Targeting Multi-Phase Chemical Reactor Networks in Biochemical Processes: A Superstructure Approach with a View to Innovation and Novel Development

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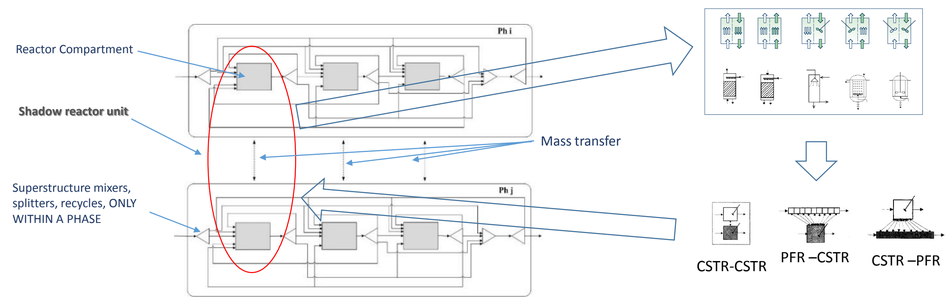
Challenges

- Chemical reactor is perhaps the most important unit to optimize within a chemical process plant.
- The growing demand for "green products" has contributed to the rapid development of biorefineries. The fractionation of biomass and its conversion to products is the objective of recently developed chemistries which are still under research in order to be optimized.
- The new objectives are centered around clean technology and are namely: (1) to give as far as possible only the desired product, (2) to reduce by-products and pollution, (3) to minimize the inhibition factors, and (4) to intensify processing in order to improve economics.
- The design of contemporary biochemical reactors is still mainly based on the existing experience and heuristics in conventional reactors.
- Bioreactor design based on conventional rules of reactor design could fail; apart from the fact that the kinetic 'constants' are no longer constants but functions of everything that characterize the biochemical system, mass transfer and the general hydrodynamic behaviour of the system becomes crucial.
- The diversity of biomass feedstock, along with the complicated activity of the microorganisms used, imposes new uncertainty factors for the design of the bioreactors.
- The feed distribution patterns of enzymes can be viral for economics and yield and can assist in reverse engineering the process and help with the design of the biocatalyst.
- This study proposes a **complete superstructure framework** for the full conceptual design and optimisation of different integrated biorefinery processes.

Superstructure Representation

Systems approach: Shadow Reactor Superstructure Model

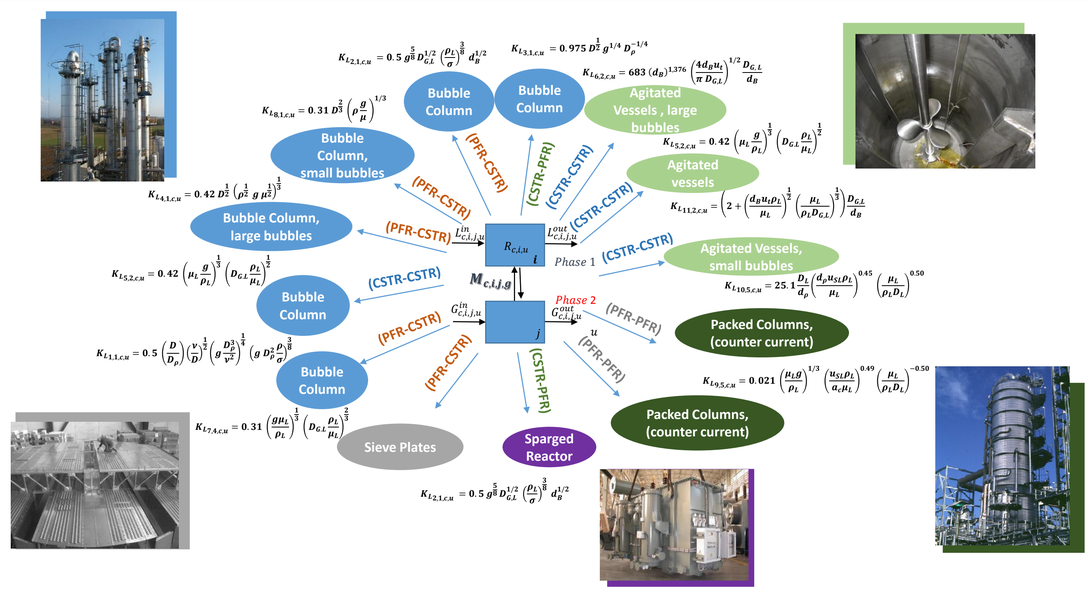


An improved version of the **systematic framework** for the optimization of a superstructure representation of ideal reactor units involving CSTRs and PFRs, firstly introduced by Mehta (1998), for the full conceptual design of multiphase chemical and biochemical reactors.

