CHAPTER II

SIMULATION

Simulation has been defined as the process of developing a computerized model of a system(or process) and conducting experiments with this model for the purpose of either understanding the behavior of the system or evaluating strategies for the operation of the system[1]. In the chemical process industries (CPI), engineers use a process simulator (software package) as a tool to deal with a process at all of its life cycle, from synthesis to design, construction, startup, modification and retirement (Figure 2.1) [2]. By performing flowsheeting calculation on a computer, manpower and design costs can be saved. Process modeling reduces the cycle time for new-process development by identifying problems and opportunities in the early stages of research, and spot operability problems due to equipment malfunction and to debottleneck a process. Therefore, simulation is the use of one system to imitate the actions of another for design of new operations, revamps of existing operations, analysis and improvement of current operation, troubleshooting plant operation and training engineers and operators[3].

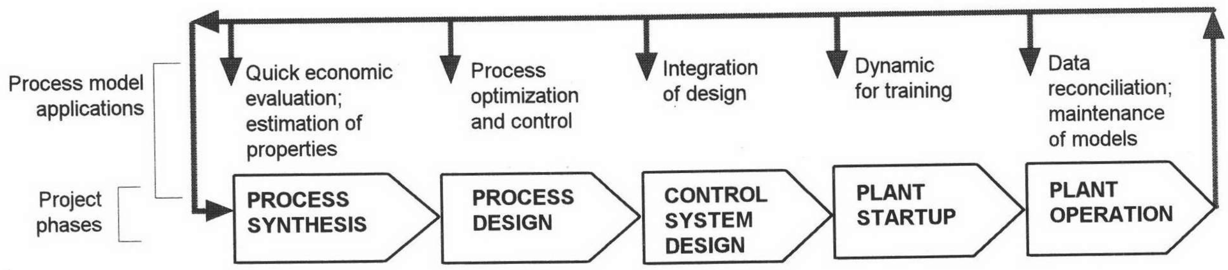

Figure 2.1 Process model application for chemical process[2].

The mathematical model being the heart of simulator divides simulators into two types as dynamic and steady-state simulators[1]. Steady-state simulators -- time independence -- are generally modeled as sets of algebraic equations, so they are easier to be solved than dynamic simulators. Three approaches employed in simulators are sequential modular, equation-oriented and simultaneous modular approaches[4]. Sequential modular approach calculates unit operations in intact modules as sequentially as the actual process flow. Each module simulates one type of unit operation, for instance, the heat exchanger module for modeling only heat exchanger, and a large flowsheet could be constructed simply by combining modules. Figure 2.2 shows a simplified structure for sequential modular simulators. At the top level, the executive program accepts input data, determines the flowsheet topology, and derives and controls the calculation sequence for the unit operations in the flowsheet. The executive then passes control to the unit operations level for execution of each module. Finally, the executive and unit operations levels make frequent calls to the physical property level for routine tasks such as enthalpy calculations and calculation of phase equilibrium and other stream properties. Although this approach is not suitable for solving the recycle structure of the flowsheet and external design specifications which create awkward iteration loops in the calculation sequence, it is usually used in the popular current commercial simulators such as PRO/II(used in this work), ASPEN PLUS, HYSIM, and DESIGN II.

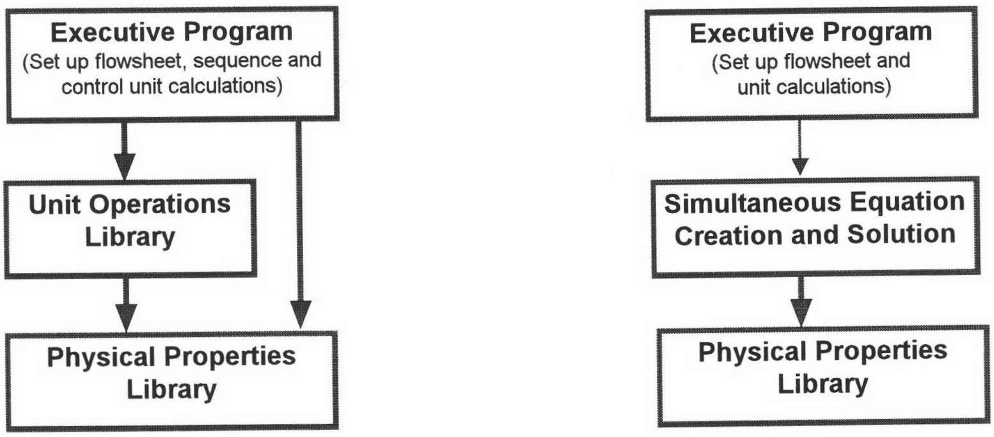

Figure 2.2 Structure of process simulators. Left, sequential modular architecture; right, equation-oriented architecture[4].

For equation-oriented approach, process equations are treated by a general purpose solution strategies (e.g., Newton-Raphson) and often solved simultaneously. As seen in Figure 2, the executive performs a slightly different function in that it organizes the equations and controls the general purpose equation solver. With nested recycle loops and additional "design" constraints at the flowsheet level, the equation-oriented simulators are much more flexible in terms of solving problems. They also allow the application of much more sophisticated optimization strategies. However, this approach is limited by capabilities of the equation solver. Equation-oriented flowsheeting problems require large-scale numerical algorithm, good initialization strategies, and reliable options to prevent convergence failure. This tendency to fail is aggravated by a set of nonlinear physical property equations. To overcome this problem, equation-oriented simulators have been modified to incorporate low-level modules for calculating nonlinear physical properties similar to sequential modular systems. Examples of equation-oriented simulators are SPEEDUP, ASCEND, and QUASILIN.

Simultaneous modular methods are developed from sequential modular approach where unit operations modules, for the most part, remain intact but stream connections(at the flowsheet topology level) are solved simultaneously. In this manner, complicated recycles and flowsheet constraints could be solved together. This development is aids for simultaneous modular methods by application of Broyden-type method, having a much faster convergence rate than sequential modular recycle algorithms. Examples of simultaneous modular simulators include FLOWPACK and MPFPL.

Dynamic simulators -- time dependence -- require an exercise of the system mathematical models as the solutions of sets of differential equations or their equivalents in finite difference equations, matrix equations or statistical expressions. They are suitable to improve safety and control features, engineer debottleneckings and startups, and train plant operators for emergency response[5]. However, they require more time and higher computer-power than steady-state simulators. The commercial dynamic simulators are, for example, SPEEDUP(can perform steady-state as well as dynamic simulation), PROTISS, OTISS, and OPTISM[6].