KT Consortium: Current Status

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KT Consortium: Mission

To provide member companies state-of-the-art CAPE/PSE methods and tools, and the technologies for future chemical and biological processes.
KT Consortium: Vision

Objectives
- Develop and use a computer aided systems approach
- Solve and analyze problems
- Product-Process Modelling, Simulation, Synthesis, Design, Analysis, Control, & Operation
- Chemical, Petrochemical, Pharmaceutical, Agrochemical, Food and Biochemical Industries.

Focus
- Development of generic methods and tools through the use of a systems approach.
- Application domain is wide and cover several industrial sectors.
- Dissemination of research results through the industrial consortium members and collaboration partners from academia
Faculty (4): Rafiqul Gani (SPEED); Georgios Kontogerogis (CERE); Xiaodong Liang (CERE); John M Woodley (KT)

Post-docs (3): Alay Arya, Teng Zhou, Hongliang Qian (July 2017)

PhD-students (16): SPEED: Olivia Perederic, Xinyan Liu, Spardha Jhamb, Rebecca Frauzem, Maria-Ona Bertran, Nipun Garg, Yuqui Chen (Sept 2017); CERE: Andre Vinhal, Mauro Torli, Edgar Vergara, Li Sun, Anders Schlaikjer, Arne B Gladis, Susana Almeida; Visiting: Daneila Damaceno, Alessandro Rosengart

MSc & Bsc students (6): Anders Jaksland, Evangelia Koumaditi, Jacob M Jensen, Maria do Carmo, Tereza Kolaiti, Nooshin Shahlari (visiting)

Administration (1): Eva Mikkelsen
SPEED

Application of PSE methods & tools

Sustainable Product-Process Engineering for Evaluation & Design

Modelling (properties, product, process, computer-aided tools)

Product Synthesis, Design & Analysis (single molecule, mixtures & blends, formulations, devices, ....)

Process Synthesis, Design, & Analysis (separation processes, process intensification, processing route optimization, .....)

Integration (sustainable product-process design, biorefinery, CO2 capture-utilization, ICAS: Integrated Computer Aided System, ....)
• Property modelling* (pure component & mixture) – GC$^{\text{plus}}$ approach
  • Revision & extension of MG-method parameters
  • Comprehensive parameter tables for systems involving lipids (PhD1, PhD2)
  • Computational algorithms* (PhD3)
  • Development of new property models (PhD4, P6, P7)
• Gas solubility (data & models) in ionic liquids (PhD5)
• Process modelling (simple & rigorous)
  • Biphasic reactors & biochemical reactors
  • Gas separation process modules (PhD5)
  • Reaction-separation process modules (P2, P5)
  • Detailed membrane-based separation modules

• Computer-aided modelling tools & models
  • Modelling template and large collection of model library (PhD7, PhD8, PhD9, PhD10)
  • Model parameter estimation
Energy efficient separation process design
  - Solvent based separations
    - Gas separations (PhD5, P3)
    - Azeotropic separations
  - Synthesis of separation schemes
Downstream separation: bioreactors (P2, P5)
Superstructure based process network (processing route) synthesis
  - CO2 to chemicals (PhD6, P3); Biomass to chemicals* (PhD7, PhD9, PhD10); Waste water treatment; chemical processing; ….
• Single molecule chemical products (PhD4, PhD5)
  • Solvents*, surfactants, lipids, amino acids, process fluids (refrigerants, ORC, heat pumps, ..)
• Tailor-made blends
  • Surrogate fuels and lubricants
• Formulations
  • Detergents, cosmetics, …
• Chemical substitutes (PhD4)
  • Formulations, organic synthesis, food, …
• Process integration & intensification
  • Phenomena-based method (PhD10)
  • Application examples (visiting students)
• Sustainability (PhD5-PhD10, P1, P4)
  • Sustainable process synthesis-design method
    • Applications (chemical process; biorefinery; CO2 capture-conversion; ....)
• Integrated computer aided system (ICAS)*
• Model-based frameworks - collaboration
  • Computer-aided flowsheet design
  • Computer-aided product design
### PhD projects: Poster presentations

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<th>PhD Students</th>
<th>Project Descriptions</th>
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<tr>
<td>P6 Edgar Camacho</td>
<td>Inhomogeneous fluid behavior: density functional theory approaches</td>
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<td>P7 Li Sun</td>
<td>Modeling CO2 semi-clathrate hydrate related systems: literature review and database</td>
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<td>P8 Anders Schlaikjer</td>
<td>Development of CPA for electrolyte mixtures</td>
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<td>P9 Mauro Torli</td>
<td>The SYNFERON project</td>
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<td>P10 Arne B. Gladis</td>
<td>Upscaling of enzyme-enhanced carbon capture process</td>
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<tr>
<td>P11 Susana Almeida</td>
<td>Predictive modeling of gas diffusion and solubility in polymers for offshore application</td>
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## Current projects

