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Editorial

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Chemical Reactors and Process Modelling

Nawaz Z*

Sabic Technology and Innovation, Saudi Basic Industries Corporation (SABIC), PO Box 42503, Riyadh 11551, Saudi Arabia

***Corresponding author:** Nawaz Z, Sabic Technology and Innovation, Saudi Basic Industries Corporation (SABIC), PO Box 42503, Riyadh 11551, Saudi Arabia, Tel: +966114999769; Fax: +966114999639; E-mail: zeeshan@sabic.com

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Editorial

The chemical and allied industries are of greatest importance for the modern society but their paradigm is changing due to the harsh economic conditions, limited feedstock and high demand of their products. Much emphasis and efforts were devoted to design inherently safer and economic conceptual design, process imagination, process intensification, revamps, energy optimization, and sustainability. The creative efforts/innovations were evaluated against substantial economic advantages and overall sustainability impact. From last two decade, a major shift has begun for above tasks in chemical industry, since there is a need of software tools to help optimization, integration, intensification, sustainability, etc., for design and operation in chemical process industry. Approaches to address and solve problem may differs for the same task, platform (software/language) may be different, problems and objectives can be different too, but todays industry is centered on modeling and simulation. This editorial focuses and reviews how modelling and simulation plays role in modern process industry and available tools.

Since designing stage at conceptual process design (CPD) or Process Design Package (PDP), the job of a chemical engineer is challenging as he has to integrate a large number of constraints, and to deal often with contradictory aspects; e.g., selection of the suitable chemistry, selection of appropriate reactor design, safety, economics, energy consumption, environment, operation and installation compatibilities, etc., The design of complex processes implies the availability of adequate science, modelling and simulation using powerful computer-based tools [1-10]. A systematic approach can provide the guidance's in identifying bottlenecks, feasible scenarios, several alternative possibilities, optimum solution, economics, etc., leading to decision. With respect to problems and mode of information required, different types of mathematical models, different numerical analysis and solution strategies are needed. In general, algebraic systems for steady-state models, ordinary differential algebraic equations for dynamic models and partial differential algebraic equations for distributed models are involved.

Chemical reactors and process modelling includes kinetics, reactor performance equation, mass and energy balance of unit process and/or operations, interpret process flowsheets to simulated flowsheet, simulate individual unit operations, locate malfunctions, and solve to predict the performance. The model is a replacement of the real system of sufficient fidelity for performing optimization tests those cannot be performed safely in shortest possible time in real systems. The systems formalism is generally seen in every problem that can be tackled using generic view by posing set of known variables and leaving others to be estimated. However, the preliminary considerations around problem statement and necessity to decision-making are common elements despite the modelling life cycle. In the area of mathematical modeling there is minor progress, while describing the dynamics of engineering systems has great importance and number of ways. Now a days much emphasis are given to below topics:

- Equation oriented reactor and process modelling
- Computer-aided product and process flowsheet simulation
- Optimization technology for reactor, process and materials design
- Shortcut modeling approaches
- Revamping options of commercial simulation and optimization
- Environmental process modeling

The model verification is generally a debugging activity; checking the model implementation, equations, code, etc., against the conceptual description of system. It gives confidence whether the model is well structured as per need and accurate representation of the conceptualization and save lot of time during implementation/validation. In order to avoid significant rework it is always recommendable to review the modeling methodology, assumptions and their justifications, sequential coding, suitable data for modelling and validation, etc., Before using the model or simulation for prediction model needs to be validated and it provide confidence that, the model is a reasonable representation of the actual system. At this stage, someone may need to fine-tune it with actual data, kinetic parameters, heat capacities, etc., In case of dynamic modelling, the actual data organization approaches initially via statistical parameter estimation and providing initialization for validation [2,5].

