation in a trickle bed reactor (TBR) using mixed microbial consortia has reached a technology readiness level of 4–5 for biomethane production. Understanding the rate-limiting step—whether mass transfer or microbial growth kinetics—is crucial to optimize scaling up. This work presents a model able to simulate microbial growth, biofilm formation, and mass transfer in TBR. The model was validated using experimental results and it predicted enhanced CO conversion efficiency with biofilm formation, both in lab- and pilot-scale TBR. The model also revealed a threshold liquid Reynolds number of 35, where mass transfer limitations shift to microbial growth limitations.

Introduction

Syngas and CO₂ biomethanation in TBR using mixed microbial cultures has reached a technology readiness level of 4–5 [1]. While this technology has great potential not only for biomethanation but also for syngas biological conversion to higher-value liquid products, scaling-up has been more intuitive than calculation-based. Optimizing mass transfer and microbial kinetics is key. Thanks to our previous work [2,3], the volumetric mass transfer coefficient may be predicted as a function of TBR operational and geometric characteristics, and the mass transfer regime may be simulated using a dynamic model able to predict mass transfer in TBR as a function of reactor operational parameters. The next step is integrating microbial growth and biofilm formation kinetics into the model.

Syngas biomethanation in a TBR using mixed microbial consortia (MMC) is highly efficient and advantageous, as it eliminates the need for sterilization and avoids contamination risks. Various microbial groups, readily available from biogas plants, support the anaerobic conversion of syngas to methane (CH₄) via diverse metabolic pathways. Hydrogenotrophic methanogens convert H₂ and CO₂ into CH₄, while carboxydrotrophic methanogens directly convert CO to CH₄ and carboxydrotrophic hydrogenogens convert CO to H₂ and CO₂ (biological water-gas shift reaction) [4]. Temperature significantly influences microbial

activities and interactions. MMC enriched under thermophilic conditions (60°C) exhibit higher CH₄ productivity and a simplified metabolic network where CO is first converted through the biological water-gas shift reaction and then hydrogenotrophic methanogens convert H₂ and CO₂ to CH₄ [5]. The present study focuses on the rate-limiting biological water-gas shift reaction.

Specific Objectives

- Development of a model able to simulate the growth and biofilm formation of carboxydrotrophic hydrogenogens together with hydraulic and mass transfer behavior of TBR and experimental validation of it.
- Comparison of CO conversion efficiency in a conventional gas-sparged chemostat (CSTR) and TBR with microbes growing in suspension and (only for TBR) in biofilm.
- Investigation of the effect of operating parameters on the overall performance of the TBR.

Results and Discussion

The already developed dynamic TBR model for the hydraulic and mass transfer behavior of the TBR [3] was expanded with the inclusion of microbial growth (and biofilm formation (carboxydrotrophs) on the packing material of the reactor (Figure 1). The expanded model was validated by comparing the model-predicted CO conversion efficiency with experimental data from literature [5] and used for



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the simulation of pilot-scale and lab-scale TBR where biological water-gas shift reaction took place.

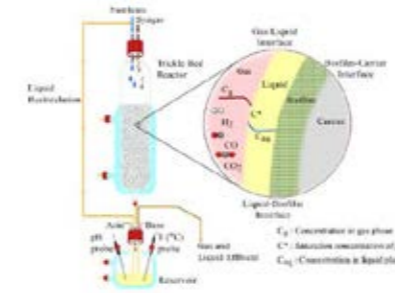


Figure 1: Schematic diagram showing biofilm formation within the TBR.

Figure 2 illustrates the experimental values and model-predicted values of CO conversion efficiency with empty bed residence time (EBRT). It was observed that the model accurately predicted the CO conversion efficiency with an R² of 0.98 (for pilot-scale TBR) and 0.99 (for lab-scale TBR).

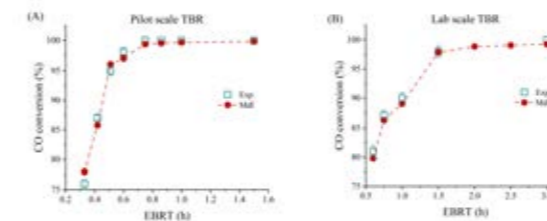


Figure 2: Comparison of experimental (Exp) and Model (Mdl) estimated values of CO conversion vs EBRT for pilot-scale TBR (A) and lab-scale TBR (B).

The model was further used to simulate a lab-scale TBR (0.22 L packed bed volume), a pilot-scale TBR (5 L packed bed volume), and a CSTR (5 L liquid volume) at the same EBRT of 45 min and liquid retention time of 8 days with attached growth in biofilm for the pilot- and lab-scale TBRs and in suspended growth for the CSTR. Figure 2 shows that the pilot-scale TBR outperformed both lab-scale TBR and CSTR based on CO conversion efficiency. Additionally, the lab-scale TBR with 22 times lower working volume than the CSTR, reached 4 times higher CO conversion efficiency. Finally, the simulations for CO conversion efficiency in the pilot- and lab-scale TBR under variable liquid flow through the bed revealed that at Re_L values higher than 35, the CO transfer rate becomes higher than the CO consumption rate (Figure 3) i.e., microbial growth became the rate-limiting step in place of mass transfer.

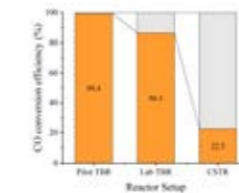


Figure 2: Comparison of CO conversion efficiency of pilot-scale TBR, lab-scale TBR, and CSTR.

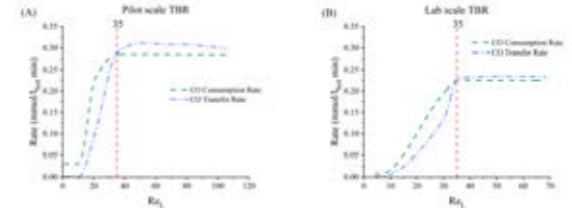


Figure 3: Simulated CO consumption rate and transfer rate in pilot-scale TBR (A), and lab-scale TBR (B) under various liquid Reynolds numbers (Re_L).

Conclusions

This study resulted in the development of a dynamic model for TBRs. The model combines microbial growth kinetics, biofilm formation, hydraulic behavior, and mass transfer phenomena and was able to simulate the biological water-gas shift reaction in TBR. The model can be applied to various reactor scales and operating conditions for the biological conversion of syngas and CO₂ to valuable chemicals.

Acknowledgement

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Chemical resistance and solvent absorption characteristics of coatings for sustainable fuels

(May 2024 – April 2027)

9 INDUSTRY, INNOVATION AND INFRASTRUCTURE



Contribution to the UN Sustainable Development Goals

Industries adopting sustainable fuels like methanol will require advanced solutions to safeguard their metal infrastructure from the corrosive effects of this energy source. Development of methanol-resistant epoxy coatings will lead to more durable fuel storage facilities and will thereby enable wider adoption of sustainable fuels, resulting in reduced environmental impact and advancement towards sustainable industrial practices. To achieve that, understanding how solvent absorption causes chemical and structural changes is crucial.



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Abstract

The upcoming shift towards sustainable fuels will require the modification of engines, storage tanks and other components of existing systems. Moreover, industries are facing new challenges due to the corrosive properties of sustainable fuels such as methanol, free fatty acids, or ammonia, which can create harsh environments. To mitigate these effects and protect metallic surfaces, the use of chemically resistant epoxy coatings is of particular interest. Therefore, the primary goal of the project is to gain a deep fundamental understanding of the chemical processes triggered by various sustainable fuels in different epoxy systems and to develop new coatings that can withstand aggressive environments.

Introduction

Global greenhouse gas emissions have been a matter of concern for the last few decades, due to their negative impact on the environment. For instance, maritime transportation accounts for 2,6 % of worldwide greenhouse gas emissions [1]. Consequently, the International Maritime Organization has imposed increasingly stringent international regulations to reduce greenhouse gas emissions from global maritime shipping operations by at least 50% by 2050.

To achieve this goal, sustainable fuels, including methanol, ammonia, hydrogen, or free fatty acids, have emerged as pivotal solutions. These fuels offer lower carbon emissions and contribute to cleaner air. For example, the shipping industry has shown keen interest in methanol (CH_3OH). This simple alcohol with a high hydrogen-to-carbon ratio stands out as a low-carbon, clean-burning fuel. In fact, Maersk is already starting to use methanol in Denmark, having produced the world's first container vessel powered by methanol, as shown in Figure 1 [2].



Figure 1: The first methanol-powered ship [2].

However, methanol is a polar molecule with conductive properties that can cause galvanic corrosion on metal surfaces, creating risks for carbon steel tanks. This corrosion in fuel storage tanks leads to billions of dollars in annual costs for repairs and replacements. In this context, barrier coatings play a crucial role in protecting metallic structures from aggressive environments, prolonging their lifespan, particularly important in challenging environments like chemical storage tanks.

Among the various types of barrier coatings, epoxy coatings offer one of the most effective solutions for corrosive environments and have proven to have high chemical resistance [3]. In particular, bisphenol-based epoxy-amine systems

and epoxy novolacs are known for their strong chemical resistance, making them ideal for protecting surfaces in chemically harsh environments. The chemical resistance of epoxy is determined by a combination of many factors, where crosslinking density, free volume and polarity seem to be the most important properties to control in a coating [4].

However, when a coating is exposed to an aggressive chemical, degradation will take place. There are two types of degradation, physical and chemical, which can occur separately or simultaneously. Physical degradation involves the diffusion of the penetrant through a coating, causing swelling, loss of flexural strength, blistering, delamination, etc (Figure 2). In contrast, chemical degradation involves the reaction of the aggressive chemical with the coating network. The common assumption is that physical degradation is the determinant factor of degradation, followed by chemical degradation [5].



Figure 2: Coated steel surface exhibiting a blistering defect [6].

While significant progress has been achieved in understanding the degradation of organic coatings exposed to chemicals, gaps in knowledge still exist in this field. Most existing research has predominately focused on water and electrolyte-induced degradation, with less attention paid to the effects of organic molecules like methanol, which has been proven to be particularly aggressive towards epoxy coatings. Therefore, understanding the degradation mechanism and interactions between methanol and epoxy coatings is essential for developing more durable, high-performance coatings capable of meeting the demands of future industrial applications.

Specific Objectives

The objectives of this project are:

- Understand the interactions between methanol and the epoxy coating
- Develop a method to track the chemical changes suffered by the coating after methanol exposure
- Investigate the effect of different sustainable fuels in the epoxy coatings,

such as ammonia and free fatty acids-based fuels

- Optimize the performance of epoxy coatings used for methanol exposure

Acknowledgements

This project is funded by the Hempel Foundation for Coating Science & Technology and is in collaboration with Hempel A/S Denmark and Hempel A/S Spain.

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Silicone-Glycerol Foams for Treatment of Chronic Cavity Wounds

(March 2022 – March 2025)

3 GOOD HEALTH AND WELL-BEING



Contribution to the UN Sustainable Development Goals

Globally, close to 50 million people suffer from chronic wounds. The patients experience a reduced quality of life [1], a high mortality rate, and a risk of amputation [2]. This work focuses on developing a silicone-glycerol foam for the treatment of chronic wounds. The foam improves the treatment of patients by delivering a perfect fit to the wound bed, absorbing exudate, and retaining the fluid in the dressing upon removal. Improving treatment of chronic wounds promotes UN sustainability goal 3 which is focused on ensuring good health and well-being for all.



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Abstract

This work introduces a novel approach to chronic wound treatment: A silicone-glycerol foam wound dressing. The silicone-glycerol formulation is applied directly into a wound cavity, whereafter it foams and cures. After curing, the foam has been shown to absorb artificial wound fluid corresponding to $76 \pm 13\%$, $126 \pm 7\%$, and $180 \pm 9\%$ by weight after 1 day, 3 days, and 7 days, respectively. The foam retains $98 \pm 0.5\%$ of the absorbed liquid during a 50% compression, indicating that the foam will retain the fluid during removal of the dressing. The in-situ foaming technique ensures a perfect fit to the wound bed, and the absorption prevents exudate pooling in the wound.

Introduction

Cavity wounds are a sub-group of chronic wounds consisting of deep, hard-to-heal wounds. This work focuses on developing a wound care dressing tailored to cavity wounds. Conforming the wound dressing to the wound bed prevents wound exudate pooling since a well-fitted dressing absorbs exudate instantly. Avoiding exudate pooling is important since pooling can lead to maceration and worsening of the wound. Furthermore, a well-fitted dressing reduces biofilm formation and thus lowers the risk of infection [1]. Current solutions for treating cavity wounds include the products 'Exufiber' produced by Mölnlycke and 'Biatain' from Coloplast. Exufiber is folded into the wound bed; when the dressing absorbs exudate, it swells up and turns into a gel. The expansion and increased flexibility of the dressing improves the fit to the wound [3]. The Biatain wound dressing is applied on top of the wound. When exudate pools up and reaches the dressing, the dressing expands into the wound. However, Biatain can expand a maximum of 2 cm [4]. Neither of the dressings conforms to complex wound shapes.

In this work, we developed a silicone-glycerol foam to improve the fit of the wound dressing to the wound bed. The developed foam is applied as

a viscous liquid via a multicomponent syringe. The mixture is applied directly into the wound cavity, where it foams up, fills out the cavity, and cures in situ, ensuring a perfect fit to the wound bed and efficient exudate absorption. The dressing can be removed in one piece while retaining exudate.

Specific Objective

The specific objective is to develop a wound care dressing that improves the treatment of cavity wounds. The dressing should:

- Conform fully to the wound cavity
- Absorb wound exudate
- Retain wound exudate in the dressing upon dressing removal

Results and Discussion

Conforming to the cavity

The conformity of the wound dressing to a wound bed was tested on a piece of pork belly bought in the supermarket. Superficial cavities of less than 1 cm in depth and deep cavities of more than 2 cm in depth were cut.

The silicone-glycerol formulation was added to the cavities cut in the pork belly in liquid form. The formulation cured in 30 minutes at 35 °C. The foam was solid and could be removed from the

cavities in one piece without leaving residue in the wound. The foam conformed to both the superficial wounds and the deep cavities, as shown in Figure 1.

Furthermore, the curing in the presence of water was investigated by filling the cavities with water before applying the formulation. The results showed that the silicone-glycerol formulation could cure under wet conditions, replicate the shape of superficial and deep cavities, and be removed in one piece without leaving residue in the wound.

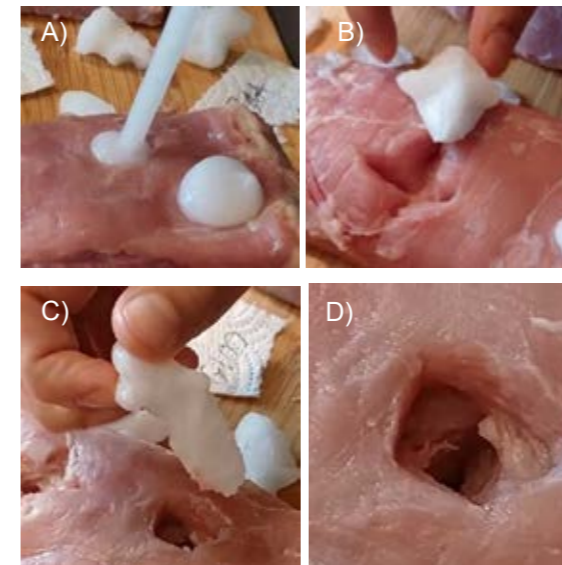


Figure 1: A) The application of the wound dressing, B) the dressing after removal showing perfect conformation to superficial wounds, C) the dressing removed from a deep wound, and D) the deep wound after removal showing no residue left in the wound.

Exudate absorption

The absorption properties of the foam were examined in a free swelling test. A free swelling test is an absorption test where the sample has no dimensional constraints, allowing for expansion in all directions. 2 g silicone-glycerol foam samples were immersed into artificial wound fluid (composition: 0.368 g CaCl₂ and 8.298 g NaCl dissolved in 1 L demineralized water). The weight increase of the foams was measured after 1, 3, and 7 days, simulating a wear time of up to 7 days. The foams absorbed $76 \pm 13\%$, $126 \pm 7\%$, and $180 \pm 9\%$ of the initial weight after 1 day, 3 days, and 7 days, respectively, indicating the ability of the foam to absorb wound exudate over extended time.

Exudate retention

The liquid retention in the silicone-glycerol foam was investigated to ensure that wound exudate does not come in contact with healthy skin or the wound during the dressing removal. The foams

absorbed artificial wound fluid in a free swelling test as described under the Exudate Absorption section. The foam was removed from the artificial wound fluid after 3 days of absorption, the surface was dried with tissue paper, and the weight was recorded. The foam was compressed 50% of the sample height by using an ElectroForce 3220 from TA instruments. After compression the foam was dried with tissue paper and the new weight was recorded. The foam retained $98 \pm 0.5\%$ of the absorbed liquid during compression, illustrating the foam's excellent fluid retention properties.

Conclusion

It was demonstrated that a silicone-glycerol foam could provide a perfect fit to a simulated wound bed due to the in-situ foaming and curing. The foam replicated the shape of superficial and deep cavities in a pork belly both in dry and wet conditions. The formulation cured in 30 minutes at 35 °C and could be removed in one piece without leaving residue in the wound bed. The foam could absorb $76 \pm 13\%$, $126 \pm 7\%$, and $180 \pm 9\%$ of the initial weight after 1 day, 3 days, and 7 days, respectively, illustrating the absorption capabilities of the foam. During a compression of 50% of the sample height, the foam retained $98 \pm 0.5\%$ of the absorbed fluid, indicating good fluid retention properties.

Funding

This project was funded by DTU proof of concept, SPARK Denmark, and NNF Pioneer.

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Characterization and modification of pore size distribution in epoxy intumescent chars

(May 2022 – May 2025)



Contribution to the UN Sustainable Development Goals

Intumescent coatings serve as passive fire protection systems for steel structures used in buildings and offshore platforms. Ensuring a correct performance of these coatings is essential for safeguarding people's security in the event of a fire. The heat-insulation properties of the intumescent char rely heavily on its internal porous structure. Gaining a deep understanding and control of the morphology of the char will aid in the formulation of reliable products which can contribute to build safer places for society.



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Abstract

Previous studies demonstrate the significance of pore morphology on the thermal insulation properties of intumescent chars. Developing methods for analyzing, from a quantitative perspective, the porous structure of intumescent chars can provide meaningful information for understanding and optimizing their performance in real fire scenarios. In this project, a new method, based on image-processing techniques and pore-identification algorithms, has been developed to quantify the porous structure of intumescent chars. The method has been used to examine the effects of parameters such as heating rate and testing conditions. Currently, experiments in a novel set up available at CoaST are being performed to evaluate coating-formulation strategies to modify the structure of intumescent chars.

Introduction

One of the major risks during a fire is the collapse of buildings and other platforms. Steel beams supporting a structure can lose about 40 to 60% of its load bearing capability when exposed to temperatures above 500 °C. Hence, it is important to establish an effective fire protection measure for the structural steel to enhance its resilience in the event of a fire [1]. Intumescent coatings are one of the most interesting solutions. When they are exposed to high temperatures, they swell due to a series of chemical reactions. As a result, the coating transforms into a porous char that insulates thermally the steel beam [1].

Interestingly, a high expansion of the initial coating does not guarantee a good insulation performance [2]. Other structural parameters, such as porosity and pore size, influence significantly the thermal behavior of these materials. Micro-size pores are excellent for reducing the thermal conductivity [3]; however, an excessive coating expansion can enlarge considerably the pores. Achieving the ideal char appears to involve finding a balance between pores size, shape, porosity, and expansion.

The goal of this project is to quantify the porous structure of intumescent chars. The research output would provide valuable insights into

achieving the optimal balance between pore size, porosity, and char expansion. Furthermore, this information would offer guidance on effectively controlling char growth.

Methodology

Simulation of fire scenarios

The intumescent coatings in this project are exposed to standardized heating rates which replicate specific types of fire. Examples of this are the UL-1709 or the ISO 834 standard fire curves. Additionally, the coatings are exposed to non-standard heating curves.

For this purpose, the CoaST fire set up, developed by CoaST group in DTU is used. A more detailed explanation can be found in the work carried out by Jochen et al. [4]. Lab-scale electric furnaces are also employed in this project. The CoaST group adapted an electrical furnace, which can achieve standardized heating curves

Characterization of the internal structure

Image recording techniques are used to map and quantify the internal structure of intumescent chars. The method proposed in this project is fluorescent microscopy, as it has been proven to be an effective method [5]. Results are compared with other image recording techniques such as Scanning Electron Microscope.

Results and discussion

The images captured from the fluorescent microscopy show the complexity and the high interconnectivity among pores in intumescent chars. The challenge arises during the identification of each pore unit, because there does not exist a universal definition to delineate pore boundaries [6]. There are available automatic algorithms that interpretate the pore space in different approaches. Nevertheless, they show some limitations related to the lack of pore shape estimation or the oversegmentation of long elliptical pores, highly present in intumescent chars. The former restriction is represented in the pore size map depicted in Figure 1a.

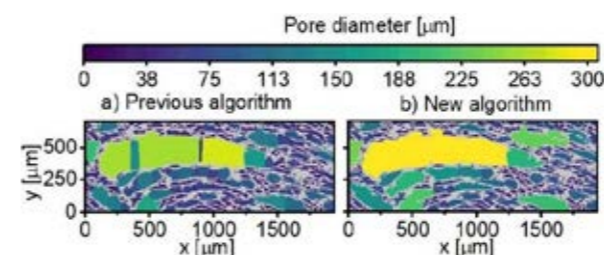


Figure 1. Pore diameter map obtained by the two methods. Each color represents a pore unit except the grey colored areas, which depicts the pore walls

To represent the pore space more realistically from a structural point of view, we propose a new method based on previous models [6]. Figure 1b shows the results of this method. It is noticeable that the oversegmentation has significantly decreased, especially in the big area colored yellow in Figure 1b.

This method allows a better and more realistic recognition of the morphology of long elliptical pores, which theoretically has significant contributions in both thermal and mechanical properties of the intumescent chars. Besides, the method is capable to measure a wide variety of pores, ranging from 1 μm to 8 mm.

The new method has been used to analyse different intumescent chars generated at different heating rates. This allows a deeper understanding of how these materials behave in different fire scenarios. Figure 2 illustrates the outcomes from this analysis.

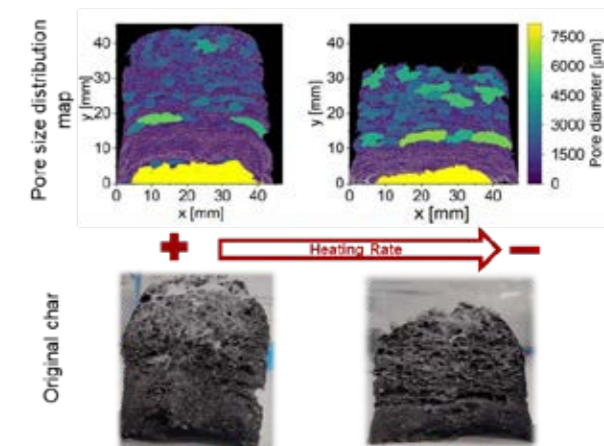


Figure 2. Pore diameter map and original images of two intumescent chars generated at different heating rates.

The results reveal the stratified structure of intumescent coatings, showing the largest pores in the top layers. The influence of heating rate varies depending on the layer analyzed. The pores in top layer decrease in size under fast heating rate while the effect in the pores of the bottom layer is the opposite. The exact mechanisms driving this phenomenon remain unclear.

Conclusions and future work

In this project, a new model has been developed to quantify the porous structure of intumescent chars, with potential applications to other porous materials. The automatic recognition of each pore improved compared to previous methods.

This technique has been employed to examine the influence of heating rate on these materials. Future work will focus on linking the pore growth with the chemistry of the initial coating.

Acknowledgements

The authors acknowledge the financial support of the Hempel Foundation and Hempel A/S.

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Digitalization of downstream process design and development

(May 2022 – May 2025)



Contribution to the UN Sustainable Development Goals

Digitalization of downstream processes can yield significant reductions in production costs and utilities as it can enable state-of-the-art process concepts such as real-time optimization and model predictive control. It can also ease implementation of more complex continuous processes. One area where the potential of continuous processes has not been reached is chromatography. Being an essential unit operation in the biopharmaceutical industry, most chromatography units are run in batch-mode despite the many benefits from running in continuous mode, eg. reduced utilities. This project aims to show how digitalization of continuous chromatography can be realized.



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Abstract

Chromatography is essential for purifying biopharmaceutical products and proteins. Continuous chromatography offers increased productivity and reduced solvent usage compared to traditional batch methods, but its implementation is complex, requiring multiple columns in series or parallel configurations. Modeling continuous chromatography is computationally intensive due to the need to solve partial differential equations (PDEs), particularly for simulated moving bed (SMB) systems. To address this, advanced solvers like the Discontinuous Galerkin spectral element method (DGSEM) have been developed. While C++ provides high computational performance, it is complex to program. Julia, a high-level language that generates fast machine code, offers a balance of ease of use and performance. The CADET-Julia package simplifies the implementation of new isotherm models for chromatography, facilitating rapid prototyping and high-performance computation.

Introduction

Chromatography plays a pivotal role in the purification of biopharmaceutical products and proteins. Continuous chromatography stands out as a promising approach to boost productivity while minimizing solvent usage compared to traditional batch chromatography. However, the implementation of continuous chromatography is notably intricate. It necessitates the utilization of multiple columns arranged in series and/or parallel configurations within open or closed loops (Schmidt-Traub et al., 2020).

While modeling can guide the design and operation of continuous chromatography, it is essential to acknowledge the computational challenge posed by solving the underlying partial differential equations (PDEs). The simulation time required for these models can be substantial. Notably, for the simulated moving bed (SMB), the simulation time can become

significant as all columns must be solved simultaneously until cyclic steady state (He et al., 2020).

The prolonged simulation times underscore the need for fast solvers. To address this challenge, Meyer introduced an arbitrary order Discontinuous Galerkin spectral element method (DGSEM) for solving the general rate model in batch chromatography (Meyer et al., 2020). Recently, Breuer derived a slightly different DGSEM variant and implemented it using C++. The resulting code is open-source and publicly accessible through the CADET-Core software (github.com/modsim/CADET) (accessed 28/02/2024) (Breuer et al., 2023; Leweke & von Lieres, 2018).

While C++ is a programming language renowned for its high computational performance, it is a low-level compiled language and thus

demands more programming expertise compared to languages such as Python. In contrast, Python is a dynamic high-level programming language that is easy to use but at the expense of lower computational performance. Meanwhile, the programming language Julia leverages the advantages of C++ and python as it is a dynamic, high-level programming language that simultaneously generates fast, low-level machine code. Furthermore, Julia has a broad range of Ordinary Differential Equations (ODE) solvers for stiff problems (Rackauckas & Nie, 2017), which are often encountered in chromatography modelling (Kumar & Lenhoff, 2020).

The CADET-Core is a fundamental system solver with various unit operations including chromatography columns, crystallization, filtration, reactions etc. It supports arbitrary sequence and networks of unit operations, tubes, valves, tanks etc. Given the extensive functionality and complex codebase, there is a need for more agile and accessible code. For example, the two most used isotherm models, the steric mass action isotherm for ion-exchange chromatography and the Langmuir isotherm, cannot always explain resulting chromatograms (Kumar & Lenhoff, 2020). Especially for complex chromatography modes with various adsorption phenomena present, such as mixed-mode chromatography, the knowledge base and selection of isotherm models available is limited (Kumar & Lenhoff, 2020). Thus, to mathematically describe the adsorption behavior accurately, new isotherm models are needed. To implement isotherm models easily while maintaining high performance computation of chromatography models, the CADET-Julia package was developed. The Julia package has implemented the DGSEM for chromatography models in a simplified codebase with ease of implementation of new models for rapid prototyping and customized isotherms. The ease of implementing new isotherms is demonstrated by the fact that specifying the analytical Jacobian is not necessary to achieve very high solver performance. Hence, the isotherm models can be specified arbitrarily and take many factors into account. The CADET-Julia code can be found on Github (github.com/cadet/CADET-Julia) (accessed 28/02/2024).

Conclusion

Continuous chromatography represents a significant advancement in the purification of

biopharmaceuticals, offering enhanced productivity and reduced solvent usage. However, its complexity and the computational challenges associated with modeling necessitate advanced solvers. The development of the DGSEM and its implementation in Julia through the CADET-Julia package addresses these challenges by providing a high-performance, user-friendly platform for rapid prototyping and customization of isotherm models. This innovation not only simplifies the implementation process but also ensures high computational efficiency, making it a valuable tool for advancing chromatography techniques.

Acknowledgements

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Liquid coatings without the use of solvents

(April 2022 – March 2025)



Contribution to the UN Sustainable Development Goals

Due to the extensive surface areas, industrial coatings, such as those used for ships, are typically applied via spraying. To facilitate spraying, volatile organic compounds (VOCs) are incorporated into the coatings to reduce the viscosity. Upon drying, the VOCs evaporate, releasing toxic compounds into the environment. This project proposes a strategy to incorporate low-viscosity cyclic siloxane into siloxane coatings, thereby reducing viscosity without using VOCs. The cyclic siloxane will remain part of the dried coating, ensuring no emission of harmful substances.

Abstract

The main challenges in the study of cyclic polymers are their synthesis and the verification of their structure. This study proposes a method to synthesize single cyclic siloxane as well as concatenated ring elastomers. Subsequently, techniques to confirm the cyclic nature of the products are discussed. End-group analysis and hydrodynamic volume is suggested as analysis methods for single cyclic siloxanes. For networks, analysis of tensile properties is proposed as a method to determine if the elastomer is concatenated rings as they should be softer than classical elastomers.

Introduction

Cyclic polymers, also known as ring polymers, are polymers without chain ends. The lack of chain ends results in an endless structure that significantly alters the dynamics of cyclic polymers compared to linear polymers. For linear polymers, the movement of end groups, known as reptation, plays a crucial role in their mobility. However, cyclic polymers are incapable of reptation. This affects their mobility and results in unique properties [1], such as lower viscosity and reduced hydrodynamic volume [2,3].

Siloxane polymers are typically viscous and can be chemically crosslinked to form a network structure, resulting in an elastic material known as an elastomer. An intriguing aspect of cyclic polymers is the type of networks they can form. One can envision a network composed entirely of cyclic polymers, where the polymers are crosslinked through physical constraints arising from the concatenation of cyclic molecules, see Figure 1. Additionally, a network combining linear and cyclic polymers, where linear polymers thread the cyclic polymers, can also be envisioned. Over the past decades, there has been considerable debate regarding the impact of incorporating cyclic polymers into an elastomer and how the resulting properties will be affected. However, cyclic polymers can only be produced in small scale, thus experimental research in this area has been minimal [4,5].



Figure 1: A concatenated ring elastomer.

One of the main challenges in working with cyclic polymers is proving their cyclic nature. The chemical difference between a linear polymer and a cyclic polymer is the presence of end-groups. In polymers with many repeating units and only two end-groups, these end-groups can be difficult to detect using techniques like nuclear magnetic resonance spectroscopy (NMR) and Fourier-transform infrared spectroscopy (FT-IR). For cyclic polymers not part of a network, a lower hydrodynamic volume can indicate ring structures. Proving the existence of rings within an elastomer is more challenging. No definitive method exists, and the best evidence comes from analyzing the mechanical properties of the elastomers.

Specific Objectives

The objectives for this project are:

- (1) Synthesis of cyclic siloxane.
- (2) Development of a method to incorporate cyclic siloxanes into elastomers.
- (3) Investigate the properties of concatenated ring elastomers in terms of application in coatings.



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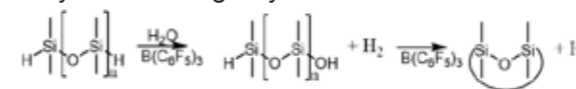
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Results and Discussion

Synthesis and analysis of cyclic siloxanes

The Piers-Rubinsztajn reaction, described in J. Tran's work [6] and shown in Scheme 1, was used to synthesize single cyclic siloxane.



Scheme 1: Ring formation by Piers-Rubinsztajn reaction.

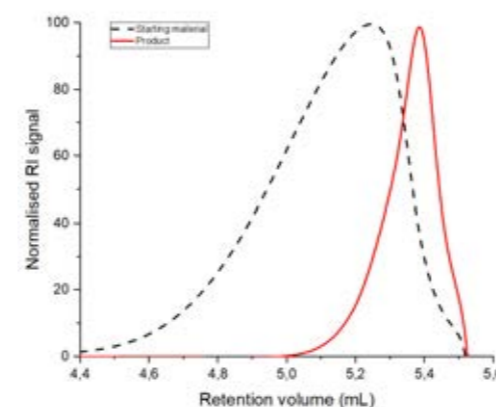


Figure 2: SEC results of product from the Piers-Rubinsztajn reaction.

Figure 2 presents the results from size exclusion chromatography (SEC) of the starting material and the product of the reaction displayed in Scheme 1. The retention volume of the product is higher than the starting material meaning that the hydrodynamic volume is lower, indicating cyclic polymers. Additionally, no end-groups were detected in either NMR or FT-IR analyses. The absence of end-groups combined with the reduced hydrodynamic volume provides strong evidence for the presence of cyclic polymers.

Concatenated ring elastomers

A divinyl-telechelic siloxane polymer and a dihydride-telechelic siloxane polymer were mixed with a platinum catalyst and cured into an elastomer. Theoretically, two difunctional polymers should not result in a cured elastomer but in a long polymer chain with a viscous nature. The formation of a concatenated ring elastomers, as shown in Figure 1, would explain this phenomenon, and in Figure 3, the proposed reaction scheme is shown.

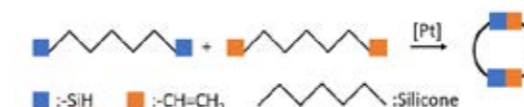


Figure 3: Ring formation by a platinum-catalyzed reaction between dihydride-telechelic siloxane and divinyl-telechelic siloxane.

It has been proposed [7] that concatenated ring elastomers are softer and more stretchable than classical elastomers due to their bonds being physical constraints rather than chemical bonds. The ultimate elongation of the prepared elastomer with cyclic siloxanes was determined from tensile

testing and compared to a classical chemically crosslinked network. The results are shown in Table 1. The maximum elongation results show that concatenated ring elastomers can be stretched more than 2000 %. Furthermore, when comparing Young's moduli for the two types of elastomers, the concatenated ring elastomers prove much softer than the classical elastomer. These results indicate a network structure consisting of cyclic polymers.

Table 1: Tensile testing of a concatenated ring elastomer and a classical elastomer.

Type of elastomer	Young's Modulus [MPa]	Maximum elongation [%]
Classical	0.207	150
Ring	0.073	2260

Conclusion

Single cyclic siloxane that are not bound in a network can be analyzed using end-group analysis and SEC. Proving the structure of a concatenated ring elastomer is more complicated. Here, the first indication that the prepared materials indeed consist of concatenated rings is that they stem from starting materials that should not be able to form networks. Further, the mechanical properties show extreme softness and stretchability compared to a classically elastomer, indicating a material based on a ring structure.

Acknowledgments

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Electrochemical regeneration of solvents for CO₂ capture

(January 2023–December 2026)



Contribution to the UN Sustainable Development Goals

One of the keys to ensure that society reaches UN's 13th sustainable development goal of climate action is to lower carbon emissions. The emissions from the use of fossil fuels are one of the main factors driving climate change, which needs to change. Carbon Capture and Storage (CCUS) may be one of many key components of limiting these emissions. This project investigates a novel technology of regenerating the solvent that is used for carbon capture, which lowers the energy requirements of a CCUS setup as well as increases the flexibility. By combining it with renewable energy, this technology may help to increase sustainable consumption of overproduction by renewable energy sources.



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Abstract

A novel setup, which regenerates solvent for CO₂ capture electrochemically has been built. This setup is a scale-up based on previous laboratory experiments. The electrochemical cell has an area of 100 cm², whereas the previous setup has one of 10 cm², approximately, i.e., the setup has been scaled up by around 10 times. The setup has been through initial tests with pure CO₂ as a gas inlet showcasing the ability to capture CO₂ and release it in the electrochemical cell. Two different experiment types has been run; one with constant gas inlet and one without.

Introduction

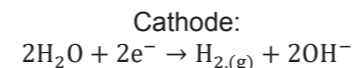
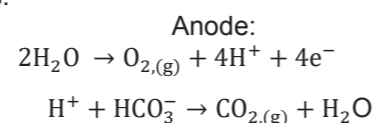
The increasing amount of carbon dioxide in the atmosphere and with it climate change is an ever increasing concern, and while green energy sources are becoming increasingly viable, problems such as overproduction, reliability and scarcity in some parts of the world still remains. Therefore, the market for hydrocarbons, e.g., for fuel or heating, will not cease to exist, due to their viability and thus mitigation of these emissions is needed to combat climate change. One way of mitigation is by capturing the carbon emissions or finding other sources for hydrocarbons. Upgrading biogas with the purpose of putting it into the gas network is an option and the process of replacing natural gas with biogas has already been started in Denmark. At the end of 2021, biogas accounted for about 25% of gas consumption in Denmark and it is expected to account for 100% of gas consumption in 2034 [1].

As biogas contains 25-35% CO₂, CO₂ removal is necessary and thus research in this area synergises well with CO₂ capture technologies. CO₂ capture can be achieved with various techniques such as adsorption, membrane separation or scrubbing. Amongst scrubbing, physical scrubbing utilises that CO₂ is more soluble than CH₄, while chemical scrubbing uses the relative reactivity of CO₂ to increase mass transfer rates and the loading capacity of the

solvent.

To decrease operational costs, the solvent is recirculated after the captured CO₂ has been desorbed and the process is repeated. The method in which the CO₂ is released varies greatly. It can either be done thermally or recent research has shown that electrochemically induced pH-swing is also a possibility, especially when combined with Power-to-X (PtX) applications [2].

This project investigates a technology that uses electrochemistry for regeneration of carbon capture solvent. This project is built on technology has been tested in a laboratory scale reactor. Parameters such as solvent flow rate, gas flow rate, pH of solvent and power induced in battery to the solvent in performance have been tested. The electrochemical cell used was a two-chamber cell separated by a membrane. In the anode chamber a mix of CO₂ and O₂ is produced, whereas H₂ is produced in the cathode chamber. This project investigates a bigger setup than previously tested, while also aiming to optimise operating conditions as well as investigate the validity of the findings in the smaller setup. The half-cell reactions are as follows.



The theory of electrochemical regeneration in regards to pH values throughout the system can be seen in Figure 1.

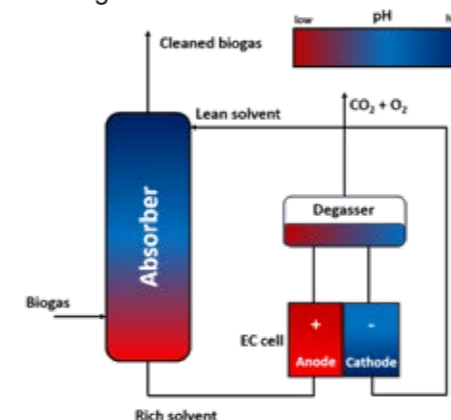


Figure 1: Schematic overview of pH in the setup.

Specific Objectives

The objectives of this project is to build a CO₂ capture setup utilizing electrochemically regenerated solvents that has the ability to capture up to 5 kg/h CO₂. Furthermore, the project aims to show robust and stable operation of up to 1000h.

Results and Discussion

The setup was building an initial tests were performed to see whether the setup had CO₂ capture capabilities. The results of a saturated CO₂ solvent without constant inlet gas can be seen in Figure 2.

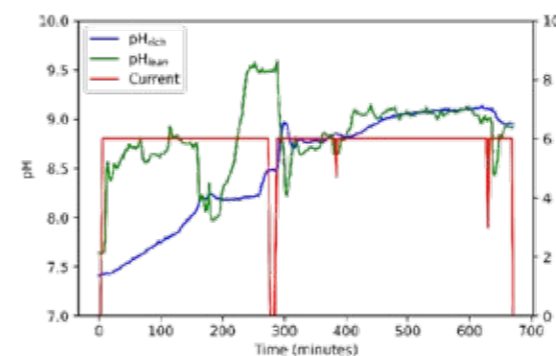


Figure 2: pH in top (lean) and bottom (rich) of scrubber as a function of experiment time.

Initial results are very promising and show that the pH in the system generally increases over time. This shows that the setup is able to desorb CO₂ in the electrochemical cell as the only possible source of such a pH change is located there.

The effect of current on the CO₂ desorption capabilities were also tested. Three different current densities were tested. From Figure 3 it can be seen that all current densities have around the same pH of the CO₂ rich solvent, whereas the pH of the CO₂ lean solvent is increasing with current density, therefore showing a higher desorption rate. This is to be expected as the more electrons

available to drive the reactions detailed earlier, the more reactions will occur.

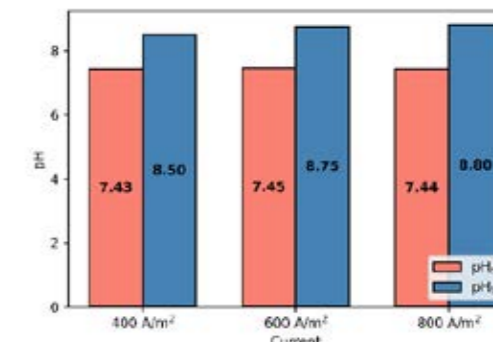


Figure 3: pH in top (lean) and bottom (rich) of scrubber with different current densities.

Finally, Figure 4 shows the CO₂ concentration in the degasser as a function of experiment time. The graph shows that increase in current density yields to faster desorption of CO₂ in the cell.

