Advance Process Modelling to Support Vision 2050 Reaction Engineering Roadmap

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Highlights

- Rigorous multi-scale reactor modelling via standardized model libraries
- Efficient workflows for model validation using experimental data from various scales
- Model centric approach to scale-up, design and optimization of catalytic reactors.
- Reactor designs with quantified uncertainty

1. Introduction

Although Chemical Reaction Engineering is widely considered as a mature field, efficient application of its concepts and methodologies to practical problems of the day and future still poses challenges. A recent publication [1] by leading practitioners from industry and academics reviewed the key challenges and research needs to address them. Advanced process modelling (APM) of the reactor systems and sophisticated model-based calculations play a key role in supporting practitioners to deal with the complexity of reaction engineering problems. The publication also outlined key expectations from APM tools to support its vision 2050 reaction engineering roadmap. The authors indicated that commercial process modelling platforms designed for general purpose process engineering tasks are not suited for the needs of reaction engineering practitioners. Such platforms generally cannot handle rigorous modelling of complex catalytic reactor systems incorporating detailed kinetics, interphase mass transfer, intrapore diffusion, heat transfer in catalyst pellet and bed etc. They also do not support efficient ways to perform parameter estimations using data from experiments of various scales and associated statistical qualification of the parameters.

This presentation is as a response to outline how the APM software such as gPROMS can currently fulfill a major part of these expectations to accelerate innovation and improve R&D efficiency of reaction engineering problems.

2. Methods

Traditional approach for reactor engineering problems heavily relies on experimentation, specialist experience and heuristics. Such approaches require a large number of experiments to solve the problem. Opportunities for exploration of the complete design and operational space to identify optimization possibilities are limited with these approaches. Designs and operational policies based on traditional approaches could be overly conservative and hence more expensive.

All the challenges mentioned above can be addressed with a model centric approach. Unlike the traditional approach, the model centric approach coupled with targeted experimentation is very effective for efficient reactor scale up and design. Experimentation is used to support the construction of a high-fidelity predictive model of the process rather than directly establish performance aspects of the industrial-scale equipment. Once a model of sufficient accuracy is established, the model is used to scale up, optimize the design and operation. The model centric approach involves the following key steps:

- Build reactor models of different scales
- Model validation by evaluating model parameters based on lab/pilot plant data
- Optimize reactor design and operation together with the process around it

Practical application of the model-centric approach needs a state-of-the-art APM tools with features such as:

- high fidelity reactor model libraries with all the relevant phenomena (kinetics, heat & mass transfer, pore diffusion, deactivation) to represent complex reactors & chemistry.

- user-friendly modelling platform enabling efficient construction of reactor system models and state of the art solvers for various model-based calculations.
- efficient custom modelling capabilities to incorporate proprietary knowledge such as reaction & deactivation kinetics including detailed microkinetics to rigorous reactor models.
- ability to build hybrid models when necessary, by incorporating data driven model elements such as neural networks along with first principle models.
- efficient workflows to link experimental data from multiple scales with relevant models and perform parameter estimations using all the data simultaneously.
- high performance computing capabilities to accelerate calculations involving large models.
- calculation of statistical significance of estimated parameters to quantify their uncertainty.
- design of model targeted experiments to reduce the uncertainty in model parameters.
- simultaneous optimization the reactor and the process around it
- ability to perform uncertainty analysis to quantify the risk associated with industrial scale designs due to the uncertainty in model parameter values,
- ability to couple CFD techniques to detailed reactor models with complex chemistry to fine tune reactor designs.

3. Results and discussion

Major catalyst producers and reactor technology developers have been using the model centric approach to scale up, design and optimize catalytic reactor technologies [2]. This approach helps them to accelerate innovation and improve R&D efficiency and hence faster time to market with innovative new technologies. With the current focus of process industry towards circularity and sustainability rapid innovation and R&D efficiency is of utmost importance and the model centric approach can play a crucial role here.

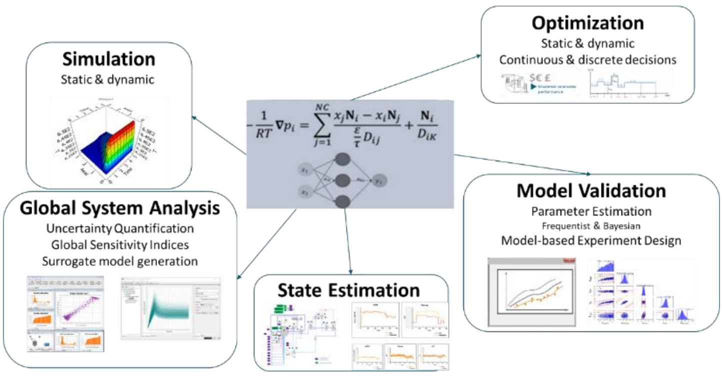

Figure 1. Equation-oriented multi-purpose modeling environment: the same underlying high-fidelity model used for different types of calculations.

4. Conclusions

Vision 2050: Reaction Engineering Roadmap [1] outlines challenges, opportunities and research needs for the coming decades. Computational tools are a major part of the reaction engineering practitioner's toolbox and the article has outlined key expectations from such tools. The main objectives of this paper are: (i) to map these expectations with the current capabilities of APM platform such as gPROMS with advanced catalytic reactor model libraries, (ii) to spread the message that a major part of these expectations can be met at the moment, and (iii) to forge collaborations to address the remaining requirements.

References

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