Chemical process modelling and simulation software's has been widely used by chemical engineers to design, test, optimize, and integrate reactors and/or process revamps. M. W. Kellogg Inc. (United States) in 1958 launched the first chemical process simulation program 'Flexible Flowsheeting' [1]. Today's chemical engineering is focused on, a) Increase productivity and selectivity through intensification of intelligent operations; b) multi scale approach to processes control; c) micro-tailoring with controlled structure; c) unique equipment design; d) process intensification; e) multiscale modelling and simulation to mimic real-system from molecular scale to the production scale. Many modeling tools are available for Process modeling and simulation, e.g., integrated Aspen Process Modelling (AspenPlus a process simulator, Aspen Custom Modeler, Aspen Dynamics, etc.), HYSYS, computer aided system (ICAS), gPROMS (process and reactor simulator), DynSim Dynamics, ChemCad, Design II, Pr-Sim, MATLAB, UniSim, computational fluid dynamics (CFD), respectively. These systems allow the conceptualization of the reactor or process by defining systems of balance volumes in the governing equations to describe the phenomena occurring within the system. Multiscale modeling poses many challenges and only few modelling platforms can handle such systems to enable integration frameworks [1-5]. There is diversity in approaches and tools used for modeling, somehow for their marketing justification, as most of the models are represented by a set of

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mathematical equations solved by similar numerical methods. The selection of numerical method depends on various factors, e.g., nature of the modelling equations being solved, desired accuracy, and computing speed/time. The summary of commonly used process modelling and simulation tools are as below:

Aspen Process Modelling is a general-purpose process simulation tool, integrated with properties databank to make accurate and reliable calculation of thermophysical properties, from AspenTech (USA) having number of modules for building large-scale flowsheets, economic analysis, reactor modelling, implement several operating procedure, perform detailed design studies, optimizing operation of individual equipment or complete process, etc., Where AspenPlus is commonly used for process flowsheet design, process and energy optimization, unit operations and reactor simulation, heat exchanger design software [8]. AspenDynamics has set of unit operations and control model library and user-oriented modeling capabilities for building dynamic simulations. AspenDynamics is mostly used for safety and controllability studies, sizing relief valves, optimizing transition, start-up, and shutdown policies, etc., It helps an engineer to estimate the relative costs of proposed designs and making decisions. Aspen Custom Modular (ACM) provides environment for building custom-based equation oriented modeling, and commonly used for reactor and other sophisticated equipment's modelling those, were not available in aspen library or available but not upto the desired sophistication level [6,7].

HYSYS was originally a product of Hyprotech (Canada) which was acquired by AspenTech in 2002. HYSYS is well-known in refinery and petrochemical process for its capabilities to perform, e.g., process safety analysis, preliminary cost estimation, control, equipment sizing and design, refinery flowsheeting, operational optimization of process bottlenecks, start-up procedures, and performing dynamic studies, etc., The built-in advanced sequential quadratic program (SQP) algorithm enables offline and online optimization of design and operation. Both Aspen Process Modular and AspenHYSYS are fully supported CAPE-OPEN compliant models.

gPROMS: A product of Process Systems Enterprise Ltd. (UK) which is characterized by the equation-based model building of any complex process and custom based equipment modelling. The tool is useful in novel technology developments, new process or equipment design having capabilities of experimental design, parameter estimation, statistical analysis, dynamic modeling, operators training, process control, safety analysis and advanced optimization. gPROMS language is a text-based powerful language, required proper description of chemical system similar to ACM, having number of solver options and has state-of-the-art model library.

Process Intensification designates the emerging techniques or equipment that can achieve significant improvement in productivity, savings in capital expenditure, energy efficiency and environmental friendliness of processes. Such as novel reactors, intensive mixing, heat transfer and mass-transfer devices, equipment size and cost reduction, safe operation, integration of reaction and separation steps in multifunctional reactors (examples: reactive distillation, membrane reactors, fuel cells), hybrid separations (example membrane distillation), alternative energy sources, and new operation modes (example periodic operations), etc. This enhances creativity and increases the number of attractive process alternatives. Creativity is a major issue in process design. In today's innovation of chemical process industries means to achieve highly efficient, economically competitive and sustainable design; and it can only be achieved using robust modelling and simulation tools [8]. In the end, an integrated conceptual design (process design) may reveal a simpler flowsheet with lower energy consumption and equipment costs, and further consists of an optimal combination of technical, economic, environmental and social aspects.

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