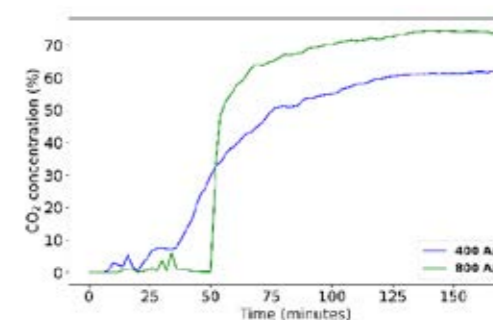


Figure 4: CO₂ concentration in degasser as a function of time with different current densities.

Conclusion

A new setup has been constructed, building on knowledge from a smaller laboratory setup. The new setup works, as it shows CO₂ absorption/desorption capabilities over time. The increase of current density shows an increase in pH difference between top/bottom of scrubber, indicating faster desorption of CO₂. This is further proved by examinations of CO₂ concentration in the degasser.

Acknowledgements

This research project has been made possible by funding by INNO-CCUS project 1-P5 ASGREEN.

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Prediction of solid-liquid equilibria in electrolyte solutions

(January 2022 – December 2024)

7 AFFORDABLE AND CLEAN ENERGY



Contribution to the UN Sustainable Development Goals

In this project, our goal is to predict thermodynamic properties crucial for modeling thermodynamics in electrolyte systems and materials containing crystalline solids. This will support efficient, informed, and innovative advancements in these areas. It is particularly important for developing better models that promote sustainable *and* cost-effective progress in the energy sector. This includes applications in heat and energy storage, carbon capture and storage, geothermal energy, and nuclear processes, where solid-state information is essential.



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Abstract

Knowledge of thermochemical properties are essential to many models of matter. Despite this experimental data are often absent or incomplete for many solids. To overcome this challenge, we have combined quantum chemistry, machine learning, experimental data and statistical data analysis. The result is a robust and highly predictive approach, which provides accurate predictions of the thermodynamic properties of solids, including enthalpy of formation ($\Delta_f H$) and Gibbs free energy of formation ($\Delta_f G$), in a rapid manner. These properties can be easily incorporated into datasets for use in e.g. electrolyte modelling, materials science etc.

Introduction

Experiments to determine formation enthalpy ($\Delta_f H$) and Gibbs free energy of formation ($\Delta_f G$) are often costly, time-consuming and complex to perform for solids, especially across wide temperature ranges. Consequently, although these properties are essential to prediction of e.g. solid-equilibria, they are unavailable for many salts. Electronic structure methods provide extensive applicability and generality but the conventional methods to calculate $\Delta_f H$ and $\Delta_f G$ are computationally costly and prone to systematic errors while machine learning predictions are often difficult to interpret and still fall short of desired accuracy. We propose the insertion of these conventional approaches into a reaction framework which enables fast and reliable predictions.

Specific Objectives

The main objectives include:

- Enhance the predictive accuracy of thermodynamic models for systems involving solids.

- Create accessible and cost-effective methods for predicting the thermodynamic properties of solids.
- Apply these predicted properties to model physical phenomena, especially in systems with electrolytes.

Results and Discussion

We have previously shown that, if the effects of thermal expansion are neglected by adhering to the harmonic approximation, we still observe very good results for the prediction of the temperature-dependence of thermodynamic properties such as G [1]. However, this model is only partially predictive because it requires an externally sourced, accurate reference value/parameter for $\Delta_f H$ to accurately predict $\Delta_f G$. For some compounds it is possible to obtain such values in literature. However, for many other compounds these values are unavailable or unreliable. To close the gap between semi-predictive and fully predictive, we have developed and employed a reaction network approach, based on DFT calculations and literature data, to predict $\Delta_f H$ at 298.15 K. Figure 1 shows the performance of our

predictions using this approach. Overall, the performance is very good (Figure 1a) compared to current methods available in literature (Figure 1c) and close to experimental uncertainty.

Conclusions

We have shown that we are able to accurately

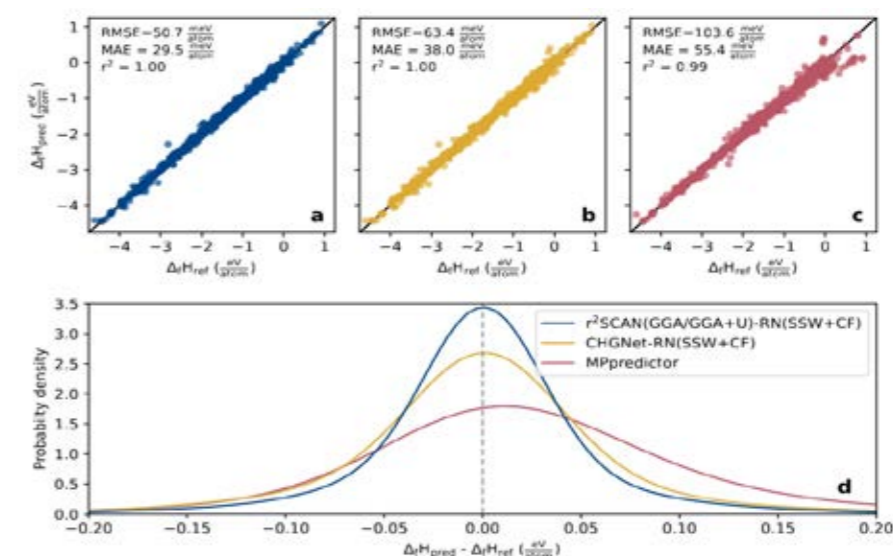


Figure 1: Detailed benchmarks of a selection of methods, for 1543 compounds. Formation enthalpies predicted using the reaction network model using: (a) quantum chemistry data [2], (b) machine learning generated quantum chemistry data [3], (c) pure machine learning predictions [4], compared to the experimental reference data [5]. (d) Kernel density estimate of the distribution of errors in data shown in (a)-(c) RMSE is the root mean squared error, MAE is the mean absolute error and r^2 is

predict the enthalpy of formation using a reaction network. This paves the way for the use of these predicted formation enthalpies, reaction networks and quantum chemistry thermodynamics to predict Gibbs free energies of formation for solids and advance applications that rely on these properties.

Acknowledgements

The authors wish to thank the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (Grant Agreement no. 832460), ERC Advanced Grant project "New Paradigm in Electrolyte Thermodynamic" and the Department of Chemical

Engineering at the Technical University of Denmark for funding this research.

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Process studies of electrically heated clay calciners

(September 2022 – August 2025)



Contribution to the UN Sustainable Development Goals

The cement industry is actively seeking methods to significantly reduce CO₂ emissions, primarily from the clinker production process. One approach is to partially substitute limestone with calcined clay, as the calcination of clay emits significantly less CO₂ compared to limestone. Another step is to replace the combustion of fossil fuels used to heat the raw material. By combining these measures, the production of clinker – and consequently cement – can become less carbon-intensive. Therefore, the implementation of an electrically heated calcined clay production process aligns with efforts to reduce the carbon footprint of cement and supports the 13th UN Sustainable Development Goal.



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Abstract

The primary CO₂ sources in cement production are limestone calcination and fossil fuel use. Using calcined clays as supplementary cementitious materials (SCMs) can significantly reduce the carbon footprint. In the current study, a simulation of an electrically heated clay calcination process is developed to explore optimal process configurations. Furthermore, the study investigates the impact of various process and design parameters on process performance such as calcination degree and energy consumption.

Introduction

Cement production accounts for around 8% of global CO₂ emissions [1], primarily from limestone calcination and fuel combustion for heating [2]. Switching to renewable electric heating can eliminate CO₂ emissions associated with traditional fuel combustion. Another strategy is to replace cement clinker with supplementary cementitious materials (SCMs) [3], like calcined kaolinitic clays, which transform into pozzolanic metakaolin when heated at 450–800 °C [3]. This work models an electrically heated flash calcination process to activate kaolinite clay. A sensitivity analysis is performed to evaluate the effect of the main process and design parameters on the process.

Specific Objectives

The objectives of this work are to:

- Develop a simulation for the electrically heated clay calcination process
- Achieve a comprehensive understanding of the calcination process to explore and identify optimal configurations
- Investigate the impact of operating conditions on calcination and energy consumption.

Process Description

Figure 1 shows the block process diagram of the electrically heated clay calcination set up. Milled and dried clay is preheated in three cyclone stages, where it exchanges heat with gas, leading to partial dehydroxylation. The preheated clay then

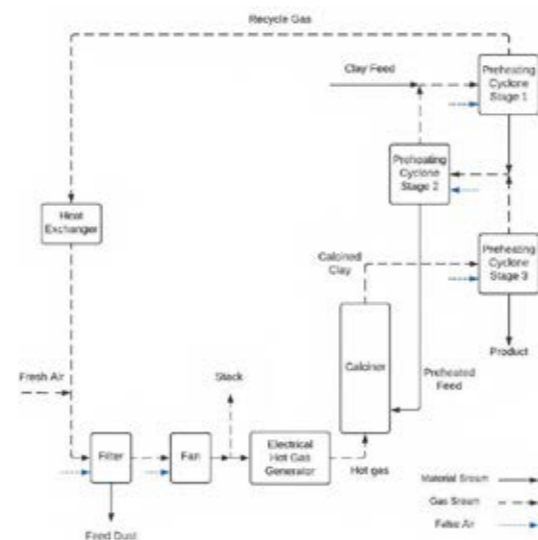


Figure 1: Block process diagram of electrically heated clay calcination process

enters the calciner, where hot gas from the Electric Hot Gas Generator (EHGG) provides energy for full calcination. The calcined clay and hot gas are separated in the last cyclone. After passing through preheating cyclones, the gas is cooled in a heat exchanger if above 400°C. The gas then passes through a bag filter and fan and is recirculated to the calciner after reheating by the EHGG.

Result and Discussion

A steady-state model of the electrically heated clay calcination process was developed. The effects of process parameters (activation energy of dehydroxylation, kaolin content, and gas flow recirculation) on calcination degree and EHGG energy input are analyzed. Lowering activation energy increases dehydroxylation in cyclones (Figure 2.a), while higher kaolinite content minimally affects calcination temperatures (Figure 2.b). Increasing gas flow rate enhances dehydroxylation in cyclone 2 due to a temperature rise (Figure 2.c).

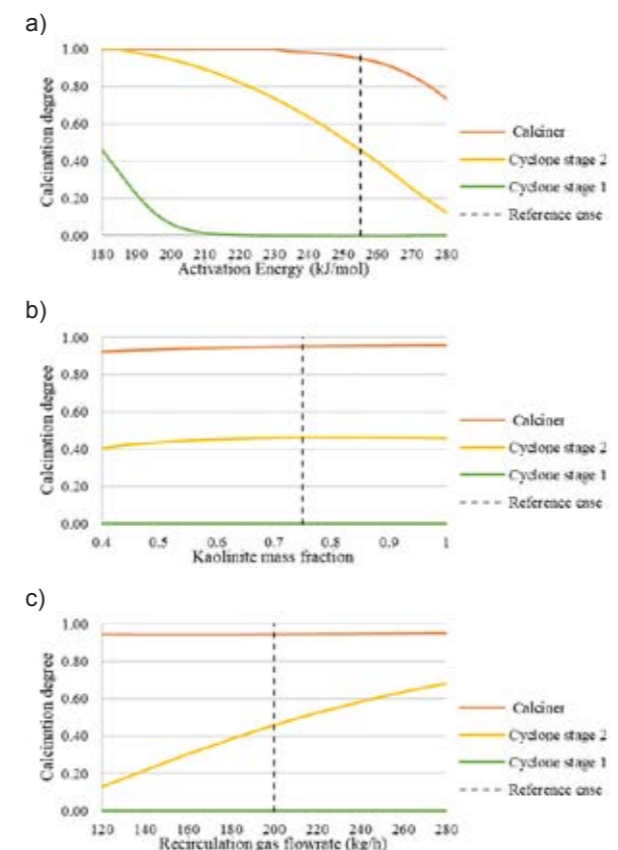


Figure 2: Impact of a) dehydroxylation kinetic b) kaolinite content c) hot gas flowrate on calcination degree

Figure 3 shows how changes in activation energy, kaolinite content, and gas flow rate impact on EHGG energy efficiency and outlet temperature. An increase in these parameters raises energy demands. By increasing the gas flowrate or decreasing the activation energy, the calcination

degree in the cyclones increases, and a smaller proportion of the reaction must take place in the calciner. Consequently, the outlet temperature of the hot gas generator decreases. Higher gas flow or lower activation energy increases calcination in cyclones, reducing the EHGG outlet temperature, while increasing kaolinite content slightly raises the EHGG temperature.

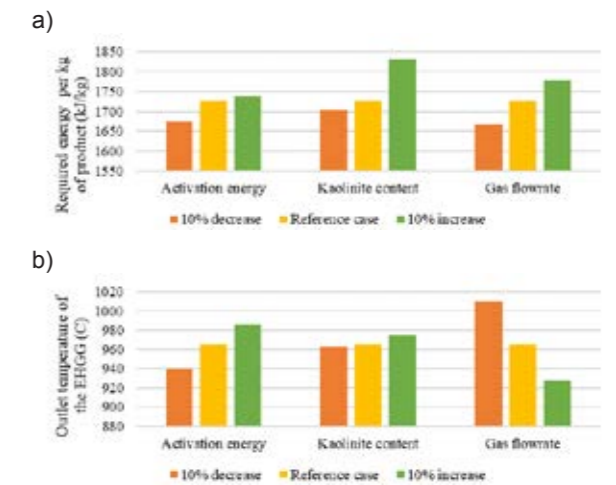


Figure 3: Impact of process parameters on a) required energy and b) outlet temperature of the EHGG

Conclusions

In the current study, a model of the electrically heated clay calcination process was developed that involves electrically heated hot gas in a flash calciner to activate the kaolinite clay. Sensitivity analysis was conducted to determine the effect of varying process parameters on the process efficiency and output. The results showed how alterations in activation energy, kaolinite content, and gas flow rate affect the energy efficiency of the clay calcination process.

Acknowledgments

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Novel inhibitive pigments for anti-corrosive coatings

(March 2023 – March 2026)

9 INDUSTRY, INNOVATION AND INFRASTRUCTURE



Contribution to the UN Sustainable Development Goals

This project, focusing on advanced corrosion protection methods, contributes significantly to United Nations Sustainable Development Goal 9: Industry, Innovation, and Infrastructure. By addressing challenges in material protection through creative solutions, it fosters sustainable industrial practices and encourages innovation in various sectors. Through research and the application of cutting-edge methods, this project not only ensures the durability of infrastructure but also promotes the growth of inclusive, innovative, and sustainable industries, aligning with the broader global agenda of fostering resilient economies and technological advancements.

Abstract

Corrosion-induced failures in metallic materials present significant challenges, demanding the development of effective protection methods. Although organic coatings are widely used, their efficacy is compromised by defects in production and application. To address this, integrating active corrosion inhibitors into coatings shows promise. However, challenges like interference with the curing process, potential inactivation, and uncontrolled consumption hinder direct addition of inhibitors. Recent advancements have focused on utilizing nanocontainers for storing corrosion inhibitors. In this project, a stable zinc-based metal-organic framework (CZIF) nanocontainer with a high specific surface area of $\sim 811 \text{ m}^2/\text{g}$ was developed and loaded with benzotriazole corrosion inhibitor (CZIF-BTA), aiming to protect mild steel. The epoxy (EP) coating containing 0.2 wt.% of CZIF-BTA showed superior barrier properties with the impedance at the lowest frequency value (0.01 Hz) of $\sim 2 \times 10^{10} \Omega \cdot \text{cm}^2$ after 71 days of immersion.

Introduction

Organic coatings represent a conventional and straightforward approach for safeguarding steel against corrosion. Among these, EP coatings, known for their commendable chemical and mechanical attributes, as well as their strong adhesion to metal substrates, stand out as one of the most extensively employed polymers. These coatings act as protective barriers, shielding substrate beneath from corrosive environments. However, achieving high-performance anti-corrosive coatings often requires innovative materials and technologies. Researchers have undertaken innovative strategies to enhance the performance of EP coatings. A noteworthy advancement in this realm has been achieved by incorporating specialized nanocontainers possessing unique capabilities such as barrier properties and high specific surface area into EP formulations. Incorporating corrosion inhibitors into specialized containers can offer coatings a multitude of advantages. These benefits include safeguarding the corrosion inhibitor from premature and uncontrolled release, preventing interference between the corrosion inhibitor and

the curing reaction, and ultimately enhancing the overall performance and durability of the coating [1].

As a new class of nanocontainers, metal organic frameworks (MOFs) have emerged as a highly promising class of materials with diverse applications, thanks to their unique properties. MOFs are crystalline porous materials comprising of metal ions or clusters and organic ligands, which can be synthesized with precise control over their structure and composition. The tunable morphology, ultra-high porosity, and well-exposed functional sites make MOFs highly attractive for various applications, from gas adsorption to catalysis and energy storage. In the field of corrosion protection, MOFs have shown great potential due to their high specific surface area, abundance of functional groups, and supramolecular characters. While MOFs have traditionally been employed as corrosion inhibitors for metal protection, recent research has explored their use in constructing corrosion-resistant coatings. Unlike traditional nanomaterials, MOFs offer a versatile platform for developing adaptive



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materials with multiple modes of corrosion protection, enabling the protection of metallic substrates from diverse corrosive agents.

Specific Objectives

This research project aims to explore the use of CZIF pigments loaded with BTA corrosion inhibitor for producing high-performance EP coatings. The goal is to investigate the loading capacity, release mechanism, and corrosion inhibition efficacy of corrosion inhibitor encapsulated CZIF, while understanding the adsorption mechanism and evaluating the anti-corrosion behavior of the coatings.

Results and Discussion

Characterization

The successful synthesis of CZIF and CZIF-BTA was confirmed through various characterization techniques. The results obtained from the X-ray diffraction (XRD) analysis revealed prominent diffraction peaks corresponding to CZIF, such as (002) and (101). On the other hand, CZIF-BTA displayed peaks at positions similar to CZIF but with reduced intensity, indicating increased structural amorphousness upon encapsulating BTA.

According to BET results, the specific surface area of CZIF decreased from $\sim 811 \text{ m}^2/\text{g}$ to $\sim 134 \text{ m}^2/\text{g}$ for CZIF-BTA, indicating the successful loading corrosion inhibitors.

Other characterization techniques such as X-ray photoelectron spectroscopy (XPS) and Fourier-transform infrared spectroscopy (FTIR) further confirmed the encapsulation of BTA into CZIF porositities.

Active inhibition of coatings

The active inhibition performance of CZIF-BTA-containing EP coating (EP/CZIF-BTA) with an artificial scratch (0.5 cm length and $120 \mu\text{m}$ width) was evaluated using the electrochemical impedance spectroscopy (EIS) test. The scratched EP coating containing 0.2 wt.% of CZIF-BTA revealed an active inhibition performance with $\sim 100\%$ enhancement in the total resistance value compared to EP/blank (Figure 1a and 1b). Furthermore, as depicted in Figure 1c, the scratched zone of EP/blank coating shows severe corrosion, evident by the presence of corrosion products, such as iron oxides. Conversely, scanning electron microscopy images (SEM) of EP/CZIF-BTA (Figure 1d) reveal a smoother surface with fewer corrosion products.

Barrier properties of the coatings

The coating containing 0.2 wt. % of CZIF-BTA showed superior barrier properties with the impedance at the lowest frequency value of $\sim 2 \times 10^{10} \Omega \cdot \text{cm}^2$ after 71 days of immersion while the impedance of EP/blank dropped to $10^9 \Omega \cdot \text{cm}^2$ (Figure 2).

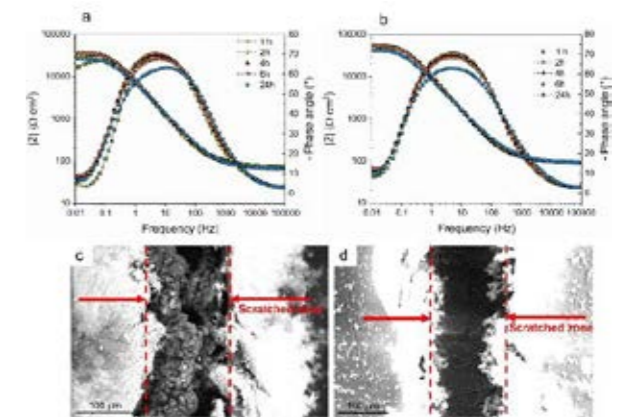


Figure 1. Bode diagrams of scratched coated steel in a 3.5 wt. % NaCl solution for 24 h: EP/blank (a), EP/CZIF-BTA (b). SEM images of scratched EP/CZIF (c) and EP/CZIF-BTA (d) after 24 h of immersion in a 3.5 wt. % NaCl solution.

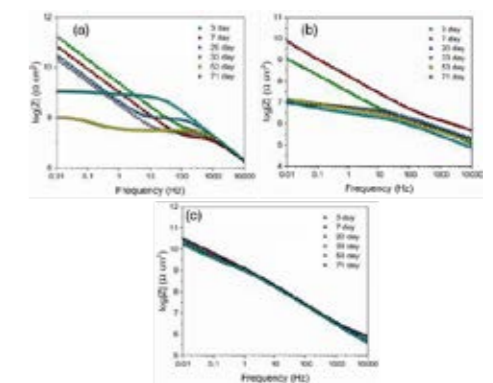


Figure 2. Bode-impedance diagrams of intact coatings during 71 days of immersion in a 3.5 wt. % NaCl solution: EP/blank (a), EP/CZIF (b), and EP/CZIF-BTA (c).

Conclusions

In this project, innovative inhibitive pigments derived from ZIF-8 were synthesized. The successful synthesis of these pigments was characterized using various techniques. Additionally, their corrosion protection capabilities were thoroughly examined via EIS analysis. The results demonstrated the significant potential of these synthesized pigments for application in EP anti-corrosion coatings.

Acknowledgements

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The ANAEROBic treasure trunk - ANAEROB

(January 2022 – December 2024)

7 AFFORDABLE AND CLEAN ENERGY



Contribution to the UN Sustainable Development Goals

Anaerobic systems, drawing inspiration from natural processes, play a pivotal role in rejuvenating ecological cycles for the betterment of both the environment and society. Their application in recycling organic waste streams aligns with the goals of achieving a circular economy. The upcycling of wastes and agricultural residues to generate materials, biochemicals, and energy emerges as a promising strategy for mitigating greenhouse gas emissions and alleviating poverty, thereby fostering a more sustainable approach to energy production and consumption.



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Abstract

The conventional cultivation approach falls short in isolating anaerobic microorganisms within complex microbial communities. Isolating microbes with specific metabolic characteristics is crucial for advancing mixed culture production in waste management. Live Fluorescence In Situ Hybridization with molecular beacons facilitates the isolation and cultivation of viable species. Incorporating conductive materials expedites anaerobic processes by enhancing direct interspecies electron transfer, overcoming the slow diffusion rates of common electron shuttles. This project integrates multiple technologies to develop a platform for synthetic mixed microbial communities in anaerobic digestion systems, augmented by conductive materials.

Introduction

Anaerobic digestion (AD), a intricate network of biologically mediated processes, relies on a diverse microbial community with varied physiological and metabolic characteristics [1]. Traditional top-down approaches are commonly employed for studying microbial communities, involving the manipulation of environmental variables to ecologically select microbiomes conducive to desired biological processes [1]. This selection phase is followed by mathematical modeling to analyze mass balances of chemicals, relevant microorganisms, and simulate rates of chemical and biochemical transformations [3]. While macro-scale processes like wastewater treatment and bioremediation have seen success with conventional top-down designs [4], limitations arise due to insufficient attention to the metabolic networks established within the microbial community and processes dependent on intricate interactions among community members [3,4].

The recognition of mutualistic synergies, such as interspecies hydrogen transfer (IHT) and the more recently described direct interspecies electron transfer (DIET), highlights their crucial roles in providing chemical energy to microorganisms in

low redox environments [5]. Metabolic exchange relations, where electron flows sustain microbial community metabolism, are expected to significantly contribute to the resilience and dynamics of these communities. The lack of understanding of these metabolic networks and interspecies transfers underscores the need for comprehensive investigation, encouraging exploration through different approaches. Recent advancements in metagenomics and microfluidics offer opportunities to adopt bottom-up approaches, focusing on the engineering of the microbiome's metabolic network [3]. A bottom-up design approach holds the potential to leverage the complexities of anaerobic microbiomes for the development of innovative platforms for bioconversion processes involving waste biomass and agricultural residues. This approach specifically aims to reconstruct microbial communities, exploiting DIET to enhance methane production in anaerobic digestion.

Specific Objectives

The main objective of the project is the development of a platform for the isolation and cultivation of anaerobic microorganisms that are non-cultivable with traditional techniques. The

target is to use the isolated micrororganisms to build synthetic microbial consortia for enhanced biomwthane production in the presence of conductive materials.

Results and Discussion

Initially, batch culture systems were established utilizing four distinct carbon sources (acetate, methanol, propionate, and H₂/CO₂) to simplify the intricate microbial community of the anaerobic digestion (AD) inoculum and enhance methanogen enrichment. Three different conductive materials, namely magnetite, activated carbon foam, and polyaniline-coated plastic, underwent testing to determine the optimal performer. Cyclic voltammetry and metagenomic analyses were conducted across all cultures to evaluate DIET processes and to identify the prevalent species. Metagenomic data pertaining to the most abundant methanogens were employed to formulate Fluorescence In-Situ Hybridization Transcript Annealing Molecular Beacons (FISH-TAMB) probes. These probes, designed for the live-FISH technique, enable the targeting of specific microbes while preserving cell viability—a departure from the conventional FISH technique. The FISH-TAMB probes were utilized to label methanogens in selected cultures and subsequently isolated using the B.SIGHT single-cell dispenser (Figure 1).

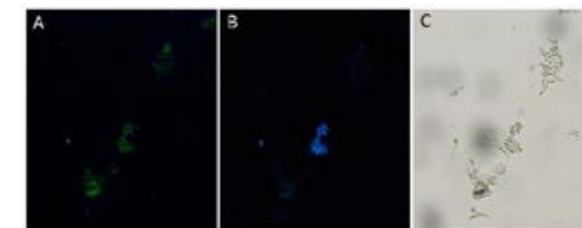


Figure 1. (A) Methanogens labeled with FISH-TAMB probe (fluorophore 5'-6-FAM, quencher Dabcyl-3'). (B) Autofluorescence of methanogens from cytochrome F420. (C) Optical microscopy of entire mixed culture.

The methanogens are presently co-cultured with randomly isolated microorganisms from the original cultures to investigate potential syntrophic relationships. Subsequently, nuclear magnetic resonance (NMR) will be employed to identify the metabolites underlying cross-feeding in the established syntrophies. These findings will inform the selection of specific combinations for constructing the synthetic microbial community and developing a flux balance analysis (FBA) model for the synthetic microbial consortia [6] (Figure 2). Following the FBA model, adjustments will be made to the initial selection, and the

synthetic microbial community will be reconstructed for model validation.

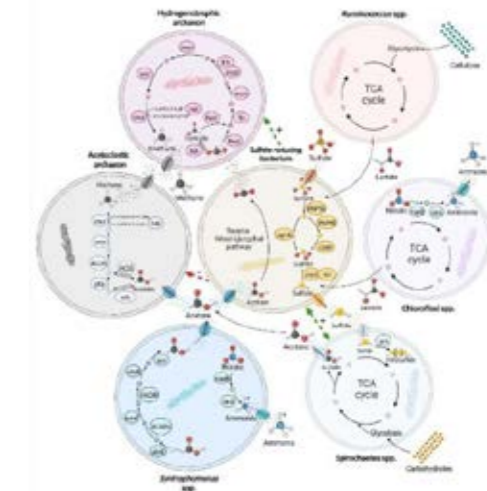


Figure 2. Example of expected FBA model to be used for the synthetic microbial consurtium reconstruction. For meget afstand

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Microbially assisted syngas biomethanation to renewable natural gas standards

(January 2023 – December 2025)

7 AFFORDABLE AND CLEAN ENERGY



Contribution to the UN Sustainable Development Goals

Methane produced from renewable sources such as dry waste biomass from agriculture or forestry is an attractive alternative to fossil natural gas. Waste feedstocks are cost-effective, the process is scalable, and its implementation can be decentralized. It can also be used as a Power-to-X application, where excess electricity during peak production from renewable sources is used to produce hydrogen. This hydrogen can then be used to achieve higher methane purity while storing the energy in a stable and flexible energy carrier for which transport and use infrastructures are already in place.



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Abstract

Syngas biomethanation offers the opportunity to convert a variety of waste feedstocks into a stable and flexible energy carrier. A popular bioreactor type for this process is the trickle bed reactor, in which the microbes form biofilm. Thus, in-depth study of the biofilm offers the opportunity to advance process understanding. The focus of this study is the protection the biofilm offers to the toxicity of carbon monoxide (CO) in syngas. Methanogens are especially sensitive to CO and the carboxydrotrophs that consume it prevent its toxic effects. 3D biofilm images show that the biofilm is stratified, and that the degree of stratification increases with increasing exposure to CO.

Introduction

Syngas (or synthesis gas) is one of the products of pyrolysis and gasification, thermochemical processes that treat dry, woody biomass. This gas is mainly composed of hydrogen (H₂), carbon monoxide (CO), carbon dioxide (CO₂), and methane (CH₄) and requires downstream processing to convert it into a recoverable, storable product, such as methane (CH₄).

The biological transformation of syngas to CH₄ can be carried out by a mixed microbial community through interconnected biochemical reactions [1]. Methanogens, who consume H₂ and CO₂ to produce CH₄, have been found to suffer from CO toxicity [2]. Carboxydrotrophs, who consume CO and produce H₂ and CO₂, have been postulated to act as CO detoxifiers in syngas fermentation, a role similar to the one they have in natural environments [3].

A popular reactor for this process is the trickle bed reactor, which relies on microbes growing attached to high specific surface area carriers, forming a biofilm. Therefore, in-depth study of the biofilm is necessary to increase process

understanding and optimization. Based on previous experiments using granules, it has been suggested that carboxydrotrophs intercept and consume CO as it diffuses into the biofilm [4]. If this is the case, a layered structure is expected in the biofilm, with CO consumers closer to the surface and methanogens beneath.

Specific objectives

Syngas biomethanation biofilms were studied using a flow cell system. This system allows the detailed study of biofilm formation and structure using confocal scanning laser microscopy. To the author's knowledge, this is the first time that flow cells have been used for anaerobic, thermophilic and gas fermenting microbial consortia.

Two different levels of CO exposure – 10 % and 90 % – were studied to investigate its influence on biofilm structure and stratification. Biofilms were cultivated in flow cell systems for two weeks, after which they were fixed and embedded to preserve the 3D structure. Fluorescent in-situ hybridization was performed targeting carboxydrotrophs (the Firmicutes phylum) and methanogens (the

Methanobacteriales order), and images taken using confocal scanning laser microscopy.

Results

After image processing, the integrated intensity of the fluorescence was used to calculate the relative abundance of methanogens. When the relative abundance nears 1, methanogens are dominant, and when it nears 0, they are practically absent. If methanogens were being physically protected from CO toxicity by carboxydrotrophs, higher methanogen relative abundance would be expected in the inner layers of the biofilm. Figure 1 shows a 3D plot of the relative abundance of a representative replicate of each condition.

Figure 1 clearly shows differences in the distribution of methanogens and carboxydrotrophs with height and CO exposure. Under 10 % CO exposure, the microbes are quite well mixed, although there is some degree of clustering. Nevertheless, there is already a concentration of highest methanogen relative abundance in the middle layers.

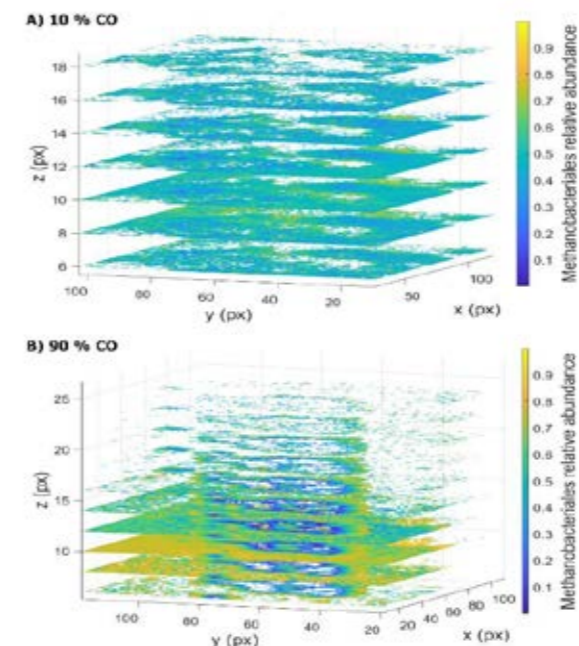


Figure 1. Three-dimensional representation of the relative abundance of Methanobacteriales (methanogens) in a flow cell under the exposure to A) 10 % CO and B) 90 % CO.

Under 90 % CO, there is clear clustering of both methanogens and carboxydrotrophs. Firstly, methanogens are most abundant in lower layers of the biofilm, showing a correlation with height that supports the idea of CO toxicity protection by carboxydrotrophs. Most interestingly, there are channels clearly visible in the biofilm, around which carboxydrotrophs are heavily clustered. In these channels flows medium saturated with CO, H₂ and CO₂. If methanogens were not affected by

CO toxicity, both methanogens and carboxydrotrophs would be present around the edges of the channels as when the CO content is 10 % (Figure 1A). The fact that the relative abundance of methanogens at the edges of the channels in Figure 1B (90 % CO) is close to zero is an indication that CO toxicity is preventing them from growing there, and that carboxydrotrophs are indeed protecting methanogens.

Overall, these results show the value of small-scale systems like flow cells for gaining in-depth understanding of process behavior.

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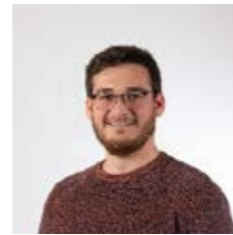
Tackling biofouling through coatings coupled with underwater cleaning

(March 2024 – February 2027)



Contribution to the UN Sustainable Development Goals

Marine biofouling presents significant economic and environmental challenges. Despite the effectiveness of fouling control coatings, fouling can still occur, making underwater cleaning a critical strategy. This project aims to develop and optimize underwater cleaning techniques, reducing reliance on harmful biocides. The development of coatings that withstand repeated cleaning without degradation further reduces the environmental impact of maintenance, supporting sustainability and compliance with stricter environmental regulations.



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Abstract

Marine biofouling, the accumulation of organisms on underwater surfaces, remains a challenge despite advances in coatings and cleaning technologies. This study focuses on optimizing underwater brush cleaning by adjusting cleaning parameters and brush geometries to improve efficiency. Cleaning effectiveness and environmental impacts were evaluated on coated samples exposed to biofouling.

Introduction

Marine biofouling, defined as the unwanted accumulation of various marine organisms such as algae and barnacles on vessels or structures immersed in natural aqueous environments, poses significant challenges [1]. The presence of biofouling results in a loss of performance, which is particularly evident in moving structures such as ships, where increased friction and structural weight lead to increased fuel consumption, greenhouse gas emissions, maintenance, and operating costs [2]. In addition, ships traveling across diverse oceans face the risk of spreading invasive species across different locations, which threaten the native ecosystems [3].

Fouling control coatings are the main solution to combat the problems and effects associated with biofouling. Incorporating biocides into the coating matrix is a commonly used strategy for antifouling coating [4]. However, growing environmental concerns about biocide accumulation and its broader impact on the aquatic ecosystems have accelerated the development of alternative biocide-free methods over the past years [5].

To improve the effectiveness of fouling control coatings and to further mitigate the effects of fouling, a variety of cleaning strategies have been developed [6]. These methods primarily involve the mechanical removal of fouling from affected

surfaces. The most commonly used cleaning strategies are rotary brushes, high-pressure water-jets and ultrasonic cleaning [7]. While some cleaning operations can be performed during dry docking or anchoring periods, the use of underwater cleaning provides a more cost-effective solution that can extend the life of a coating and minimizes the need for frequent and expensive dry docking [8].

However, it is crucial to recognize that improper cleaning poses a significant risk of coating damage [9]. Therefore, a comprehensive understanding of the fouling formation, the employed fouling control strategy, the impact of cleaning parameters on the different coating types and the environmental impact in terms of different releases during cleaning procedures is essential for effective maintenance and a prolonged lifetime.

Specific objectives

The objectives of this research project are:

- Optimizing underwater brush cleaning in terms of parameters and brushes used
 - Implementing laboratory scale underwater cleaning methods for fouling control coatings
- Compare effectiveness for multiple underwater cleaning strategies on different fouling control

coatings in terms of efficiency, regrowth and environmental impact.

Methodology

Different types of fouling control coatings were applied to test substrates using an airless spray technique, ensuring a surface finish comparable to that of marine structures like ships.

To create a realistic environment for the development of biofouling, the coated samples were submerged at a depth of 0.5 m in the Baltic Sea at the CoaST Maritime Test Center (CMTC) in Hundested, Denmark, starting on April 1, 2024. The duration of biofouling accumulation varied depending on the antifouling properties of each coating, despite uniform exposure conditions. Subsequent to different underwater cleaning procedures, the samples were re-immersed at the same location to assess regrowth behavior following the application of different cleaning procedures. The assessment of fouling resistance was conducted through visual evaluation based on image recordings of the samples at different time points, in accordance with the standard ASTM D6990-05 (2011).

Figure 1 shows the laboratory-scale rotary brush cleaning apparatus, which simulates and measures the primary parameters of underwater rotary brush cleaning, including cleaning force, brush rotation speed, and the trajectory of the brush across the surface [10].



Figure 1: Automated underwater cleaning system (AUCS) for laboratory scale simulation of underwater rotary brush cleaning

The device allows for the attachment of various cleaning brushes to conduct the cleaning procedures. For this project, the brushes were custom-built to specifically assess the effects of brush geometry and bristle fiber stiffness. Three distinct brush geometries were designed and tested for each fiber stiffness. The fiber stiffness was visually distinguished by color: red representing very stiff fibers, yellow for medium stiffness, and white for very soft fibers. Figure 2 illustrates each brush geometry, with fiber colors corresponding to the different levels of stiffness used in the tests.

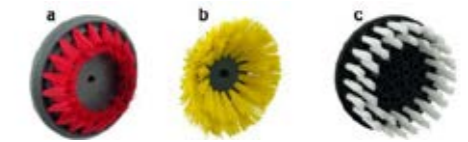


Figure 2: Different cleaning brush geometries with 45° inward oriented bristles (a), 45° outward oriented bristles (b) and 90° perpendicular oriented bristles (c) with the different stiffnesses indicated by the bristle color

Progress and future work

The study demonstrated that the efficacy of cleaning and regrowth behaviors are contingent upon the specific cleaning parameters and brush types utilized. Furthermore, these variations are also influenced by the distinctive characteristics of the coating type.

Future work will aim to establish correlations between cleaning parameters and their effectiveness, providing guidance on selecting the most suitable brushes and cleaning conditions for each coating type.

Acknowledgement

Grateful acknowledgment is given to the Hempel Foundation for their financial support.

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Upscaling and modelling of biocatalytic reactions

(December 2022 – November 2025)



Contribution to the UN Sustainable Development Goals

To ensure a more responsible production and consumption, many production processes used in industry must be improved. One improvement is to replace the chemical catalysts used, which is often harmful itself or requires harsh conditions (extreme pH, high temperature and pressure). The project introduced in this section aims to improve the usage of more sustainable biocatalysts at industrial scale. One of the challenges when working with these biocatalysts is the effect of gradient formation on the performance of the biocatalyst. The project aims to better understand the gradient formation itself but also the effect on the catalytic performance and stability.



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Abstract

Biocatalysts have a high reaction selectivity, which causes them to be of high interest to the pharmaceutical industry, where they already find application. For lower priced chemicals, biocatalysts are not yet widely applied, since the efficiency of its catalytic action is not sufficient in relation to its cost and the revenue gained from the products. One major problem in using biocatalysts is their stability in unfavorable conditions [1]. Other research has shown that in industrial scale reactors, heterogeneity will occur, producing conditions that are outside of the biocatalyst's optimum conditions [2]. This project aims to give further insight into the formation of these gradients at a pilot scale level and its effects on the biocatalyst within the reactor.

Introduction

To investigate the effect of gradients on biocatalytic reactions two model reactions were chosen in this project.

1. Ester hydrolysis by *Candida antarctica lipase B* (CalB)
2. Alcohol oxidation by unspecific peroxygenase

In this report the focus will be on the first reaction, as this has been further investigated until now.

The aim is to develop a Computational Fluid Dynamic (CFD) model which simulates a 200L bioreactor when the ester hydrolysis reaction is performed. In this reaction an acid is produced, which will decrease the pH in the bioreactor from pH 7 (starting pH) to ~pH 4 (pKa of the acid). Due to this shift in pH the lipase will lose some of its catalytic action. To counteract this drop in pH a base is added to the top of the tank, which is causing pH gradients to form.

Material and Method

To make a CFD simulation, modelling pH gradients and the biocatalytic reaction, additional equations need to be added to the simulation apart from the fluid dynamic equations.

In the case of the ester hydrolysis with pH gradients, the equations contributing to a change in pH, as well as the reaction rates, are required.

The equations to calculate the pH were concluded from the main and side reactions happening in the tank as well as reaction rates taken from literature. The reaction rates for ester-hydrolysis by CalB were measured at different pH values in a 200 ml vessel, assuming perfectly mixed conditions.

Results

The measured reaction rate for each pH value was plotted and fitted with a Gaussian equation, see Figure 1.

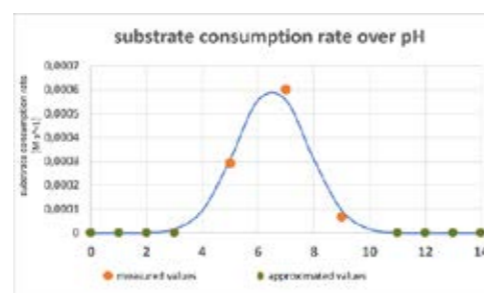


Figure 1: Substrate consumption rate over pH values, rates measured and approximated.

