Development of Advanced Polymerization Process Modeling, Simulation, Design and Optimization Tools Based on Interoperability Specifications

Krallis A., Kanellopoulos V., Chatzidoukas C., Pladis P., and Kiparissides C.

Department of Chemical Engineering and Chemical Process Engineering Research Institute,
Aristotle University of Thessaloniki P.O. Box 472, 54006 Thessaloniki, Greece

As the polymer industry becomes more global and competitive, pressures are intensifying. European polymer manufacturers recognize that computer modeling is a key enabling technology in dealing with their current urgent needs regarding environment protection, cost reduction, product quality improvement, reduction of the time-to-market for new products, improved safety, global operation and competition. In fact, many of the current decisions in industry, regarding process design and operation, are being determined by solving deterministic or statistic optimization models with the aid of generic platforms equipped with optimization algorithms and enabling model developments with a structural architecture.

The development of software packages for the simulation of industrial polymerization processes requires a Computer Aided Design (CAD) expertise as an added value to the mathematical models of process units and physical properties evaluation. This expertise encompasses a wide variety of interdisciplinary fields such as numerical analysis, for the solution of differential and algebraic equations, mathematical programming, for the solution of optimization problems and computer science, in order to carry out the model developments exploiting the computer-technology capabilities offered today. The latter might imply qualifications that range from hardware, languages (FORTRAN, C++) and operating systems knowledge, up to programming approaches (mathematical modeling) and software structure skills (modular, equation-based approach, object-oriented programming).

The software structuring expertise and the state-of-the-art problem solving tools, although they are available to the major software vendors, they are the weak point of the individual modeling experts in the diverse fields of polymer process engineering. Most early process simulators were equipped their own process models, physical properties calculations, solvers and software design methods. However, there are strong incentives for moving from the traditional stand-alone software applications, to the development of software components, so that complete interoperability between different components from different process simulation environments can be achieved.

Our scope is the development of software packages in which the design of industrial polymerization processes will be based on an object-oriented programming environment. Based on this object-oriented programming design and the Cape Open (CO) specifications, the various structural elements of the polymerization process (e.g., materials, chemistry, unit operations, etc.) which describe the phenomena occurring in the micro-, meso- and macro- scales (e.g., polymerization kinetics, diffusion phenomena, phase equilibrium, mass and energy balances, etc.), can interact with other CO-compliant objects from different process modeling environments. Furthermore, an object-oriented designed process unit (e.g., PVC batch suspension polymerization reactor, high-pressure PE tubular reactor, etc.), will be capable to be exported and plugged in another process simulation environment in which it can be connected with other upstream and downstream equipment based on well-defined interfaces.