Part-A. Process Modeling, Simulation, and Optimization

Process modeling clearly plays a central role in Process Systems Engineering as it provides a framework based on mathematical modeling for predicting and optimizing the performance of chemical process systems. As the reader will find out, most of the early work in process systems took place in the sub-area of process modeling. The core tool that has emerged from this area is process simulation, a tool that is widely used in the chemical industry. The Sequential Modular Simulator is one of the most pervasive technologies in the chemical processing industries with commercial penetration over 90%. It has also become a standard tool in the undergraduate and graduate curricula of chemical engineering education. While the early work focused on steady-state calculations, more recently it has expanded to include the dynamic calculations as well as the capability of performing optimizations. The 56 papers in this section received a total of 6,229 citations, that is, an average of 113 citations per paper, which is somewhat higher than the papers in the three other areas that are covered in the virtual issue.

We have organized the papers in Part-A. Process Modeling, Simulation, and Optimization in the following subsections:
- First Principles-Based Modeling and Simulation
- Empirical or Semi-Empirical Modeling
- Modeling Thermophysical Properties
- Numerical Methods for Steady State or Dynamic Simulation
- Optimization Algorithms and Applications
- Analysis of Process Behavior

The reader will find out from the papers in this section how the research in process modeling has evolved towards tackling larger and more complex problems. While one might be tempted to conclude that this area has become mature, we should note that the solution of nonlinear systems of equations, for the steady-state or dynamic assessment of process behavior, can still be very challenging and prone to failure. The same obviously applies when trying to perform optimization of these complex systems. Thus, the need for more robust and resilient numerical methods for simulation and optimization remains, and we hope that new ideas will emerge in the future that can build on the fine and strong tradition in this area of Process Systems Engineering, and take a quantum step further on several fronts, including: effective empirical modeling; multi-scale and multi-resolution modeling and simulation; computational processes-based (equation-free) modeling and simulation; more efficient methods for steady state or dynamic global and combinatorial optimization, and others.