The Gaussian approximation as well as the equations to calculate the pH within the CFD simulation were implemented in the simulation and the plots in Figure 2 were produced, showing the pH as well as the NaOH addition after 6,8 s.

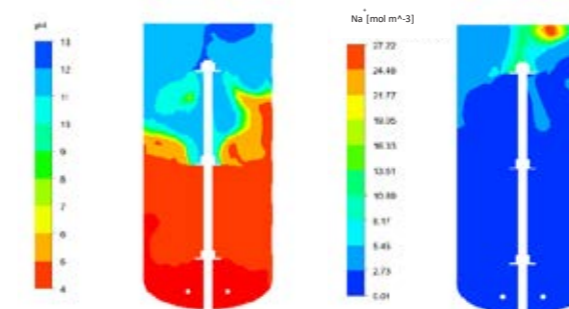


Figure 2: 200L bioreactor with ester hydrolysis and pH gradient formation simulated. The left plot shows the pH values within the tank, the right hand-side shows the Na⁺ concentration.

This CFD simulation was then used to test different scenarios in order to decrease the gradient formation. The effect of reduced enzyme concentration, increased stirrer speed as well as NaOH pulse feeding was tested, see Figure 3.

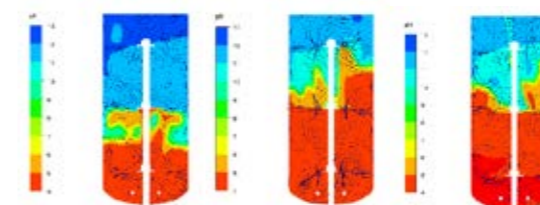


Figure 3: Different scenarios of a 200L bioreactor with ester hydrolysis and pH gradient formation simulated. The left plot shows the pH values with reduced enzyme concentration, the plot in the middle shows the pH values with increased stirrer speed (increased by 100 rpm), the right plot shows the pH values when the NaOH was added as a pulse feed instead of a continuous feed.

Discussion

From the simulations it can be assumed that there is a severe formation of pH gradients in the bioreactor. However, there are some limitations to the current state of the model that will reduce the severity of the gradients. To describe the enzyme kinetics only with a rate, which has been done in Figure 1, neglects the fact that the rate does also depend on the substrate concentration. This dependency is described in the Michaelis-Menten kinetics in Equation 1.

$$v = V_{max} * \frac{[S]}{K_m + [S]}$$

Equation 1: Michaelis-Menten kinetics, with reaction rate (v), maximum reaction rate (V_{max}), Michaelis constant (K_m) and substrate concentration ($[S]$) [3].

Including this substrate concentration dependency will reduce the reaction rate for higher substrate concentrations, slightly reducing the formation of pH gradients.

Another adjustment that needs to be made is the addition of NaOH. The current addition assumes that the reaction is occurring under optimal conditions with the highest product production rate. This causes too much NaOH to be added to the tank, causing the gradients to be too extreme.

None of the improvements mentioned are expected to remove the gradients all together, but they will influence the current results.

Future work

In order to make it easier for different v scenarios to be tested the CFD simulation will be converted into a compartment model to reduce the simulation time.

Furthermore, the current product formation rates will need to be changed into Michaelis-Menten kinetics. Additionally, the NaOH addition rate needs to be adjusted.

Once the ester hydrolysis by CalB has successfully been implemented, the second model reaction will need to be investigated and Michaelis-Menten kinetics will need to be determined to be implemented in the CFD model as well.

Acknowledgements

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Understanding the Galvanic Mechanisms in Zn-rich Coatings

(March 2024 – February 2027)



Contribution to the UN Sustainable Development Goals

Focusing on the mechanisms of zinc-rich epoxy coatings contributes to UN SDG 12 (Responsible Consumption and Production) by enhancing the sustainability and efficiency of protective coatings for steel infrastructure. By optimizing the use of zinc and improving the durability of these coatings, the project aims to reduce material waste and resource consumption. This research supports the development of coatings that require less frequent maintenance and have a longer lifespan, thereby promoting more responsible and sustainable industrial practices.



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Abstract

This project aims to investigate the protective mechanisms in zinc-rich epoxy coatings for steel, with a primary focus on sacrificial and cathodic protection processes. The study begins with the development of a mathematical model to simulate the diffusion of water and oxygen through the coating, providing insights into key parameters like zinc particle distribution, coating thickness, and porosity. This modeling approach will guide the experimental phase by predicting the conditions necessary for optimal protection and supporting further development of the coating formulation. Planned experiments will include a galvanic current measurement setup, where zinc-coated panels and steel panels are immersed in an electrolyte solution, separated by filter paper to prevent direct electrical contact. This setup, combined with advanced techniques such as Electrochemical Impedance Spectroscopy (EIS), micro-Raman spectroscopy, X-ray Photoelectron Spectroscopy (XPS), X-ray Diffraction (XRD), and Fourier-transform infrared spectroscopy (FTIR), will allow for in-depth analysis of chemical reactions and structural changes occurring within the coatings over time. Together, these methods will help clarify the mechanisms of galvanic protection, with the goal of improving the long-term effectiveness and durability of zinc-rich epoxy coatings in harsh environments.

Introduction

Zinc-rich epoxy coatings are a widely used method of corrosion protection for steel, particularly in harsh environments such as marine, industrial, and offshore applications. These coatings work through two primary mechanisms: sacrificial protection and barrier protection. Zinc serves as a sacrificial anode, corroding in place of the steel and protecting it from rust. Simultaneously, the epoxy matrix acts as a barrier that slows the ingress of corrosive agents like water and oxygen [1].

However, the performance of zinc-rich coatings depends on various factors, such as zinc concentration, particle distribution, and coating formulation. High zinc content enhances cathodic protection, but it may also reduce mechanical properties like adhesion and flexibility, as the coating becomes more brittle. Additionally, as zinc corrodes, it forms corrosion products that can block

pores in the coating, transitioning the protection from sacrificial to barrier based.

Research has shown that optimizing zinc-rich coatings requires balancing zinc concentration to maintain both protective performance and mechanical durability. The sacrificial protection provided by the zinc diminishes over time as zinc corrodes and conductivity decreases. Understanding how zinc concentration affects the initiation of protection at different depths within the coating is crucial for improving long-term performance [2].

This project investigates the mechanisms in zinc-rich epoxy coatings by analyzing how various chemical and electrochemical processes contribute to corrosion protection. The study utilizes several advanced techniques: Electrochemical Impedance Spectroscopy (EIS) will be employed to assess the coating's electrochemical behavior over time, while micro-Raman spectroscopy and X-ray

Photoelectron Spectroscopy (XPS) will help identify chemical reactions occurring at different depths, with a particular focus on zinc's oxidation states. Additionally, X-ray Diffraction (XRD) will monitor structural changes and phase formation as the zinc corrodes, and Fourier-transform infrared spectroscopy (FTIR) will be used to track chemical transformations and corrosion product development within the coating. Mathematical modeling will simulate the diffusion of corrosive agents like water and oxygen through the coating, providing a comprehensive understanding of how these coatings protect steel substrates and how the cathodic protection mechanism evolves over time. These methods collectively aim to optimize the performance of zinc-rich epoxy coatings.

Mathematical Modeling of Zinc-Rich Epoxy Coatings

To guide our understanding of the protective mechanisms in zinc-rich epoxy coatings, this project begins with a mathematical modeling approach. The model simulates the diffusion of water and oxygen through the epoxy matrix and predicts how these elements interact with zinc particles to initiate and sustain cathodic protection. By focusing on parameters like zinc particle distribution, coating thickness, and porosity, the model aims to identify the conditions under which optimal protection occurs, helping to balance corrosion resistance with mechanical durability.

This modeling phase will provide a foundation for understanding key processes, such as the formation of corrosion products and the transition from sacrificial to barrier protection as the zinc corrodes. Insights gained through modeling will inform subsequent experiments, allowing us to refine the coating formulation and focus experimental efforts more effectively. Ultimately, the model will serve as a predictive tool, supporting the development of durable, high-performance zinc-rich coatings for steel infrastructure in corrosive environments.

Experimental Setup for Galvanic Current Measurement

The galvanic current setup is designed to measure the protective effect of zinc-rich coatings. The setup consists of a zinc-rich coated zinc (Zn) panel and a steel (Fe) panel, with filter paper between them to allow ionic flow but prevent direct electrical contact. This ensures that the measured galvanic current results from corrosion rather than electrical conduction. The setup is immersed in an electrolyte solution to simulate a corrosive environment. As zinc corrodes, it protects the steel, and the electrochemical workstation monitors the galvanic

current over time to assess the effectiveness of the coating.

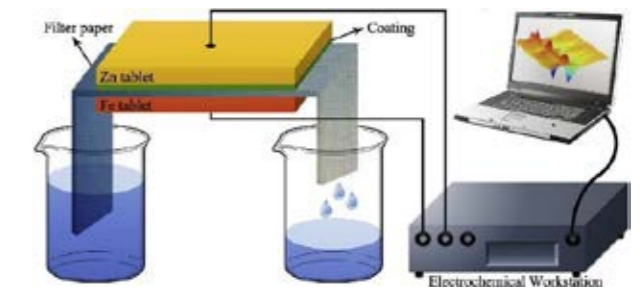


Figure 1: illustrates the experimental setup for measuring galvanic current, which is key to understanding the sacrificial protection provided by zinc-rich coatings [3].

Conclusion

This project aims to understand the galvanic protection mechanisms in zinc-rich epoxy coatings for steel. By using techniques such as galvanic current measurements, XPS, Raman spectroscopy, and XRD, along with mathematical modeling, the study will explore the chemical and electrochemical processes involved in sacrificial protection. The insights gained will help optimize the performance and durability of these coatings, contributing to more effective corrosion protection in harsh environments and longer-lasting infrastructure.

Acknowledgements

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Self-stratifying fouling control coatings

(November 2022 – November 2025)



Contribution to the UN Sustainable Development Goals

Multilayer coating systems typically demand substantial amounts of raw materials and involve intricate, time-consuming application processes, especially evident during dry-docking in the shipping industry. The technology of self-stratifying coatings can address these challenges by spontaneously forming multiple functional layers in a single application step, potentially resulting in reduced raw material usage and significantly improved operational efficiency.

Abstract

Coating systems applied to commercial ships typically consist of multiple layers ensuring the required protective and fouling control properties. However, when applying such multilayer systems during dry-docking, valuable time is lost in which the ship cannot operate. Self-stratifying coatings, coatings spontaneously forming multiple functional layers, hold great potential to bring significant ecological and economic benefits to the shipping industry. As a result of this unique property, the coating application process could become more time and material efficient, and overall improved lifetime-extending properties may be expected. This research focuses on the formulation of self-stratifying coatings while also exploring their underlying mechanisms and novel coating characterization techniques. Additional aspects include the development of coatings with other engineered morphologies.

Introduction

Seagoing ships face various environmental impacts, including harsh corrosive conditions and the growth of marine organisms on the ship hull, known as marine biofouling. The most common method to protect ships from these impacts is the application of functional organic coatings [1]. State-of-the-art coating systems typically consist of at least three layers: an anticorrosive primer, an adhesion-promoting tiecoat, and a topcoat to minimize marine biofouling [2].

Commercial merchant ships must undergo frequent dry-docking, usually every five years, for hull cleaning, repairs, or complete coating system replacement [2]. During these periods, the ship is out of water, resulting in lost operational time in addition to dry-docking related costs [3]. The coating process often dictates the overall duration of dry-docking, as each layer requires a specific drying time before the next can be applied. Unfavorable weather or logistical issues can further delay the process. Therefore, reducing the time needed for coating application is of significant ecological interest.

A well-designed self-stratifying coating spontaneously forms multiple, usually two layers as soon as the coating is applied to the substrate

(ship hull) [4]. This distinctive characteristic offers considerable advantages compared to conventional multilayer coating systems. For instance, the time required for the application process could be significantly reduced as no additional drying or overcoating intervals are required. Additionally, it has been proposed that gradient-shaped interfaces are formed between the stratified layers, potentially making the coating less susceptible to interlayer adhesion failures [5].

The comparison between a conventional multilayer coating system and the approach of self-stratifying coatings for ship hull coatings is schematically illustrated in Figure 1.

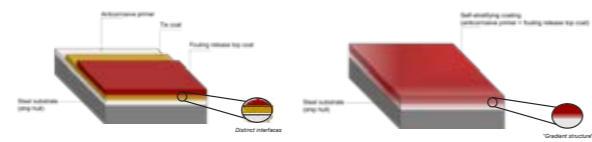


Figure 1: Schematic illustration of a conventional three-layer coating system (left) and a self-stratified coating (right) for ship hulls.

Specific objectives

The development of self-stratifying coatings and the building of a fundamental understanding of



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their underlying mode of actions as well their dependence on formulation and external parameters are key points for this research. This additionally requires the exploration of suitable characterization methods to detect self-stratification in-situ and in the final (solid) state. Moreover, feasibility studies are conducted on developing coatings with controlled morphologies and multiple functionalities, beyond "just" multiple layers.

Results and discussion

A reactive binder combination of epoxy and silicone were selectively chosen for the development of self-stratifying coatings to be used as ship hull coatings. The former binder type is commonly employed in anticorrosive primers [6] whereas silicone compounds being the main component of current fouling release coatings [3]. Therefore, the epoxy binder is intended to form the anticorrosive primer (bottom layer) adhering to the substrate and silicone the top layer during self-stratification. Figure 2 shows an exemplary cross-sectional analysis of a developed self-stratifying coating composition based on the binder combination mentioned above (in the cured state). The image was taken with a scanning electron microscope.

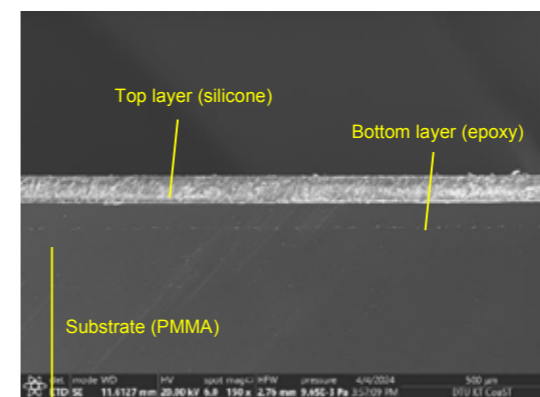


Figure 2: Cross-sectional image of a developed epoxy/silicone based self-stratifying coating applied on PMMA.

In contrast, when the same coating composition was applied to another substrate, differing in surface energy, the two binders formed a different coating morphology (see Figure 3). This behavior could be attributed to the surface tension relations, more precisely to the interfacial tensions between the binders and the surrounding interfaces (substrate and air). The design of self-stratifying coatings as well as developments of other morphologies require therefore the knowledge of

the underlying driving forces resulting from interfacial tensions.

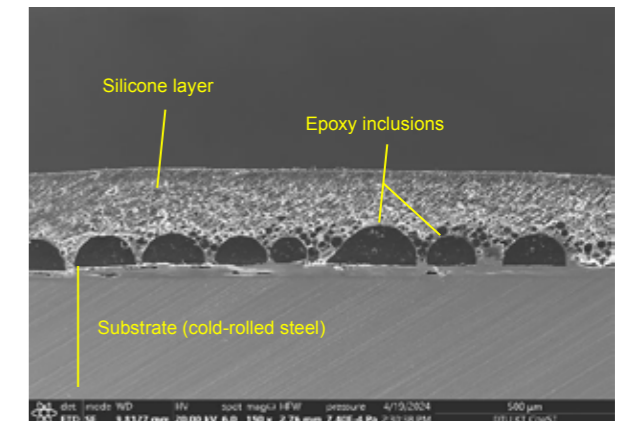


Figure 3: Cross-sectional scanning electron microscopy image of the same coating composition applied to cold-rolled steel.

Conclusions

The technology of self-stratifying coatings could offer a more sustainable alternative to multilayer coating systems. The key advantages lie in the time savings during the coating application process. Experiments have shown the feasibility of the successful production of self-stratifying coatings that form layers in the desired order. Furthermore, it has been pointed out that the knowledge of surface tension relations between the binder mixture applied and the substrate is significant for the stratification process.

Acknowledgements

Financial support from the Hempel Foundation to CoaST (The Hempel Foundation Coatings Science and Technology Centre) is gratefully acknowledged.

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Mathematical modelling of granulation processes for the manufacturing of biochemical products

(April 2024 – March 2027)



Contribution to the UN Sustainable Development Goals

This PhD project demonstrates how scientific research can support Sustainable Development Goal 9, which focuses on industry, innovation, and infrastructure. By creating a more efficient method for producing enzymatic granules, the project enhances manufacturing processes, promoting economic growth and job creation. Additionally, the development of reduced-order models for spray dryers makes complex industrial processes more accessible, fostering innovation and the adoption of advanced technologies in various industries.



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Abstract

This PhD project focuses on developing a CFD-based compartment model for multi-stage spray dryers, aiming to improve the understanding and efficiency of spray drying processes, particularly for heat-sensitive enzymatic granules. By modeling the complex interactions within the spray dryer while minimizing computational costs, the project seeks to address the limitations of existing simulation methods. Key objectives include determining particle properties, establishing a robust CFD model setup, conducting comprehensive simulations, and developing an interpolation algorithm to streamline data handling. Initial efforts have successfully replicated previous CFD results, demonstrating the viability of the approach. This research is expected to enhance process control and optimize the production of enzymatic granules, ultimately contributing to advancements in industrial applications.

Introduction

Granulation processes involve producing granular material from either fine powders or liquid solutions. It is important to maintain adequate control of the granule characteristics, such as temperature and water content, when producing enzymatic granules to prevent denaturation of the enzymes. One way of producing heat-sensitive enzymatic granules is through the process of spray drying [1]. A common method of modelling spray dryers is to model the unit at the local scale using computational fluid dynamics (CFD) as they can capture the trajectories of the air flow and the droplet particles simultaneously. However, they require high computational cost, making them incapable for real-time process control and flowsheet simulations [2],[3]. Another approach could be the systemic approach which is to model the whole spray dryer domain as a single ideal reactor with input and output or as a few virtual ideal reactors representing each phase [4]. The fluid dynamics are therefore fast and easy to solve and only take a minor number of global parameters into account. However, they are often too simple and insufficient to fully understand and

capture the dynamics within the system [5]. Another modelling approach is therefore needed for the spray dryers which can capture the complex dynamics within the spray dryer at limited computational costs.

Specific objectives

The overall objective of the PhD project is to develop a CFD based compartment model for a multi-stage spray dryer, which can capture the complex mechanisms within the spray dryer at limited computational costs. The main objectives in this PhD are:

1) Particle properties determination.

This includes conducting various experiments in which properties such as the drying rate, stickiness and enzyme denaturation properties are measured. Here, the correlation between the properties and possible uncertainties for the variables will be determined.

2) Spray dryer CFD model setup.

A CFD model for a spray dryer, both single stage and multistage, must be developed. This includes creating the spray dryer geometries and

discretizing them into multiple finite volumes (meshing). The various spray drying dynamics will be determined and modelled as to fit within a CFD model setup. This includes dynamics such as air turbulence, particle/air, particle/wall and particle/particle interactions.

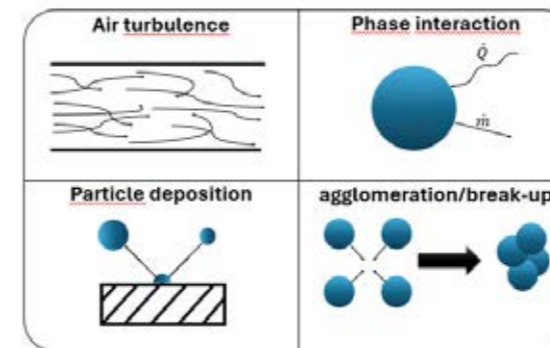


Figure 1: Illustration of the various spray drying dynamics which must be modelled.

3) Conduct CFD Simulations and develop an Interpolation Algorithm.

CFD output data for the entire input space will be generated for the spray dryers. Multiple CFD simulations must be conducted with different inputs which are chosen as to cover the entire input space. To reduce the number of CFD simulations, and to make the reduced order model independent on future CFD data output, an algorithm must be developed which will be able to interpolate between the CFD output datapoints.

4) CFD based compartment model

A CFD based compartment model will be developed for the spray dryer in which the CFD data will be used to generate the compartments of the spray dryer and to provide values for particle trajectories, heat flow, mass flow among others.

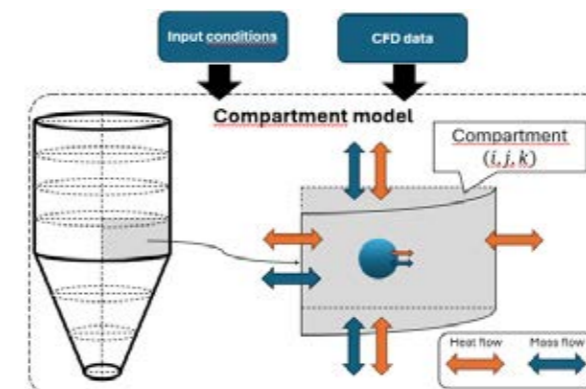


Figure 2: Overview of a compartment model for a spray dryer geometry.

Results and discussion

As this PhD has been started only recently, not many results have been gathered so far. A lot of the ongoing work so far has been to gather

experience within CFD modelling and the creation of user-defined functions (UDF) within the Ansys fluent software. This has mounted in the replication of the results from S. N Salah [6] in which he conducted a CFD simulation of a Niro atomizer. Here a UDF has been created which takes the hindered drying rate of the particles into account. The results which I have created are very similar to those of Salah, indicating that the learning progress is going satisfactorily.

Conclusions

In conclusion, this PhD project aims to enhance the modeling of multi-stage spray dryers by developing a CFD-based compartment model that effectively captures the complex dynamics of the system. Compartment models offer significant advantages, such as simplifying computational demands while maintaining essential details of particle interactions and flow dynamics. These models allow for efficient simulations, enabling better real-time process control and optimization of enzymatic granule production.

Acknowledgements

This project is funded by the Novo Nordisk Foundation and DTU Chemical Engineering.

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Towards eco-sustainability in the protective coatings industry

(October 2021 – October 2024)



Contribution to the UN Sustainable Development Goals

A sustainability model for coating systems will enable us to assess their environmental impact more effectively. By leveraging this information, we can guide the future of the coatings industry in a more eco-friendly direction. This involves minimizing the use of natural resources and hazardous materials, as well as reducing waste and pollution across all stages of a coating system's lifecycle, from cradle to grave



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Abstract

The growing desire within the coatings industry to contribute to the green transition has highlighted the need for a method to assess the environmental consequences of actions taken across the industry. This is essential to ensure that the industry moves toward a more sustainable future. Our project focuses on the protective coatings sector, establishing research and development priorities, and concludes by proposing an eco-strategy for the industry. The model we employ is based on Life Cycle Assessment (LCA) and an in-depth understanding of the protective coatings industry. It has been validated through five case studies, three of which have been published in peer-reviewed journals.

The proposed eco-strategy for the industry can be summarized as follows:

- Minimizing the release of toxic substances (red list)
- Enhancing performance (durability)
- Selecting alternatives with the lowest environmental impact, with particular focus on epoxy resins, titanium dioxide (TiO₂), acrylic resins, and zinc dust by:
 - Substituting fossil-based raw materials with bio-based alternatives
 - Reducing volatile organic compounds (VOCs)
 - Creating multifunctional coatings
 - Improving eco-efficiency
 - Encouraging reuse and recycling
 - Developing alternative production methods

Introduction

In recent years, there has been a noticeable shift in the priorities of the business world. Historically, the primary focus was on profitability, but today, there is a much greater emphasis on sustainability and taking responsibility for the future. It has been driven by growing concerns about global warming reaching a critical point. Sustainability is now a key consideration not only in our homes but also in corporate boardrooms.[1]

The coatings industry is no exception, showing a strong desire to contribute to a cleaner and more sustainable future through responsible development. To achieve this, companies must adopt a sustainability-focused approach at every level of their operations. The first step is to integrate sustainability into their corporate strategies, sending

a clear message to all stakeholders that sustainability must become an integral part of daily activities and decision-making.[2]

Sustainable development requires a company to balance its responsibilities across social, environmental, and economic dimensions. While all three aspects are crucial for determining whether a company is progressing in a sustainable direction, this project focuses specifically on the environmental aspect.

Model

The basis for the model is the Life Cycle Assessment (LCA) from cradle to grave for the coating system. This includes the raw-materials

for the individual coatings, the manufacturing, use, and also the substrate the coating is applied on. The remaining part of the life cycle is the 'end of life processes' including reuse and recycling if possible.

The inputs to the model is data describing the materials, chemicals and energy used in the processes. These data are typically proprietary data owned by individual companies. It is possible to obtain average industrial data from existing Life Cycle Inventory (LCI) databases for most of the processes, but these are often opaque and contain uncertainties making them difficult to use.

The mass balances and flows connecting the process are all calculated using standard LCA software adding up the total element flows from the processes to the environment. By use of a proper LCA methodology it is possible to compile the flows into impact categories which all have effects on human health, the environment and the use of resources.

Examples on relevant impacts categories are 'global warming', 'resource depletion', 'ecotoxicity', 'human toxicity', 'land use', 'eutrophication', 'ozone depletion' etc.

Case stories

The model is verified on five case studies of which three are published:

The case: "**Sustainability of corrosion protection for offshore wind turbine towers**" [3] evaluates hot-spots and assess alternative coating systems for an off-shore wind turbine tower. The main conclusion is that the most durable coating system is also the most environmentally sustainable.

The case: "**Assessing the Environmental Sustainability of Lignin-Based Epoxy Resins for Coating Production**" [4] evaluates if lignin-based epoxy resins are more environmentally sustainable than fossil based equivalents. The result is mixed, but it is clear that it requires more research to develop the bio-based raw-materials to a technology level similar to the fossil-based used today. A further important conclusion from the case is that standard inventory data bases used in LCA are problematic to use within especially the categories concerning toxicity.

The case: "**An eco-strategy for development of more sustainable coatings**" [5] is an attempt to create a sustainable approach for the coatings industry. It involves evaluating the total raw material consumption from global coatings production, combined with an assessment of hazardousness and the need for durability. The

result is a set of recommendations that can be summarized as follows:

- Minimizing the release of toxic substances (red list)
- Enhancing performance (durability)
- Selecting alternatives with the lowest environmental impact, with particular focus on epoxy resins, titanium dioxide (TiO₂), acrylic resins, and zinc dust by:
 - Substituting fossil-based raw materials with bio-based alternatives
 - Reducing volatile organic compounds (VOCs)
 - Creating multifunctional coatings
 - Improving eco-efficiency
 - Encouraging reuse and recycling
 - Developing alternative production methods

Acknowledgements

Financial support from the Hempel Foundation to CoaST (The Hempel Foundation Coatings Science and Technology Centre).

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Investigating the lignin barrier mechanism for anticorrosive coatings



Contribution to the UN Sustainable Development Goals

Large steel structures, including ships, wind turbine towers, and oil rigs, are safeguarded by multi-layer anticorrosive coating systems to prevent structural failure. However, these coatings are derived from fossil fuels. Consequently, substituting fossil-based materials with bio-based alternatives throughout the coating lifecycle, while reducing carbon emissions and process waste, represents a more responsible approach to resource consumption.



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Abstract

Our research focuses on developing bio-based anticorrosive coatings by utilizing lignin, the second most abundantly available biopolymer, to improve corrosion resistance, offering a sustainable alternative to fossil-based resins conventionally utilized pigments and fillers. The project aims to explore the molecular interactions between lignin and epoxy resins, which are expected to enhance coating homogeneity and barrier properties. Additionally, the study will examine how lignin will be different from conventional metal oxides influencing corrosion resistance. Overall, this research provides insights into molecular interactions, barrier mechanisms, and performance evaluation methods for lignin-based coatings.

Introduction

Heavy-duty industries, such as marine, oil and gas, and wind energy, commonly utilize anticorrosive coatings to protect against the harmful effects of corrosion in harsh environments.

These coatings are applied in several layers, including a primer, intermediate coat, and a topcoat. The primer improves adhesion and provides anticorrosive protection, while the topcoat adds aesthetic appeal and shields against weather, sunlight, and chemicals. Epoxy is commonly used for high-performance applications, with epoxy resin primers typically made from fossil-based resources like oil, coal, and natural gas. Bisphenol A (BPA) resins, a key raw material in epoxy resin production, are widely used in heavy-duty coatings [1].

Currently, most coating ingredients are derived from fossil-based raw materials like oil, coal, and natural gas. However, the rising demand for sustainable solutions and durable materials, particularly in industries exposed to harsh environments, has driven interest in renewable alternatives. As part of this shift toward sustainability, research is increasingly focused on developing eco-friendly coatings using bio-based

materials such as vegetable oils, lignin, tannins, and chitosan.

Lignin, due to its high aromaticity, and Availability is considered as a potential alternative to replace petroleum-based ingredients in the anticorrosive coating. But its complex chemical structure presents a challenge for its direct application. To enhance the uniformity, reactivity, and solubility of the lignin, a common approach involves solvent fractionation and selective modification of its functional groups, such as aliphatic hydroxyl, phenolic, and carboxylic acid groups. However, the added costs of solvent fractionation and chemical modification at an industrial scale must be considered. Therefore, a method that directly incorporates unmodified lignin particles into epoxy coatings, replacing pigments and fillers, would be highly beneficial [2], [3].

In this regard, Laxaminarayan et al. [4] explored the use of technical Kraft lignin particles as a sustainable alternative to fossil-based pigments and fillers in epoxy novolac coatings for steel structures. By grinding and sieving the lignin "Figure 1", the researchers compared the effects of sieved and unsieved lignin on the coatings' anticorrosive and mechanical properties. For the unsieved version, agglomerates were formed on

the coating surface "Figure 1", which allowed salt water to penetrate and initiate corrosion during the salt spray exposure test. Additionally, the visible agglomerates in the film with unsieved lignin indicate that the lignin is poorly miscible/soluble in the resin formulation, while sieved lignin improved film formation.

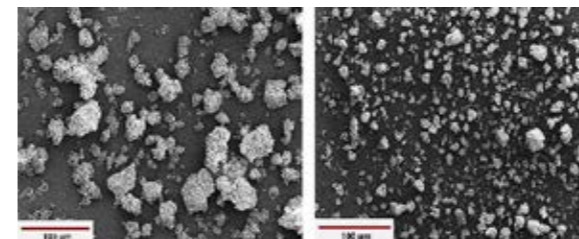


Figure 1: SEM images of (left) unsieved and (right) sieved particles of Kraft lignin at 1000× magnification.

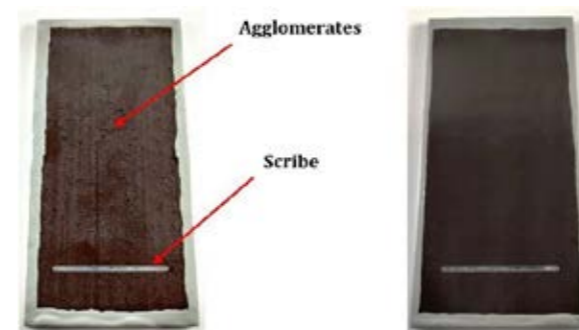


Figure 2: Film formation of unsieved (left) and sieved (right) based epoxy novolac coatings.

This study aims to investigate the molecular interactions between lignin and the epoxy resin matrix influencing corrosion resistance. A key aspect of this research is to analyze the water uptake and diffusion pathways within the lignin-epoxy matrix. Water penetration is a primary cause of coating degradation, leading to corrosion. By understanding how lignin affects the transport of water and other corrosive agents through the matrix, the project seeks to identify how the structure of lignin influences the diffusion process, important for designing lignin based anticorrosive coatings.

Specific Objectives

The specific object of this project is:

- Investigate the molecular interactions between lignin and epoxy resins to understand their role in lignin-based coatings' homogeneity and structural integrity.

- Explore lignin-based coatings' water uptake and mechanisms to gain insights into their corrosion resistance properties.

By achieving these objectives, the project seeks to advance the development of sustainable anticorrosive coatings by optimizing lignin's properties, understanding its interactions with epoxy resins, and improving barrier mechanisms compared to conventional coatings.

Acknowledgment

We are grateful to Hempel Foundation for its financial support to CoaST (The Hempel Foundation Coating Science and Technology Center).

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Development of conducting PDMS composites for soft robotic applications

(August 2023 – August 2026)



Contribution to the UN Sustainable Development Goals

Developing soft artificial muscles represents a significant stride in enhancing human health and well-being. These innovative, bio-inspired actuators emulate the mechanisms of biological muscles and have garnered attention for their potential to revolutionize several facets of healthcare and overall quality of life. They solve issues across various healthcare applications, spanning assistive devices, rehabilitation, human-robot interaction, wearable technology, and soft robotics.



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Abstract

This project focuses on developing novel highly soft actuators. Previous research has sacrificed the compliant mechanical properties of the electrode in favor of forming stable particle networks to gain high conductivities. Here, I will present the concept of utilizing novel silicone-based materials, which demonstrate extremely low values of Young's moduli and high strains, to produce soft conducting electrodes.

Introduction

Soft artificial muscles, in general

In fabricating wearable actuators, soft robotic systems can solve many challenges that traditional hard robotics fail to address. New technologies are paving the way for soft actuators that are compliant with the human body[1].

The ideal wearable actuators must provide muscle-like force when on yet be mechanically transparent when off. This apparent contradiction, from infinitely soft when off to generating useful mechanical work when needed, presents a significant challenge for soft actuators. New materials, device architectures, and ways of integrating wearables on the body are required.

Soft electrodes

Modern wearable devices need flexible, soft, and stretchable electronic components that can fit complex shapes, handle movement, and connect with biological tissues. Achieving these objectives hinges on the design and synthesis of materials that exhibit high electrical conductivity while maintaining mechanical compliance.

Various methodologies have been explored to balance electrical conductivity with mechanical compliance. Conducting polymers, such as poly(3,4-ethylenedioxythiophene) poly(styrenesulfonate) (PEDOT:PSS), exhibit notable promise owing to their flexibility and

tunable electrical properties. Doping of nanoparticles, including carbon derivatives, ionic liquids, and metal nanoparticles, offers exceptional conductivity and mechanical resilience. Emerging 2D materials like transition metal dichalcogenides (TMDs) further diversify the soft electrode landscape due to their remarkable electronic properties. Moreover, biocompatible hydrogels and elastomers, such as polydimethylsiloxane (PDMS) and polyurethane, provide soft electrodes with the requisite compliance for seamless integration with biological tissues.

Nanoparticle doping stands out as a pivotal approach due to its potential to synergistically harness the polymer matrix's mechanical properties and the nanomaterial dopant's electrical properties. This leads to a significant enhancement in electrical conductivity while preserving the mechanical compliance intrinsic to soft electrodes.

Nanoparticle doped polymers

Thus far, most studies on nanoparticle-filled polymer composites have utilized commercial polymer products and doped them with nanoparticles with the desired properties. This approach ignores the possibility of tailoring polymer properties through carefully selecting the matrix. Commercial polymers are often designed with a limited inherent softness for practical

applications and thus restrict the intrinsic softness of the resulting composites. My work will focus on custom polymer design to enhance desirable properties upon nanoparticle doping.

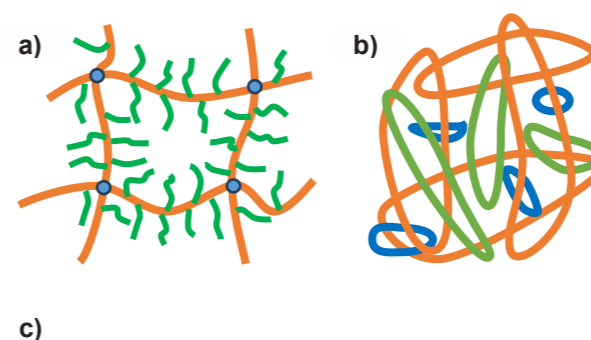
Specific Objectives

- 1) Synthesis of a highly soft electrode capable of good conductivity at large strains.
- 2) Facile fabrication of conductive material in a variety of different electrode architectures.

Results and Discussion

Novel networks

Two novel networks have been developed at the Danish Polymer Center (DPC) capable of extremely large strains before breakage and impressive softness (Figure 1).



Network type	Maximum strain (%)	Young's modulus (kPa)	Reference
Concatenated rings	2400	600	[2]
Bottle Brush	500	12	[3]
Sylgard 184	120	2050	[4]

Figure 1: a) The structure of the bottle brush networks. b) The structure of the concatenated ring networks. c) A comparison of mechanical properties between the DPC networks and a commercial network, Sylgard 184.

The bottle brush (Figure 1a) and concatenated ring networks (Figure 1b) exhibit extraordinary softness and extensibility compared to the commercial PDMS network (Sylgard 184) (Figure 1c). The incorporation of conductive nanoparticles typically increases the rigidity of conventional silicone matrices. However, the intrinsic softness of these novel materials is a significant advantage, as it allows for the addition of higher nanoparticle concentrations without making the material too stiff for practical use in compliant electrodes.

Additionally, molecules with different functionality can be grafted to the silicone backbone to form the bottlebrush polymers. This enables tuning of the networks chemical properties which can aid the dispersion of nanoparticles stopping agglomeration and improving the conductivity of the material at lower filler loadings. The size of the molecules grafted to the silicone backbone can also have an impact on the percolation of the nanoparticles through the network through changing the free space within the network. The synthesis of concatenated ring networks occurs in the absence of traditional crosslinking agents. This unconventional approach leverages a unique form of physical crosslinking, creating potential percolation pathways within the network, thus fundamentally reshaping its conduction capabilities.

Conclusions

Bottle brush and concatenated ring networks may provide a new era for soft electrode materials. These networks, characterized by exceptional softness and extensibility, surpass conventional alternatives. They have the ability to enable the introduction of conductive nanoparticles without sacrificing softness. The structural precision of bottle brush networks and unconventional crosslinking in concatenated ring networks promise transformative advancements in conduction capabilities.

Acknowledgements

This project is funded by the Novo Nordisk Foundation.

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Catalytic stabilization and upgrading of biomass pyrolysis oil to fuels for heavy transport and aviation

(August 2022 – July 2025)

7 AFFORDABLE AND CLEAN ENERGY



Contribution to the UN Sustainable Development Goals

Access to affordable, reliable, and clean energy is only possible if greener alternatives to fossil fuels are found. Biomass derived fuels are a promising alternative, and fast pyrolysis of biomass is interesting since it produces a high yield of crude bio-oil. However, this oil contains a high concentration of oxygen-rich compounds, that need to be hydrotreated before the biofuel can be used instead of conventional fossil fuels.



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Abstract

Biomass-derived fuel is a promising alternative to conventional fossil fuels. Conversion of biomass by fast pyrolysis produces a high yield of crude bio-oil. This product is however highly unstable, corrosive, and has a poor heating value due to a high oxygen content. This oxygen can be removed by catalytic hydrotreatment, but the process is difficult and challenges like catalyst deactivation and reactor plugging still need to be overcome.

Introduction

Fossil fuels are known as major contributors to the world's current high carbon dioxide emissions, and therefore greener alternatives are needed. In terms of heavy transport and aviation, it is necessary to find fuel of high volumetric energy density [1]. Liquid hydrocarbons have a high volumetric energy density and are therefore well suited as fuel for these purposes [1]. Biomass-derived liquid hydrocarbons can be produced from fast pyrolysis of biomass, which provides a high oil yield (up to 80 wt.%) [1]. Unfortunately, the resulting crude bio-oil from the fast pyrolysis has a high concentration of oxygen-rich compounds, resulting in a lower heating value, high acidity, immiscibility with conventional petroleum oils, and poor thermal and chemical stability [1]. Thus, the oxygen needs to be removed from the oil.

Catalytic hydrodeoxygenation (HDO) is a process to remove oxygen in the presence of excess H₂ gas at elevated temperatures [2]. Previously, attempts have been made to perform this HDO in a single step, however, this resulted in significant catalyst deactivation and plugging of the reactor [3]. These problems resulted in the suggestion to perform the HDO of the crude bio-oil in a two-step process: first catalytic stabilization of the oil is carried out at low temperature followed by the

actual HDO step at elevated temperature. The purpose of dividing the process into these two steps is prevention of polymerization of the bio-oil, which happens if it is heated to a higher temperature in its unstabilized form [4]. During the stabilization the unstable components in the bio-oil will be hydrogenated to more stable compounds, e.g., aldehydes and ketones will be converted to alcohols [5, 6].

Specific Objectives

The objective of this project is to develop a fixed bed reactor-based process and catalyst for stabilization and subsequent hydrodeoxygenation of the pyrolysis oil. A literature study furthered the understanding of the process. The following catalyst screening experiments lead to the identification of the most promising catalyst(s) and the most reactive species in the pyrolysis oil. Additionally, the project included participation in setting up and performing experiments on a high pressure two-stage trickle bed reactor setup for the two-step process.

As the project is part of the Innovation Fund Denmark (IFD) project, HyProFuel, collaboration with the project partners is also an important part of the PhD project.

Results and Discussion

A series of experiments using different catalysts were conducted in a 500 mL batch reactor at 180 °C, and 90 bar H₂ for 60 min. 50 g of a model compound mixture (50 wt% furfural, 40 wt% guaiacol, 10 wt% octanoic acid) was used as reactant. The conversions observed in the experiments with the model compound mix as well as the model compounds alone can be seen in Figure 1.

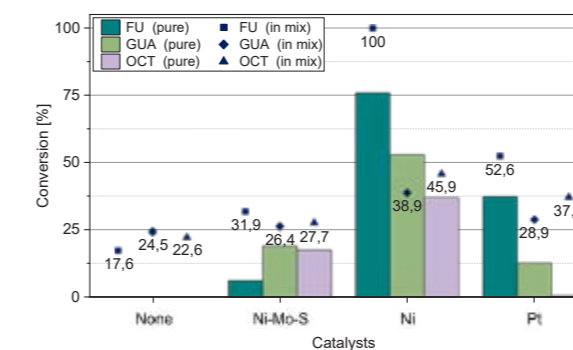


Figure 1: Conversion of furfural, guaiacol, and octanoic acid at 180 °C, 90 bar H₂, 60 min for different catalysts. The conversion in the mix is marked as a scatter plot, where the pure compounds are plotted as bars.

