Editorial

Modeling, Simulation, Optimization in Process Design and Synthesis

Guest editor: Zdravko Kravanja

At the beginning of the new millennium the market is characterized by globalization of trade and increasing competition in general, while the community strives for sustainable development of chemical and bio-chemical industries in particular. Process synthesis is for this reason a paramount importance in the integrated Process System Engineering (PSE). Because it deals with integration of process units, material and energy streams into chemical plants, and chemical plants into networks, it is concerned primarily with a part of the overall chemical supply chain on a large scale (Grossmann and Westerberg, 2000).

In the last two decades important achievements occurred in the area of synthesis, design and optimization of process systems. Methods that were established in the area differ in the way of how straightforwardly they can be used to obtain the final design: either progressively or directly. Besides, they rely on different concepts: either on heuristics (intuition, engineering experience), thermodynamics (physical insight) or mathematical programming. It is apparent that the former heuristic concept is becoming more and more redundant and that efficient optimization methods, strategies and algorithms, presently available, enable us to solve a wide range of problems arising in chemical engineering. In principle, they rely on either of two extreme approaches, a sequential or a simultaneous one. The former follows the hierarchical strategy of process synthesis, e.g. Douglas (1988) and can be easily implemented by any flowsheet simulator. However, the sequential strategy does not account for interactions between subproblems (reaction paths, separations, and auxiliary operations) and, hence, gives rise to sub-optimal solutions. To account appropriately for all interactions, all subsystems have to be considered simultaneously, which gives rise to the simultaneous type of optimization, based on algorithmic method using mathematical programming approach, e.g. Biegler et al. (1997). It should be noted that besides very important feature – the optimality, the mathematical programming approach is equally important also, because it enables the engineers to meet feasibility and integrality of the solutions. The feasibility is achieved by imposing different constraints on the models and the integrality by enlarging the scope of process optimization models and criteria, e.g. by extending conventional economic criterion optimization to multi objective optimization including different operability issues such as feasibility, controllability, safety, minimization of environmental impact, etc. In the context of the simultaneous multi optimization approach there are, however, many difficulties, e.g. the mathematical representation may become too complex and the problem cannot be solved. The hierarchical multilevel mixed-integer nonlinear programming (MINLP) can serve to decompose the problem in the sequence of smaller subproblems that are easier to solve. Disjunctive modeling with convex hull formulation of logical decisions can be used to handle combinatorial discrete decisions in more robust way. Figure 1 shows the variety of model complexity ranging from a simple LP for nominal steady state continuous process optimization to a flexible, dynamical, multiperiod, entire life-cycle, hybrid plant network optimization. Unfortunately for end-users and fortunately for the research community the current solution techniques, strategies and concepts are still insufficient to solve such very complex problems. There is thus an incentive and a great challenge of the PSE community to develop further the existing theoretical and methodological framework. The extent of the implementation of integrated CAPE tools that would enable the engineers to solve ever more complex problems, will have the key impact on the success or failure of the future sustainable development in chemical and biochemical industries. Process of de-bottlenecking and intensification is just a smaller part of the needed breakthrough. It is evident that the process synthesis can solve the task only if it is linked integrally with other task of the chemical supply chain from the molecular modeling and chemical species identification, selection of reaction paths up to the large scale industrial enterprise networking.

The area of process design, synthesis and optimization is a very vital one and among the most successful areas in PSE. International journals and meetings, such as PSE, ESCAPE and FOCAPD, are receiving increasing number of contributions. The purpose of this special issue of Chemical and Biochemical Engineering Quarterly to contribute to the area is among them, also. The following invited papers reflect some important aspects of the current state-of-the-art in the field.

The first paper by *Vasic-Racki, Kragl and Liese* describes the importance and benefits of chemical kinetics modeling. Chemical reaction system is regarded as the heart of chemical or biochemical process. Therefore, modeling of reaction system is of the key importance and should be formulated in a rigorous way, in order, to preserve appropriately in the model the interactions between the reaction system and its background.