### MSc projects: Poster presentations

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<th>MSc Students</th>
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<tr>
<td>P1 Anders Jaksland</td>
<td>Development of novel processing networks for biorefineries</td>
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<td>P2 Evangelia Koumaditi</td>
<td>Intensified reaction-separation schemes</td>
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<td>P3 Jacob Møller Jensen</td>
<td>Design of a CO2 Utilizing and neutral process</td>
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<tr>
<td>P4 Maria do Carmo</td>
<td>Food waste upgrading by an integrated biorefinery process</td>
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<td>P5 Tereza Kolaiti</td>
<td>Process design and analysis for the synthesis of glycerol to 3-hydroxypropionic acid and 1,3-propanediol</td>
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ICAS – Integrated Computer Aided System

ICAS: combines computer-aided tools for modelling, simulation, property prediction, synthesis/design, control and analysis into a single integrated system

• ICAS dedicated to manage the complexity through a systems approach
• ICAS algorithms based on a systematic solution approach.
• ICAS allows single- and multi-dimensional problems to be solved efficiently, reliably, consistently and robustly.
• ICAS improves productivity by allowing sharing of common knowledge between different groups of people.
Since July 2016

- Chemical product design (Sawitree Kalakul)
- Modelling, design & analysis of biphasic reacting systems (Amata Anantpinijwatna)
- Modelling and synthesis of pharmaceutical processes (Emmanouil Papadakis)
- Integrated process design-control (Seyed S Mansouri)

Since January 2017

- Computer-aided sustainable process synthesis-design and analysis (Anjan K Tula)
Energy efficiency versus CO2 management versus new innovative solutions
Direct & indirect CO2 emission

Power Plant

\[ I_{in} \rightarrow I_{out} \]

Manufacturing Process

\[ I_{in} \rightarrow I_{out} \]

Reduction in process utility demand
= less energy consumption, less waste and less CO2-footprint
= more profit
More than 40,000 distillation units alone in US (2005) using nearly 75 million KW of energy

Consumes half the energy except drying which is still 20% less than distillation.
Analysis of design: distillation column

Design specification versus energy cost

Decreasing driving force

Increasing driving force
Use membranes to remove from distillate the compound in the smaller amount ~ to increasing the purity of the compound in the larger amount!
Apply these hybrid modules whenever they match the design targets

Close to 50% or more energy reduction compared to original process achievable
Target: Intensify (reduce number of operations) as well as operational cost

Methyl acetate in multifunctional reactor (Eastman Chemicals)
Examples (synthesis of dioxolane products)

Landero et al. ESCAPE-27, 2017
More examples (toluene to p-xylene)

Anantasarn et al, CACE 2017 (PI Special Issue)
Find swap solvent that gives the following LLE & VLE diagrams
Innovative energy efficient separation schemes

Find swap solvent that gives the following LLE & VLE diagrams

Application: Aqueous solutions of acetone, methanol, acetic acid, ….
Future directions – Research & PSE tools

- **Modelling** (new property models; new chemical systems; extensive library of process models; …)
- **Product synthesis-design-analysis** (new innovative formulations; reliable chemical substitution; wide range of innovative products)
- **Process synthesis-design-analysis** (energy efficient hybrid schemes; reaction-separation; novel processing routes, …)
- **Integration & Sustainability** (innovative intensified solutions; integrated biorefineries; sustainable product-process design)

*New state of the art PSE methods and tools*
The chemical product tree

Question of what, why & when (how)?

Refined chemicals & Consumer products (~3000)
- Plastics, Pharmaceuticals, Dyes, Solvents, Fertilizers, Fibres, Dispensers, Cosmetics...

Intermediate Products (~300)
- Methanol, Vinyl chloride, Styrene, Urea, Formaldehyde, Ethylene oxide, Acetic acid, Acrylonitrile, Cyclohexane, Acrylic acid, ...

Basic Products (~20)
- Ethylene, Propylene, Butadiene, Benzene, Synthesis gas, Acetylene, Ammonia, Sulfuric acid, Sodium hydroxide, chlorine, ...

Raw Materials (~10)
- Petroleum, Natural Gas, Biomass, Roack, Salt, Phosphate, Sulfur, Air, Water, ...

High | Low

Product price | Molecular size | Number of alternatives | Production rate

Low | High