From the figure, it can be deduced that furfural is the easiest convertible compound of the three while using the Ni or Pt catalyst. Overall, the Ni catalyst shows the highest conversion for all three compounds, both alone and together. It should be noted that a higher conversion of the model compounds when in a mix vs. by itself, as observed in several cases in Figure 1, may warrant two different explanations. It may be due to the initial lower amount of the three different compounds in the mixture, but it could also be due to cross-reactions between the different compounds. Likely, it is a mixture of the two. To further investigate this, it is interesting to look into the products formed in the mixtures in the four different cases (no catalyst, Ni-Mo-S catalyst, Ni catalyst, or Pt catalyst), see Figure 2.

As previously stated, the purpose of the stabilization step is to hydrogenate aldehydes and ketones to alcohols. While the condensation reactions observed in Figure 2 are not undesirable during the stabilization step, as they do stabilize the unstable compounds, the production of larger molecules will in general also lead to a higher viscosity, which may be a problem in the two-stage setup. As the Ni/Al₂O₃ catalyst resulted in the most non-condensation products, it seems to be the most promising candidate.

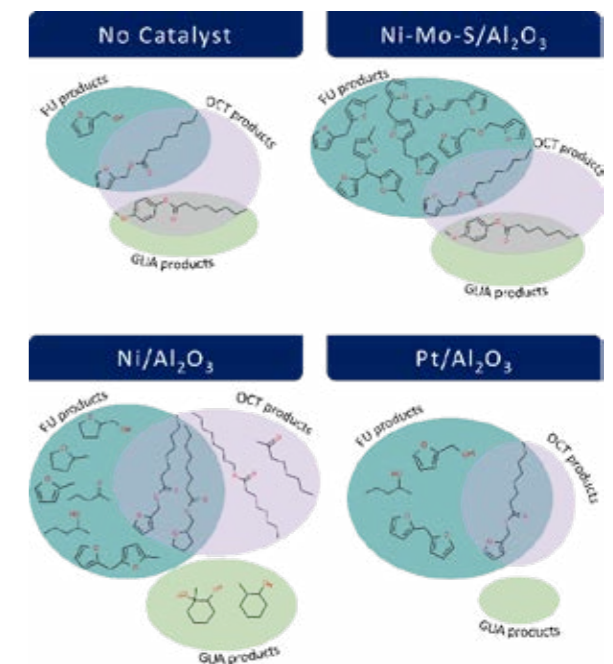


Figure 2: Products observed by GC-MS/FID for the different mix experiments.

Conclusions

It can be concluded that the products for the different experiments depended on the catalyst used. As the Ni catalyst not only resulted in the highest conversion but also had the highest selectivity towards the desired products, this seems to be the best candidate for further stabilization experiments. However, the long-term catalyst stability with real bio-oil has not been uncovered in this experimental series, which is a key aspect of the optimal stabilization catalyst and will be studied in further work.

Acknowledgements

This project has been funded by Innovation Fund Denmark (project # 0224-00029A), and the Department of Chemical Engineering, DTU.

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Mathematical modeling of intumescent coating chars

(October 2023 – October 2026)

9 INDUSTRY, INNOVATION
AND INFRASTRUCTURE



Contribution to the UN Sustainable Development Goals

Enhancing the understanding of intumescent coatings fosters sustainable development and economic growth by mitigating fire-related economic losses and enhancing the production and testing efficiency of these protective materials. This research paves the way for a circular economy by potentially increasing the understanding of their inner workings to the degree where the recyclability of expanded coatings would be possible, thus promoting environmental stewardship and technological innovation. Additionally, it supports the goal of inclusive industrialization and resilient infrastructure, particularly in conflict-affected regions, by improving safety standards for buildings and production facilities worldwide.



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Abstract

Intumescent coatings expand when heated, forming insulating barriers against fire. This project aims to develop predictive mathematical models tailored to CoaST's testing equipment to deepen our understanding of them. In previous work, a one-dimensional model based on experimental data and CFD simulations incorporates factors like conductivity, radiation, and heat loss and has effectively replicated experimental data. Ongoing work focuses on developing models that account for chemical reactions and the progression of the reaction front within the char.

Introduction

Intumescent coatings are a passive fire protection system primarily used to protect structural steel in buildings [1]. When the structural steel exceeds 500°C, it loses most of its load-bearing properties, which can lead to the building collapse [2]. Intumescent coatings can delay the time for the steel to reach this critical temperature from minutes to, in some cases, several hours [2].

The most commonly used intumescent coatings are organic intumescent coatings [1]. While some suggestions of the reactions that happen in them have been proposed in the literature (Cite some papers), the precise mechanism remains a mystery.

In order to fulfill the requirements posed by the government, the coatings must be tested in large industrial furnaces following international standards [3]. Such tests are expensive and require large setups, making them not widely available [4]. Many attempts have been made to reduce the costs of the tests and increase their availability [3]. One notable such attempt has been the development of the CoaST-FIRE made in-house by our research group [5].

Modeling of intumescent coatings has been ongoing since 1975 with varying degrees of success [6]. A wide variety of intumescent coating models exist. These models have been developed with various purposes in mind, for which they have been optimized. Most currently existing models are based on data from cone calorimeters, with some being based on small gas fire furnaces. The models include various combinations of physical phenomena, including but not limited to conductive and radiant heat transfer, chemical reaction, coating expansion, and gas mass transfer. Until now, no single model has been developed that reliably predicts the performance of intumescent coatings.

The project preceding this one has shown that a one-dimensional engineering mathematical model can be used to model the data obtained from small-scale electrical furnaces. Figure 1. illustrates the results obtained from the model [7].

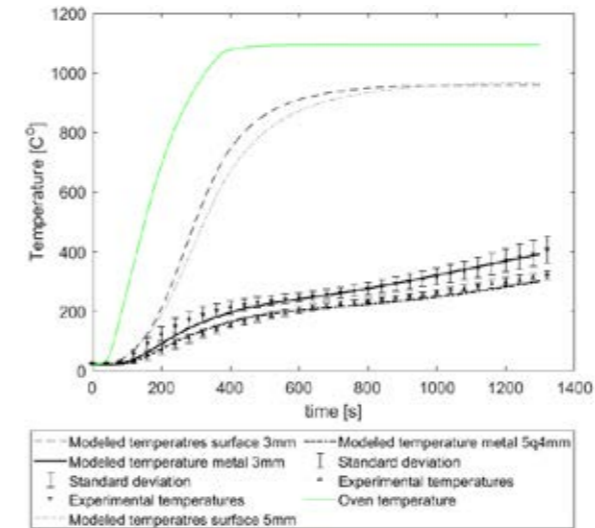


Figure 1. Model results for predicting intumescent coating performance [7].

Specific objectives

This project focuses on further developing models to predict the behavior of the intumescent coatings in small-scale test setups. The goal is to understand their behavior and ultimately explain the differences from the tests conducted in the large industrial furnaces. The hope is to relate the small-scale tests to the big-scale ones, potentially eliminating the need for the big-scale tests. In addition, the goal of the PhD is to further our understanding of the intumescent coatings.

Results and Discussion

Currently there are as of yet no publishable results to discuss. Currently the work is ongoing in an attempt to characterize and describe the reactions which are happening inside of the intumescent coating and use them to develop a model which will describe the propagation of reaction fronts through the intumescent coating during reactions.

Conclusions

Currently, there are no publishable results to discuss. Presently, the work is ongoing in an attempt to characterize and describe the reactions happening inside the intumescent coating and use them to develop a model that will describe the propagation of reaction fronts through the intumescent coating during reactions.

Acknowledgements

The author would like to thank the Hempel Foundation for funding this project.

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Post-combustion electrochemical CO₂ capture (ECC) for cement plants

(February 2023 – January 2026)

13 CLIMATE ACTION



Contribution to the UN Sustainable Development Goals

CO₂ is a major contributor to climate change, with the cement industry being one of the main sources of global CO₂ emissions. The research focuses on improving CO₂ capture process using potassium hydroxide as the solvent, with a modified electrochemical regeneration approach. By enhancing both the absorption and regeneration steps, the project has achieved improvements in efficiency and reduced energy consumption. This method contributes to UN SDG 13 by providing a scalable, energy-efficient solution to reduce industrial CO₂ emissions.



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Abstract

The project aims to improve CO₂ capture from flue gas using KOH absorption and a modified electrochemical cell (ECC) for solvent regeneration. By increasing background electrolyte concentration (0.4 m K₂SO₄ vs. 0.05 m) and feeding the rich solvent to the exit flow instead of the acid compartment, CO₂ bubble formation was eliminated, reducing potential drop between membranes to 1.47 V/cell pair and increased current efficiency to 81% at 400 A/m², thus lowered specific energy consumption to 4 GJ/ton CO₂. The improvements optimize CO₂ desorption and KOH regeneration, making the process more energy-efficient and scalable for industrial applications.

Introduction

Climate change is one of the most urgent global challenges, driven largely by rising levels of greenhouse gases, particularly carbon dioxide (CO₂). Among industrial sources, the cement industry is a major contributor, accounting for about 8% of global CO₂ emissions [1]. The flue gas from cement plants typically contains 15% CO₂, making it a significant target for CO₂ capture technologies. Addressing emissions from this sector is critical to achieving international climate goals and mitigating the adverse impacts of global warming.

In recent years, electrochemical processes have emerged as promising alternatives for CO₂ capture due to their potential for lower energy consumption compared to traditional thermal methods. Unlike conventional approaches that require high temperatures for CO₂ desorption, electrochemical systems can operate at lower temperatures and integrate directly with renewable energy sources, enhancing their sustainability. However, despite this potential, the adoption of electrochemical CO₂ capture has been limited by high specific energy consumption (SEC). For meget mellemrumThe minimum

thermodynamic energy required for CO₂ separation is below 2 GJ/ton CO₂ [2]. Yet, many studies on electrochemical CO₂ capture report SEC values exceeding 4 GJ/ton CO₂, even at low current densities [3]. These figures highlight the gap between the theoretical potential and current performance, indicating substantial room for improvement. The high SEC is often attributed to factors such as inefficient solvent regeneration, significant potential drops across membranes, and challenges related to CO₂ bubble formation within the electrochemical cell.

The focus of this research is to develop an optimized electrochemical CO₂ capture system. One of the objectives is to reduce the specific energy consumption (SEC) by addressing inefficiencies in system design and factors causing high overpotential, creating a more energy-efficient process suitable for industrial applications.

Experimental work

The experimental work was conducted using an electrochemical cell configured in a four-chamber setup: anode-BPM-CEM-BPM-cathode, where BPM is a bipolar membrane and CEM is a cation

exchange membrane. The electrodes are 10 × 10 cm in size. The background electrolyte concentration was increased from 0.05 m, as in previous studies [3], to a range of 0.2-0.4 m in the current study. Figure 1 shows the process diagram of the CO₂ desorption and solvent regeneration of the electrochemical cell.

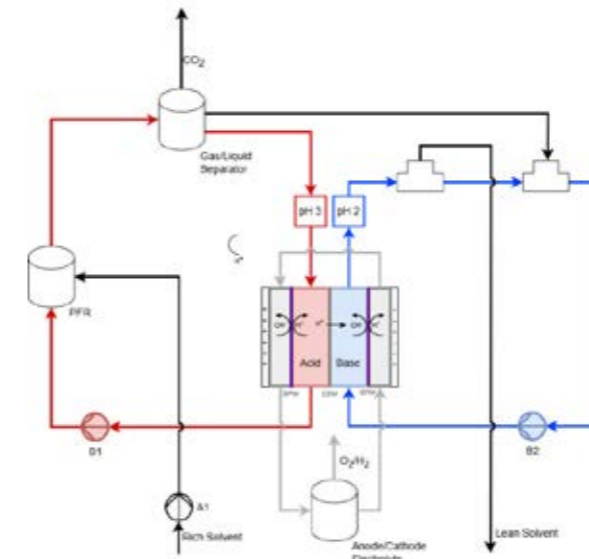
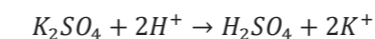
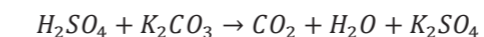
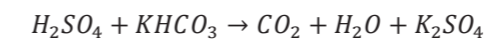


Figure 1: Process flow diagram of the CO₂ desorption and solvent regeneration of the electrochemical cell

Upon applying an electrical current, K⁺ ions migrate through the CEM from the acid chamber to the base chamber. Meanwhile, SO₄²⁻ ions remain in the acid chamber and react with H⁺ ions generated by the BPM, producing sulfuric acid as the following reaction:



The sulfuric acid produced in the acid chamber is then mixed with the CO₂-rich solvent feed from the absorption column, leading to the release of CO₂ through the following non-reversible reactions:



The released CO₂ is separated in a gas-liquid separator for further utilization or storage, while the K₂SO₄ solution is recirculated back to the acid chamber. A portion of this solution exits the acid chamber via an overflow and is directed into the base chamber.

In the base chamber, K⁺ ions combine with OH⁻ ions generated by the BPM, regenerating KOH, which is recycled back to the absorption column through a second overflow unit. Simultaneously, the oxygen evolution reaction (OER) occurs at the anode, and the hydrogen evolution reaction (HER) takes place at the cathode. The O₂ and H₂ gases

produced are diluted and safely vented to the environment.

Results and Discussion

The modified process successfully reduced the potential drop across the membrane to 1.47 V per cell pair at a current density of 400 A/m². This improvement is attributed to moving CO₂ production outside of the electrochemical cell (ECC), which prevents CO₂ bubble formation within the cell. Bubble formation can increase the potential drop because bubbles disrupt the uniform flow of ions, create localized resistances, and reduce the effective surface area of the membrane, thereby hindering ion transport.

Additionally, increasing the K₂SO₄ concentration raised the K⁺ ion concentration, improving current efficiency to 81.1% at 400 A/m². As a result, a specific energy consumption (SEC) of 4 GJ/ton CO₂ was achieved at 400 A/m². This marks a significant improvement over previous studies, where such a low SEC could only be achieved at a much lower current density of 150 A/m²

Acknowledgements

We would like to thank INNOVANDI for funding this research under the research program "post-combustion electrochemical CO₂ capture (ECC) for cement plants".

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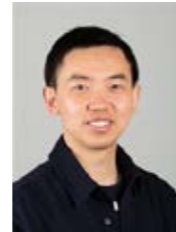
Development of Digital twInS to optimize chemical addition on inTegrated uRban watEr SystemS (DISTRESS)

(April 2023 – April 2026)



Contribution to the UN Sustainable Development Goals

In recent years, the issue of greenhouse gas (GHG) emissions in wastewater treatment plants (WWTPs) has become increasingly concerning, primarily due to the production of nitrous oxide (N₂O). This project uses plant-wide modelling approach to predict the operation costs and GHG emissions of wastewater treatment systems. The model will serve as a valuable tool for optimizing the processes and operations of WWTPs, contributing to a more sustainable future.



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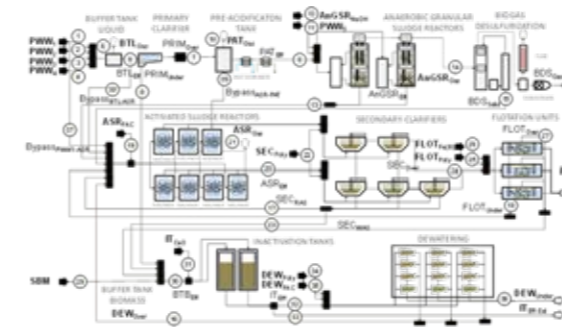


Figure 1: Flow diagram of the WWTP under study. Black/White arrows are inputs/outputs to the whole system [1,2].

Model Structures

This plant-wide model integrates three key components:

- 1) biological models,
- 2) physio-chemical models, and
- 3) model interfaces

The biological model (BM) encompasses two critical aspects: an anaerobic digestion model (ADM) and an activated sludge model (ASM). The ADM accounts for influent conditions and processes in anaerobic lines, while the ASM covers the aerobic lines. Within the ASM, N₂O biological pathways are explicitly considered, including the NH₂OH oxidation pathway (NN pathway), AOB nitrifier denitrification pathway (ND pathway), and heterotrophic denitrification pathway (DEN pathway). The physio-chemical model (PCM) includes an aqueous phase plus

precipitation model and a gas transfer model. Interfaces are used to connect those models [1,2,3].

Data Collection and Analysis

A five-week measuring campaign was conducted to compare full-scale measurements and model predictions. Sensor data monitors high frequency dynamics within the ASR. Data was dynamically reconciled using a four-steps methodology based on:

- 1) definition of the identity matrix,
- 2) curation, processing, cleansing and data analysis,
- 3) estimation of the missing fluxes, and
- 4) calculation of optimal flows using Lagrange multipliers.

Conclusion and Expected Outcomes

Regarding the expected outcomes, the model will be able to predict the key aspects during operation conditions under different time resolutions. The model will undergo further calibration and validation with the high-resolution dynamic data from both aqueous phase and gas phase N₂O sensors and new measurement campaigns.

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Abstract

The upcoming change of legislation in some European countries like Denmark where wastewater facilities will start to be taxed based on direct greenhouse gas (GHG) emissions will force water utilities / industries to take a closer look at nitrous oxide (N₂O) production. In this project, a set of mathematical tools are developed together to (dynamically) predict N₂O emissions in a full-scale industrial wastewater treatment plant using a plant-wide model. The model will support verifying hypotheses about the fundamental mechanisms of N₂O production and emissions and will serve as a valuable tool for optimizing the processes and operations of WWTPs.

Introduction

N₂O is a major contributor to GHG emissions in WWTPs, with a global warming potential 296 times greater than that of CO₂. The industrial partner in this project, Novozymes A/S, is currently facing challenges in reducing GHG emissions from their industrial WWTP. Accurate measurement and accounting of N₂O production in Novozymes A/S' industrial WWTP are essential for developing effective strategies to mitigate emissions and improve plant performance.

Objectives

The objective of this project is to focus on the development of digital twins (DTs) that serve as virtual replicas of the full-scale industrial WWTP. Through the creation of accurate models that capture the N₂O production pathways / processes and the identification of key factors influencing N₂O production, this project aims to enhance understanding and provide a mathematical description of N₂O production in the industrial WWTP. By leveraging the insights gained from the DTs, process operators / engineers will be able to

conduct in-silico experiments, enabling them to make informed decisions regarding the operation and optimization of GHG emissions reductions.

Furthermore, the accurate description of N₂O pathways provided by the DTs can enable their applicability to other WWTPs with appropriate modifications. This broader utilization of the DTs can contribute to carbon-neutral goals on a global scale and make a significant impact in the broader context of sustainable wastewater treatment.

Plant Configuration

A plant-wide model has been developed to comprehensively depict the design and operational conditions of the WWTP under examination, as shown in Figure 1. Flow diagram and model parameters are adjusted to reproduce the influent, effluent, and process characteristics.

Mathematical Modelling of digital twins for fermentation processes

(October 2023 – September 2026)



Decreasing the energy consumption of energy costly fermentation processes

Fermentation processes are already considered a more sustainable way to produce chemicals, pharmaceuticals, etc. compared to the chemical industry. However, when having a closer look at industrial fermentations one realizes quickly, that the highest cost of such a process is the energy consumption. Without a huge amount of energy that is needed e.g. to stir the fermentation, many fermentations would not be feasible. This project aims to deploy models, a digital twin to e.g. decrease the energy of such processes.



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Abstract

The work presented in this article aims to introduce the field of mathematical modeling of filamentous fungal fermentation. An attempt is made to provide an insight into one of the most important, although still not comprehensively grasped, topics of a fermentation process, the oxygen transfer rate and more specifically the volumetric oxygen mass transfer coefficient (K_La). A novel hybrid K_La model is shown, which seems promising but still needs further validation.

Introduction

Filamentous fungi such as *Aspergillus oryzae* can secrete large amounts of proteins, including amylases, proteases, phytases and lipases, into the surrounding medium, which makes them very well suited for industrial production. Such production, e.g. of amylase is done in an industrial scale by companies around the globe and can be referred to as a fermentation process. Newest publications state a market value of \$100 billion for products created with precision fermentation and biomanufacturing. Furthermore, demand for products using biological processes is growing due to the need for sustainable manufacturing and reduced carbon emissions. Nearly 200 nations at COP28 pledged to move away from fossil fuels and petrochemicals, while over 4,100 large companies have set emissions reduction targets. The White House aims to produce 30% of the US chemical demand through sustainable biomanufacturing within 20 years. Fermentation processes are a pivotal technology in achieving those targets. However, it is believed that there is still huge potential to reduce the cost of fermentation processes, which is why bioproduction must be made commercially

profitable through precision fermentation on a commercial scale, while yields must increase.

One besides many other cost-reducing strategies is to digitalize and automate the bioproduction and transit towards industry 4.0. Improving the efficiency, reliability and optimization of the entire manufacturing process is desired to be achieved by a digital twin. The concept of a digital twin plays a central role in the transition digital and can be defined as “a virtual representation that serves as the real-time digital counterpart of a product, process and/or physical object”, as presented in.

The hope is anchored in the desire to cope with the inherence of a bioprocess, which includes a certain degree of batch-to-batch variability, caused by system and population heterogeneities. Additionally, the digital twin is meant to be used in controlling the physical production based on the model's suggestions. In order that this becomes reality in a production facility, one needs 1) a mathematical description of the process that can describe the process accurately enough for the entire operational range and 2) the scientist's acceptance and trust of that model. This project, which is being realized in collaboration with the fermentation pilot plant of Novonesis and PROSYS, KT attempts to implement such a digital

twin for fermentation processes of Novonesis. A well-studied and modeled process is taken as a foundation, refined and further developed into a hybrid model that is supposed to be suitable for a digital twin. The digital twin should e.g. assist in predicting the start fill of a fermentation tank or guide in energy-related decisions.

K_La correlation

The physical oxygen volumetric mass transfer coefficient (K_La) has been studied intensively, due to its correlation to e.g. the energy demand of a fermentation process. The empirical correlation, as seen in eq. 1 must be related to each specific process and production equipment. This was done in a novel approach in which the experimental effort of a DoE (three-factor full factorial design) was reduced from traditionally 10 fermentations to only 2. This was done by shifting from one DoE corner point to another and collecting online data along those two fermentations.

The resulted parameter of eq. 1 with an R^2 -fit of 0.92 can be found in tab. 1. The K_La correlation in eq. 1 has been found, where the viscosity represent the online viscosity measurement in the upper Newtonian region.

$$K_{L,a} = C * \left(\frac{Power}{Volume}\right)^v * v_g^c * Viscosity^b \quad (1)$$

Table 1: parameter of equation 1.

parameter	Value
C	10.9
v	0.5
c	0.48
b	-0.7

Hybrid model

Viscosity is often considered a negligible parameter when describing bioprocesses, as it is often assumed to be comparable to water. However, this assumption should not be followed when it comes to high biomass concentration in the fermentation broth. As this is given in this case, an approach to model the apparent viscosity of the bioreactor was already presented in a study by Albeak et al. This mechanistic approach did not lead to satisfactory predictions for the OTR shifting experiments conducted in this project, prompting a new solution: a hybrid model.

A machine learning algorithm called Light Gradient Boost Machine (LGBM) was selected based on the best prediction compared to the training data as well as the lowest computational cost for training and applying the model. The

model features and training dataset were comprehensively and carefully selected based on SHAP values, residual analysis and a learning curve. In this approach, a hybrid model is developed in which the viscosity is predicted based on the trained data-driven model, as shown in Figure 1. Multiple fungal fermentations from production and the pilot plant were used to train the model with a randomly selected data set (80%-20%, training - testing), also containing the data

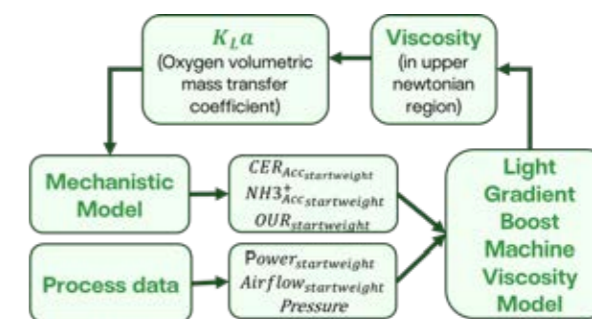


Figure 1: K_La of 4 different operated fermentation in respect to OTR.

from reactors 1, 3 and 4 in Figure 1.

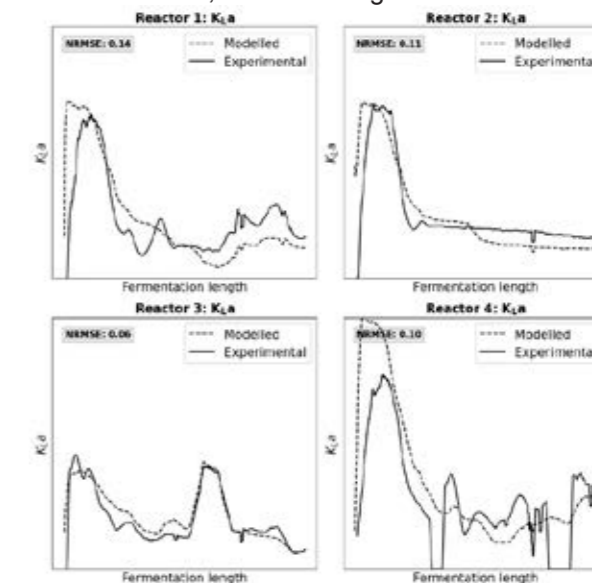


Figure 2: CERacc, NH3+, OUR, Power, Airflow, Pressure are taken as features for the LGBM to model the viscosity, which is looped back to the K_La and mechanistic model.

The results of the hybrid K_La – model are shown in Figure 2. An NRMSE between 0.06 and 0.14 can be seen, depending on the reactor.

The next steps include validating the model on production batches, evaluating the model performance, and optimizing the parts of the model that are not accurate enough to use it as described in the Introduction section.

Progressing Towards Non-Biocidal Antifouling Coatings

(February 2024 – February 2027)



Contribution to the UN Sustainable Development Goals

The elimination of biocides in marine antifouling coatings directly supports SDG 14. Biocides in traditional coatings can leach into the ocean, causing toxic effects on marine life, disrupting ecosystems, and reducing biodiversity. By developing biocide-free alternatives the release of harmful chemicals is minimized, promoting healthier marine ecosystems and preserving the quality of ocean waters. This approach aligns with SDG 14's objectives to prevent marine pollution and sustainably manage and protect marine and coastal ecosystem.



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Abstract

Marine biofouling poses significant challenges to structures and vessels, resulting in damage and increased operating costs. Despite environmental concerns, biocidal antifouling coatings remain widely used for their effectiveness. To protect aquatic ecosystems, biocide-free alternatives like hydrogel coatings are being explored. Hydrogels can repel fouling, extend biocide retention, and can be easily formed in water atop an antifouling coating without further ado by adding powders or liquid gel builder to antifouling coatings. They are easy to implement, cost-effective, renewable, and reduce biocide use. Ongoing research focuses on optimizing gel building and coating properties to improve this technology.

Introduction

Marine biofouling poses significant economic and environmental challenges, not only by causing structural damage to marine infrastructure, but also by increasing ship drag. Even biofilms increase the drag while macrofouling worsen the penalty dramatically, leading to increased fuel consumption, pollution and operational costs [1], [2]. To address these issues, fouling control coatings are essential with two main approaches to achieving antifouling performance.

The first approach is to use Fouling Release Coatings (FRCs), which are typically non-biocidal and designed to minimize organism adhesion with their smooth, hydrophobic surfaces. Low surface free energy allows them to remove foulants with water shear or cleaning [3]. Common binder materials include silicones and fluoropolymers, often combined with surfactants [4]. However, FRCs are prone to mechanical damage, require an additional adhesion layer, and face other challenges. Also, they often lack long-term antifouling efficacy in idle periods [5]. This is why high performance FRC often include biocides.

As a result, biocidal antifouling coatings have been the industry standard for decades due to their proven efficacy and ease of use. These

coatings typically feature an ablative self-polishing mechanism, where a hydrolysable binder gradually dissolves in seawater, continuously releasing biocides like cuprous oxide (Cu_2O) along with other organic biocides that enhance its effect [6].

Heavy maritime traffic in the Baltic Sea, including approximately 2,000 ships at any one time [7] and nearly two million recreational boats, makes biocidal antifouling paints a major concern [8]. Of the 1,560 tons of copper released annually, 37 % (575 tons) comes from shipping and boating. Copper-based biocides harm non-target marine life, accumulate in ecosystems and cause toxicity that often exceeds safe levels in heavily trafficked port areas, which is particularly pronounced in semi-open waters such as the Baltic Sea [9]. To protect the marine environment, it is therefore essential to reduce or eliminate the reliance on biocides in antifouling coatings.

Recent commercial developments by Nippon Paints are leading the way towards biocide-free antifouling coatings although their effectiveness has yet to be proven in extended field tests [10]. This shows that the fundamentals of hydrogel coating technology need to be further investigated

in order to develop an advanced and functional biocide-free antifouling coating.

Hydrogel Technology Approach

Hydrogels are a promising way to minimize biocides in antifouling applications because they mimic the wet, soft surfaces of marine organisms to naturally resist fouling. Hydrogels can hold large amounts of water and swell significantly. However, current methods for crosslinking hydrogels, such as UV [12], [13], are impractical for large-scale hull applications due to the complexity of application and curing, high cost, and environmental factors. In addition, an adhesion-promoting tie coat, similar to FRC, must be applied, making it even more impractical [13], [14]. Researchers have addressed the problem of the complex curing process by pre-polymerizing hydrogel precursors and making hydrogel coatings sprayable by curing them via chemical reactions in the sol state [14], [15]. However, this still requires an adhesion-promoting pretreatment and has not been proven to be effective as a marine antifouling.

Butschle et al. [16] introduced a hydrogel that is built in-situ on top of the AFC without external curing, allowing a 50 % reduction of Cu_2O content without compromising antifouling efficacy. Dry hydrogel building particles were mixed during the production of the coating. Since the solvent does not hydrate the particles in-situ gel formation occurs only when the coated surface approaches water due to the self-gelling properties of the particles. Polysaccharide-based hydrogel is renewable, biodegradable and inexpensive. However, they lack strong adhesion, mechanical strength and homogeneity. This simple approach is promising, but further investigation of the gel formation and the interplay with the dissolution of the coating is needed to improve the effectiveness of the coating.

Conclusion

Antifouling coatings are necessary to protect marine vessels and structures from fouling. Biocides, especially Cu_2O , must be ultimately avoided to protect marine ecosystems, especially semi-enclosed waters with heavy shipping traffic such as the Baltic Sea. Ablative antifouling coatings are effective and can be improved using hydrogel technology.

Specific Objectives

To address the environmental concerns of biocides, hydrogel approaches could be explored as an alternative to eliminate or reduce their use. The ease of application and repair capabilities of traditional antifouling coatings should be maintained, along with their durability. Improvements in gel formation and a deeper understanding of the influencing factors will help to advance hydrogel technology towards effective biocide-free solutions.

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List of publications

M. Butschle, S. Lindner, M. Schackmann, and K. Dam-Johansen, *Prog. Org. Coat.* 188 (2024) 108197

Recycling of crosslinked elastomer systems

(May 2023 – April 2027)

12 RESPONSIBLE CONSUMPTION AND PRODUCTION



Contribution to the UN Sustainable Development Goals

Elastomers are used in various applications and environments, from heavy mining industries to medical devices inside human bodies. Some examples are seals and gaskets, tires, conveyor belts, implants and catheters, footwear, and roofing membranes. As of today, there are no recycling processes for elastomers that are efficient enough to fit them in a circular economy. This project investigates solutions to this problem.



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Abstract

The manufacturers of crosslinked elastomers face a significant challenge in finding efficient recycling processes for their products. The difficulties derive from these materials' superior stability and crosslinked nature. This project investigates how diffusion properties can be utilized to develop new recycling processes. A method to automatically and continuously analyze the swelling behavior of polymer networks has been developed.

Introduction

Crosslinked elastomers, or rubbers, have a network structure formed by chemical and/or physical crosslinks between the polymer chains. The density and type of crosslinks will determine the characteristic mechanical properties of the material. Chemically crosslinked materials are called thermosets. The chemical crosslinks alter the mechanical properties of these types of materials and give them superior chemical and thermal stability, which complicate recycling at their end of life. [1]

Due to their chemical and thermal stability, unique mechanical properties, and biocompatibility, silicone elastomers are used in various applications, ranging from biomedical devices to construction machinery. Their backbone consists of alternating silicon and oxygen atoms with different organic groups attached to the silicon. The most common structure is polydimethylsiloxane (PDMS), with two methyl groups attached to each silicon. [2]

A crosslinked polymer will not dissolve when immersed in a solvent. Instead, the polymer network will swell if their cohesive energy densities are similar. The solubility is, therefore, measured by the degree of swelling. [3]

Swelling is often measured by the gravimetric measurement of a sample that has been

immersed in a solvent, following the standard ISO 1817. According to the standard, the procedure is to immerse a sample of known mass in a solvent of interest for a certain amount of time, often 72 hours. The mass of the sample is then measured again after removing the sample from the solvent and removing surplus solvent from the surface. The degree of swelling is then calculated using Eq. 1. [4]

$$\% \text{ Swelling} = \frac{(m_t - m_1)}{m_1} * 100\% \quad (1)$$

Where m_t is the mass of the sample after immersion in a solvent for time t , and m_1 is the mass of the sample before immersion. Triplicates are needed to report a reliable value. [4]

There are, however, uncertainties in the gravimetric measurements stemming from the evaporation of the volatile solvent(s) when the sample is removed from the solvent for the weighing. To avoid this problem, the standard also covers surface area measurements to evaluate the degree of swelling. This is done by measuring the diagonal length of a sample in a transparent glass vial, without removing the sample from the solvent, before and during immersion in a solvent. Similar methods have successfully been used for PDMS elastomers to evaluate its solvent compatibility. [3] [4]

Specific objectives

The overall objective of this project is to widen the knowledge of how to recycle crosslinked elastomers. Specifically, the project aims to develop an understanding of how the diffusion behavior of different solvents and reagents in a crosslinked polymer network can be utilized to enable recycling.

Experimental methods

Knowledge of swelling behavior is the foundation for understanding the diffusion of solvents and reagents inside crosslinked elastomers. Therefore, a method was developed to follow the swelling in a facile and precise way.

A portable microscope, *Dino-Lite AM4115ZT - EDGE*, was mounted vertically at a suitable distance from the table surface to capture the image of six different Petri dishes of borosilicate glass. In each dish, 17 mL solvent was added together with a 15 mm diameter and 2 mm thick PDMS-based silicone elastomer sample. Images of the samples were collected continuously using the software *DinoCapture2.0*. The collected images were analyzed using a script written in the macro language used in the software *FIJI*, a further developed version of *ImageJ*. The image analysis's outcome was the samples' surface areas at different times. The degree of swelling was calculated using Eq. 2.

$$\% \text{ Swelling} = \frac{(a_t - a_1)}{a_1} * 100\% \quad (2)$$

Where a_t is the sample's surface area during immersion in a solvent at time t , and a_1 is the sample's surface area before immersion. Each measurement was triplicated.

Results and discussion

Figure 1 displays the results from the automatic surface area measurements. The results show that the swelling of the elastomer reaches a plateau after approximately 6 hours for all solvents but toluene, which takes around 13 hours to reach a plateau. The differences seen among the solvents can be explained by the different intermolecular forces between the solvents and the silicone elastomer [3].

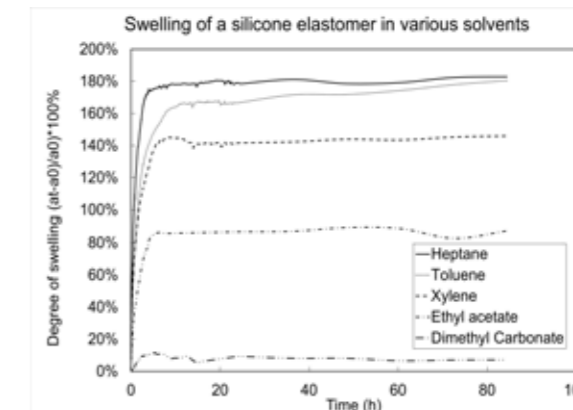


Figure 1. Swelling (Eq. 2) of a PDMS-based elastomer in various solvents as a function of time.

Conclusions

A method to continuously follow the swelling behavior of crosslinked elastomers has been developed. The technique utilizes the fact that the surface area of a crosslinked sample will increase as the degree of swelling increases. The surface areas of elastomer samples immersed in solvents of interest are automatically analyzed with a script in the image processing software *FIJI* that scans images captured with the portable microscope *Dino-Lite AM4115ZT - EDGE* and its software *DinoCapture2.0*.

The developed method will be used to explore how the swelling of crosslinked polymers in different solvents can be utilized, in combination with suitable reagents, to enable the recycling of such networks.

Acknowledgements

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Inorganic particle formation and deposition in thermal conversion of biomass and waste

(December 2021 – November 2024)

7 AFFORDABLE AND CLEAN ENERGY



Contribution to the UN Sustainable Development Goals

Biomass and waste can be used in power plants as a substitute for coal. This increases the stability and reduces the CO₂ emissions for energy and heat production. However, the increased inorganic content in biomass and waste leads to an increased ash formation and deposition at boiler and heat exchanger surfaces. This limits the electrical efficiency and increases the cleaning activities. A fundamental understanding of formation and deposition processes helps finding countermeasures and thereby supports the transition from fossil fuels to biomass and waste.



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Abstract

During combustion, the vaporizable inorganic content of biomass and waste particles is released into the gas phase. The gaseous species cool down and condense directly on heat exchanger surfaces or form aerosol particles which are then transported toward and stick to these surfaces. Aerosol formation happens through nucleation when the flue gas is supersaturated. The most dominant deposition mechanisms are inertial impaction, thermophoresis and condensation. This project aims to gain fundamental knowledge of the aerosol formation and particle deposition processes.

Introduction

Biomass is regarded as a renewable, sustainable and environmentally friendly alternative to fossil fuels. In the 2018 Energy Agreement, Denmark sets the target to phase out coal in electricity production by 2030 [1]. Biomass is seen as a replacement in pulverized fuel-fired power plants. To facilitate a successful transition from fossil fuels to biomass fuels in combustion processes, several challenges, including pre-preparation, firing, and ash-related issues, have to be addressed [2]. Ash-related issues result from the large amount of inorganic species composed mainly of alkali metals, silicon, chlorine and heavy metals accumulated in biomass and waste fuels [3]. Ash from biomass and waste leads to increased slagging, fouling and corrosion in boilers compared to coal ash. Deposit formation on heat exchanger tubes due to slagging and fouling hinders the heat transfer to the steam cycle and thus reduces the boiler efficiency [4]. Increased cleaning activities and plant shutdowns are the consequences. Understanding and predicting the ash deposition helps finding preventative measures and thereby supports the transition from fossil fuels to biomass fuels [5]. To

understand ash deposition several steps included in the process have to be examined:

1. Release of critical ash-forming elements
2. Formation of aerosol particles
3. Formation of coarse fly ash particles
4. Transport of ash species
5. Sticking and rebound of ash species
6. Sintering, consolidation, erosion, shedding

Complex interactions among fuel chemistry, fuel particle morphology and surface properties, conversion path, deposition mechanism, reactor design and operation conditions make it difficult to describe the individual steps [6]. In this work, the focus is on the formation and deposition of aerosol particles. In biomass and waste combustion, alkali species that are released as vapors (e.g. potassium chloride) act as precursors for aerosol particle formation [7]. The most important mechanisms for aerosol particle deposition in biomass and waste combustion are inertial impaction, thermophoresis and condensation. The larger the particle the more dominant inertial impaction becomes. The smaller the particle and the higher the vaporized content in the gas phase

the more important thermophoresis and condensation are [5].

Methods and Materials

To examine the influence of aerosol particles on the deposition of fly ash, a two-step experiment with an entrained flow reactor (EFR, Figure 1) is performed. First, a fine deposit layer from aerosol particles is generated on a steel tube [8]. Second, the steel tube with the deposit layer is exposed to a stream of fly ash. To simulate the aerosols, potassium chloride (KCl) is employed, while for the fly ash, silica (SiO₂) is used.

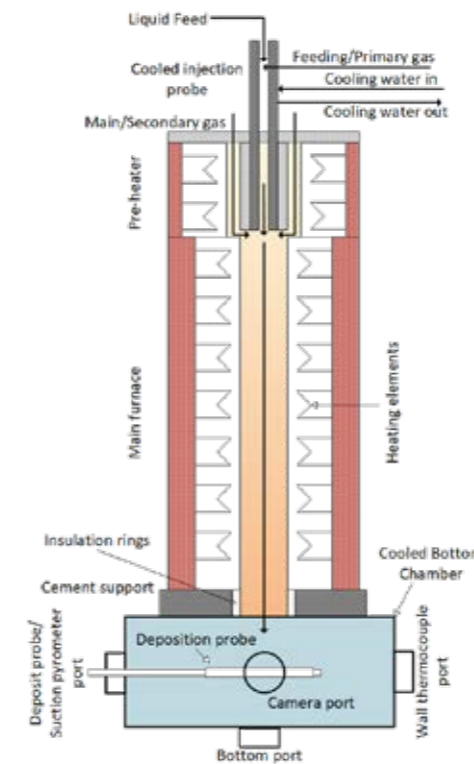


Figure 1: Schematic drawing of the EFR.

For both steps, the influence of the surface temperature of the steel tube and the time it was exposed to the respective chemicals was examined. After each experiment, the amount of SiO₂ on the probe was measured.

