INTENSIFIED REACTION-SEPARATION SCHEMES

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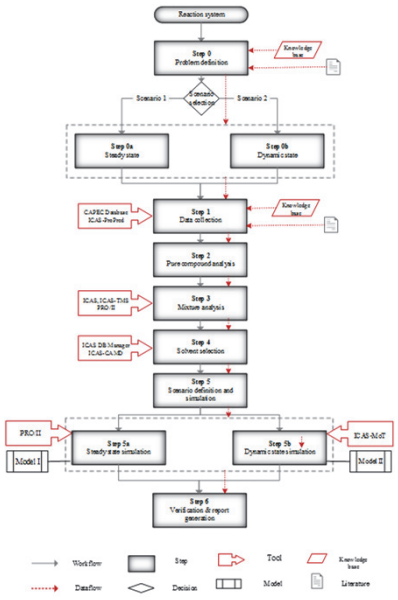
INTRODUCTION

- *Bioprocess* is the transformation of raw materials into a product by the use of a biocatalyst (cell or enzymes).
- Despite the advantages over conventional chemical synthesis pathways, biocatalysis comes with limitations needed to be overcome:
  - Substrate/product inhibition, which results in low yield.
  - Water-dependent reactions lead in highly diluted products, resulting in difficult downstream separations.
- Integration of reaction and separation can increase the product yield and reduce the separation steps.

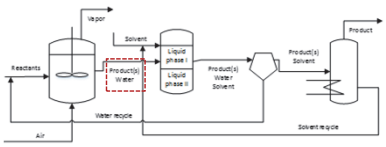
OBJECTIVES

- Development of a systematic design method for reaction-separation schemes.
- Two Scenarios are considered: 1) Steady state and 2) Dynamic state.
- Scenario 1 evaluates the feasibility of the product recovery.
- Scenario 2 evaluates the feasibility of increasing the production yield.
- Downstream in both of the Scenarios are phase equilibrium based.
- Liquid-liquid equilibrium is considered by using a solvent to generate it.
- The method should be applicable for any enzyme, with low substrate concentration, resulting in diluted product.

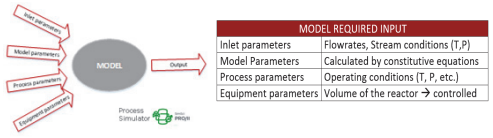
METHODOLOGY



SCENARIO 1: Steady state



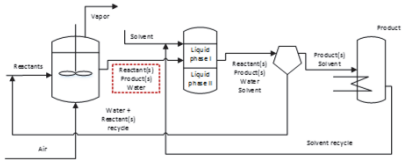
- Steady state → complete conversion of reactants.
- Water exists due to enzymatic requirements.
- Water-immiscible solvent → LLE.
- Product recovery by evaporation.



MODEL REQUIRED INPUT	
Inlet parameters	Flowrates, Stream conditions (T,P)
Model Parameters	Calculated by constitutive equations
Process parameters	Operating conditions (T, P, etc.)
Equipment parameters	Volume of the reactor → controlled

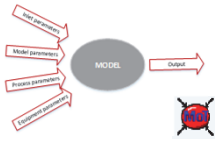
- Simulations were performed in PRO/II.
- Based on the algorithm the input of the model needs to be specified.
- T, P, V : constant by controller
- For a reacting system, only the process parameters are free to change (2 DoF).

SCENARIO 2: Dynamic state



Reactor mass balance:

$$\frac{dn_i}{dt} = F_1 x_{1,i} - F_2 x_{2,i} + \gamma_i rV - (F_{air} y_i - \vartheta_i^V F_{air} y_i + \vartheta_i^L n_i)$$



- Continuous product removal in the reactor.
- Dynamic state simulation of the reactor.
- Steady state simulation of the downstream.
- Water-immiscible solvent → LLE
- Vapor exists due to possible aeriation demands.
- No vapor-liquid equilibrium.