Degrees of freedom and objective:

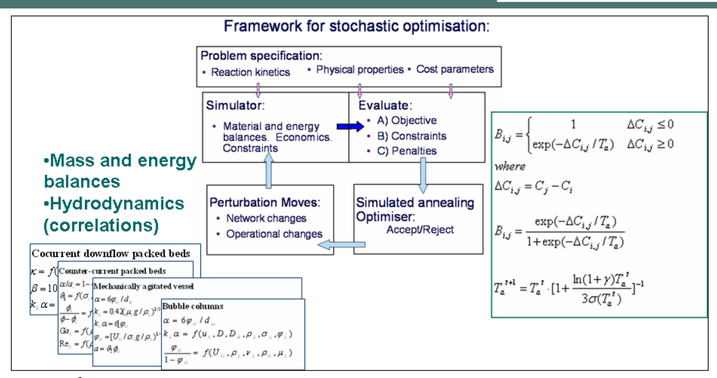
- ✓ Type of mass transfer favored - Reactor configuration
  - ✓ currently a list of 12 options each suggesting an experimental rig
  - ✓ possible inclusion of experimental, bespoke correlations
- ✓ Type of mixing in the shadow reactor compartment (CSTR, PFR, macro-mixed PFR)
- ✓ Comprehensive macro-mixing and micro-mixing options among shadow reactor compartments
- ✓ Reactor hold ups, Reactor volumes, flowrates, connectivities, feed distribution patterns, In-situ product recovery (ISPR) patterns
- ✓ **Optimization objectives** (as usual): yields, selectivity, (occasionally) cost

Mass Transfer



The examination of the impact of different mass transfer correlations on the real design of bio-reactors running different biorefineries examples based on recently developed or under research technologies using the synthesis framework embedded with appropriate mass transfer correlations for the best approximation of mass transfer between phases for each type of reactor.

Optimisation Technology



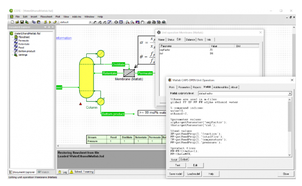
Synthesis framework:

1. **Targeting stage:** creation of initial structure of the superstructure representation using the shadow reactor superstructure
2. **Screening and design stage:** evaluation of the results of the targeting stage and screening of the options that have a positive impact on the system
3. **Analysis stage and validation**: the implementation of **a generic probabilistic metaheuristic global optimization method**

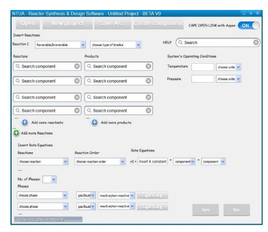
Evolutionary optimisation is employed utilising **Simulated Annealing (SA)** algorithm, on FORTRAN programming language, for the synthesis, design, optimization and superstructure representation of complex reaction network systems (Kokossis & Floudas, 1990).

The approach as a software

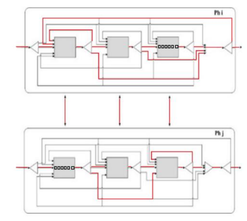
➢ ***INPUT:***
- ❑ *Reaction system*
- ❑ *Reaction kinetics*
- ❑ *Design objective*



➢ ***CAPE - OPEN Link:***
Link with CAPE-OPEN and Aspen Plus for a very accurate chemical properties calculation and fast feed re-characterization.



➢ ***OUTPUT:***
- ✓ *Yield, Selectivity*
- ✓ *Reactor configurations, Reactor volumes*
- ✓ *Macromixing and micro-mixing patterns*
- ✓ *Enzymes/catalyst feed distribution patterns*
- ✓ *In-situ product recovery (ISPR) patterns*
- ✓ *Actual performance limits of the system*



➢ ***INTERPRETATION OF RESULTS:***
(illustration of superstructure)
✓ *Recommendation for the real design*
✓ *Strong Link to Innovative (non-conventional/novel) designs*
(Significant evidence that non-conventional reactors bring key benefits)

Conclusions and Work in Progress

- ✓ The proposed method can be applied for the synthesis, design, and optimization for both, conventional and non-conventional processes since it is fully adjustable to any type of process.
- ✓ Reliability of the framework to adapt with flexibility and high level of accuracy reconfirmed by the results of the case studies.
- ✓ Enables reactor design of the conventional chemical processes with linear simple kinetics
- ✓ Facilitates the synthesis and design of biochemical processes with complex reaction mechanisms.
- ✓ Optimizing various microorganisms & enzymatic reaction systems was proven the Michaelis –Menten kinetics & Monod equation which applies to most biochemical processes can be accurately simulated.
- ✓ The latest version of the framework proposed enables the real design of biochemical reactors with interactive mass transfer coefficients adapted for each case.
- ✓ The great importance of the framework is that it identifies the maximum achievable efficiency of the resulting optimum reactor network, providing useful information about: (1) The number and type of reactors, (2) The desired mass transfer correlation for each type of reactor, (3) The volumes of reactors, (4) The appropriate feeding, mixing, recycling and bypassing strategy and (4)The optimal values of the flowrates, compositions and yields.
- ✓ Work in progress is aiming to make available online this framework as web tool enabling the user to input fast and easy any set of chemical/biochemical reaction equations and kinetics choosing the objectives.

References

A.C. Kokossis and C.A. Floudas, 1990, Optimization of complex reactor networks: Isothermal operation. Chem. Eng. Sci., 46, 1361.

V. Linek, T. Moucha, F. J. Rejl, M. Kordač, F. Hovorka, M. Opletal, & J. Haidl, 2012, Power and mass transfer correlations for the design of multi-impeller gas–liquid contactors for non-coalescent electrolyte solutions. Chemical Engineering Journal, 209, 263-272.

P. Linke, & A.C. Kokossis, 2003, On the robust application of stochastic optimisation technology for the synthesis of reaction/separation systems. Computers & chemical engineering, 27(5), 733-758.

L.V. Mehta, 1998, Synthesis and Optimization of Multiphase Reactor Networks, University of Manchester, Institute of Science and Technology, Dept. of Process Integration, PhD Thesis.

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