Results and Discussion

Figure 2 shows the steel tube at different points during the experiment. In the beginning, the tube is clean, without any deposit. After the KCl deposition, two regions are visible. An outer one, where the KCl formed a fine powder of spherical particles, and a central one, where the KCl formed coarse, crystal-like dendrites. The SiO₂ deposit appears as a brown layer on top of the KCl deposit. The majority of SiO₂ is deposited in the center where the KCl formed the crystal-like dendrites.

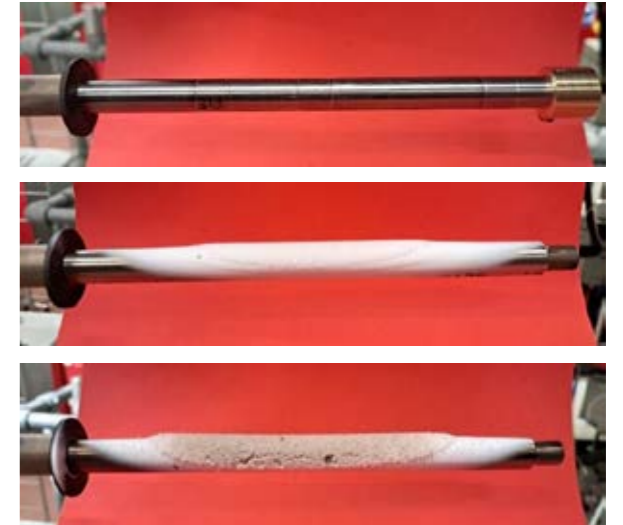


Figure 2: Steel tube: 1) before the experiment; 2) after KCl aerosol deposition; 3) after SiO₂ deposition.

The more KCl was deposited on the tube prior the SiO₂ deposition, the more SiO₂ stuck to the tube afterward. At low amounts of KCl, the probe temperature highly influenced, the amount of SiO₂ sticking to the probe. While at high amounts of KCl, the probe temperature had no influence.

Acknowledgments

The project has received financial support from the Sino-Danish Center for Education and Research.

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Next generation of deNO_x technology for WtE plants

(May 2023 – April 2026)

7 AFFORDABLE AND CLEAN ENERGY



Contribution to the UN Sustainable Development Goals

By 2050, the world is expected to generate 3.40 billion tons of waste annually, increasing drastically from today's 2.01 billion tons. Waste-to-energy (WtE) plants are an effective option for recovering energy from waste, helping the world's population to access renewable energy. However, when solid waste is combusted, nitrogen oxide is emitted, becoming an environmental concern. Currently, most deNO_x processes in WtE plants suffer from environmental variability. The aim of this project is to develop a deNO_x technology that is more resilient to these changes.



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Abstract

Due to the increasingly stringent emission limits, the control of nitrogen oxide emissions in waste incineration plants has become a significant technical challenge. Selective non-catalytic reduction has proven to be an effective strategy to mitigate NO_x emissions during combustion. However, the effectiveness of this strategy is affected by fluctuations in temperature and gas composition. In light of this, the aim of this project is to develop a more robust NO_x control technology.

Introduction

Selective non-catalytic reduction (SNCR) is an effective strategy to mitigate NO_x emissions during combustion. Its benefits include its simplicity, the absence of a catalyst (and therefore other associated challenges) and the ease of installation in existing plants. Additionally, it is applicable to all types of stationary-fired equipment's, has lower capital and operating costs, and can be used in conjunction with other NO_x emission control technologies [1]. The process involves the injection into the flue gas of a reducing agent, which reacts with NO_x to form mainly N₂ and H₂O. The reaction takes place in a temperature window between 1213 and 1423 K.

In most full-scale applications, the reagents of choice are either ammonia or aqueous urea. The injection of aqueous urea instead of ammonia is of interest because it offers a safer and more convenient option for storage, handling and transporting [2]. Several groups have reported on the effectiveness of the urea SNCR process on a laboratory scale [3]. However, the kinetic models developed present some uncertainties, mainly related to the behavior of urea under high temperature conditions. This challenge arises from the limited data available on urea decomposition at high temperature and high heating rates.

To improve SNCR efficiency, current research also focuses on extending the operational

temperature window by injecting various additives alongside urea or ammonia. Studies have shown that substances such as hydrogen, hydrogen peroxide, hydrocarbons, alcohols, carbon monoxide and other additives can shift the active temperature towards lower temperatures. However, these additives can lead to potential side effects such as increased CO emissions, formation of by-products and, in some cases, reduced optimal NO_x control efficiency [4].

Further research is crucial to make the process more robust and to successfully extend the temperature window.

Specific Objectives

The main objective of the project is to develop deNO_x technology, which is more robust towards the fluctuating environment in a WtE plant. This objective will be achieved using alternative reducing agents, agent mixtures, or additives that can shift the process temperature window as needed. A key focus will be on better understanding the chemistry of urea decomposition at high temperatures and heating rates in order to improve existing kinetic models.

Experimental Set up and Modeling Approach

The setup shown in Figure 1 was used to investigate urea decomposition under SNCR temperature conditions. The experiments were conducted within a temperature range of 973 to 1473 K, with a total flow rate of 2 NL/min and residence time of 104/ T (k). The urea-water solution was dosed with an atomizer, and the decomposition of urea was evaluated at oxygen concentrations of 0, 5 and 100 %.

The concentrations of NO, N₂O, H₂O, NH₃, HNCO, CO₂ and CO were continuously monitored by on-line FTIR spectroscopy.

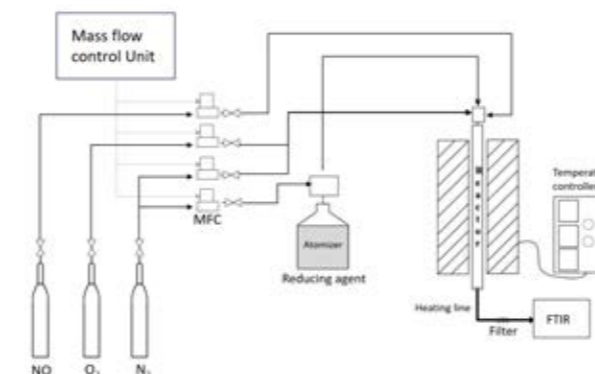


Figure 1: Schematic illustration of the flow reactor setup.

A chemical kinetic mechanism, based on the model of Glarborg et al. [5] and recently updated by Jian et al. [6], was developed and validated with CHEMKIN PRO assuming ideal plug flow reactor conditions.

Progress and Future Work

Urea decomposition and oxidation was investigated at high temperatures and heating rates. The results showed that at temperatures above 973 K, urea decomposes into NH₃ and HNCO with no other species identified, supporting the reaction pathway $\text{CO}(\text{NH}_2)_2 = \text{NH}_3 + \text{HNCO}$. Both products remained stable over the investigated temperature range. The decomposition experiments were consistent with the theoretical rate constant for gas-phase urea decomposition of Honorien et al. [7], which deviates significantly from previous values used in modelling SNCR with urea. The presence of oxygen (Figure 2) enhanced the consumption rate of NH₃ and HNCO, leading to the formation of NO, CO₂ and N₂O. The modeling predictions were in good agreement with the experimental data from this study, as well as with the data reported in literature.

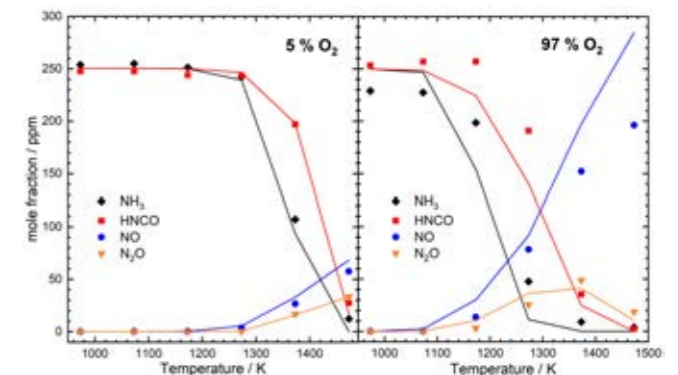


Figure 2: Urea decomposition under oxidizing conditions. The symbols denote experimental data, while the solid lines denote modeling predicted values. Inlet conditions include 250 ppm $\text{CO}(\text{NH}_2)_2$, 3.2 % H₂O, 5 % O₂ (left figure) and 97 % O₂ (right figure), balance N₂.

Future work will assess the effectiveness of various additives used in combination with urea, focusing on their resistance to temperature fluctuations and CO levels.

Acknowledgements

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Understanding the mechanism of the Adhesion of Waterborne Epoxy Coatings

(January 2024 – January 2027)

9 INDUSTRY, INNOVATION AND INFRASTRUCTURE



Contribution to the UN Sustainable Development Goals

This research on waterborne epoxy coatings contributes to several United Nations Sustainable Development Goals (SDGs) by enhancing the performance of environmentally friendly coatings that reduce VOC emissions. By improving the durability and sustainability of coatings used in industries like construction and automotive, the project aligns with goals for innovation and infrastructure, responsible consumption and production, climate action, and health and well-being. The study promotes sustainable industrial practices, minimizes environmental pollutants, and supports efforts against global warming, while also protecting human health by reducing exposure to harmful chemicals.



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Abstract

The research investigates the adhesion mechanisms of waterborne epoxy coatings on steel substrates, focusing on understanding and characterizing the covalent and physical bonds at the interface. The study aims to enhance adhesion while preserving the environmental advantages of waterborne coatings. It addresses challenges such as surface preparation, wetting behavior, and the impact of contaminants like oil and rust on interfacial chemical bonds. Initial findings indicate that optimizing surface interactions and chemical bonds during the curing process can improve adhesion strength, thereby enhancing the longevity and effectiveness of waterborne coatings in industrial applications. Key objectives include characterizing covalent and physical bonds using techniques such as X-ray Photoelectron Spectroscopy (XPS), Atomic Force Microscopy (AFM), and Attenuated Total Reflection Infrared Spectroscopy (ATR-IR). The study also explores how contamination impacts these bonds and seeks to elucidate the mechanisms behind insufficient surface tolerance in waterborne epoxy coatings. Additionally, integrating wettability characterization with mechanical testing will provide a comprehensive understanding of the adhesion mechanism.

Introduction

The use of waterborne coatings has become increasingly popular due to their environmental and health benefits, particularly in reducing volatile organic compound (VOC) emissions compared to traditional solvent-borne coatings. Despite these advantages, waterborne epoxy coatings face significant challenges in achieving robust adhesion to steel substrates, particularly in industrial settings where contaminants such as oil, rust, or dust are present [1]. Strong adhesion is essential to ensure the durability of the coating and its ability to protect against corrosion. Although solvent-borne coatings have a proven history of good adhesion, the industry's shift towards more sustainable options has highlighted the need for enhanced performance in waterborne coatings. This project focuses on understanding the molecular mechanisms of adhesion in waterborne epoxy coatings. Specifically, it examines the formation and breakage of chemical

bonds, such as hydrogen and covalent bonds, during the curing process. Functional groups in the epoxy resin chemically react with the steel, forming strong bonds that are crucial for adhesion. As illustrated in Figure 1, steel surfaces naturally form a thin layer of iron oxide that contains hydroxyl (OH) groups. These OH groups, formed by the dissociative chemisorption of water, create acid and base-type hydroxyl groups that increase the surface's chemical reactivity and improve adhesion [2].

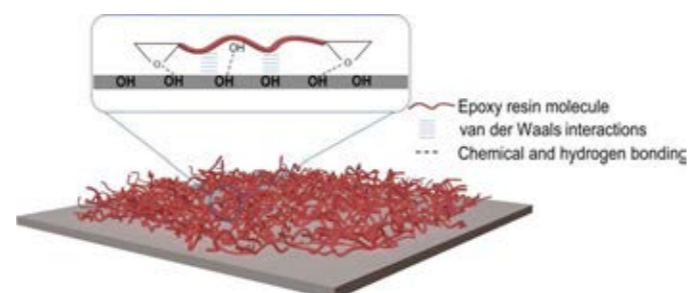


Figure 1. Epoxy resin adhering to a steel

substrate through van der Waals forces and chemical and hydrogen bonds with surface hydroxyl groups, enhancing adhesion strength.

Regarding the interaction between epoxy resin and steel as shown in Figure 2, hydrogen bonds (green) are depicted as weak interactions between the molecules and the steel surface, while chemical bonds (red) represent strong connections that directly link the molecules to the steel surface, thereby enhancing the overall structural integrity of the coating.

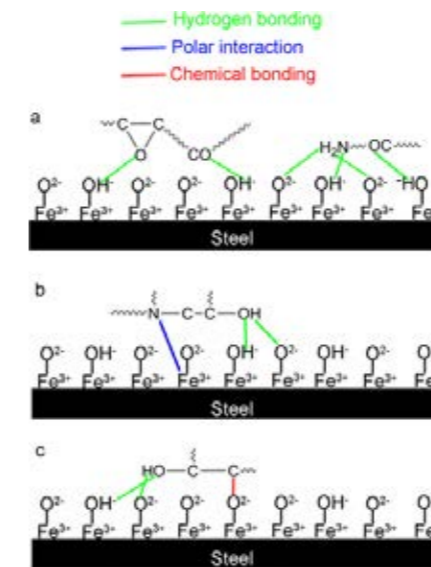


Figure 2. Interfacial interactions between the cured epoxy formula and steel surface. (a) Hydrogen bonding (green lines) between the groups (epoxide, ester, amine) of uncured epoxy formula and ions (O_2^- , OH^-) on the steel surface. (b) Additional hydrogen bonding [3].

Objectives

The objectives of this project include:

The project aims to elucidate the adhesion mechanism of waterborne epoxy coatings to steel substrates. Key objectives include:

Wetting Investigation: Evaluate the initial spreading and adherence of the epoxy on steel surfaces.

Adhesion Development and Its Mechanism: Analyze the formation of chemical and mechanical bonds at the interface.

Adhesion Degradation during Exposure: Assess how environmental factors impact the adhesive bond over time.

Effect of Contamination on Adhesion: Investigate the impact of surface contaminants on adhesion performance.

Analytical Techniques

X-ray Photoelectron Spectroscopy (XPS): XPS can be utilized to identify the elemental composition and chemical states at the interface of the epoxy coatings and steel substrates. This analysis provides insights into the chemical bonds contributing to adhesion.

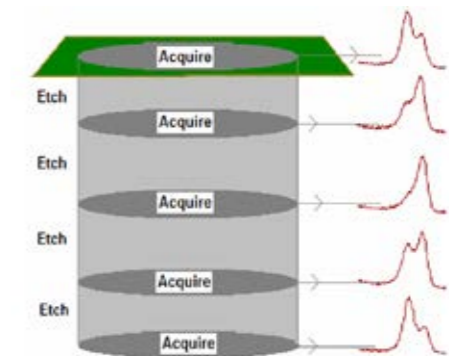


Figure 3. Segment of an XPS depth profile [4].

Progress and future work

Fourier Transform Infrared Spectroscopy (FTIR): FTIR analysis can be conducted on both types of epoxy coatings to evaluate the functional groups present at the interface. This technique aids in understanding the molecular interactions that influence the adhesion mechanism. The test can be performed close to the interface to ensure precise measurements in order to evaluate the conversion at the interface.

Acknowledgment

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Silicone elastomers with cyclic polymers: synthesis and functionalization

(January 2023 – January 2026)

3 GOOD HEALTH AND WELL-BEING



Contribution to the UN Sustainable Development Goals

In recent years, silicone elastomers have received considerable interest for their use in stretchable electronics, medical devices, and soft robotics. Silicone elastomers consisting of a network of cyclic polymers will provide improved mechanical properties than their linear counterparts. The novel network also facilitates the enhancement of the dielectric permittivity, which improves actuation properties. Integrating these silicone elastomers into textiles can revolutionize the production of soft wearables and lightweight exoskeletons. These devices can help users with reduced mobility regain independence and improve their overall quality of life.



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Abstract

Silicone elastomers have received vast attention for their use in stretchable electronics, implants, and medical devices. There has been a growing interest in developing elastomers with properties resembling human tissue in terms of softness and elasticity for integration into soft robotics. In this study, a novel polydimethylsiloxane (PDMS) polymer with carbon-carbon double bonds was synthesized. This polymer was used to create elastomers with a network of concatenated cyclic polymers and preserved carbon-carbon double bonds. These elastomers display unique properties compared to their linear counterparts, making them interesting for mechanical devices and soft robotics applications.

Introduction

Silicone elastomers have gained considerable attention due to their versatility across various industries, including emerging fields like stretchable electronics, where they are employed to create flexible and adaptable electronic components [1,2]. The growing interest in elastomers that combine mechanical stability with softness and elasticity, similar to human muscles, is driven by their potential use in advanced technologies such as soft robotics and exoskeletons [1,2]. Recently, an extremely soft elastomer was produced using α -monovinyl- ω -monohydride terminated PDMS and a platinum catalyst, achieving 1270% elongation and 96% strain recovery after three deformation cycles. [2] From these observations, we can exclude the possibility that a conventional crosslinked elastomer is present. This is because elastomers (materials known for their flexibility and stretchability) usually need cross-links—connections between their molecules—to quickly return to their original shape after being stretched. If an elastomer doesn't have these cross-links, it is unlikely to have such a strong ability to bounce back after being stretched. [2,3]. The elastomer structure includes chain-extended linear PDMS

from intermolecular reactions and cyclic concatenated PDMS from intramolecular reactions (Figure 1) [2,3]. The main advantage of these elastomers lies in their exceptional softness and stretchability.



Figure 1: A concatenated ring elastomer network.

This work aims to synthesize a PDMS polymer with internal carbon-carbon double bonds (Figure 1).

When cured into an elastomer, this polymer has the potential to allow post-cure functionalization via a thiol-ene click reaction. This approach takes inspiration from the highly extensible cyclic network and offers similar mechanical benefits while enhancing the electromechanical properties of the elastomer, enhancing their potential for use in soft robotics and smart materials.

Experimental

The polymer (PDV) was synthesized via hydrosilylation between telechelic hydride-terminated PDMS (DMS-H11, Mn=1100 g/mol) and 1,5,9-decatriene at room temperature (Figure

1a). After the reaction, the platinum catalyst was removed, and the product dried using a rotavapor. For elastomer synthesis, PDV was cured with DMS-H11 (Mn=1100 g/mol) and DMS-H21 (Mn=5500 g/mol) in the presence of a platinum catalyst. Post-curing functionalization involved a thiol-ene reaction with 3-chloro-1-propanethiol and 2-chlorothiophenol. Elastomers were swollen in THF with DMPA and thiols, then exposed to UV-Vis light.

Results and discussion

The structure of the polymer (PDV) was identified by $^1\text{H-NMR}$, and the completeness of the reaction was confirmed by the disappearance of the Si-H peak at 4.7 ppm and the appearance of the signals from the decatriene molecule between 5-5.5 ppm, as shown in Figure 2b.

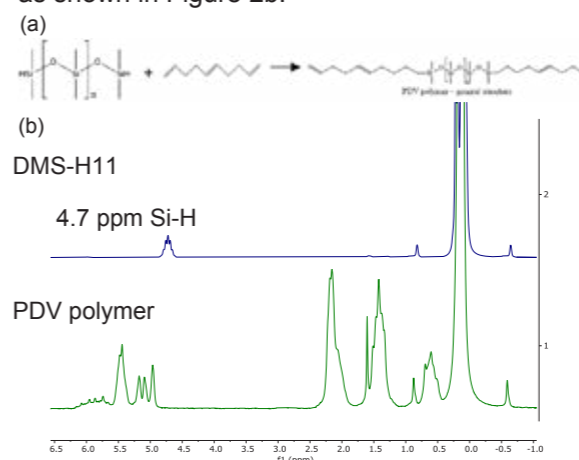


Figure 2: (a) reaction scheme; (b) $^1\text{H-NMR}$ spectra of the DMS-H11 and the PDV polymer.

The synthesized polymer was then cured to obtain an elastomer with a network of concatenated cyclic polymers.

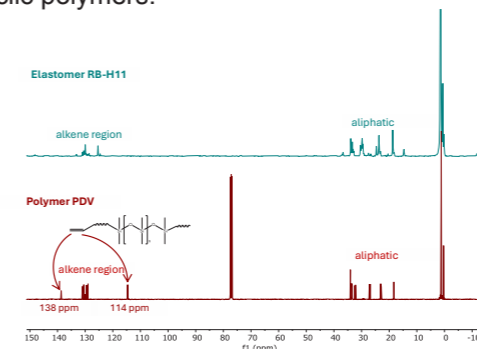


Figure 3: Solid state $^{13}\text{C-NMR}$ spectra of the resulting elastomer RB-H11 (blue, top) and the polymer PDV (red, bottom).

Solid-state $^{13}\text{C-NMR}$ spectroscopy confirmed the completion of the reaction, revealing the disappearance of resonances at 114 ppm and 138 ppm, indicative of the complete reaction between

the vinyl end groups in the PDV polymer and the hydride from DMS-H11 (Figure 3).

The available internal carbon-carbon double bonds were further functionalized with 3-chloro-1-propanethiol and 2-chlorothiophenol to increase the dielectric permittivity of the prepared elastomers. The permittivity results are shown in Figure 4. The functionalization of the elastomer prepared from the pre-polymer PDV, with 2-chlorothiophenol (E-CITP), revealed an increase in permittivity up to 3.2, corresponding to a +14% increase compared to a silicone elastomer reference. The elastomer functionalized with 3-chloro-1-propanethiol (E-CIPT) showed a permittivity of 3.8, corresponding to a +25% increase compared to the reference.

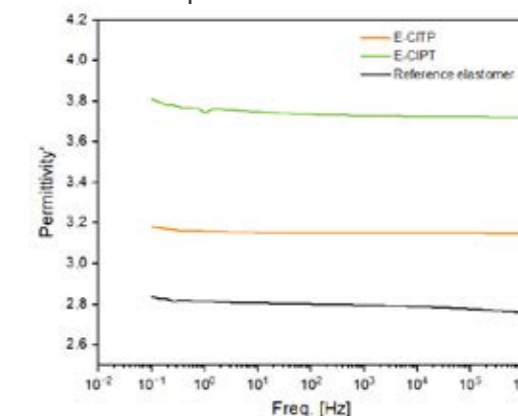


Figure 4: Relative dielectric permittivity of the functionalized elastomers.

Conclusions

In this work, a telechelic vinyl siloxane polymer with internal carbon-carbon double bonds was synthesized. The obtained polymer was used to prepare silicone elastomers through hydrosilylation with commercial telechelic hydride-terminated polydimethylsiloxanes. The preservation of the internal carbon-carbon double bonds permitted the functionalization of the cured elastomers by thiol-ene addition, which improved the dielectric permittivity.

Acknowledgments

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Optimized Modular Paint Production

(August 2022 – July 2025)



Contribution to the UN Sustainable Development Goals

This project provides a new perspective to the traditional paint production operations. It aims to change paint manufacturing system from "full formula production" to "modular production with intermediates including inline production equipment" so, unnecessary logistics, work force, and material use can be reduced, production times can be shortened and some of the energy can be saved.



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Abstract

Modular paint production targets more efficient processes by creating intermediates as building blocks for the final products. By doing so, unnecessary logistics, labor force, and cleaning time can be decreased, and less energy usage can be achieved by optimizing the dispersion processes. For each intermediate, target-oriented solutions for process optimization and quality control methods can be developed. The project centers on exploring the advantages of implementing modular paint production with intermediates. It places particular emphasis on activation of rheological additives and continuous monitoring of fineness of grind.

Introduction

In traditional paint production, raw materials undergo a series of unit processes such as premixing, grinding, and let-down, to be converted into finished products like primers, topcoats, and varnishes [1]. However, in modular production, intermediates are first created, and the final products are manufactured using these intermediates which can be pigment/filler slurries, additive solutions, or binder solutions. The shift from conventional paint production to a modular approach with intermediates offers several advantages, notably the centralization of complex operations such as powder handling, pigment dispersion, and the activation of rheology modifiers. By adopting this strategy, challenges associated with these operations are confined to the intermediate production stage, avoiding the need to address these difficulties for each product batch. Moreover, shift to the modular production with intermediates allows specific solutions for relevant intermediates and creates opportunities for "do it yourself products" and specialized production facilities.

This project aims to explore and optimize modular paint production and facilitate the moving journey towards it. Furthermore, it places a closer look on the selected intermediates and quality control methods:

- **Activation of Rheology Modifiers:** Rheology modifiers are essential for controlling flow behavior, allowing for the monitoring of aspects such as leveling, sagging, settling, or thixotropy. Some rheology modifiers require activation, and this project will delve into understanding the activation mechanisms of these materials. The aim is to reduce both energy consumption and the quantity of rheology modifiers needed.
- **Measurement of Fineness of Grind:** Determining the fineness of grind is a crucial aspect of quality control for pigment dispersions. The traditional grindometer method has significant limitations. As part of this project, an innovative method for objective measuring the fineness of grind will be developed, addressing the shortcomings of traditional approaches.

This research endeavors to enhance paint production efficiency, minimize energy consumption, and improve the overall quality control processes, ultimately advancing the field of modular paint production.

Experimental Activity

Modular production

In the laboratory, a pilot study case will be undertaken to compare factory operations conducted using both conventional and modular production systems. The optimization of

intermediate formulas that align with the principles of modular production will be the initial step of experimental activity. For this purpose, various formulas for TiO₂ and filler intermediates were created and assessed in terms of rheology, fineness of grind, hiding power, color, stability, and producibility. Effect of powder loading, amount of rheological modifier, and process parameters such as rotation speed were tested in order to achieve optimum formula that fits the concept of production with intermediates.

Activation of rheology modifiers

Bentonite and amide waxes are used as rheological agents in paint formulation. To understand their activation mechanism and propose a method for the optimum activation, an in-depth study will be conducted on bentonites and amide waxes. Figure 1 simply shows the activation mechanism of polyamide waxes and bentonites. Experiments were carried out to optimize formula and production. The effect of the amount of rheological agent and polar activators and type of the polar activator were optimized. Shear level, dispersion equipment, dispersion time, pre-and post-conditioning, were studied to find the best process. By optimizing the activation procedure, the applicable paint film thickness increased 78% without using any additional bentonite. The research also suggests that optimizing activation processes can substantially cut down both production time and energy consumption.

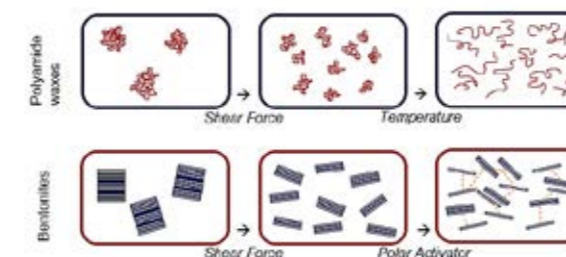


Figure 1. Activation mechanism of polyamide and bentonite rheology modifiers

Measurement of Fineness of Grind

One of the most common quality control methods for pigment dispersion is the assessment of fineness of grind, typically executed using a Hegman gage. The measurement technique relies on the visual assessment of particles on the surface of the paint which is applied with varying film thickness [4]. Despite its simplicity and cost-effectiveness, the grindometer method is plagued by certain drawbacks. Primarily, it remains a subjective technique, requiring a high degree of technical expertise for the evaluation of appearance on the grindometer. To mitigate these challenges, a novel method for measuring the fineness of grind continuously has been designed

and a prototype device has been manufactured. Preliminary studies were completed with various commercial paints and proof of concept was accomplished. Results show that there is a good agreement between the particle / scratch pattern on Hegman gage and continuous grindometer. It was seen that the fineness of grind development during dispersion process can be tracked by continuous grindometer. Moreover, image processing techniques can be used to analyze scratch patterns and finds fineness of grind.

Future Work

In the pilot modular factory case, intermediates and products will be designed and produced in the laboratory to facilitate a comparative analysis of various parameters between conventional and modular paint production. Various dispersion methods, including the use of an in-line disperser, will be conducted. The quality of the products will be analyzed and the production performance parameters, such as logistic times, production times and energy consumption, will be assessed and compared to the conventional productions.

For fineness of grind measurements, experiments will be repeated with more paint samples. An upgraded prototype device will be manufactured and tested.

Acknowledgements

The invaluable financial support provided by the Hempel Foundation and the material and advising contributions from Hempel A/S are greatly appreciated.

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Fast and reliable test of intumescent coatings

(December 2021 – March 2025)



Contribution to the UN Sustainable Development Goals

Intumescent coatings are tested in industrial scale gas fired furnaces in order to be commercially available in the market. This testing method consumes great amount of fuel, energy, product, and labor hours. Furthermore, since it is quite expensive to run these tests, it is not feasible to be done in coating development phase. Finding correlations between lab scale and industrial lab scale methods and potentially developing a new lab scale method will allow to lower these consumptions rates.



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Abstract

Intumescent coatings are exposed to time-temperature curves defined in national and international standards for commercialization. These standards use industrial scale furnaces which are fueled by gas and test real size structural elements. Since this type of testing is very costly, energy intensive, and time consuming, various lab-scale methods are adopted in academia. These methods can be used to compare different coating materials with each other in one set-up. However, variations of conditions between methods make it difficult to compare coatings tested in different set-ups and there is no agreed technique to correlate them. The project aims to develop precise correlations between various lab-scale and industrial-scale test methods for intumescent coatings and to modify current methods for faster and less resource demanding screening/testing of new formulations.

Introduction

Steel is a commonly used building material for architectural structures[1]. It has a high melting point and is nonflammable, however when exposed to high temperatures (around 500°C) its strength and stiffness decrease and this would eventually end in collapses of buildings in a fire[2]. Thus, fire protection measures must be taken e.g., to provide people with more time to evacuate the buildings.

Intumescent coatings are one of the most preferred passive fire protection materials with their high flexibility, rapid application and pleasant aesthetics[1], [3]. These coatings can expand up to 100 times of their original thickness at elevated temperatures, and with the expanded thickness they create a thermal insulation of the underlying steel[4].

Fire can be classified in two different types, namely cellulosic and hydrocarbon fire. Cellulosic fire shows slow temperature increase and takes place in residential and commercial buildings where fuel is mostly paper, textile and wood. Hydrocarbon fire shows rapid temperature increase and takes place in petrochemical or offshore industry where fuel is a combustible hydrocarbon[5].

Intumescent coatings must be tested according to standards such as ISO 834-1, UL 1709, ASTM E119-18c, EN 1363-1 in order to be commercially available. Figure 1 shows the time – temperature curves of the common standards. These standards utilize cubic meter sized industrial furnaces for the final approval of intumescent coatings which are time and energy consuming and also costly[6]. Therefore, there is a need to develop precise correlations between various test methods and to modify current methods to allow fast screening of performances and consequently be less costly and lead to safer coatings.

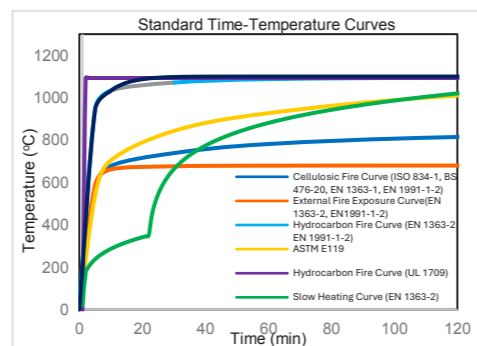


Figure 1: Time-temperature curves of commonly used standards.

Specific objectives

- Investigating different types of testing equipment (Electrical furnace, radiative heater, CoaST Fire set-up, industrial scale furnace) to find correlations to the industrial scale furnace and to develop a method to predict industrial scale behavior through lab scale data.
- Evaluating the differences (heat capacity, side effects etc.) between testing equipment and how they affect time-temperature values and char structure.
- Testing different parameters (coating thicknesses, substrate thicknesses, fire conditions) for various commercial intumescent coatings to see how they influence fire protection behavior.

Results and discussion

Experiments were conducted with various equipment using epoxy-based hydrocarbon intumescent coating under EN 1363-2 hydrocarbon fire curve. These experiments utilized samples with section factors of 200 m⁻¹ for flat plates in CoaST-Fire, small electric furnace, and industrial furnace and 333, 100 and 75 m⁻¹ for CoaST-Fire specific tests.

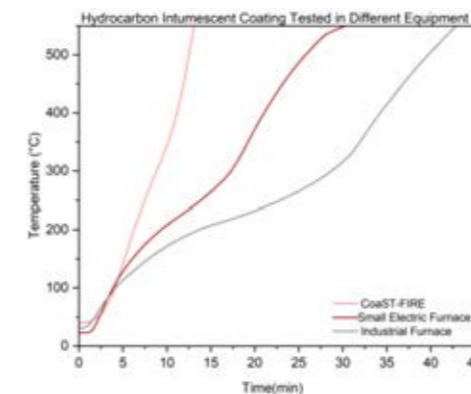


Figure 2: Time-temperature curves of flat plates tested in different equipment.

Tests on flat plates revealed a significant difference in time to failure, with the CoaST-Fire sample showing the shortest critical time. These results contradict existing literature, indicating that samples with the same section factor heat up differently in various equipment. Additionally, the CoaST-Fire sample reaches critical time the fastest.

In the previous yearbooks, the effect of insulation material and DFT were discussed. The current study examines the effect of section factor, with results shown in Figure 3. Results indicate that increasing the section factor leads to shorter time-to-failure, and that time-to-failure and section factor are not directly proportional.

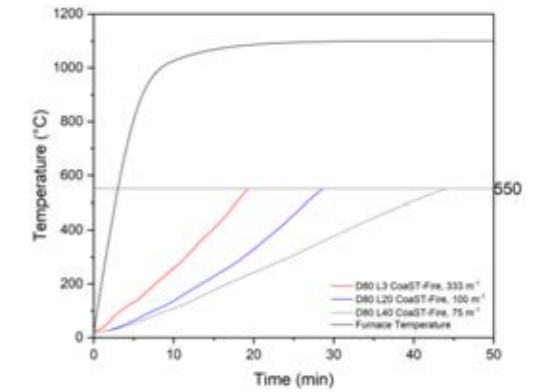


Figure 3: Time-temperature curves of flat plates with different section factors tested in CoaST-Fire.

Conclusion and future work

These experiments underscore the importance of section factor and heat exposure across various equipment types. This systematic study, alongside prior research on insulation materials and DFTs, seeks to refine lab-scale testing conditions.

Future efforts will focus on testing samples with varying thicknesses and section factors in CoaST-Fire, aiming to establish a correlation between CoaST-Fire and the industrial furnace.

Acknowledgement

The authors would like to acknowledge the financial support from Hempel Foundation Coatings Science and Technology center (CoaST).

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Dynamic Fouling Control Tests

(May 2021 – December 2024)



Contribution to the UN Sustainable Development Goals

Biocides are used in marine coatings to inhibit fouling on ship hulls, thus improving the fuel efficiency as drag and total weight of the ship is reduced, but also impede the translocation of invasive species. However, aquatic life is affected by the biocides released from the marine coatings. Determining the lower critical amount of biocides in an antifouling coating could allow reducing the amount of incorporated biocides. Additionally, the evaluation of fouling release coatings with no biocide release could prove the effectiveness equal to conventional antifouling coatings.



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Abstract

Evaluation of marine coatings has commonly been performed by static immersion tests to obtain data before application. However, these tests are limited as the coatings are not subjected to the hydrodynamics and fouling conditions present in voyaging ships. Different dynamic test methods have been used to mimic a ship underway by introducing these parameters. The purpose of this project is to establish the next generation of dynamic test setups, aiming to illuminate how a coating performs in a real-life scenario, which can aid in the selection of an appropriate coating for optimal performance for the ship's traveling schedule.

Introduction

Marine vessels are subjected to biological fouling on the hull by bacteria, algae, and marine animals [1]. The accumulation of biofouling increases fuel costs because of added weight and drag, which inevitably elevates the environmental concern due to the growth of emitted CO₂, SO₂, and NO_x [2]. Subsequently, the translocation of invasive species, which when introduced to a new environment can threaten the ecosystem leading to a potentially irreversible effect on wildlife [3]. Aiming to limit the environmental impact antifouling coatings have been utilized to reduce drag by impeding biofouling growth, maintain the structural integrity, and prolong the smoothness of the hull. Commonly, immersion of samples tested statically, in strategically advantageous sites, has been applied as small-scale experiments to evaluate various parameters such as skin friction, leaching rate, fouling growth, polishing rates, etc. Several advantages are present in small-scale experiments. Cost-effectiveness combined with the sample capacity allows the evaluation and comparison of multiple fouling control coatings, which can facilitate the determination of lifetime, fuel-saving capabilities, and growth mechanisms. However, the small-scale experiments are challenging to convert into full-scale as larger vessels rarely lay idle in ports. Specific Objective

- Establish the next generation of dynamic test methods for fouling control coatings.
- Increase the traditional output from dynamic test to high throughput by big sample capacity and extensive data monitoring.
- Increase the reliability of data by obtaining additional datasets and more data points with higher precision and accuracy.
- Optimize the timeframe for when mechanical cleaning is necessary for ships in more or less constant movement.

Method

The release rate measurement setup (Figure 1R) consists of a concentric cylinder, immersed in a glass beaker, which is filled with artificial seawater. A disperser drives water motion. The sample is attached to the beaker wall and copper released from the coating is measured in the water using a complexing agent with subsequent absorbance measurements.

The on-site cylindrical rotor setup, which is shown in Figure 1L is one of 8 in use. It consists of a rotating cylinder located in a raft at the harbor in Hundested. The rotational speed can be adjusted in the control box, which also controls the rotational intervals.

The specific objectives of this project are:

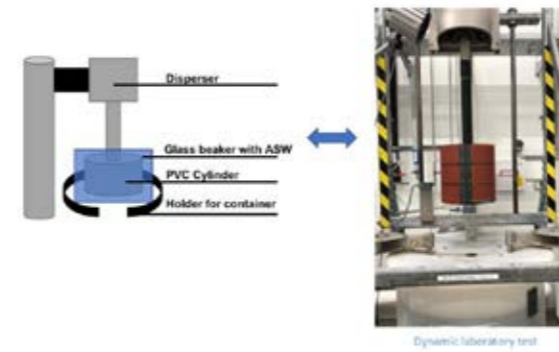


Figure 6: Left) Release rate measurement setup. Right) Cylindrical rotary setup and static samples in Hundested harbor.

A dynamic copper release rate comparison was conducted on two reference samples. The samples were formulated based on a CoaST reference formulation. One formulation was a rosin-based copper coating and the second was a rosin/acrylic-based copper coating. The panels were immersed for 4 weeks with weekly visual inspection and release rate measurements. After the last release rate measurement, the leached layer thickness was measured using optic microscopy.

Results and Discussion

Figure 2 illustrates the difference in release rate over 4 weeks of dynamic exposure of the two samples. This was conducted to establish if the release rate testing procedure would show valid results.

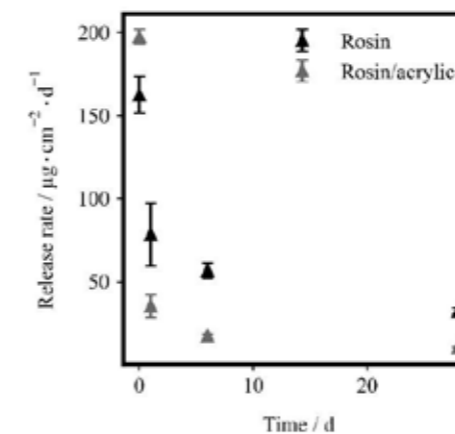


Figure 2: Comparison of release rates between different binder ratios over time during dynamic exposure

In accordance with Figure 2 hydrophobic co-binders are recognized for their ability to enhance resistance to water penetration, thereby reducing the rate of copper release. Conversely, increasing the concentration of hydrophilic resins, such as rosin, is anticipated to elevate the biocide release rate. The phenomenon was observed using the setup. The rosin/acrylic system has a significantly lower release rate than the pure rosin coating after one day.

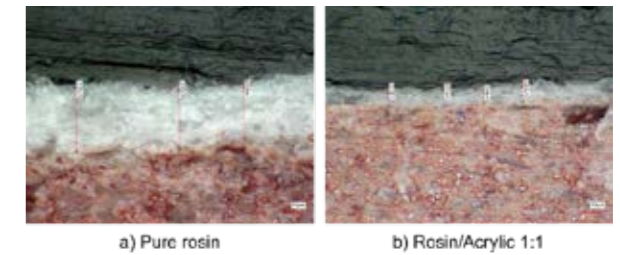


Figure 3: Thickness of the leached layers of the two coating systems after 4 weeks of dynamic immersion.

As seen in Figure 3. The leached layer is approximately three times thicker for the pure rosin coating, 35 μm (rosin) and 11 μm respectively. In relation to the release rate in Figure 2, A thicker leached layer means that the biocide has been leaching faster. Furthermore, the high hydrophilicity of rosin allows water to penetrate the coating beyond the outer layer, hence cuprous oxide is dissolved from deeper layers in the coating matrix.

Conclusions

The results from Figs. 2 and 3 demonstrate that the inclusion of hydrophobic co-binders in the coating formulation effectively reduces the release rate of copper by limiting water penetration, as seen in the lower release rate of the rosin/acrylic system. In contrast, the pure rosin coating exhibited a higher release rate and a significantly thicker leached layer, indicating faster biocide leaching. The high hydrophilicity of rosin contributed to deeper water penetration and dissolution of cuprous oxide from the coating matrix. These findings validate the testing procedure and highlight the impact of binder composition on fouling control performance.

Acknowledgement

Financial support from the Hempel Foundation to CoaST (The Hempel Foundation Coating Science and Technology Center).

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Physiological bioprocess control

(September 2023 – September 2026)



Contribution to the UN Sustainable Development Goals

Applying advanced control strategies to the cultivation of microbial cells enables a more efficient and sustainable production of a wide range of products. A focus on the physiology of the cells promises more or higher quality products with less raw material input. Gaining more control over the process can furthermore reduce the risk of failed batches and the resulting loss of material and energy input. Therefore, the methods and results of this work contribute towards the responsible production cultivation products.