METHODOLOGY APPLICATION

- The design method was applied to 6 reacting systems of the general form:

$$A + B \rightarrow C + D$$

- The reaction class is oxidation of alcohols to aldehydes.

#	Case study	Reaction
1	Oxidation of 1-propanol to 1-propanal	$C_3H_8O + ½\ O_2 \rightarrow C_3H_6O + H_2O$
2	Oxidation of 1-butanol to 1-butanal	$C_4H_{10}O + ½\ O_2 \rightarrow C_4H_8O + H_2O$
3	Oxidation of 1-pentanol to 1-pentanal	$C_5H_{12}O + ½\ O_2 \rightarrow C_5H_{10}O + H_2O$
4	Oxidation of 1-hexanol to 1-hexanal	$C_6H_{14}O + ½\ O_2 \rightarrow C_6H_{12}O + H_2O$
5	Oxidation of 1-heptanol to 1-heptanal	$C_7H_{16}O + ½\ O_2 \rightarrow C_7H_{14}O + H_2O$
6	Oxidation of benzyl alcohol to benzaldehyde	$C_7H_8O + ½\ O_2 \rightarrow C_7H_6O + H_2O$

- The reacting systems are catalyzed by the enzyme GOase.
- The methodology was applied to each reacting system for both of the Scenarios.
- Scenario 1 results in the binary mixture water+aldehyde.
- Scenario 2 results in ternary mixture alcohol+water+aldehyde.
- Each case study requires a different solvent.

RESULTS

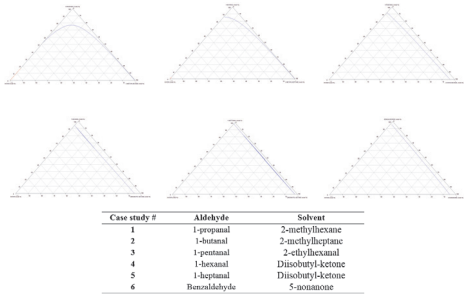
➢ SCENARIO 1: Steady state

Objective: Product recovery

Performance indicator: Percentage of recovered product.

Solvent characteristics:

- Liquid state → Tm<Top<Tb
- Water-immiscible
- No azeotrope formation with the aldehyde
- Non-volatile
- Large distribution coefficient.



Case study #	Aldehyde	Solvent
1	1-propanal	2-methylhexane
2	1-butanal	2-methylheptane
3	1-pentanal	2-ethylhexanal
4	1-hexanal	Diisobutyl-ketone
5	1-heptanal	Diisobutyl-ketone
6	Benzaldehyde	5-nonanone

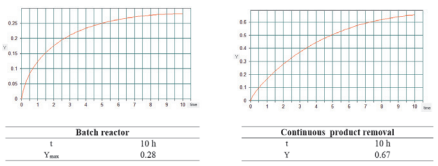
➢ SCENARIO 2: Dynamic state

Objective: Increase of product yield

Performance indicator: Product yield

Solvent characteristics:

- Liquid state → Tm<Top<Tb
- Water-immiscible
- No azeotrope formation with the aldehyde
- Non-volatile
- Large distribution coefficient
- Alcohol affinity in solvent << Alcohol affinity in water



- Simulation of a batch reactor showed that the maximum yield is Y=0.28 and is achieved at 10h. After 10 h the yield decreases.
- Simulation of continuous removal and feed showed that at 10 h the yield is Y=0.67.

ACHIEVEMENTS

- Implementation of the steady state scenario in the six case studies and solvent selection for each case study.
- Development of a systematic method for the design of reaction-separation schemes.
- Implementation of the dynamic state in MoT.
- Verification of the objectives of the two scenarios.

FUTURE WORK

- Report generation for each case study with all the results.
- Sensitivity analysis of different variables in the product yield.
- Simulations of dynamic state for different variables that affect product yield.
- Implementation of solvent selection method in case studies in dynamic-state.
- Verification of the results according to the performance indicator of each scenario.