Equations	Linear	Nonlinear	Finite difference	Differential	Combination
Models, e.g.	Steady	state	Multiperiod	Dynamical	Integrated Hybrid
Examples, e.g.	Continuous	process	Life-cycle	Batch process	Plant networks
Certain variables			Nominal		
Continuous, *x*	LP	NLP	e.g.	e.g.	
Discrete, *y* 0-1	ILP	INLP			
Logical, *Y*	DisLP	DisNLP			
x, *y*	MILP	MINLP			
x, *Y*	MDisLP	MDisNLP			
Independent variable, *t*			Mul. MINLP	Dyn. MINLP	Mul. Dyn. MI(Dis)NLP
Uncertain parameters, θ		**Flexible**		e.g. Flexible	Mul. Dyn. MI(Dis)NLP

Notation: Dis-disjunctive, Dyn.-Dynamic, I-integer, L-linear, N-non, M-mixed, Mul.-multiperiod, P-programming

Fig. 1 – *Systematic nomenclature of mathematical programming*

In the second paper *Fermeglia, Pricl and Longo* give us a nice review of the state-of-the-art of molecular modeling applications ranging from engineering correlations and estimations, property prediction in development of new products, prediction of mixture properties, polymers, sorption thermodynamics and even nanotechnology, where molecular modeling is used as an alternative laboratory tool to run virtual experiments rather than to perform time and money expensive laboratory experiments.

Next paper by *Emtir, Mizsey, Rev and Fonyo* represents an example of integrated approach to the process synthesis. In particular, five different energy-integrated distillation schemes, two of them being heat-integrated, one fully thermally coupled Petlyuk column and the forward and backward heat integrated sloppy sequences, are simulated and optimized rigorously for the minimum total annual costs, and finally tested for controllability. The investigation shows that 37 % of the costs could be saved if the direct sequence with backward heat integration was selected rather than the conventional scheme. However, it shows worse controllability features. The example clearly indicates that controllability issues should be considered simultaneously with the selection of the appropriate heat-integrated configuration.

Next paper by *Eglue, Le Lann, Cabassud, Prat and Cezerac* describes the importance and advantages in the synthesis of fine chemical or pharmaceuticals of using simultaneous or global optimization approach vs. the sequential or dissociated one. Inherent interactions between subsystems can only be explored if different aspects of process synthesis are performed simultaneously, as a total system to assess the effects of the aspects on the overall performances. In their SQP application to a batch synthesis of a propylene glycol process they found 9 to 14 % of reduction in an operating time when compared to one of the sequential approach. The benefits comes from the appropriate consideration of interactions between the reaction and the separation subsystems resulting in a faster reaction and an earlier separation, which could not be gained if the sequential or dissociated approach was applied.

The paper by *Narodoslawsky* reviews new challenges for process integration, synthesis and sustainable development in a field of renewable resource utilizations. It is stated that process integration must be directed towards integration of reaction processes with other process steps, e.g. integration of biochemical reactions and storage steps like silage as in the Green Bio Refinery Concept, or integration of reaction and separation steps, e.g. in membrane reactors. Even more challenging than the integration is the need for revision of the current synthesis methods to be applied to process networks utilizing renewable raw materials in order to develop technologies adequate for decentralized raw material production, seasonal nature, high cost and complexity of raw material. It is claimed that the optimization based network synthesis is characterized with non-technical and non-economic multi objectives, especially with consideration of ecological sustainability issues. Case studies of the utilization of meat and bone meal and the Green Bio Refinery Concept serve to generalize the underlying ideas.

The paper by *Reneaume and Niclout* describes discrete and parameter optimization of plate fin heat exchanges. It is an example of performing rigorous synthesis of process equipments by detailed economic objective function and detailed MINLP model in order to increase the profitability of the equipment manufacture. Authors applied relaxed SQP, MINLP Simulated Annealing (SA) and MINLP Branch and Bound algorithms to solve different case studies, resulting to cost reduction from 14 to 21 %. The best solutions were usually achieved by SA, however, with the largest consumption of CPU time.

Another paper by *Vasquez-Alvarez and Pinto* describes a mixed-integer linear programming (MILP) model for the synthesis of protein purification processes, considering product loss, simultaneously with the optimization of the process rather than to assume the complete recovery of the protein. The objective is to calculate the minimum number of chromatographic steps at specified purity and amount of recovered proteins. The model formulation is based on a convex hull representation. Since the product is recovered in discrete percentage levels, the model is linear. Global optima solutions can thus be obtained and the appropriate trade-off between product purity and quantity, can be achieved.

The last paper by *Kravanja, Ir~iè-Bedenik and Pahor* is also devoted to discrete and parameter oprimization, now applied to the synthesis of reactor-separator networks. The synthesis step by MINLP is upgraded by the analysis step in an economic attainable region to verify the MINLP solution and to propose in the feedback loop, any profitable superstructure modifications for the next MINLP. The main motivation of using the combined MINLP/analysis approach is to overcome the drawback of the conventional superstructure approach, so the search for the optimal solution is within the reach of an abundance of proposed alternatives. The objective of the integrated synthesis is to obtain an appropriate trade-off between reaction selectivity and separation cost. It has been shown, that intermediate separation becomes attractive only when its costs are considerably smaller compared to the ones of the final separation.

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