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Abstract

Microbial bioprocesses are often run with fixed recipes for feeding profiles and simple control algorithms focusing on general technical parameters. Shifting the focus towards creating process models that consider the physiological state of the cells can benefit the understanding and design of industrial bioprocesses. Putting these models to use in advanced and predictive control algorithms opens the way to more productive and efficient cultivations. Simultaneously, they pose as a real-time monitoring tool for the current cell conditions inside the bioreactor and its predicted trajectory. This is showcased for the control of the dissolved oxygen level inside the broth for an intermittent fed-batch process of *Escherichia coli* producing green fluorescent protein after induction.

Introduction

The ability to control biotechnological processes at their optimal state accurately and automatically is of considerable interest to many fermentation industries. Providing cells with ideal physiological conditions for the respective task can improve the production of the targeted metabolic products in higher quantities and qualities, while also reducing the process and material costs [1].

The highly dynamic and non-linear nature of bioprocesses poses great difficulties with bioprocess monitoring and bioprocess control approaches to ensure such conditions in the reactor. Therefore, mechanistic models are developed that can capture this behavior without introducing too much mathematical complexity to achieve robust and fast predictions. These models are then parameterized with experimental data and further deployed in model-based control algorithms to optimize a process for a respective goal. Special attention will be placed on biomass specific rates including nutrient uptake, oxygen consumption, carbon dioxide production as well as inducer consumption and production rates. The ability to control these biomass specific rates does not only lead to higher productive and better scalable processes but they can also stabilize

production and therefore enable continuous biomanufacturing [2].

Model predictive control (MPC) algorithms emerge as a viable option to ensure optimal physiological conditions throughout the process due to their predictive nature. By using mechanistic models with a focus on cell physiology, they can capture the deviations in the trajectory of key process indicators from a limited set of online signals [3]. The project investigates the application of such controllers for an *Escherichia coli* cultivation for the production of recombinant proteins such as green fluorescent proteins.

MPC Application for dissolved oxygen levels

The level of dissolved oxygen (DO) in the broth plays a pivotal role here, as limitations cause shifts in the metabolic activity of the cultivated organisms, byproduct accumulation or even cell death. Simple controllers such as PIDs keep the DO level above a defined threshold by acting on the agitation, air flow and oxygen partial pressure, where many are based on PID algorithms [4]. But when faced with abrupt changes in nutrient addition, their purely reactive nature struggles, which can be observed for intermittent feeding profiles in high-throughput small scale multi-

reactor systems [5]. A MPC algorithm on the other hand can anticipate the next feed addition and proactively start to ramp up the oxygen supply to meet the increased uptake rates in time.

Methods

The process uses an *Escherichia coli* strain with green fluorescent protein encoded into the expression system. Experiments were conducted in a 5L bioreactor setup.

The oxygen uptake is modeled through the metabolic activity of an aerobic microbial process by employing simple growth kinetics and elemental balances. This demand is met with the oxygen transfer rate, which is connected through a $k_L a$ model [6] to the two actuators of the control loop, the agitation speed and the aeration rate.

The parameters of the resulting models are estimated, using a combination of online and offline signals. The model is then implemented and assessed first *in-silico* in form of a simulation study before being tested as a soft-sensor during a process that simulates an intermittent feeding profile. Finally, it was incorporated as an MPC algorithm and evaluated by comparing it to a conventional PID controller.

Results and discussion

The simulation study showed that the predictive nature of the MPC is able to mitigate the sudden drops in dissolved oxygen. This can be observed in Figure 1 where it is shown against a simple PID algorithm. It was then further applied in the laboratory setup and tuned with the experimental conditions. Similar results could be achieved where the oxygen depletion time after the shot-wise substrate addition could be reduced compared to the conventional PID. Further analysis of the produced data is necessary to assess the implications on the physiological state of the cells and the overall process benefits in avoiding the oxygen depletion times.

Conclusion

Model-based control algorithms outperform conventional reactive controllers at certain tasks. Thereby, they present a promising strategy for small scale reactor systems with intermittent feeding or processes with harsh phase transitions. Since the model is using only simple growth kinetics, it is generically applicable to aerobic cultivations at different scales after parameterizing the reactor specific $k_L a$ model.

For future work, these benefits of the MPC are to be applied to the optimization of protein production for two feed systems where the induction agent itself is also a metabolizable substrate.

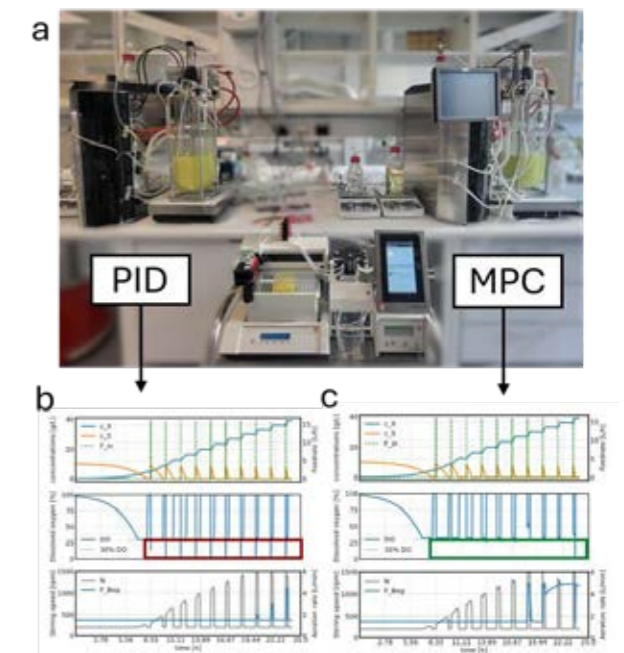


Figure 1: a) Lab-Reactor setup for verification of advanced control algorithms. b) classical PID control of DO with O_2 limitation periods after feed addition (red rectangle) c) Model-Predictive Control (MPC) with reduced O_2 limitations (green rectangle).

Acknowledgements

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Deciphering the anaerobic microbiome for construction of robust microbial consortia for mixed culture fermentations

(May 2024 – April 2027)



Contribution to the UN Sustainable Development Goals

Advancing the development of biofuels and bioproducts through anaerobic fermentation, this project focuses on creating comprehensive metabolic models of mixed-microbial communities to optimize the production of medium-chain fatty acids. These fatty acids can find many applications substituting fossil-based fuels and products, alternative to fossil fuels and reducing greenhouse gas emissions. The use of microbial consortia enhances the efficiency and scalability of the fermentation processes. This approach supports the transition to renewable energy sources, reducing carbon footprints and fostering a sustainable energy future.



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Abstract

This project aims to develop a comprehensive mathematical model of the metabolic reactions occurring within mixed-species cultures of anaerobic microorganisms, specifically focusing on taxa involved in chain elongation. This research will involve the development of a laboratory protocol for the chain elongation of volatile fatty acids, investigation of microbial consortia interactions, and the generation of community genome-scale metabolic models. The objective is to establish synthetic mixed microbial cultures capable of efficiently producing medium-chain fatty acids. This work will advance the field of microbial community dynamics and contribute to the development of sustainable biofuel production processes.

Introduction

Anaerobic fermentation represents a pivotal sector in biotechnology, contributing significantly to the green transition. The deployment of anaerobic microorganisms is particularly advantageous due to their capacity to produce secondary metabolites in substantial quantities, which are extensively utilized in industrial applications. Prominent examples include the biosynthesis of lactic acid [1] and volatile fatty acids [2].

The application of single-species anaerobic cultures for the bioremediation of heterogeneous and toxic compounds is impractical, as such conditions inhibit microbial proliferation. An effective alternative is the utilization of mixed-species cultures, comprising microbial species that engage in synergistic interactions. These mixed cultures exhibit superior adaptability to environments characterized by extreme

thermodynamic conditions, such as fluctuations in pH and temperature, compared to single-species cultures [3].

The selection of appropriate microbial species capable of establishing a robust microbial community in environments with heterogeneous and toxic organic wastes is crucial. This can be assisted by developing models that describe the metabolic reactions occurring within microbial communities of different species. An efficient approach to modeling microbial metabolism is the creation of genome-scale metabolic models (GSMMs). GSMMs are *in silico* representations of the metabolic reactions within a cell, including the enzymes that catalyze these reactions [4]. The design of GSMMs relies on information from published metabolic maps found in databases. With the increasing number of publications related to high-throughput sequencing, GSMMs now

integrate data from various -omics sources, enhancing their predictive accuracy [5].

GSMMs are often combined with Flux Balance Analysis, a mathematical method that calculates the flux of metabolites within a metabolic network [6]. This combination allows for the estimation of microbial growth rates and the production rates of specific metabolites.

In conclusion, the knowledge generated during the project will create the know-how to build faster and more efficient synergistic mix species microbial communities, capable of successfully transforming different raw materials into high-value chemicals.

Specific Objectives

The aim of this project is to develop a comprehensive mathematical model of the metabolic reactions occurring in mixed-species cultures for improving capacity and specificity of chain elongation process. The species to be modeled will be selected based on their collaborative mutualistic properties in chain elongation conversion processes. Metabolic models will be constructed to provide a complete understanding of the microbial community. These single-species models will be used to establish mixed-species microbial communities in the laboratory. The appropriate culture conditions will be explored to ensure the successful growth of the resulting microbial community.

The specific objectives of the project are:

1. Development of a laboratory protocol to perform chain elongation of volatile fatty acids using microbial consortia
2. Investigate the interactions of the microbial consortia
3. Generate community Genome Scale Metabolic Models
4. Establish synthetic mixed microbial cultures

Materials and Methods

Lab-scale batch experiments will be conducted under anaerobic conditions. Enrichment cultures will be established with various carbon sources to perform chain elongation. The production metabolites will be monitored regularly. Upon observing a significant increase in the production of medium-chain fatty acids, comprehensive taxonomical and functional analyses will be performed. These analyses will aim to elucidate the structural composition and metabolic activities of the involved microbial communities, utilizing high-throughput sequencing. By integrating this data, *in silico* genome-scale metabolic models will be developed to describe the microbial community

responsible for the chain elongation of short-chain fatty acids to medium-chain fatty acids. The species constituting these communities will be isolated using molecular tools, cultured separately, and subsequently utilized to create synthetic mixed microbial cultures that will produce the desired products.

Acknowledgement

This work was financially supported by European Research Council Advanced Grant Project "The ANAEROBic treasure trunk" (Grant agreement No. 101098064)

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Oxygen affinity in biocatalytic oxidation

(January 2023 – December 2025)

12 RESPONSIBLE CONSUMPTION AND PRODUCTION



Contribution to the UN Sustainable Development Goals

Traditional oxidation processes consume large quantities of energy and require polluting compounds such as metal salts and organic solvents. Biocatalysis is an alternative and sustainable route since it consumes less energy, uses renewable compounds and the waste produced is non-toxic. However, oxidative biocatalysis still has some major bottlenecks before it can become fully implemented. This project aims to tackle the challenges associated the presence of oxygen in the reaction to achieve economically feasible biocatalytic processes.

Abstract

Many relevant chemicals are produced through the oxidation of a feedstock via chemical oxidation. One alternative route is biocatalysis which conveys enormous benefits such as superb selectivity under mild conditions. Oxidative biocatalysis requires a constant bubbling of air to achieve high levels of dissolved oxygen in the media. However, the bubbling compromises enzyme stability, hence the activity measurements become not accurate. To characterize enzymes and avoid the destabilization effect of the gas-liquid interface we have developed a device that is able to supply oxygen without a gas-liquid interface: the Tube-in-Tube Reactor system.

Introduction

Many products we use in our daily life contain modified organic chemicals (from flavors to the plastic used for packaging). These compounds must be manufactured by a serial of (often catalytic) steps and it is common that one of these steps is oxidation.

Metal-based catalysts are traditionally used to oxidize chemicals to produce valuable products. This process involves the mining and processing (curation) of the metals by using organic solvents before they can be used as catalysts. During the catalysis, high temperatures (up to 500°C) and pressures are applied, requiring a big expense of energy. Large amounts of catalyst are used in the reaction and end up becoming hazardous waste difficult to discard.

Biocatalytic oxidation provides a sustainable, safe, and highly selective alternative to chemical catalysis. This is, enzymes are produced by bacteria which grow on renewable materials and produce only organic waste (which can even be upcycled or easily disposed). In biocatalytic reactions molecular oxygen is used as the final electron acceptor (oxidizing agent) instead of metals.

In industrial setups, oxygen is typically provided to the reaction mixture by bubbling air since it is cheap, widely available and non-toxic [1].

Oxygen transfer and bubbles

Oxygen is unfortunately, a quite insoluble gas: the maximum concentration of oxygen in water in equilibrium with air is 250 μM (at 30 °C and ambient pressure). The fact that it is a gas implies that it must be constantly bubbled to keep up with the oxygen demand of enzymes and its low solubility implies that oxidative processes are often oxygen-limited.

A high rate of air bubbling is a double-edged approach: while a larger supply of air increases the oxygen transfer to the liquid, bubbles create a gas-liquid interface which adsorbs enzymes and compromises their stability (Figure 1).

The deactivation mechanism of enzymes by the interaction with the gas-liquid interface is not well understood yet. This is because many parameters that are difficult to dissect experimentally can affect the enzymes in different ways. These parameters are (but not limited to): interfacial area, time of exposure to the interface, size and shape of the bubbles, speed of the bubbles rising and type of gas.



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In order to study the pure kinetics of an enzyme while avoiding its activity loss as a result of the adsorption to the gas-liquid interface, we have developed a unique tool: the Tube-in-Tube Reactor system.

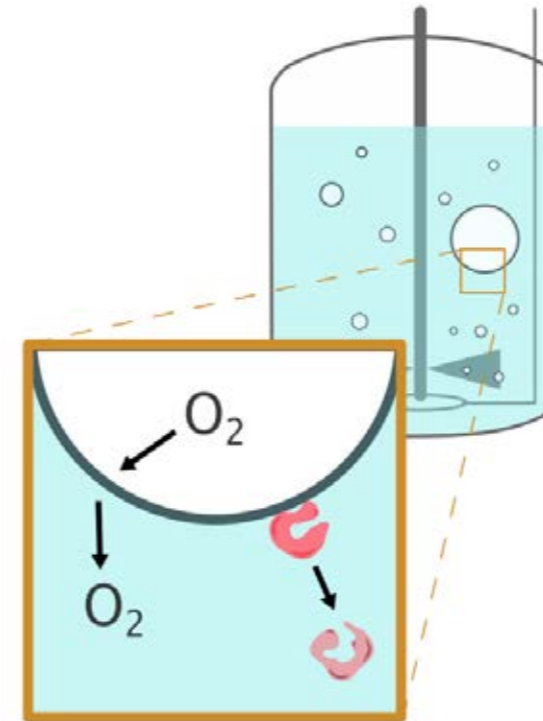


Figure 1. The reactor is sparged with air, which creates bubbles. The oxygen must get transferred from the gas bubble to the liquid and only then it will be available for the enzyme. At the same time, the enzymes that get adsorbed to the bubble end up losing their structure and getting deactivated.

Tube-in-Tube Reactor system

The Tube-in-Tube Reactor system is a novel tool that allows to study oxygen transfer avoiding the presence of bubbles, hence, avoiding the gas-liquid interface [2].

The Tube-in-Tube Reactor is composed by a gas-permeable tube encased in a gas-impermeable tube [3]. The liquid phase flows through the inner tube and the gas flows in the outer tube, diffusing through the inner tube wall and gets solubilized in the liquid phase. Hence, the inner tube wall becomes a solid membrane-like barrier between the gas and liquid phase that prevents the oxygen to form bubbles in the inner tube (Figure 2).

The Tube-in-Tube Reactor system is a complex tool that allows to achieve concentrations of oxygen in water up to 12 mM through the tuning of the oxygen partial pressure (which can go from 5 – 100%) and the absolute pressure (which can go from 0 – 10 atm). Moreover, the system operates automatically thanks to a software which combines all the parts. Samples are taken in-line also automatically.

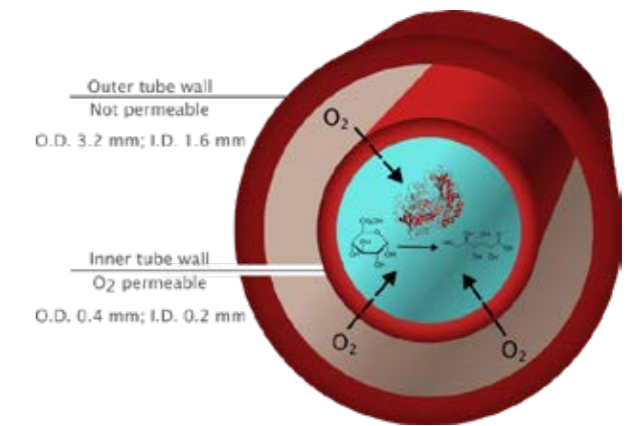


Figure 2. Cross section of the Tube-in-Tube reactor.

Conclusions

It is crucial to address the challenges derived from the presence of oxygen in the reaction media in biocatalytic oxidations. Unfortunately, there is a lack of tools to dissect the parameters affecting the enzymes in a bubbling reactor. Now, the Tube-in-Tube Reactor system can provide enormous amounts of oxygen to the system while avoiding the gas-liquid interface.

The kinetic data obtained from the experiments carried out in the Tube-in-Tube Reactor system will contribute to a better understanding of the potential of oxidases and its limitations. This information will be also valuable to biochemists and enzyme engineers who want to develop better enzymes to be used as biocatalysts in industry.

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Novel membrane structures for improved performance of immobilized enzymes

(September 2022 – August 2025)

13 CLIMATE ACTION



Contribution to the UN Sustainable Development Goals

Multienzymatic reactions open possibilities for new routes of sustainable production of chemicals from renewable bio-based feedstock. However, existing reactor designs do not enable simultaneous exposure of each enzyme to their individual optimal conditions and thereby result in low reaction rates. In this project, we aim to develop novel membrane supports that would allow to modify and optimize the microenvironment of immobilized enzymes. We expect that the improvement of activity and stability of biocatalytic cascade systems will help to boost the industrial enzyme applications.



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Abstract

Immobilization of enzymes is an efficient strategy to promote stability, selectivity, recovery, and reuse of a biocatalyst. Fixation of enzyme molecules can be performed on a variety of solid supports, and a polymeric membrane is one of them – in addition allowing a continuous process with simultaneous reaction and product removal. In this project, we focus on the systematic study and development of enzymatic membrane reactors (EMRs) using membrane modification as a tool. Our aim is to develop new membrane modification strategies (with inorganic and organic coatings) so we can simultaneously advance enzyme activity, enzyme stability, and permeability of the reactor, as well as understand the interconnection between various EMR properties.

Introduction

EMR (also known as enzymatic or biocatalytic membrane) is a type of catalytic membrane which employs immobilized enzymes as a source of catalytic activity (Figure 1) [1]. The recent developments in the field highlight large potential of EMs for applications in the biotechnological, chemical, food, and pharmaceutical fields, with a particular focus on degradation of environmental micropollutants, carbon capture and utilization, and use in biosensors [2,3]. Enzyme immobilization can significantly advance specific enzyme properties compared to free biocatalyst; however, at the same time it can cause a lot of undesired effects (high loss of enzymatic activity mass transfer limitations, high extra costs associated with the immobilization process itself and disposal of deactivated biocatalyst) [4]. Thus, only systems which demonstrate overall desirable qualities are considered for implementation in the practical settings; and there is a large demand for new enzyme immobilization strategies which can achieve that.

One way to improve the overall performance of EMs lies in modification of the membrane support prior to immobilization. Polyelectrolytes (PEs) – macromolecules containing a (large)

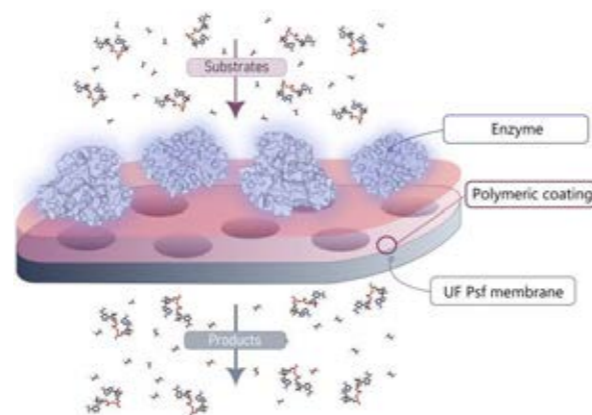


Figure 1: Graphical illustration of the EMR system

number of positively and/or negatively charged groups - can be used as efficient mediators in the synthesis of EMRs as they can have a positive effect on properties of both immobilized enzyme and membranes (single PEs and layer-by-layer (LbL) PE assemblies can be used to improve chemical stability, fouling resistance, and selectivity of membranes for various applications and provide more binding sites for enzyme immobilization) [5–6].

Specific objectives

1. Study of the interconnection between structure of the nanoscale LbL assemblies and biocatalyst efficiency.
2. Tailoring the properties of membrane supports to optimize performance of individual enzymes and multienzymatic cascade systems.

Results and Discussion

Our recent results underline the significance of optimization of membrane modification protocol for advancement of EMR performance. Figure 2 indicates the trade-off between biocatalytic activity, enzyme loading, and water permeability of the reactor - which can be resolved by using alternative surface chemistries [7]. Figure 3 shows how chemistry of the employed polyelectrolyte affects immobilization yield and immobilization efficiency – two main indicators of the immobilization process [8]. Table 1 presents the results of linear regression analysis aimed to investigate statistically significant relationships between properties of the modified membrane support and enzyme performance [8].

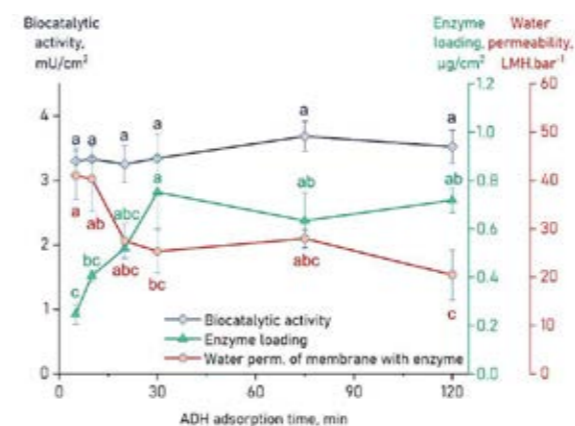


Figure 2: Interconnection b/w biocatalytic activity, enzyme loading, and water permeability in EMR systems upon different time of enzyme adsorption.

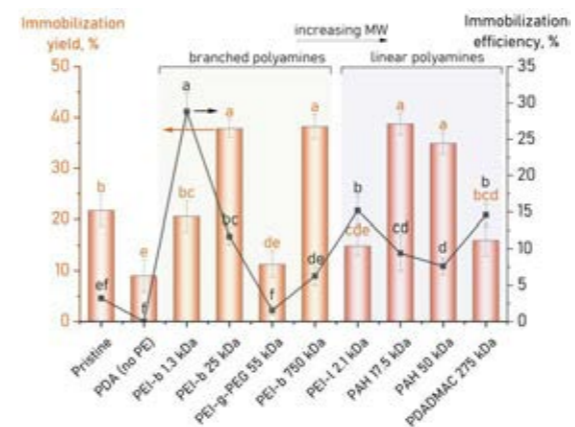


Figure 3: Immobilization yield and immobilization efficiency (activity recovery) values for EMRs modified with different polyamine in the support.

Table 1: The regression coefficients and corresponding p-values for the linear regression

models quantifying relationships between membrane and enzyme properties in EMR.

Covariate	Biocatalytic activity, mU/cm ²	Activity recovered in the retentate to total activity, %	Immobilization yield, %	Immobilization efficiency, %
MW of polyamine, kDa	-0.0091 (p = 0.28)	0.25 *** (p = 7.1·10 ⁻⁴)	-0.038 (p = 0.11)	-0.0072 (p = 0.69)
Water permeability, LMH.bar ⁻¹	0.061 (p = 0.45)	-2.9 *** (p = 4.3·10 ⁻⁵)	0.15 (p = 0.61)	0.11 (p = 0.67)
WCA (10 s), °	-0.055 (p = 0.35)	-1.6 ** (p = 0.0072)	N/A	-0.29 ** (p = 0.0062)
ZP (at pH 8.80), mV	0.07 * (p = 0.012)	-0.28 (p = 0.43)	0.45 *** (p = 2.6·10 ⁻⁵)	0.04 (p = 0.71)
Isoelectric point	1.2 * (p = 0.020)	-3.0 (p = 0.64)	8.7 *** (p = 1.9·10 ⁻⁷)	0.07 (p = 0.97)

Conclusions

The presented results may be used as a promising platform for further study and development of biocatalytic LbL assembly structures for immobilization of commercial enzymes. Modification of membranes with PEs using proposed techniques can be used as an efficient strategy to simultaneously reuse biocatalyst, promote its activity, and retain high permeability of the membrane.

Acknowledgements

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Functionalization of PDMS via click chemistry for dielectric elastomers

(January 2023 – January 2026)

7 AFFORDABLE AND CLEAN ENERGY



Contribution to the UN Sustainable Development Goals

Silicone elastomers are attractive materials for developing wearable electronics. While most current applications focus on their benefits as soft wearables for life improvement and health benefits, silicone elastomers can also be applied as a material for triboelectric generators, converting mechanical energy into electric energy from sources like wind and tidal energy. This versatility makes silicone elastomers promising candidates for innovative energy-harvesting applications in addition to their established wearable roles.



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Abstract

A facile synthetic route of converting a commercial polydimethylsiloxane (PDMS) to a prepolymer capable of non-metal-catalyzed cross-linking *via* Thiol-Michael addition is presented. Two prepolymers and their respective cross-linked networks are thus compared: Maleimide (MI)-terminated PDMS, and maleamic acid amide (MA)-terminated PDMS. We argue for the potential of maleamic acid amide functionalities in particular as a good platform for construction of dielectric elastomer actuators, due to their improved dielectric properties and self-healing.

Introduction

Polydimethylsiloxane (PDMS) is a flexible polymer with a low glass transition temperature. It is widely used as a silicone elastomer in applications like soft robotics and dielectrics. When forming a network, PDMS is normally cured in the presence of a metal catalyst (e.g., Pt).

Metal-free silicone elastomers are cured under mild conditions, enhancing their application and recyclability and reducing metal-related conductivity issues, where the presence of a metal catalyst can lead to unwanted conductivity of the dielectric [1]. Michael addition, a type of click chemistry, involves coupling a nucleophile (thiol) with an unsaturated bond (vinyl), known for rapid, selective reactions with minimal use of catalysts.

In this study, aminopropyl-terminated PDMS (APDMS) is converted to maleamic acid amide-terminated PDMS (MA) and then to maleimide-terminated PDMS (MI) through a two-step process (Scheme 1). These prepolymers are cross-linked via Thiol-Michael addition using triethyl amine as a catalyst, making the process metal-free and oxygen-insensitive.

Specific Objectives

The primary objective of this project is to:

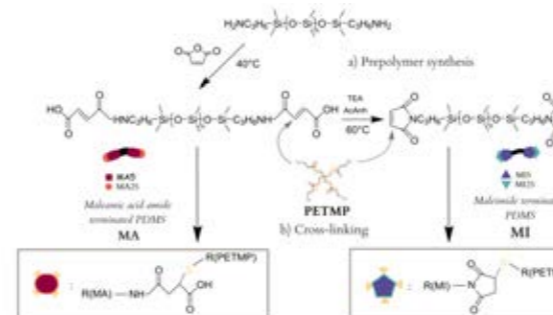
- Develop a facile and robust methodology for synthesizing PDMS networks using metal-free cross-linking.
- Adapt the network by using novel additives for improved dielectric properties.
- Produce dielectric elastomer actuators or triboelectric nanogenerators.

Current progress has met the first point, while work on the latter two is ongoing.

Results and Discussion

The MI and MA networks formed from their respective prepolymers (as shown in Scheme 1, in two molecular weights, named based on the chain length of their prepolymer, 5 kDa and 25 kDa) show an increased dielectric permittivity. While they possess higher permittivity in the entire spectra compared to a commercial reference (Sylgard™ 184, $\epsilon_r = 2.73$), only the more polarizable MA system shows a major increase in permittivity at low frequencies (Figure 1). This is particularly beneficial for their applications as actuators or generators, considering that most of

the energy harvesting devices are in the frequency range below 15 Hz [2].



Scheme 1. The reaction scheme of the synthesis and cross-linking of the MA and MI prepolymers.

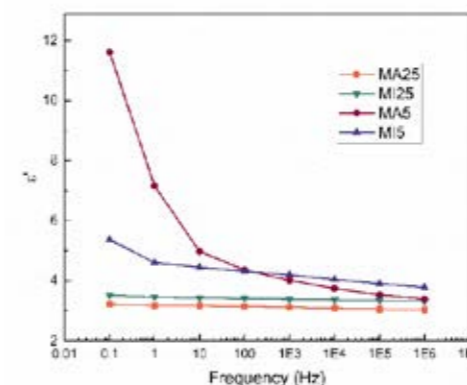


Figure 1: Dielectric permittivity as a function of frequency for MA and MI networks (5kDa, 25kDa).

MI and MA elastomers were assembled as a simple dielectric elastomer, a 25 mm thin film disc with an applied carbon grease electrode on each surface. Both MI and MA networks show electric breakdown comparable to commercial products (Sylgard™ 184, $E_{BD} = 130 \text{ kV mm}^{-1}$), irrespective of their type and the molecular weight of the prepolymer (Table 1). This is an excellent basis for further improvement, considering no additives were used to achieve these properties, unlike commercial products.

Table 1: Electric breakdown strength averaged over eight samples for the long-chain MA/MI25 and short-chain MA/MI5.

SAMPLE	$E_{BD}, \text{KV MM}^{-1}$
MA5	64.5 ± 16.3
MA25	64.2 ± 9.39
MI5	77.3 ± 27.3
MI25	93.3 ± 15.6

Finally, the MA5 and MA25 networks are self-healable, even at room temperature. This is due to the abundant hydrogen bonding allowing for

intermolecular organization and reorganization after inflicted damage. Since MI networks only possess hydrogen bonding acceptors, they do not show self-healing. This attractive feature can improve the actuator's real-world performance by healing the pinhole damage from a potential electric breakdown. The self-healing efficiency, as defined by the ratio of tensile strength after healing and tensile strength of pristine material, is 85% for both networks (Fig 2.).

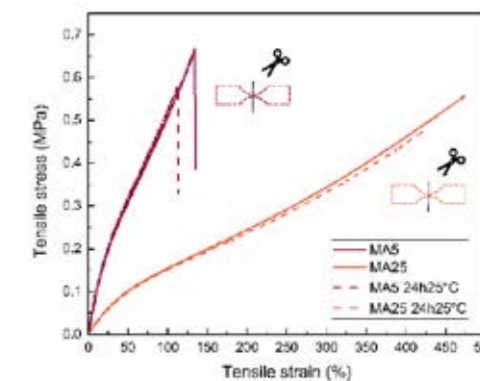


Figure 2: Stress-strain test of pristine (line) and self-healed (24h25C, dashed) MA5 and MA25 networks.

Conclusions

Two different cross-linked networks based on Michael-addition were prepared from modified commercial PDMS. Both networks showed improved dielectric permittivity and promising electric breakdown strength. MA networks are particularly of interest for their self-healing and low-frequency performance, due to their increased intermolecular bonding.

Acknowledgments

The authors would like to thank the Novo Nordisk Foundation for funding this project.

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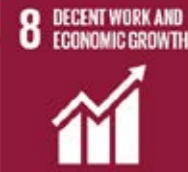
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List of Publications

P. Ramah, L. Yu, A. E. Daugaard, A. L. Skov, *RSC Appl. Polym.* **2024**, *2*, 891–904.

Artificial Intelligence in Process System Simulation and Control

(November 2021 – January 2025)



Contribution to the UN Sustainable Development Goals

The introduction of Artificial Intelligence in the modeling of process systems enables opportunities for modeling processes that have not previously been possible to model accurately. This project works towards applying artificial intelligence in the modeling of process systems for optimization and control applications. Artificial intelligence-enabled process optimization can positively contribute to SDG 8 “Decent work and economic growth” through profit maximization or minimization of utility and raw material consumption.



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Abstract

Over the previous years a surge in the applications of AI tools has occurred with ChatGPT leading the way in bringing AI to everyday use. Applying AI for (Bio)Chemical engineering applications have however proved a challenge due to the characteristics of the data available from the production lines. More promising is the use of hybrid approaches combining process knowledge and data-science. In this project different hybrid approaches are investigated, comparing the prediction accuracy, extrapolative capabilities, and ease of interpretation.

Introduction

As data is becoming more easily accessible in the (bio)chemical industry, there is a renewed interest in leveraging data-based methods for the improvement of process operations [1]. Even though vast amounts of data are available for said processes, it is often serially correlated and with low variation due to the operation of the processes at specified set points. As a result “purely” data-driven modeling approaches are often inadequate in predicting process outcomes, and there is a high risk of the models extrapolating when used for process optimization. As a way of mitigating these problems, a priori process knowledge can be incorporated into the development of data-based models.

Modeling Methods

Process knowledge and data-driven methods can be combined in “hybrid semi-parametric modeling” (hereinafter referred to as hybrid modeling) [2] (Figure 1). Over the last 30 years, hybrid modeling has been gaining popularity and a large number of applications of hybrid modeling have been published [3]. Hybrid modeling offers the possibility to model well-known phenomena using a parametric model, such as first principles equations, while unknown or uncertain phenomena are modeled using a nonparametric model, e.g. neural networks. In typical applications

of hybrid modeling, feedforward neural networks are used for predicting mass transfer coefficients in material balances for bubble column aeration [4] or for predicting kinetic parameters for population balances in flocculation processes [5].

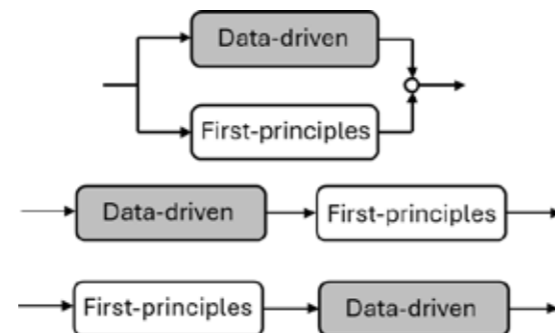


Figure 1: Hybrid semi-parametric model structures

A new and promising way of including process knowledge in data-driven modeling is using “Physics-informed Neural Networks” [6] (Figure 2). In physics-informed neural networks, physical knowledge about the system is implemented in the cost function used for training the neural networks, rather than enforcing the mathematical structure

as done in hybrid models. Physics-informed neural networks can be used for approximating both ordinary differential equations (ODEs) and partial differential equations (PDEs), using automatic differentiation for differentiating the neural networks. Through the cost function, both boundary/initial conditions and the mathematical structure of the ODE/PDE are imposed for the neural network to learn these system characteristics. Physics-informed neural networks have been used for solving lumped kinetic models for chromatography processes [7] and for model predictive control of CSTR systems [8].

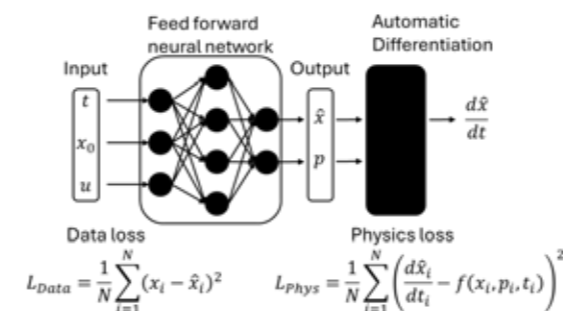


Figure 2: Physics-informed neural network

Case Study

In this project, a comparative study of hybrid modeling and physics-informed neural networks has been performed based on the same pilot-scale bubble column aeration case as used in [4]. Both modeling approaches were applied to the same data obtained from experiments performed at the pilot plant at the Technical University of Denmark. The bubble column is used for investigating oxygen mass transfer using the hydrogen peroxide-catalase method to determine the oxygen transfer rate and volumetric mass transfer coefficient ($k_L a$). The physical knowledge included in both modeling approaches were based on species conservation balances, while $k_L a$ were considered as the unknown phenomenon. Furthermore, a sensor drift was observed for the dissolved oxygen sensor in the bubble column, meaning that the models had to be able to account for a sensor bias, which is different depending on the time the experiment was performed. The study was seeking to investigate strengths and weaknesses in the two modeling approaches, comparing the prediction accuracy, extrapolative capabilities, and ease of interpretation.

Conclusions

All hybrid model approaches proved capable of modeling the pilot-scale bubble column unit with high accuracy. For the PINN models, a trade off was observed between the data loss and the physics loss as a result of the multiobjective optimization problem. The physics-informed models proved to be less prone to overfitting compared to a purely data-driven model. The

hybrid semi-parametric model overall represented the system best as it had both a high accuracy in prediction and showed greater respect for the physics equations, as these equations were hard-coded into the model structure. PINNs have shown great promise in surrogate modeling instead of complex PDE systems, however they Trondhjem, Norge should be used with care as they are not necessarily better for all problems.

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Microfluidic measurement tools for enzymes

(January 2023 – January 2026)



Contribution to the UN Sustainable Development Goals

The project aims to significantly reduce water consumption in the chemical sector, thereby minimising environmental impact, optimising enzymatic processes and reducing the use of energy and raw materials. By bridging the gap between academia and practical innovation, this research promises to contribute substantially to the SDG 12 objectives by conserving resources, improving sustainability and aligning with global development goals.



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Abstract

Microfluidic devices have emerged as a promising technology for optimizing biocatalysis, offering advantages over traditional methods, such as improved mass and heat transfer rates, cost reduction, enhanced yields, and suitability for enzyme screening. However, scaling down bioprocesses using microfluidic devices, especially for multi-parameter fluctuations, is still being explored. The aim of this project is to investigate the potential of novel technologies in testing enzyme stability, which can be correlated with data from lab-scale processes.

Introduction

Biocatalysis has gained a relevant role as a prominent green alternative to replace conventional petrochemical processes, primarily for its capacity for cost process reduction and its contribution to minimising the impact of climate change and energy resources. Therefore, optimising the performance of a biocatalyst is crucial to guarantee competitive processes from an economical and sustainable point of view^[1].

According to Dias Gomes and Woodley, product concentration, productivity, and enzyme stability are 3 key parameters to accurately assess the scalability of an enzymatic process^[2]. However, the comprehension of the enzyme stability in bioreactors continues to be a bottleneck for the scale-up due to their sensitivity to different stress factors; one is the interaction between enzymes and interfaces with distinct hydrophobic properties. These interfaces could be a surface or material that promotes the interaction of the enzyme with hydrophobic regions. For instance, the interface gas-liquid generated due to the air/oxygen supply in bioreactors offers an environment for hydrophobic interaction, in which enzymes are adsorbed and added to the bubble surface, losing their activity^[3–5].

Another example of that occurs during Hydrophobic Interaction Chromatography (HIC), where it has been reported that the protein's interaction with HIC media ligands may promote partial conformational changes of proteins upon adsorption^[6]. Therefore, understanding and controlling the conformation of adsorbed proteins at surfaces could be a critical point in maintaining their stability and predicting behaviour at various interfaces^[7,8].

On the other hand, microfluidic devices have emerged as a promising and sustainable approach for biocatalysis^[9]. These devices offer several advantages over traditional methods^[10,11], e. g., high mass and heat transfer rate, reduced cost and time-product development with low waste generation, improved yields, and usage for enzyme screening. However, despite these advantages, few published studies have reported using microfluidic devices to scale down biocatalytic processes, for the collection of performance data.

Specific objectives

The main objective of this work is to develop new methods, which involve designing microfluidic devices and studying the interaction of enzymes on hydrophobic surfaces for scaling-down and enzyme stability studies.

Methodology

To achieve this purpose, the project was divided into two parts. The first part describes the study of the enzyme stability effects due to the presence of a hydrophobic interface; meanwhile, the second part consists of designing a microfluidic device to simulate the enzyme performance on a chip based on the Hydrophobic Interaction Chromatography principles.

Part 1. Effect of hydrophobic interfaces on the enzyme stability

In this section, we evaluate the stability of 4 variants of NADPH oxidase (NOX) by correlating the adsorption phenomena between the gas-liquid interface in a bubble column with the performance of this enzyme exposed to a hydrophobic solid phase (HIC).

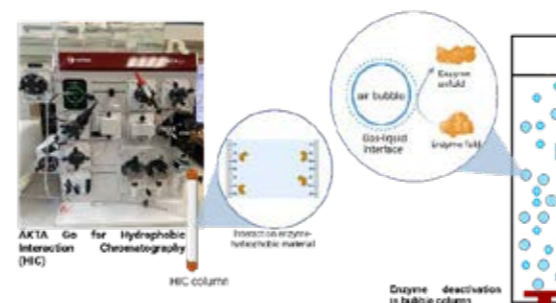


Figure 1. Methodology to evaluate the impacts of hydrophobic interfaces on enzyme stability.

Part 2. Scale-down process from lab-scale bioreactor to microfluidic device

Development of an innovative platform able to mimic the enzyme stability data derived from lab-scale reactors to a microfluidic chip using Hydrophobic Interaction Chromatography (HIC-ON-A-CHIP) technology.

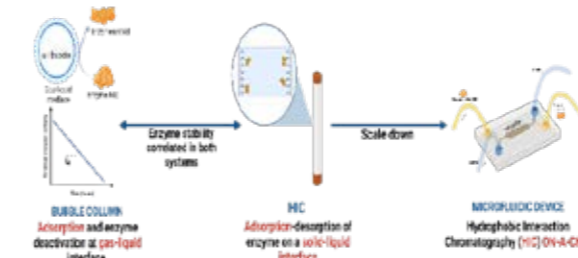


Figure 2. Description of the steps to achieve the scale-down process from lab-scale to microfluidic devices.

