

### **37c Development of Mrdsim, Multiphase Reactor Design Simulator**

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The reactor is the heart of a chemical process. Therefore, it is crucial to know and apply the key concepts such as selection, scale-up and proper design of chemical reactors to maximize the process efficiency. Development of educational software-based simulation packages that can be friendly used by engineers, operators and students are needed to illustrate the key concepts in reactor design and operation. In the poster, we will present our efforts to develop educational user-friendly software-based simulation packages for various types of multiphase reactors. The simulation package guides the user through the key concepts needed in the reactor design. It allows the user to examine quickly the effect of operating and design variables and to identify which are the important parameters affecting the reactor performance. The role of mass transfer parameters is also included in the simulation. The packages are system specific and are expected to cover a wide range of commercially important processes. The first simulation package focuses on the modeling of liquid-solid circulating reactor for solid catalyzed alkylation processes. Much research has been devoted to study the alkylation processes using acid based solid catalyst as they are environmentally benign in order to avoid the use of HF and other liquid phase catalysts reducing the wastewater generated. The simulation package covers key factors in the reactor design. Simulation platform is designed for Windows using Excel Visual Basic (for the user interface) and Fortran (for the simulator). The user starts the simulation by specifying several parameters needed in the reactor design calculations. Once all the needed parameters are specified, the user starts the simulator to solve the 1D axial dispersion model or the core-annulus model to get conversion, selectivity and catalyst deactivation. The concentration and catalyst deactivation plots as a function of dimensionless bed length are also provided. Since this module is for educational purposes, a detailed explanation of the parameters is also provided. A second simulation package for methanol synthesis in a three-phase slurry reactor is in progress. It is hoped that these packages would be used as a supplementary material in undergraduate senior level reaction engineering courses.