Computational models will also be developed to simulate the performance of the enzyme in both systems.

Expected results and future perspectives

- ✓ Establish novel methods for enzyme screening, which can simulate the effects of the dynamic environment of bioreactors on enzyme stability.
- ✓ Development of an innovative platform able to correlate enzyme stability data derived from microfluidic devices with lab-scale processes.
- ✓ Impacts on the Sustainable Development Goals through the implementation of the new technology.

Acknowledgements

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Optimal Dynamic Operation of Power to Ammonia Processes

(August 2022 – July 2025)



Contribution to the UN Sustainable Development Goals

Transition to renewable energy sources, eg. wind and solar power, are the basis of a future clean and carbon-neutral energy sector. However, the intermittent nature of renewable power makes these energy sources unsuited for a demand-driven energy market. Power-to-Ammonia (P2A) offers the most energy dense chemical storage medium where the energy can be returned to the electrical network without carbon emission. Furthermore, ammonia is intensely researched as a fuel for marine engines expected to decarbonise maritime transportation. Replacing conventional ammonia production for agriculture with P2A can reduce global CO₂ emission with about 1%.



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Abstract

The project investigates the flexible operation of an ammonia synthesis loop for Power-to-Ammonia (P2A). Due to the intermittent nature of renewable sources, the ammonia reactor is required to operate flexible over a wide operating window between 20% to 120% of the nominal load. A dynamic model for a three-bed adiabatic quench-cooled ammonia reactor with a feed-effluent heat-exchanger has been formulated. Steady-state stability analysis of the reactor system revealed a significant unstable operating range. Open-loop simulations of the synthesis loop subjected to varying electrical energy (feed flow) pushed the reactor system into the unstable operating range. Hereby, severe temperature oscillations of up to 300 K arose in the system. Thus, for flexible operation of the ammonia synthesis loop, a control structure is required for stabilising the reactor system. In this work, a simple regulatory PI controller has been implemented, which yielded efficient system control.

Introduction

Ammonia is the second most produced chemical in the world and production contributes about 2% of total global CO₂ emissions. Additionally, ammonia is perceived as one of the most promising mediums for chemically based storage on renewable energy sources, e.g. wind and solar power. In P2A, electrical energy from renewable sources is used to generate the reactants, hydrogen via electrolysis and nitrogen via air separation. Therefore, P2A plants need to comply with a fluctuating energy supply from intermittent renewable sources [1]. This defines entirely new requirements for the operation of ammonia reactors, which are conventionally supplied with a stable and reliable flow of reactants from steam-methane reforming. Furthermore, studies have shown that ammonia reactors exhibit highly non-linear dynamics, and process disturbances such as varying reactant supply may cause severe temperature oscillations in ammonia reactor systems [2]. Thus, a detailed understanding of the dynamics of ammonia

reactors is paramount to ensure safe and flexible operation of P2A plants.

Specific Objectives

This study aims to set up a reliable dynamic model of an ammonia synthesis loop. With the model, steady-state stability analysis and optimization of the reactor system can be performed. Additionally, a control structure capable of ensuring flexible and stable operation of the synthesis loop is desired.

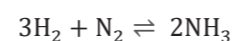
Mathematical model

Each reactor bed is modelled as a 1D adiabatic packed bed plug flow reactor. The material and energy balance are given by two PDEs,

$$\frac{\partial c_i}{\partial t} = -\frac{1}{A_c} \frac{\partial N_i}{\partial t} + R_i \quad (1)$$

$$\frac{\partial u_R}{\partial t} = -\frac{1}{A_c} \frac{\partial H}{\partial t} \quad (2)$$

The ammonia production follows the overall reaction scheme,



Results and Discussion

The steady-state (SS) of the reactor system is solved by setting the time derivative in Eq. (1) and (2) equal to zero and solving concurrently with the equation for the feed-effluent heat-exchanger. For a given reactor feed temperature three possible steady states were identified; One ignited state, one extinguished state, and one unstable intermediate state. The region of multiple steady states can be mapped by solving the SS-problem for varying parameters, e.g. the feed temperature as illustrated in Figure 1.

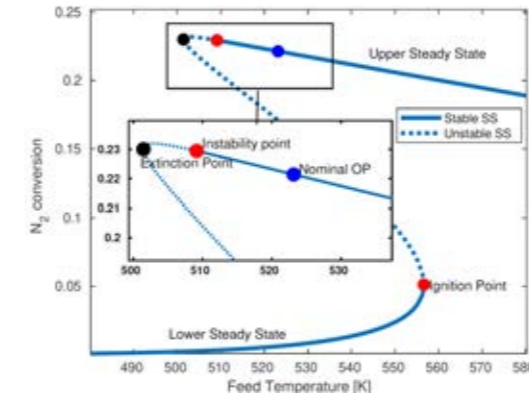


Figure 17: Mapping of the possible SS solutions for the reactor outlet temperature by varying feed temperature.

Furthermore, Figure 1 shows the stable and unstable operating range of the reactor system as well as the location of the conventional operating point. Clearly, the conventional operating point is located at a substantial safety margin from the reactor instability point. However, greater conversion can be achieved closer to the instability point and even inside the unstable range.

From the steady-state, dynamic simulations can be performed. Figure 2 shows the response of the ammonia reactor system to step changes in the feed temperature. For the initial decrease of 10 K the reactor system remains within the stable range defined in Figure 2 and shows an asymptotic response with damped oscillations. However, the second step decrease in feed temperature moves the reactor to the unstable range, which results in severe temperature oscillations. Temperature oscillations as observed in Figure 2 are highly undesirable as the porous catalyst structure is easily damaged.

In P2A plants the changing reactant feed flow risks pushing an uncontrolled reactor into unstable oscillations. Thus, flexible and stable operation is not possible without a properly designed control structure. Figure 2 displays closed loop simulations of the entire synthesis loop. The normalized electrical input, load factor (LF), is varied over the entire operating window from 20% to 120% of nominal load at a stepwise ramping of 10% per 10 min.

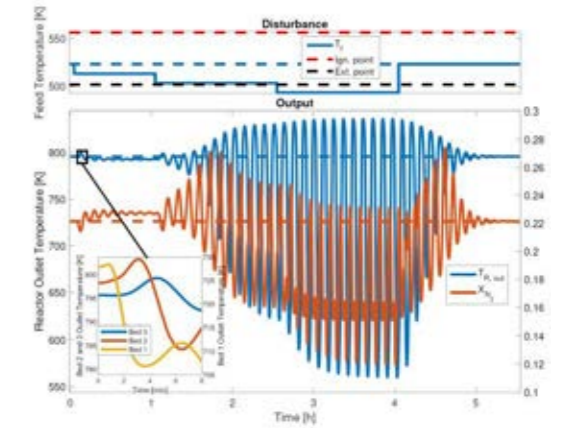


Figure 2: Reactor outlet temperature and N₂ conversion response to step disturbances in the reactor feed temperature.

For each change of the load factor, the reactor system is optimized for the reactor inlet temperature, $T_{1,in}$. The inlet temperature is used as setpoint for a PI controller, which Figure 3 shows to yield rather efficient system control.

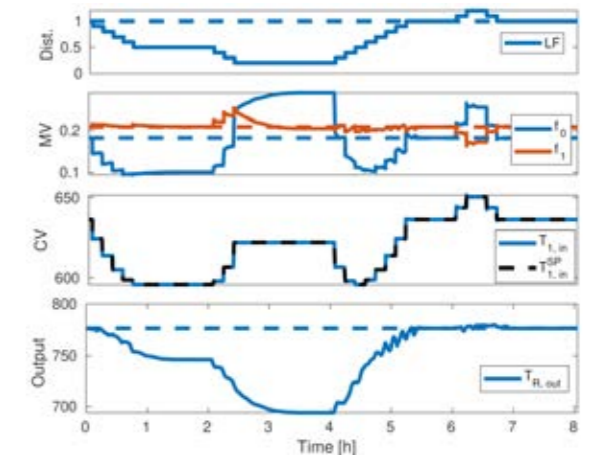


Figure 3: Closed loop simulation of the synthesis loop subjected to ramp changes in the load.

Conclusion

A dynamic model of an ammonia synthesis loop has been developed. Steady-state stability analysis predicted regions of unstable operation, which was confirmed by dynamic simulations as severe temperature oscillations arose from the unstable states. By implementing a simple PI control structure, the system was well controlled for changing electrical loads.

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Process studies of electrically heated clay calciners

(September 2022 – August 2025)



Contribution to the UN Sustainable Development Goals

The cement industry is actively seeking methods to significantly reduce CO₂ emissions, primarily from the clinker production process. One approach is to partially substitute limestone with calcined clay, as the calcination of clay emits significantly less CO₂ compared to limestone. Another step is to replace the combustion of fossil fuels used to heat the raw material. By combining these measures, the production of clinker – and consequently cement – can become less carbon-intensive. Therefore, the implementation of an electrically heated calcined clay production process aligns with efforts to reduce the carbon footprint of cement and supports the 13th UN Sustainable Development Goal.



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Abstract

The primary CO₂ sources in cement production are limestone calcination and fossil fuel use. Using calcined clays as supplementary cementitious materials (SCMs) can significantly reduce the carbon footprint. In the current study, a simulation of an electrically heated clay calcination process is developed to explore optimal process configurations. Furthermore, the study investigates the impact of various process and design parameters on process performance such as calcination degree and energy consumption.

Introduction

Cement production accounts for around 8% of global CO₂ emissions [1], primarily from limestone calcination and fuel combustion for heating [2]. Switching to renewable electric heating can eliminate CO₂ emissions associated with traditional fuel combustion. Another strategy is to replace cement clinker with supplementary cementitious materials (SCMs) [3], like calcined kaolinitic clays, which transform into pozzolanic metakaolin when heated at 450–800 °C [3]. This work models an electrically heated flash calcination process to activate kaolinite clay. A sensitivity analysis is performed to evaluate the effect of the main process and design parameters on the process.

Specific Objectives

The objectives of this work are to:

- Develop a simulation for the electrically heated clay calcination process
- Achieve a comprehensive understanding of the calcination process to explore and identify optimal configurations
- Investigate the impact of operating conditions on calcination and energy consumption.

Process Description

Figure 1 shows the block process diagram of the electrically heated clay calcination set up. Milled and dried clay is preheated in three cyclone stages, where it exchanges heat with gas, leading to partial dehydroxylation. The preheated clay then

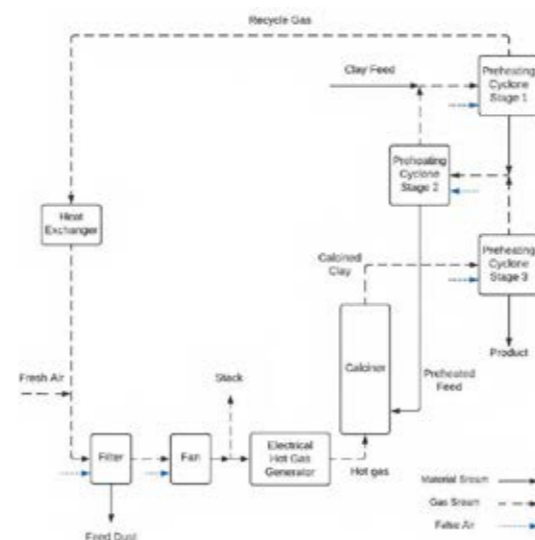


Figure 1: Block process diagram of electrically heated clay calcination process

enters the calciner, where hot gas from the Electric Hot Gas Generator (EHGG) provides energy for full calcination. The calcined clay and hot gas are separated in the last cyclone. After passing through preheating cyclones, the gas is cooled in a heat exchanger if above 400°C. The gas then passes through a bag filter and fan and is recirculated to the calciner after reheating by the EHGG.

Result and Discussion

A steady-state model of the electrically heated clay calcination process was developed. The effects of process parameters (activation energy of dehydroxylation, kaolin content, and gas flow recirculation) on calcination degree and EHGG energy input are analyzed. Lowering activation energy increases dehydroxylation in cyclones (Figure 2.a), while higher kaolinite content minimally affects calcination temperatures (Figure 2.b). Increasing gas flow rate enhances dehydroxylation in cyclone 2 due to a temperature rise (Figure 2.c).

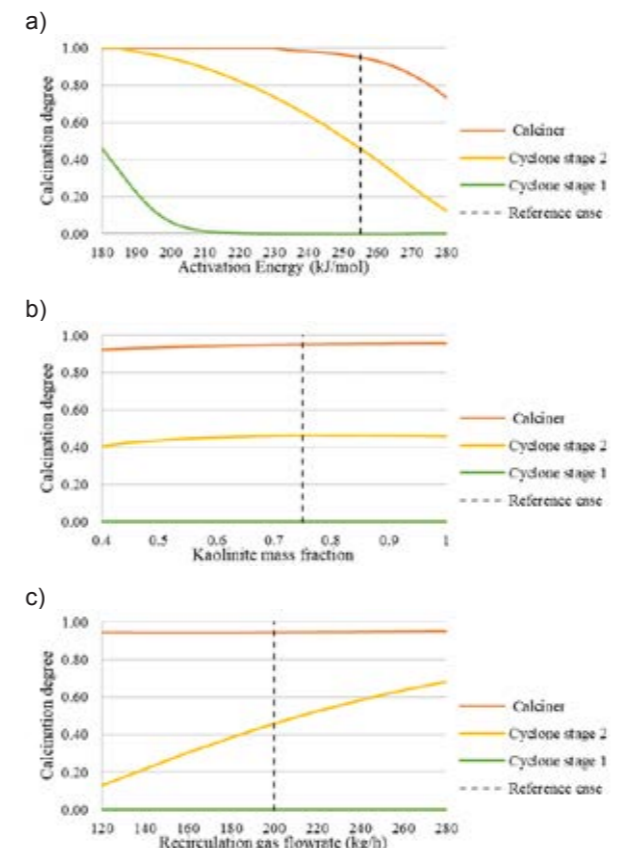


Figure 2: Impact of a) dehydroxylation kinetic b) kaolinite content c) hot gas flowrate on calcination degree

Figure 3 shows how changes in activation energy, kaolinite content, and gas flow rate impact on EHGG energy efficiency and outlet temperature. An increase in these parameters raises energy demands. By increasing the gas flowrate or decreasing the activation energy, the calcination degree in the cyclones increases, and a smaller proportion of the reaction must take place in the

calciner. Consequently, the outlet temperature of the hot gas generator decreases. Higher gas flow or lower activation energy increases calcination in cyclones, reducing the EHGG outlet temperature, while increasing kaolinite content slightly raises the EHGG temperature.

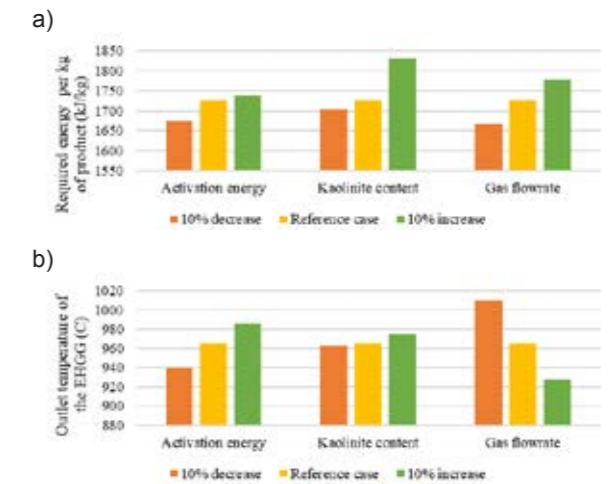


Figure 3: Impact of process parameters on a) required energy and b) outlet temperature of the EHGG

Conclusions

In the current study, a model of the electrically heated clay calcination process was developed that involves electrically heated hot gas in a flash calciner to activate the kaolinite clay. Sensitivity analysis was conducted to determine the effect of varying process parameters on the process efficiency and output. The results showed how alterations in activation energy, kaolinite content, and gas flow rate affect the energy efficiency of the clay calcination process.

Acknowledgments

This work is supported by the ECoClay project: Electric Calcination of Clay funded by EUDP, in collaboration with FLSmidth, Danish Technological Institute, Chemney lab, Cementos Argos, VICAT, RONDO, and the Technical University of Denmark.

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Mechanism investigation of corrosion protection and coating degradation

(April 2023 – March 2026)



Contribution to the UN Sustainable Development Goals

It is estimated that corrosion costs 3 trillion US dollars annually, which translates to more than 3 percent of global GDP. In addition to this heavy economic cost, corrosion also imparts the material and environmental cost as well. Understanding degradation and protection mechanisms of organic coating would help mitigating these effects. Understanding the corrosion and coating degradation mechanism will help guide the coating formulations design with improved corrosion protection performance, thereby prolonging the lifetime of protected structures and products, directly lowering consumption of raw materials used in their manufacturing.



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Abstract

The results of corrosion and failure modes of coating protection are known and internalized by the academy and industry professionals. But the distinct mechanisms that led to those failure modes are not that clear. Anti-corrosive coating formulations, by their nature, take considerable time in development and especially testing. Knowing how the coating protects & fails and understanding the mechanism behind it would provide significant guidance for the new coating formulation development and facilitate the coating performance improvement. In light of this, the project is on the fundamental understanding of the protection and degradation mechanism of anti-corrosive coatings and the key factors affecting the coating performance, thereby providing guidance to the coating formulation improvement.

Introduction

In most fundamental terms, metallic corrosion is the degradation of the metals due to outside conditions, humidity, chemicals, and similar factors. Corrosion affects every aspect of modern life and has important consequences. Corrosion costs around 3.4% of the global gross economic product annually [1].

One of the ways of mitigating the effects of corrosion is organic coatings. Organic coatings are widely applied on marine and offshore structures for corrosion prevention. The results of corrosion and failure modes of coating protection are well known, namely what happens when materials corrode. But distinct mechanisms that led to those failure modes are not that clear. Investigations on the mechanism for corrosion protection and coating degradation have been ongoing for decades. However, until today, there is no such clear understanding of how coating provides corrosion protection and degrades.

If the coating completely restricts the oxygen, water and ionic species transfer, corrosion reaction could not take place. This situation is

rarely the reality. Aggressive species find their way into the substrate, even though the seemingly intact coatings.

In the most basic terms coatings fail due to their characteristics and / or due to their defects. These defects can be in the coating itself, on the substrate or on the interface. But in the absence of defects, coating will fail due to their insufficient characteristics.



Figure 1: Degradation of protective organic coating through accelerated exposure test (neutral salt spray test ASTM B-117) – An example

In this case the chronology of failure will follow basic steps, first corrosive species water, oxygen and ionic species will transfer through coating to the substrate interface, then underfilm corrosion will progress. Finally, this will result in visible corrosion. These steps are shown schematically in the figure 1.

For structures coated with organic coatings, corrosion can occur in damaged as well as intact areas. There are variety of approaches to explain the corrosion initiation under seemingly intact coatings, ionic resistance, adhesion, barrier effects [2]. It is not possible to assert one encompassing mechanism, rather different mechanisms seem to play a part depending on the conditions and coating properties.

For characterizing corrosion under the coating, transport processes of three main factors must be known: water, oxygen, and ionic species. Transport processes must be related to fundamental formulation parameters like stoichiometric ratio, presence of certain compounds and like.

While almost never the limiting factor, water is the essential factor for corrosion [3]. Water is peculiar in terms of its hydrogen bonding ability. It has differing effects on the polymeric network according to this. Therefore, its characterization inside polymeric matrix must and has been done according to its hydrogen bonding state [4]. The general methodology for this is shown in the Figure 2.

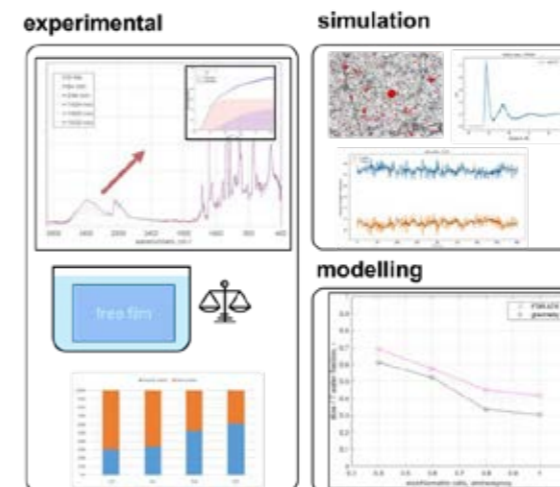


Figure 2: Schematic illustration of water-epoxy interaction investigation

Anti-corrosive coating formulations, by their nature, take considerable time in development and especially testing. Knowing how the coating protects & fails and understanding the mechanism behind it would provide significant guidance for the new coating formulation development and facilitate the coating performance improvement. Modelling of the underlying processes would give more robust and efficient support for coatings formulation development.

Future Work

Absorbed water within the epoxy network was characterized according to its persistence and diffusion behavior. A working molecular model was constructed to investigate processes at

atomic level. Analysis and modelling water interactions are ongoing.

Further work will be carried out to investigate the effect of resin structures, ingredients and application conditions on the basic performance parameters of model coatings.

Acknowledgements

Financial support from the Hempel Foundation through CoaST (The Hempel Foundation Coatings Science and Technology Centre) is greatly appreciated.

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Synthesis and applications of bio-based poly (4-hydroxyphenylacetate)

(March 2022 – February 2025)



Contribution to the UN Sustainable Development Goals

As the plastic crisis intensifies, the polymer sector is turning its attention to bio-based alternatives. These sustainable alternatives are emerging as a promising solution, steadily gaining popularity across multiple areas of polymer science. Project UPLIFT aims to target this issue, addressing the entire lifecycle of plastics - from the initial synthesis of monomers to the final end-of-life (EoL) treatment. The research includes evaluating both traditional and microwave polymerization techniques, to valorize bio-based monomers that are downstream from fermentation processes. The ultimate goal is to create polymers that are suitable for large-scale industrial implementation.



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Abstract

The plastics industry is showing increasing interest in integrating bio-based polymers. However, these materials currently face limitations in replacing fossil-based commodity plastics due to their low thermal stability and lack of recycling methods. To address this challenge, the EU project UPLIFT is concentrating on producing monomers through biological processes. These monomers will serve as building blocks for innovative polymers, with a strong focus on their recyclability and end-of-life management. The project explores two synthesis methods at the laboratory scale; conventional heating and a more sustainable microwave heating pathway. The resulting polymers must be suitable for industrial upscaling while meeting the two critical criteria, compliance with food and drink packaging standards, and recyclability. By tackling these aspects, UPLIFT aims to enhance the viability of bio-based polymers in replacing traditional plastics.

Introduction

The plastics industry has experienced substantial growth in contemporary economies and societies. While plastics offer numerous advantages in global markets, including facilitating efficient and cost-effective mass production, their disposal and management pose significant environmental and health risks. Given the projected increase in plastic demand, it is imperative to address the recycling and substitution of commonly utilized petroleum-based plastics. This strategy aims to conserve valuable resources and mitigate plastic pollution in the environment.

There is a growing need to explore alternative raw material sources for plastic production, with particular emphasis on bio-based materials as a promising solution. Polymers derived from renewable bio-sources demonstrate considerable potential as sustainable alternatives in the plastics industry. However, to meet the stringent requirements of sectors such as packaging, these bio-based polymers necessitate substantial

enhancements in their properties and production scales.

Moreover, it is essential to develop innovative recycling methods that promote the efficient and responsible utilization of bio-based polymers, particularly after their initial use. This objective necessitates the creation of bio-based polymers amenable to conventional recycling techniques or biological degradation processes, thus enabling diverse waste management approaches.

The EU project UPLIFT focuses on the depolymerization of non-recyclable post-consumer fossil- and bio-based plastics through enzymatic and biological methods. This process aims to produce fully bio-based monomers that will be used for synthesizing new bio-based polymers that are suitable for food and drug packaging applications, ensuring non-toxicity. (Figure 1) These monomers must also effectively manage impurities from previous processing stages, exhibit optimized thermal properties and maintain durability and reprocessability. Among the

monomers synthesized within the UPLIFT project, 4-hydroxyphenylacetic acid (HPA) is of particular interest since it can be produced from biological processes as described by [B.Wynands et al.] and possesses highly interesting properties for polymer synthesis due to its aromatic nature.

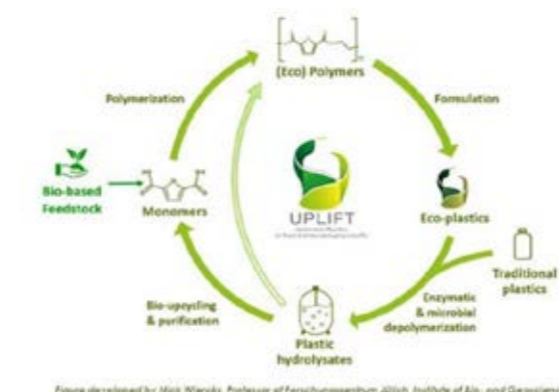


Figure 1: Methodology of project Uplift.

Methods

As a hydroxy-acid, 4-HPA can condense into a polymer with promising thermal and mechanical properties. The polycondensation reaction can be performed by conventional heating, and by applying appropriate heating temperatures and sufficient vacuum, the oxidation of the aromatic phenol of 4-HPA can be tackled and yield poly (4-hydroxyphenyl acetic acid), PHPA, a polymer of relatively low molecular weight but of high processability. Such polycondensation reactions generally demand extended polymerization times at elevated temperatures and often the use of high vacuum, making these processes both energy-intensive and time-consuming. Typically, condensation polymerization can take up to two days, which poses a significant limitation in the production of various grades and the validation of catalysts. To address this, the use of microwave radiation for polymer synthesis as an alternative to conventional heating was explored. (Figure 2) This approach has shown great promise in reducing both the energy and time required for polymerization, thus further reducing the carbon footprint of the synthetic procedure of this bio-based polymer.

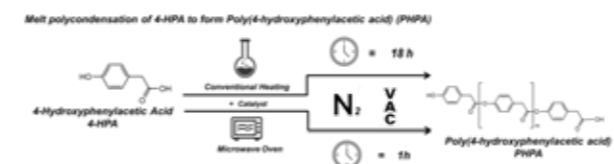


Figure 2: Reactive pathways of 4-HPA to PHPA

Due to its processability at relatively low temperatures, poly(4-hydroxyphenylacetic acid), PHPA is eligible to be used for copolymer synthesis by performing transesterification

reactions with other bio-based polyesters, such as PLA. The resulting copolyesters inherit characteristics from both the aromatic and aliphatic segments of the parent polymers, exhibiting accelerated degradation rates in aqueous solutions and via enzymatic degradation, while not significantly affecting mechanical properties. This improvement is particularly valuable in the food and drink packaging industry, where achieving biodegradability while maintaining mechanical strength is the desired outcome and a significant challenge.

Acknowledgements

Project UPLIFT is financially supported by the EU Horizon 2020 research and innovation program under grant agreement N° 953073.

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Chemical and Catalytic Conversion of Lignin to Organic Coatings

(September 2023 – August 2026)

12 RESPONSIBLE CONSUMPTION AND PRODUCTION



Contribution to the UN Sustainable Development Goals

By replacing BPA in epoxy resins with lignin, this project offers a sustainable alternative to a petroleum-based and potentially harmful chemical. Lignin, a renewable byproduct of the paper industry, promotes the use of bio-based materials and reduces reliance on non-renewable resources. This approach contributes to more environmentally friendly production processes and encourages the efficient use of industrial waste. By addressing these issues, the project supports SDG 12: Responsible Consumption and Production.



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Abstract

This research addresses the environmental concerns associated with Bisphenol A (BPA) by exploring the potential of lignin, a renewable biomass byproduct from the pulp and paper industry, as a sustainable alternative. Annually, approximately 70 million tons of lignin are produced, yet about 98% is incinerated. By substituting BPA with high-purity aromatic molecules derived from lignin, we can significantly reduce greenhouse gas emissions—lignin-based epoxy resins produce around 3 kg CO₂ equivalents compared to over 9 kg for BPA-based resins. The conversion process begins with the kraft pulping method, yielding black liquor, rich in organic compounds, which can be processed to extract kraft lignin. This lignin can then be converted into bio-oil and epoxidized for use in high-performance polymers. Overall, this project aims to promote a circular economy while aligning with Sustainable Development Goals focused on innovation and responsible production.

Introduction

The increasing awareness of environmental sustainability has highlighted the harmful effects of Bisphenol A (BPA), a chemical primarily derived from fossil fuels. BPA is not only costly but also poses serious health risks, including endocrine disruption, which can lead to reproductive issues and other health problems in humans and animals [1],[2]. In light of these concerns, our research seeks to replace BPA in epoxy resin formulations with aromatic molecules sourced from lignin, a renewable biomass byproduct. This innovative approach not only addresses the toxicity associated with BPA but also aligns with several Sustainable Development Goals (SDGs), specifically SDG 9 (Industry, Innovation, and Infrastructure), SDG 12 (Responsible Consumption and Production), and SDG 13 (Climate Action).

Lignin is produced in vast quantities as a byproduct of the pulp and paper industry, generating approximately 70 million tons annually, with around 1.4 billion metric tons of black liquor produced in 2022 alone [1],[2]. Despite its

abundance, about 98% of lignin is incinerated for energy recovery, representing a significant waste of a valuable resource[1]. The pulp and paper industry has also experienced a compound annual growth rate (CAGR) of 2% over the past 60 years, indicating a stable demand for lignin-derived products.

Recent studies have shown that utilizing lignin-based materials can lead to reduced greenhouse gas emissions, producing greenhouse gas emission compared to traditional petroleum-based products [3],[4]. For instance, lignin-derivable bisphenols have demonstrated significantly lower estrogenic activity than BPA, achieving a reduction in harmful effects by up to 110-fold [2]. By harnessing the unique properties of lignin through innovative chemical modifications and processing techniques, we can develop sustainable alternatives that not only mitigate the environmental impact associated with BPA but also contribute to a more sustainable industrial framework prioritizing renewable resources. This project will explore the feasibility and benefits of substituting BPA with lignin-derived aromatic

compounds, emphasizing their potential to revolutionize material science while addressing pressing global sustainability challenges. Through this research, we aim to demonstrate that lignin can serve as a viable feedstock for high-performance polymers that meet or exceed the properties of traditional BPA-based materials while promoting environmental stewardship.

Global Warming Impact

The results indicate that lignin-based epoxy resins lead to a substantial reduction in CO₂-equivalent emissions compared to standard BPA-based epoxy resins. The global warming potential for lignin epoxy resins is approximately 5 kg CO₂-equivalents, with epichlorohydrin production being the major contributor. When using industry-scale epichlorohydrin, emissions are reduced further to less than 3 kg CO₂-equivalents. In contrast, BPA-based epoxy resins result in over 9 kg CO₂-equivalents. This demonstrates that replacing BPA with lignin-derived compounds in epoxy resins significantly decreases their carbon footprint, contributing to more sustainable material production [5].

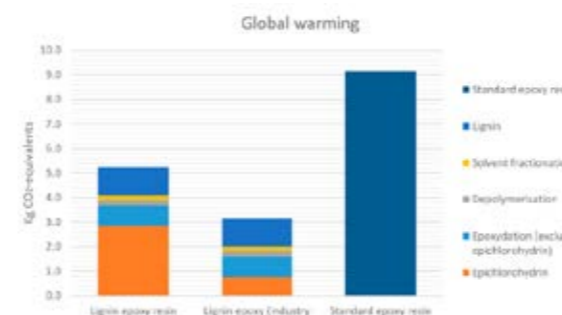


Figure 1: Global warming emissions from producing 1 kg standard epoxy and 1 kg lignin epoxy resins [5].

Strategy

The process of converting lignin into high-purity aromatic molecules begins with the kraft pulping method, a widely used technique for producing wood pulp from lignocellulosic materials. In this process, wood chips are cooked in a pressurized digester using an alkaline solution of sodium hydroxide (NaOH) and sodium sulfide (Na₂S). This treatment effectively breaks down the lignin that binds cellulose fibers together, allowing for the separation of cellulose from other wood components.



The result is a solid pulp along with a liquid byproduct known as black liquor, which consists of two-thirds of organic compounds: dissolved lignin, hemicellulose, and other organic compounds, and one-third of inorganics.

From black liquor, we can extract lignin through various techniques, allowing us to isolate and purify kraft lignin, which serves as a valuable precursor for further chemical transformations. Once extracted, the kraft lignin can be converted into bio-oil, that can afterwards be epoxidized to introduce reactive epoxide groups, facilitating its use in the production of epoxy thermosets.

By leveraging this process, we not only create sustainable alternatives to BPA but also promote a circular economy by valorizing a byproduct of the pulp and paper industry.

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Thermodynamic and physical properties as basis for digitalization of glycol processes

(July 2021 - November 2024)



Contribution to the UN Sustainable Development Goals

Develop facilities that can operate remotely. Reach new places impossible for humans, but not for machines. Imagine how this can expand our exploration, production, and creation capabilities. Unmanned processing units are already a reality in the oil and gas industry, and with more accurate data and models, these processes can be increasingly larger and more efficient. This is how we intend to contribute to technological innovation in industrial sectors, boosting economic growth

Abstract

Recent technical advances have seen an increase in unmanned processing installations. However, the process design of these facilities requires accurate models, which depend on reliable equilibrium and physical properties data. This work focuses on obtaining experimental data and developing models for glycol processes in unmanned facilities. This will involve both experimental and modeling work, improving the numerical robustness of the Cubic Plus Association model.

Introduction

Triethylene glycol (TEG) is a very relevant chemical in the oil and gas industry nowadays as it is used in about 95% of the natural gas dehydration units [1]. However, despite the importance of measurements of physical and thermodynamic properties for the process design of these facilities, there is still a lack of TEG-related data sets available in the open literature and some of the published data are questionable. For the binary TEG + Methane, for example, while the methane solubility in pure TEG shows the same trend in the work of different authors, the TEG concentration in the methane vapor phase reported by Jerinić et al. [2] and in our previous work [3] is in considerable disagreement. It is important to note that the experimental mole fractions of TEG in the vapor phase for this binary system are extremely low, with measurements in the order of ppm. These concentrations pose a significant challenge in the experimental procedure, requiring a meticulously designed setup and procedure for accurate sampling and analysis. Nevertheless, another possible cause for the discrepancies between Jerinić's dataset [2] and ours [3] is the presence of water in our system. From the thermodynamic modeling point of view, the Cubic-Plus-Association (CPA) equation of state has been showing good performance for natural gas

dehydration applications. In essence, the model keeps the relative simplicity of the Cubic's, ideally suitable to describe interactions between alkanes, while specific interactions between molecules such as water and glycols, are accounted for by the association term.

Specific Objectives

Aiming to extend the accurate thermophysical characterization of glycols, we have measured new vapor-liquid-equilibrium (VLE) data for the binary TEG-Methane using pure glycol at 323.15 K and pressure ranging from 5.0 to 18.0 MPa. The 4C association scheme (where two proton donors and two proton acceptors are assumed on every molecule) previously estimated by Derawi et al. [5] was used for correlating the experimental data generated in this work.

Results and Discussion

The data reported by Jerinić et al. [2] are in between ours and Soroondan et al. [4] measurements at 323.15 K (Figure 1), supporting investigations that Jerinić's dataset presents unsuitably high values for the reported temperature (298.15 K). The experimental challenge of these ppm-scale measurements needs to be stressed.



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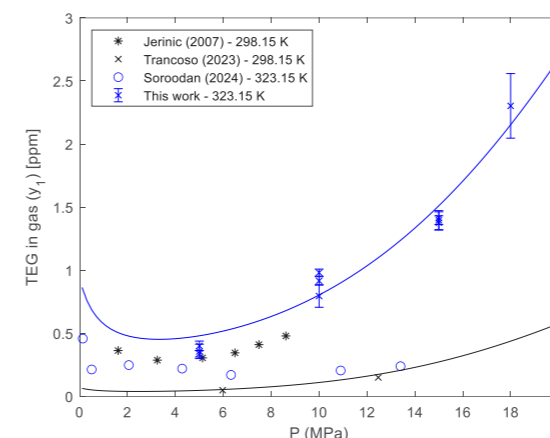


Figure 1: Experimental data for TEG content in the methane gas phase (y_1) of Jerinić et al. (*) [2] and Trancoso et al. (x) [3] at 298.15 K, and Soroondan et al. [4](o) and this work (x) at 323.15 K. Lines represent CPA modeling at 298.15 K (black) and 323.15 K (blue).

In addition to the differences between singular experimental points, the divergence in the experimental trends is notable. Our measurements follow the characteristic "bowl shape" dew-line predicted by CPA, where the concentration of triethylene glycol reaches a minimum. This behavior is typical for gas mixtures that follow a retrograde condensation behavior and has been previously reported for similar systems. Soroondan's dataset, however, is almost pressure independent. Figure 1 also shows the direct effect of pressure and temperature on the glycol vapor fraction (y_1). The 25 K increase between the evaluated temperatures results in an order of magnitude increase of TEG content in the vapor phase, while another order of magnitude increase of y_1 is seen when pressure increases from 5.0 to 15.0 MPa at 323.15 K. The average standard deviation of our measurements is determined as ± 0.07 and an overall uncertainty of ± 0.07 (maximum 0.15). The CPA model provides a satisfactory description of the new experimental data with a total AARD = 15%.

Conclusions

The phase behavior of natural gas dehydration systems is of great interest to the oil and gas industry. In this context, the 323.15 K isotherm from 5.0 to 18.0 MPa was measured for TEG-Methane. The phase distributions have been quantified using gas chromatography for the vapor phase, and a combination of process changes, liquid sample mass, density, and water content measurements for the liquid content. The relative experimental uncertainty range observed was $u_r = (0.01-0.17)$, with the highest uncertainties for glycol (y_1) in the vapor.

Experimental measurements and modeling show that the TEG content in the gas phase is directly proportional to pressure and temperature. The new

measurements for the binary TEG-Methane support our previous work [3] and the recently published Soroondan et al. [4] data, being also in disagreement with the dataset presented by Jerinić et al. [2] for TEG concentration in the vapor phase. Here, the challenges in the experimental procedure for accurate sampling and analysis in the ppm-scale study were stressed.

From the modeling perspective, no parametrization was done in this work, being all pure component and interaction parameters taken from the literature and used here to predict the phase behavior of the studied systems at new conditions. CPA with the well-established 4C association scheme for TEG and only one interaction parameter has provided qualitative good performance for all cases evaluated, with AARD ranging from 3-54%.

Acknowledgements

The author gratefully acknowledges the financial and technical support from the Department of Chemical Engineering, Technical University of Denmark, and Equinor A/S (Norway).

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Fermentation of carbon monoxide to chemical precursors

(November 2023 – October 2026)



Contribution to the UN Sustainable Development Goals

The increasing global population and rising fossil fuel consumption necessitate the development of technologies that produce commodity chemicals from renewable resources. Valorizing renewable feedstocks, such as residual biomass and industrial by-products like carbon monoxide and carbon dioxide, can significantly advance sustainable development. Gas fermentation presents a circular model by integrating waste management with chemical production, thereby reducing greenhouse gas emissions associated with fossil fuel use.



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Abstract

Syngas, consisting mainly of CO, H₂ and CO₂ and generated from biomass gasification can be used to produce a wide range of commodity chemicals and fuels. However, biological conversion of syngas is still a challenge because of the sensitivity of microorganisms to high CO gas content, resulting in low growth and consequently production rates. In this study, adaptation of mixed microbial consortia to high CO gas content was investigated in trickle bed reactors, TBR, operated in continuous mode under mesophilic (37 °C) conditions and ambient pressure.

Introduction

With a growing global population and increasing consumption of fossil fuels, there is an urgent need to develop technologies that can produce commodity chemicals from renewable resources [1]. Gasification of biomass, along with the subsequent biological conversion of the generated syngas (mainly a mixture of CO, CO₂, and H₂), gains growing interest [1]. However, its biological conversion is still challenging since most microorganisms are sensitive to high CO gas content, resulting in low growth and production rates. Adaptive laboratory evolution (ALE) is a promising method to overcome these adverse effects and to create efficient microbial cell factories [2]. Although it has shown high potential, studies using the ALE approach in CO-rich gas fermentation are scarce.

Apart from microbial communities, important consideration has also been given to the bioreactor configurations that can enhance the mass transfer rate of the sparingly soluble gas components [3]. Trickle bed reactor (TBR) exhibits enhanced gas-to-liquid mass transfer rates combined with low power consumption. So far, TBR has been extensively investigated for biomethanation processes [4]. However, studies on its use in production of chemicals are scarce,

yet this technology has great potential for liquid bioproducts.

This present work focuses on the long-term adaptation of mixed microbial cultures in a trickle bed reactor for effective bioconversion of CO to valuable chemicals. Here, a stepwise ALE strategy was applied to develop the CO-tolerant microbial consortia by increasing the CO content of the gas stream.

Specific Objectives

- Long-term adaptation of mixed microbial consortia to CO-rich gases.
- Achieving high CO conversion rate and metabolite productivity.
- Identifying responsible and functional microbial communities.

Results and Discussion

The trickle bed reactors were operated continuously under mesophilic (37 °C) conditions and ambient pressure. The initial gas mixture (Phase I) fed into the reactors consisted of 20% CO, 45% H₂, 25% CO₂, 10% N₂. Subsequently, the gas mixture gradually changed to higher CO content with simultaneous elimination of H₂ and CO₂ and it was 40% CO during Phase II, 60% CO during Phase III and IV and 90% CO during Phase V. As the reactors exhibited very high CO

conversion efficiency, the gas flow rate, Q_g, was increased from 2.5 ml·min⁻¹ (120 min EBRT) in Phases I, II and III to 3.6 ml·min⁻¹ (82 min EBRT) in Phase IV and V to allow for a wider observation window. The reactors operational parameters were kept constant until a steady state was achieved in each experimental phase.

At the steady state reached in Phase I, the average CO consumption rates achieved were 3.8 mmol·l_{bed}⁻¹·h⁻¹ for TBR1 and 3.5 mmol·l_{bed}⁻¹·h⁻¹ for TBR2. Further increase in CO gas content during Phase II and III resulted in a significant enhancement of the CO consumption rate for both TBR1 and TBR2 (Figure 1). At the same gas inflow rate (2.5 ml·min⁻¹), the highest CO consumption rates were reached at Phase III steady state for both reactors, and it was 10.7 mmol·l_{bed}⁻¹·h⁻¹ for TBR1 and 10.9 mmol·l_{bed}⁻¹·h⁻¹ for TBR2. Furthermore, the CO conversion efficiency was considerably stable during the first three phases.

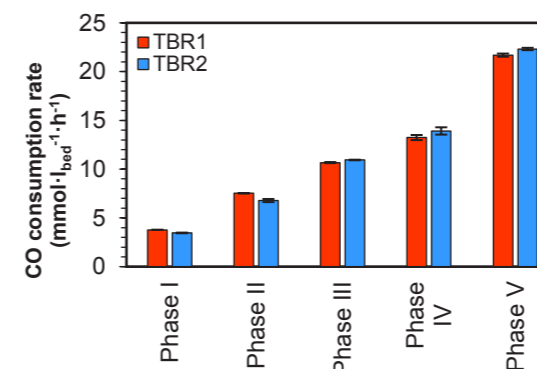


Figure 1: Average CO consumption rates of the gaseous substrates

When passing from phase III to phase IV, the composition of the gas mixture was not changed; instead, the gas inflow rate was increased from 2.5 ml·min⁻¹ (120 min EBRT) to 3.6 ml·min⁻¹ (82 min EBRT). This change enhanced the CO consumption rate by 23% in TBR1 and 41% in TBR2. The highest CO consumption rates during Phase V steady state were 21.7 mmol·l_{bed}⁻¹·h⁻¹ for TBR1 and 22.3 mmol·l_{bed}⁻¹·h⁻¹ for TBR2. This was 58% and 45% enhancement in CO consumption rates compared to Phase IV. Acetic acid and butyric acid were the primary metabolites produced in all phases during the present study. The highest acetic acid concentration of 8.7 g·l⁻¹ and 8.2 g·l⁻¹ for TBR1 and TBR2 respectively was achieved at Phase I steady state. The increase in inflow CO percentage during the operation caused a slight decrease in the acetic acid levels, yet acetic acid productivity remained considerably high (Figure 2). On the other hand, from Phase I to V, butyric acid productivity was remarkably increased in both reactors, resulting in 1.2 g·l⁻¹·d⁻¹ and 0.9 g·l⁻¹·d⁻¹ for TBR1 and TBR2, respectively at the steady state of Phase V.

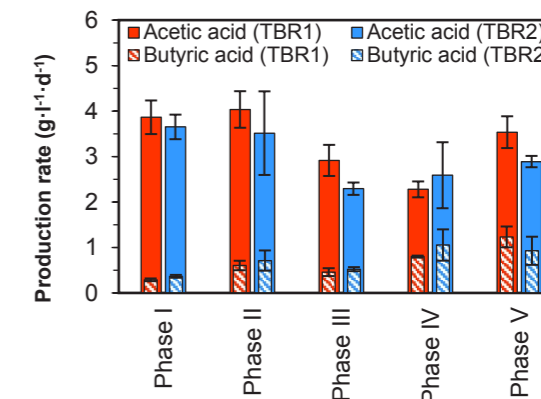


Figure 2. Average production rate of acetic acid and butyric acid at steady state conditions

Conclusion

The results revealed that the gradual increase of CO concentration led to the successful adaptation of CO-consuming microbial consortia. Enriched consortia exhibited efficient CO conversion primarily to acetic acid, with high consumption rates and product selectivity.

Acknowledgement

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Investigation of dry and semi-dry mineral carbonation process at high temperatures

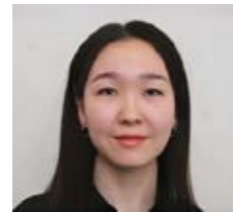
(April 2023 – March 2024)

13 CLIMATE ACTION



Contribution to the UN Sustainable Development Goals

The cement industry is responsible for 8% of global anthropogenic CO₂ emissions. Reducing these emissions is a key goal for the industry in mitigating climate change. Mineral carbonation of solid sorbents, such as naturally occurring minerals, industrial wastes and cementitious materials, represents one of the perspective technologies to cease carbon dioxide content of the flue gases, while forming stable carbonates. These carbonated products can later be used as concrete fillers or as partial substitutes in cement composition, thereby contributing to the circularity of the process.



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Abstract

This study explores post-combustion CO₂ capture using solid sorbents in cement production, focusing on the carbonation of CaO, Ca(OH)₂, recycled cement fines (RCF), and wollastonite under dry and semi-dry conditions. Carbonation experiments were performed at temperatures ranging from 300–700°C with a gas mixture containing 25% CO₂, examining the effects of adding 10% water vapor. Results indicate that Ca(OH)₂ has the highest CO₂ uptake at 700°C, while CaO's efficiency triples with water vapor addition. In contrast, wollastonite showed limited carbonation potential. Surface area, rather than particle size, significantly influenced CO₂ uptake. Future project studies will focus on optimizing process conditions for RCF CO₂ capture and use these findings for providing recommendations for efficient CO₂ capture from cement flue gases.

Introduction

Post-combustion CO₂ capture using solid sorbents is a promising method to reduce greenhouse gases, particularly as an integrated part of sustainable building materials. Reaction of solid sorbents, including natural minerals, demolition and industrial waste materials, with CO₂ to form stable carbonates is called mineral carbonation. This research focuses on dry and semi-dry routes of this process, investigating the effects of carbonation conditions and feedstock properties on the carbonation outcome. The objective is to optimize carbonation conditions, such as temperature, atmosphere, and particle properties, to enhance CO₂ capture. Studies on the carbonation of cementitious materials at elevated temperatures have shown promising results [1]. Previously, in the literature high temperatures in the range of 300–700°C were reported to be beneficial for carbonation, with optimal one being 600°C [2].

Objective

Various materials' carbonation behavior will be explored, with further assessment of their potential

use as supplementary cementitious materials (SCMs) or fillers, and designing an efficient CO₂ capture reactor for cement plants (Figure 1). Engineering models will be used to analyze and interpret experimental data.

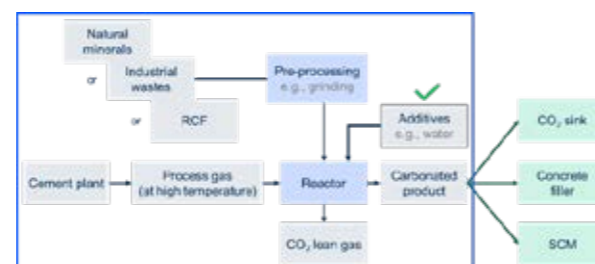


Figure 1: A CO₂ sequestration procedure using high temperature carbonation technology.

Materials and methods

Materials rich in Ca and/or Mg were tested for carbonation potential. CaO and Ca(OH)₂ were chosen as model compounds, with RCF showing the next highest CO₂ uptake. Wollastonite samples were included for comparison with wet carbonation test results. An STA instrument (STA

449 F3 – Jupiter) was used for initial carbonation experiments and CO₂ uptake analysis, and later upgraded with a humidity generator to study carbonation at humid conditions.

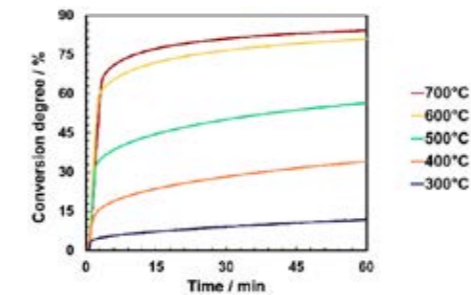


Figure 2: Carbonation efficiency of Ca(OH)₂ at different temperatures.

Results and discussion

Carbonation experiments were conducted at different temperatures for 1 h with a gas containing 25% CO₂. Prior to the experiments materials were subjected to heat pretreatment to 1000°C, thereby removing the LOI. This simplified the further calculations of CO₂ uptake by the material. As shown in Figure 2, reaction rates increase with temperature, as the rate constant follows the Arrhenius relationship. Although pretreatment generates surface area, elevated temperatures can cause sintering, reducing surface area and collapsing pore structures.

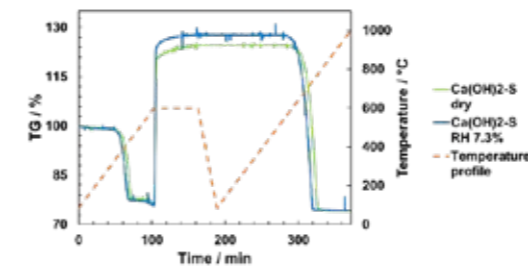


Figure 3: Carbonation of Ca(OH)₂ in dry and semi-dry (10% vol water vapor) conditions.

Addition of 10% vol water vapor to the system slightly improved the CO₂ uptake for Ca(OH)₂ as shown in Figure 3, while for CaO it increased the uptake by 3 times. To compare the influence of particle characteristics, BET and particle size distribution (PSD) analysis were conducted to measure the surface area and particle size of the samples, respectively. Conversion degree is calculated as a ratio of CO₂ uptake measured in TGA to the theoretical uptake possible for each material based on its oxide composition using the Steinoor equation. Table 1 presents the Ca and Mg content of the materials, along with their particle size and surface area measurements. It also includes their theoretical uptake potential and the calculated conversion degrees. Notably, neither higher Ca content nor smaller particle size show a clear positive effect on the carbonation

process. Conversely, materials with larger BET surface area measurements exhibit increased carbonation performance, suggesting that surface area may play a more significant role.

Table 1: Comparison of different materials' properties and conversion degrees.

Material	CaO (%)	MgO (%)	D50 (µm)	BET (m ² /g)	Theoretical max (%)	Conversion (%)
Wollastonite	52.69	1.38	17.80	6.32	36.36	0.71
CaO	98.84	0.57	6.95	6.94	78.57	4.73
RCF	36.30	1.28	21.40	7.51	20.10	16.07
Ca(OH) ₂	98.04	1.42	22.40	49.37	78.57	80.94

Conclusion

Results indicate that pure Ca(OH)₂ achieves a high degree of conversion to stable calcium carbonate, while other materials show limited carbonation degree under the applied conditions. Natural minerals like wollastonite exhibit particularly low CO₂ uptake. Particle size does not seem to be the key parameter governing CO₂ uptake for CaO, Ca(OH)₂, Wollastonite and RCF, according to PSD results. However, as the materials with larger surface areas demonstrate the highest conversion degree, a large surface area seems to indicate a higher conversion. The addition of vapor enhances carbonation for CaO and Ca(OH)₂. Further research is required to understand the limitations and controlling mechanisms of carbonation.

Acknowledgement

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Effect of biochar's pyrolysis conditions on anaerobic digestion and microbial composition

(August 2023 – July 2025)



Contribution to the UN Sustainable Development Goals

This project involves enhancing the anaerobic digestion of sulfate-rich waste streams for biogas production through agricultural waste-derived biochar. This approach contributes to efficient resource use, waste reduction, green energy generation, and responsible management of organic materials, thereby advancing a more sustainable and environmentally conscious world.



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Abstract

Anaerobic digestion provides a sustainable solution for energy production and waste management. Biochar addition has emerged as a promising green solution to boost biogas yields. Despite its growing popularity, its role in the digestion process, particularly as a biodegradable carbon and nutrient source, remains poorly understood. This project aims to bridge this knowledge gap by investigating biochar's function and influence in anaerobic digestion. The findings clarify its contribution as a bio-based material, shedding light on how biochar affects digestion efficiency and methane production.

Introduction

Anaerobic digestion (AD) is a key enabler of the circular bioeconomy, addressing the pressing need for sustainable energy sources and effective management of the ever-increasing organic waste streams [1]. In pursuit of economic growth, biogas facilities are actively exploring strategies to maximize biogas yields of treated waste.

Recently, biochar, a highly versatile, low-value bio-based carbon material, has been proposed as an effective green additive to improve digestion and increase methane production. Its physicochemical properties allow it to promote adsorption of inhibitory compounds, pH regulation, microbial immobilization, or even stimulate direct interspecies electron transfer (DIET) [2]. Numerous studies have shown that the addition of biochar can improve the stability and efficiency of AD. However, there is limited understanding of the role of biochar as a biodegradable carbon and nutrients source and its significance in enhancing methane production.

This project investigated the role of biochar in the AD process, taking into account its potential biodegradability. Biochars produced from different feedstocks and pyrolysis conditions were

evaluated in terms of methane yield during cellulose digestion and biodegradable organic content. This was followed an analysis of their physicochemical properties, as well as studies on biochar dosage and microbial distribution during AD cultivation.

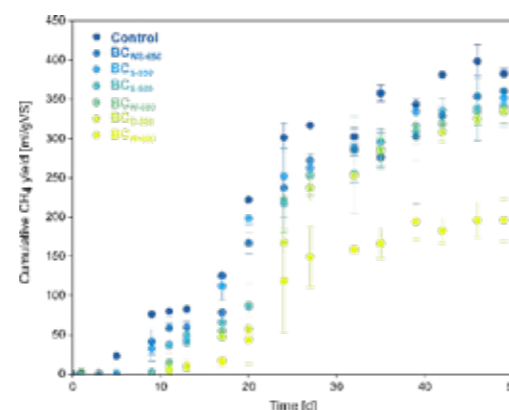


Figure 1: Cumulative methane yield at 15 g/L biochar addition [3].

Results and Discussion

Tested biochars showed great variations in their physicochemical properties. Although some biochars appeared to have properties highly favorable to the digestion process and led to an increase in the relative abundance of the methanogenic community, most of the tested biochars showed no positive effect on methane yield, regardless of the concentration added, contradicting existing literature [3]. An inhibitory to the process biochar was also observed, with inhibition being attributed to its feedstock and high-temperature production conditions [3,4]. Microbial results also reflected this inhibitory behaviour, showing an overall decrease in microbial diversity. Finally, additional methane yield was observed when using biochar containing residual biodegradable organic matter, attributed to the low-temperature and incomplete pyrolysis conditions [3].

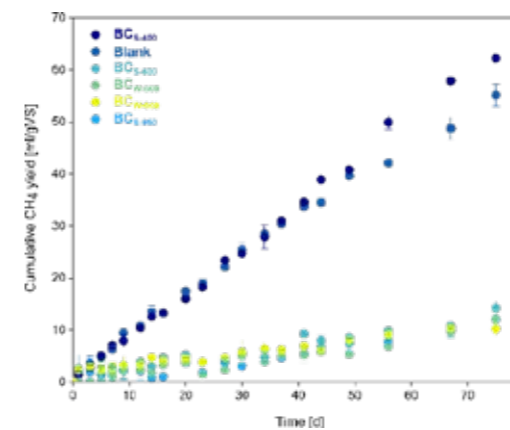


Figure 2: Cumulative methane yield of biochar-controls (no substrate) at 5 g/L addition [3].

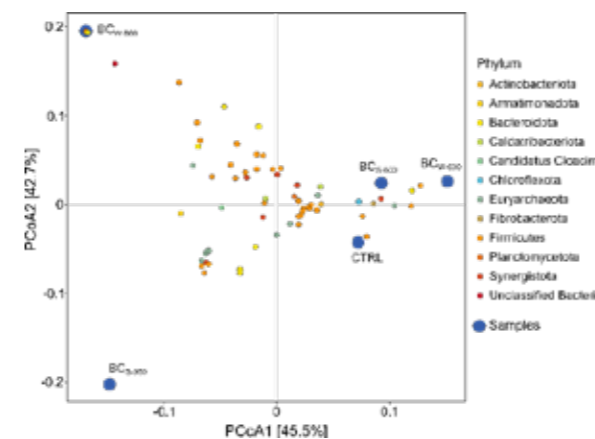


Figure 3: Principal coordinates analysis (PCoA) plot representing the microbial distribution at family level of the most abundant ASVs in the samples at 10 g/L biochar addition [3].

Conclusions

Biochar comprises a diverse group of carbon materials whose properties are largely determined by pyrolysis conditions. High-temperature pyrolysis can potentially generate or release toxic compounds that inhibit the digestion process, while low-temperature pyrolysis may not fully stabilize the treated biomass, producing biochar that contributes to methane production through its content of residual biodegradable organic matter. In any case, once the under-digestion substrate has been completely biomethanized, the addition of a well-stabilized biochar cannot lead to further methane regardless of its physicochemical properties [3].

Acknowledgements

This work was supported by the Novo Nordisk Foundation under the project framework DIET-Syntrophy [program No. NNF21OC007139]; and the European Union's HORIZON-MISS-2022-SOIL-01 under the project framework FENIX [grant agreement No. 101113002].

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Optimization of an Industrial Tubular Photobioreactor through Model-Based Control

(November 2023 – November 2026)



Contribution to the UN Sustainable Development Goals

As the world struggles to reduce greenhouse emissions and minimize the use of natural resources, microalgae can be of great utility in both areas. Their high content in protein and fatty acids makes them outstanding candidates for human and animal consumption, while their cultivation can be very efficient in terms of land use and carbon footprint, as they uptake CO₂ to perform photosynthesis.



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Abstract

Microalgae technology has recently gained interest due their capacity to absorb and fix carbon dioxide while still producing high-value compounds. However, the ability of light to penetrate into the bulk of the liquid becomes a limiting factor when attempting to upscale this technology to large-scale production, as dark and unproductive volumes appear. In our project, we have mechanistically characterized how transitions from well-illuminated to dark regions and vice versa affect algal metabolism, with the overall goal of understanding and optimizing the performance of large-scale tubular photobioreactors.

Introduction

In the current scenario of climate crisis, the development of sustainable alternatives for a multitude of processes and products is more urgent than ever, to reduce emissions of greenhouse gases and mitigate the degradation of natural environments. In this context, microalgae can prove to be a valuable ally. Similar to higher plants, microalgae perform photosynthesis to grow, fixing carbon dioxide into organic molecules, and releasing molecular oxygen in the process. On top of having a high content of protein and fatty acids, some species and strains can produce different valuable compounds, such as EPA, a fatty acid in the group of omega-3, or paramylon, which is considered to have anti-tumor and anti-HIV activity [1]. In addition, microalgae cultivations are much more efficient land-wise than traditional plant crops, the protein productivity of a hectare of algae cultures, even after factoring in ancillary equipment and utilities, is calculated to be 20 times larger than that of soybean [2].

Yet, there is room for improvement. As microalgae grow and divide, and the cell density increases, so does the volumetric productivity and the substrate consumption. Thus, efficient distribution of the limiting

substrate becomes a key priority. In the case of microalgae, however, the limiting factor is not a chemical compound, as it is the case with oxygen or the carbon source in yeast and bacterial fermentations, but light, and specifically, how much it can penetrate into the medium. As algae absorb and scatter light, in dense cultures only the few millimeters closest to the light source are properly illuminated, while the bulk of the medium remains in darkness, unproductive.

This factor constrains the design of cultivation systems, and limits the operational biomass concentration. Overcoming this limitation requires ingenious design of the number, power and location of the light sources, the reactor geometry and the flow patterns in the reactor, so that microalgae are circulated efficiently between illuminated and dark areas. It also requires good understanding of how the algae metabolism is impacted under fluctuating light conditions. In our project, we have focused on the last point, our goal being to characterize the key metabolic pathways that are involved in the photosynthesis, through a mechanistic approach, and analyze how the dynamic illumination conditions impact it.

Model development

We have focused in creating a model for the two main pathways that characterize photosynthesis, the electron transport chain (ETC), and the Calvin cycle. The former comprises the set of redox reactions that start with the light absorption, and overall lead to the oxidation of water into molecular oxygen, and the production of the metabolic vectors for energy (ATP) and reductive capacity (NADPH). The latter covers the cyclic set of enzymatic reactions that consume ATP and NADPH to fix CO₂ into an organic carbon backbone, output a basic organic building block and regenerate the original backbone.

For the ETC, we focused on its limiting step, which is the initiation of the transport chain [3]. This takes place at a molecular complex (photosystem II), which contains chlorophyll molecules bound to its structure. These pigments absorb the light and transfer the energy to the reaction center of the complex. There, a special type of chlorophyll is oxidized, releasing an electron. However, this chlorophyll is photosensitive, and can be damaged under strong illumination. Thus, the overall rate of the transport chain is determined by the number of photosystem II units that have not been damaged and can therefore initiate the chain.

We modelled the likelihood of this damage based on the probability of a photon being absorbed at the molecular complex, the availability of electron acceptors, the presence of reactive oxygen species and the photoprotective role of some pigments bound to the photosystem II. On the other hand, we assumed the repair process to be enzyme-mediated, and proposed a Michaelis-Menten type of kinetic.

Regarding the Calvin cycle, we focused on those reactions where external metabolites are incorporated to the cycle and consumed, and considered the overall rate of the cycle to be that of the slowest kinetic.

Preliminary results

We have so far successfully simulated the kinetics of damage and repairation of the photosystem II units, under fluctuating light conditions, and made some preliminary findings. In fact, our equations suggest that the rate of damage of the photosystem II units should be proportional to the fraction of functional units, and quasi-linear linear with respect to light intensity. This non-linearity appeared as a consequence of the influence of the photoprotection mechanisms, which can minimize the damage up to a certain extent, before becoming saturated as light intensity increases. For very strong illuminations, the rate of damage is almost proportional to light intensity.

We simulated how the fraction of functional photosystem II units, θ , evolved over time, under

binary light conditions (ON – OFF), until it reached a dynamically stable steady state, θ_{ss} (Figure 1); and then we compared the values of θ_{ss} for different light intensities (Figure 1). We found out that regardless of the intensity, θ_{ss} was always lower in discontinuous illumination compared to its continuous counterpart, because the frequent dark periods allowed the cells to recover from some of the damage induced by light. This means that microalgae grown under fluctuating light have a larger pool of functional photosystem II units that can absorb a greater fraction of the incoming light intensity, thus increasing the overall productivity of cultivation system per energy input.

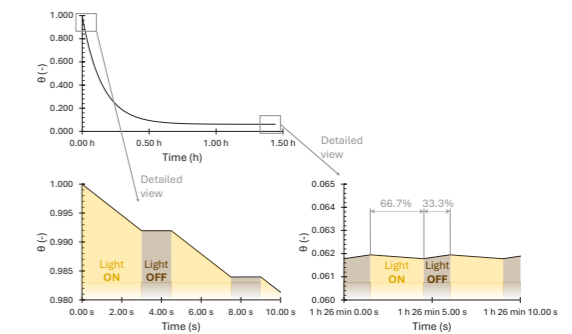


Figure 1: Evolution of θ under fluctuating light.

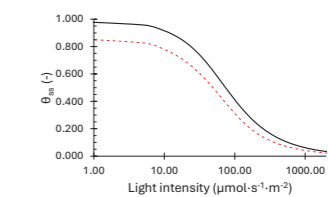


Figure 2: Impact of light intensity on θ_{ss} .

Further work

We expect to incorporate the Calvin cycle kinetics to our simulation soon, in order to achieve a full picture of the metabolism under fluctuating lights. In the medium term, we will integrate this model with other models that we are currently developing, which will describe the light field inside a tubular photobioreactor and the particle lifelines to be traced by microalgae cells under a given flow condition. Combining these, we aim to put forward a highly detailed characterization of the impact of light availability in high cell density tubular photobioreactors, and eventually analyze and determine the optimal operational conditions for such a system.

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Reactor characterisation methods for gas dependent bioprocesses

(May 2023 – April 2026)



Contribution to the UN Sustainable Development Goals

Many chemical processes impact the climate in various ways. Therefore, more sustainable and green technologies need to be implemented. One of the ways to solve some of the problems is by the use of biocatalysts. Biocatalytic oxidation provides a sustainable and safe alternative, operating very selectively. Moreover, using a biocatalyst is a much faster process compared to fermentation, meaning the production time will be significantly minimised. To ensure the lowest impact on the environment, the processes need to be fully optimized, especially regarding the oxygen supply.



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Abstract

Biocatalysis has started to overtake chemical processes to enhance the sustainable aspects of production. However, many biocatalytic processes are oxygen dependent, which comes with challenges, such as low oxygen solubility in water. Therefore, new bioreactor configurations must be tested to enhance the oxygen mass transfer. This project aims to test new impeller and sparger configurations to optimise bioprocesses concerning bubble size distribution and mass transfer.

Introduction

The increasing population, climate changes, geopolitical instabilities, and supply chain problems all mean we must adapt to production with a greater degree of green and sustainable technology. [1]

However, many processes are already well-optimised, meaning an entirely new synthesis is required, which is a demanding development process. A potential route would be the use of biocatalysis, which means enzymes are used as chemical catalysts in an isolated format. [2]

Numerous biocatalytic reactions have already been implemented in industry, especially enzymes such as lipases and dehydrogenases. These biocatalytic reactions have significant benefits, such as superb selectivity under mild conditions and very high reaction rates compared to fermentation. [3]

Oxidation is one of the most critical targets in the potential next generation biocatalysis. Oxidation is essential for industrial organic chemistry but comes with several challenges. One of the greatest challenges is the fact that the enzyme reactions often use molecular oxygen, which is

limited by the low water solubility, around 250 μM under ambient conditions. [4]

Specific objectives

The project's primary objective is to evaluate alternative bioreactor configurations to overcome the challenges of the kinetics of biocatalytic gas-dependent reactions. A particular focus will be placed on oxidation using molecular oxygen. To try and overcome the solubility challenges that affect mass transfer and enzyme stability, gas bubble size distribution will be a primary factor.

Experimental work will investigate the bubble size distribution using the most conventional bioreactor type used for industrial organic chemistry, the stirred tank reactor (STR). Different sparger and impeller setups will be tested and evaluated compared against the standard ring sparger and Rushton turbines

Experimental setup

A new reactor has been built in collaboration with the KT workshop to explore the options for different reactor configurations. The reactor is shown in Figure 1. The reactor is equipped with a ring sparger, four equal baffles, four Rushton turbines, and four oxygen probes attached to one

of the baffles to ensure a homogenous oxygen distribution.



Figure 1: Pilot scale reactor, with a working volume of 180 L. Equipped with standard ring larger, Rushton turbines, and baffles.

Moreover, six blue inlets on the side of the reactor were placed at different heights to ensure measurements of the local gas bubble size by using an inline Shadowscope. This allows for detecting the gas bubble size distribution at different heights, following the bubble's size changes throughout the reactor.

With a focus on oxygen mass transfer, some essential parameters that will be tested are the volumetric mass transfer coefficient, $K_L a$, local and overall gas holdup, and bubble size distribution.

Bubble size distribution

An inline ShadowScope (Dantec Dynamics, Denmark) determines local gas bubble size, proving images as shown in Figure 2.



Figure 2: Use of Shadowscope in the reactor and an example of an analysed bubble image.

To capture the images, a high-speed camera connected to the inline endoscope allows capturing up to 1600 frames per second. This means that the endoscope not only provides the

size of the individual bubble but also allows following a bubble between the frames, thereby providing the direction and velocity of the bubbles. This can help understand the liquid flow. Moreover, the images can be used to count the bubbles and determine the bubble volume, which can be used to specify the local gas holdup.

Combining all the knowledge we can get from the endoscope, it will be possible to establish the specific process for which impeller setup and reactor configuration would be the most optimum in case of oxygen mass transfer.

Conclusion

Based on the experimental work and implemented models, The project aims to establish the most suitable bioreactor configuration for oxygen-dependent biocatalytic reactions.

Acknowledgements

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme. (Grant agreement No. 101021024) and DTU. Thanks to the KT workshop for building the reactor and making the use of inline Shadowscope at pilot scale possible.

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Modifying electrical properties of PDMS membranes for electrostatic actuators.

(March 2023 – March 2026)

10 REDUCED INEQUALITIES



Contribution to the UN Sustainable Development Goals

This PhD project is a contribution to the Novo Nordisk Foundation (NNF WeAreAble project). The general scope of the project is to promote advancement in the technology of soft and wearable robotics. A possible benefit is the development of light exoskeleton-type devices, which could be used in medical and social care applications. This could potentially reduce inequalities by assisting people with mobility issues.



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Abstract

This study explores enhancing dielectric permittivity in polydimethylsiloxane (PDMS) elastomers for dielectric elastomer actuators (DEAs) by incorporating choline-based ionic liquids (ILs) and crosslinking under a 1 kV DC electric field. IL variants were synthesized and added to a photocurable PDMS system. Results showed all IL variants increased permittivity compared to the PDMS control, with choline glycolate showing the highest increase. However, cross-linking under an electric field did not enhance permittivity. Choline itaconate-IL-based PDMS films exhibited unique properties at lower frequencies post-electric field curing, suggesting further investigation potential. The study found no significant advantage in curing IL PDMS films under an electric field but highlighted choline itaconate's potential as an additive.

Introduction

Dielectric elastomer actuators (DEAs) are composed of two compliant electrodes with a dielectric elastomer (DE) material in between, creating a flexible, variable capacitor. Their lightweight and flexible nature makes DEAs ideal for wearable robotics. However, they require high voltages (around 1-10 kV) to produce significant strain. The force generated by a DEA is influenced by the dielectric permittivity of the DE, Young's modulus of both the DE and electrodes, the applied voltage, and the electrode separation

Equation 1 shows the simplified actuator equation. Here, ϵ_0 is the vacuum permittivity, ϵ_r is the relative dielectric permittivity, Y is Young's modulus, V is the applied voltage, and d is the film thickness. S_{max} is the maximum achievable electromechanical force.

$$S_{max} = \frac{\epsilon_0 \epsilon_r}{Y} \left(\frac{V}{d} \right)^2 \quad [1]$$

Equation 1 shows that the DE may be optimized by reducing Young's modulus, increasing the

dielectric permittivity, or increasing the electrical breakdown strength.

Polydimethylsiloxane (PDMS) elastomers are ideal for DEs due to their suitable dielectric permittivity, low Young's modulus, and high breakdown strength. Previous studies have demonstrated that incorporating charged molecules into the PDMS matrix enhances the dielectric permittivity of a DE. Ionic liquids (ILs), particularly those based on imidazolines, can achieve this at low concentrations without significantly reducing breakdown strength or increasing Young's modulus [2,3].

This project aims to incorporate ILs into the PDMS matrix and achieve charge separation by crosslinking the reagents under an external electric field. Choline derivative-based ILs have been selected due to their successful integration into similar polymer systems [5,6].

Specific Objectives

The specific objectives of this project are:

- (1) To investigate if cross-linking PDMS with IL under an electric field enhances.

dielectric permittivity compared to without an applied field.

- (2) To determine whether the choline-based IL additive positively affects the dielectric permittivity.

Experimental

Initially, IL variants were prepared from the acid/base reaction of choline bicarbonate with itaconic acid, glycolic acid, and 4-(hydroxymethyl)benzoic acid (Merck), forming choline glycolate, choline itaconate, and choline 4-(hydroxymethyl)benzoate, respectively. Each IL was dried for 24 hours in a vacuum oven before use.

The ILs were incorporated into a photocurable PDMS system in a concentration of 20 wt%. The PDMS system consisted of the commercial material Momentive UV Electro 225-1 with a 100:2 catalyst ratio. All samples were speed-mixed for 2 minutes before use. Films (0.5 mm) of each variant were blade cast onto a polyethylene terephthalate (PET) film. Control samples were immediately exposed to UV (365 nm) for 10 minutes to crosslink the system.

Test samples were placed in the electrical cell (see Figures 2 and 3) and exposed to a 1 kV DC external electrical field for 10 minutes before UV lamp exposure. The field was maintained during the subsequent 10-minute crosslinking period. All films were then characterized for electrical permittivity.

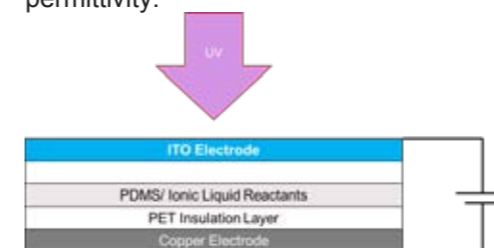


Figure 1: Composition of the PDMS cell. Initially, 1kV is applied to the uncured PDMS/IL resin. Finally, the UV lamp is applied to the indium-doped tin oxide (ITO) glass window to crosslink the network.

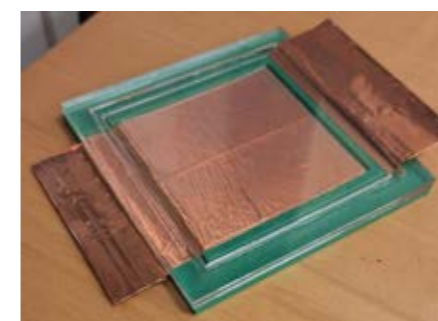


Figure 2: Assembled cell. The base is 3D-printed PET-glycol. The top is ITO glass in an acrylic frame.

Results and Discussion

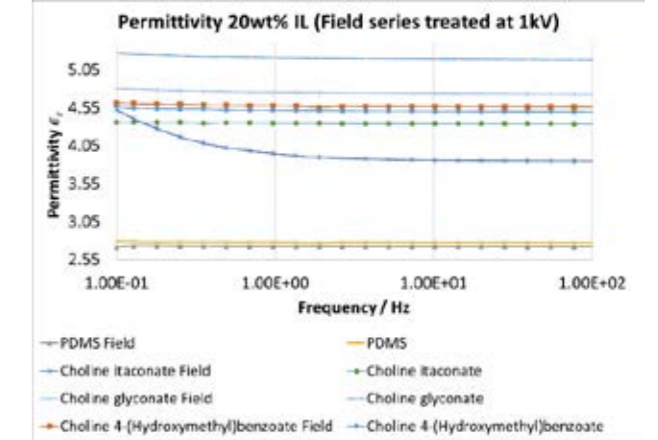


Figure 3: Dielectric permittivity ϵ_r results for each variant crosslinked with and without an external electric field.

All variants exhibited increased permittivity compared to the PDMS control, with choline glycolate showing the highest increase. Cross-linking in the electric field did not show increase of permittivity compared to without. Choline itaconate-IL PDMS showed a significant lowering of ϵ_r for frequencies greater than 0.1 Hz after field treatment.

Conclusion

Treating the PDMS-IL variants with a 1 kV external field during cross-linking showed no significant increase in permittivity. Choline itaconate exhibited the most difference, increasing ϵ_r at 0.1 Hz vs cross-linking without a field and warrants further investigation.

Acknowledgments

This project is funded by the Novo Nordisk Foundation.

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Phosphorus Chemistry in Pyrolysis of Biomass

(January 2023 – January 2026)

12 RESPONSIBLE CONSUMPTION AND PRODUCTION



Contribution to the UN Sustainable Development Goals

Biomass, as a renewable resource, could be converted to bio-oil and char through pyrolysis, with a potential for replacing fossil fuel-based products. Adding phosphorus additives in biomass is an effective approach to promote the selective production of high-value organics, increasing the content of furan and anhydrosugars in bio-oil. However, phosphorus undergoes transformation in char and influences its physical, chemical and thermal properties. The aim of this work is to investigate the release, transformation, and distribution of phosphorus species during biomass pyrolysis.



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Abstract

Phosphorus additives have been employed in biomass pyrolysis to promote the selective production of furan and anhydrosugars in bio-oil. However, the transformation mechanisms of phosphorus additives during pyrolysis is not fully understood. In this work, we investigated the transformation and distribution of three commonly used phosphorus additives, $\text{NH}_4\text{H}_2\text{PO}_4$, $\text{Ca}(\text{H}_2\text{PO}_4)_2$, and NaH_2PO_4 , during the pyrolysis of pine wood and wheat straw at 550°C . Two types of model compounds, potassium species and phosphorus additives were employed to study the interactions between phosphorus and potassium species during biomass pyrolysis. The char produced from the pyrolysis of pine wood and wheat straw was further devolatilized at 800°C to study the release, transformation, and distribution of phosphorus and potassium species.

Introduction

The consumption of fossil fuels leads to a series of environmental pollution problems [1]. Biomass, as a renewable resource, could be converted to bio-oil and char through pyrolysis, with a potential for replacing fossil fuel-based products [2]. However, due to the poor selectivity of conventional fast pyrolysis, most of the high-value organics in the bio-oil are of very low content, thereby making it difficult for further separation and refinement [3]. Adding phosphorus additives in biomass is an effective approach to promote the selective production of high-value organics, increasing the content of furan and anhydrosugars in bio-oil [4]. However, phosphorus undergoes transformation in char and influences its physical, chemical and thermal properties. Some studies have reported that phosphorus species react with inorganic ash species in biomass during pyrolysis [5]. Carbothermic reactions of phosphorus occur above 800°C , leading to its release into the gas phase as elemental phosphorus [6]. Although phosphorus release and transformation have gained a great interest, the mechanisms are still far from clear, and the phosphorus distribution in char has seldom been discussed. Furthermore, the influence of phosphorus on char properties requires further investigation.

Specific Objectives

The overall objective of this PhD project is to provide an improved understanding of the high-temperature phosphorus chemistry in pyrolysis of biomass. More specifically, the objectives of this project are to:

- Understand experimentally the transformation and distribution of phosphorus in biomass pyrolysis.
- Establish knowledge on the interactions of phosphorus species and potassium species.
- Understand experimentally the release, transformation, and distribution of phosphorus in char devolatilization.

Materials and Methods

Two typical woody and herbaceous biomasses, pine wood and wheat straw, were used in this study. The chemical properties of biomass are given in Table 1.

Three anhydrous phosphorus additives, $\text{NH}_4\text{H}_2\text{PO}_4$ ($\geq 99.99\%$, product no. 467782), $\text{Ca}(\text{H}_2\text{PO}_4)_2$ ($\geq 95\%$, C8017), and NaH_2PO_4 ($\geq 99.0\%$, S0751), were purchased from Merck. The phosphorus additives were mixed with biomass in a mortar mechanically for 10 mins, with biomass at a PO_4^{3-} /biomass mass ratio of 1/20 to prepare pine wood-

phosphorus additive and wheat straw-phosphorus additive mixtures.

Table 1: Proximate and ultimate analysis of pine wood and wheat straw.

	Biomass	Pine wood	Wheat straw
Proximate analysis (wt.% ad)	M	8.28	10.05
	A	0.25	4.29
	V	77.7	69
	FC	13.77	16.66
Ultimate analysis (wt.% ad)	C	0.06	0.35
	H	48.24	43.72
	N	6.21	6.03
	S	0.04	-
	O*	45.21	45.6

Note: "ad", "-" and "*" represented air dried, not detected and by difference, respectively.

Pyrolysis of three types of feedstocks, phosphorus additives, biomasses, and their mixtures, were carried out with a fixed-bed reactor. The diagram of the equipment is shown in Figure 1. In each run of experiment: a corundum boat containing 2 g sample was placed into a water-cooling section; the carrier gas of N_2 with a flow rate of 3 NL/min was introduced to purge air; the horizontal reactor was then heated to 550°C by $10^\circ\text{C}/\text{min}$; after 30 minutes of oven temperature stabilization, the corundum boat was swiftly pushed into the reactor from cooling section, the heating rates of feedstocks were higher than $100^\circ\text{C}/\text{min}$; after 40 minutes' reaction, the corundum boat was pulled out into water-cooling section for fast cooling with the presence of N_2 . The residues in the corundum boat were weighed and collected for further analysis.

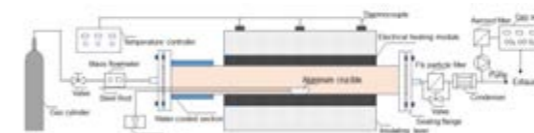


Figure 1: The diagram of fixed-bed reactor

Char oxidation was conducted in a TGA (STA-449C, Netzsch Germany). 10 mg of char was placed in an corundum crucible in each run of experiment; the char was heated from 30°C to 800°C by $10^\circ\text{C}/\text{min}$ in a N_2 atmosphere (200 mL/min), then held 30 minutes for devolatilization, in order to eliminate the influence of volatiles on the subsequent oxidation; the residue was then cooled to 100°C by $20^\circ\text{C}/\text{min}$, followed by 15 minutes of system stabilization; the carrier gas was switched from N_2 to a mixture of 5% O_2 and 95% N_2 (200 mL/min), then held 15 minutes for system

stabilization; afterwards, the residue was heated to 1000°C by $10^\circ\text{C}/\text{min}$ for oxidation.

Crystal phase transformations of solid products were characterized with XRD (Huber G670) over a 2θ range of 5° to 90° by $1^\circ/\text{min}$ using $\text{Cu K}\alpha_1$ radiation ($\lambda = 1.54056 \text{ \AA}$). Micro-morphologies of solid products were observed with SEM, while the elemental distribution and elemental composition were determined with EDS (Thermo Scientific). Ultimate analysis of biomass and char were performed with an elemental analyzer (Eurovector EuroEA3000) to investigate the influence of phosphorus on carbon and hydrogen release.

Preliminary results

The results indicated that the addition of $\text{NH}_4\text{H}_2\text{PO}_4$ and $\text{Ca}(\text{H}_2\text{PO}_4)_2$ to pine wood increased the yield of char. The release ratio of carbon decreased while that of hydrogen barely changed with the addition of phosphorus additives. XRD analysis revealed that all three phosphorus additives dehydrated and reacted with potassium species in biomass to form K-P compounds during pyrolysis, with the exception of the phosphorus in pine wood- $\text{NH}_4\text{H}_2\text{PO}_4$ -char, which remained amorphous. EDS analysis showed that the phosphorus from $\text{NH}_4\text{H}_2\text{PO}_4$ and $\text{Ca}(\text{H}_2\text{PO}_4)_2$ was distributed homogeneously on the surface of char. $\text{Ca}(\text{H}_2\text{PO}_4)_2$ partially converted to $\text{Ca}(\text{PO}_3)_2$, while NaH_2PO_4 primarily converted to NaPO_3 .

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