USER FRIENDLY MODULES FOR MULTIPHASE REACTORS MODELING

I-36. Developing User Friendly Modules for Modeling Multiphase Reactors

A. Problem Definition

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. Educational user-friendly software-based simulation packages that can be used by engineers, operators and students are important tools to illustrate the key concepts in reactor design and operation.

B. Research Objectives

The goal of this project is to develop educational user-friendly software-based simulation packages for multiphase reactors. The simulation package is designed to deliver the key concepts of reactor design for a diverse background of potential users both in terms of discipline and experience.

C. Research Accomplishment

Last year, we worked on developing two simulation packages that focused on the modeling of liquid-solid circulating reactors: One for the modeling of liquid-solid circulating reactor for solid catalyzed alkylation process and the other for the modeling of trickle bed reactor for phenol oxidation. The simulation packages cover key factors in the reactor design. The simulation platforms are designed for Windows using Excel Visual Basic (for the user interface) and Fortran (for the simulator). The first step in both of the simulations is to specify several parameters needed in the reactor design calculations. These parameters include *reactor parameters* such as diameter and length, *operating parameters* such as liquid and solid flow rates, *catalyst parameters* such as catalyst diameter and density, *transport parameters* such as solid-liquid mass transfer coefficients and *kinetic parameters*. Figure 1 illustrates the parameters to be specified by the user for the alkylation simulation. Figure 2 shows the individual parameters. Once all the needed parameters are specified, the user starts the simulator to solve the 1D axial dispersion model to get conversion, selectivity and catalyst deactivation. The concentration and catalyst deactivation plots as a function of dimensionless bed length are also provided. Figure 3 shows an example of the output page. Since this module is for educational purposes, a detailed explanation of the parameters is also provided.

Our recent work involves improving the user interface and further developing the simulation packages to cover more reactor types.

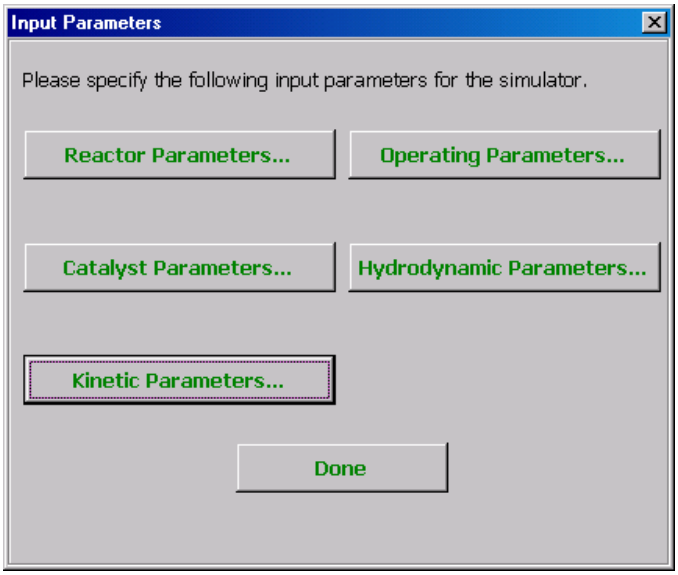
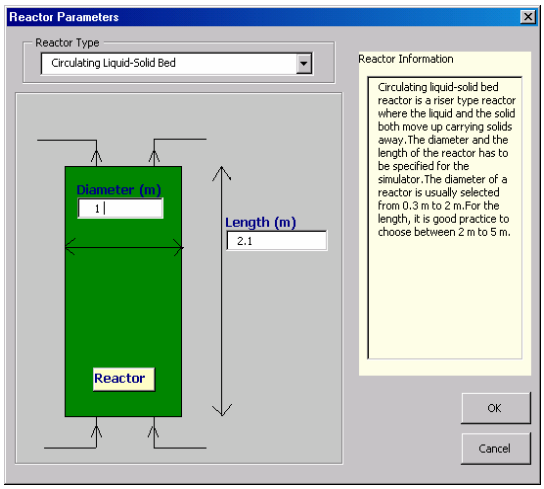


Figure1. Input parameters to the software.



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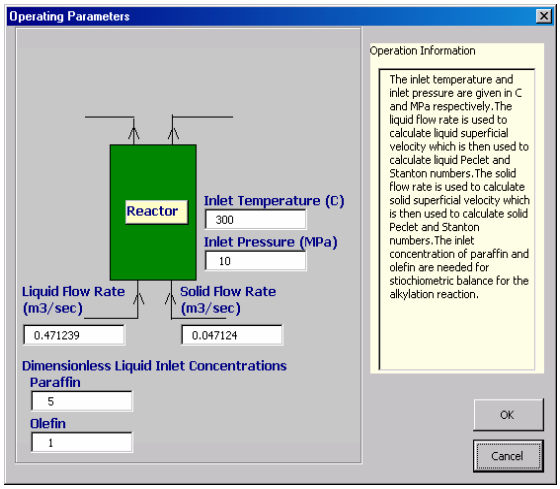

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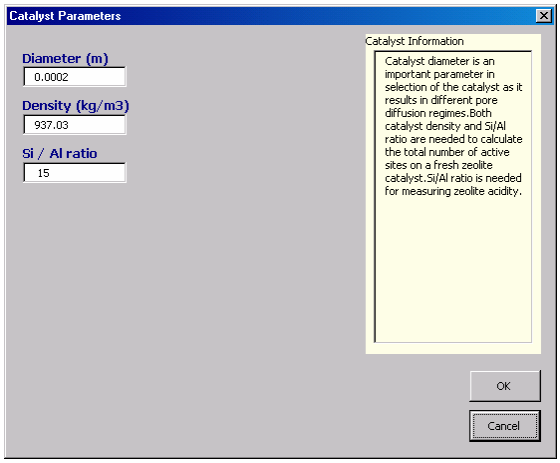

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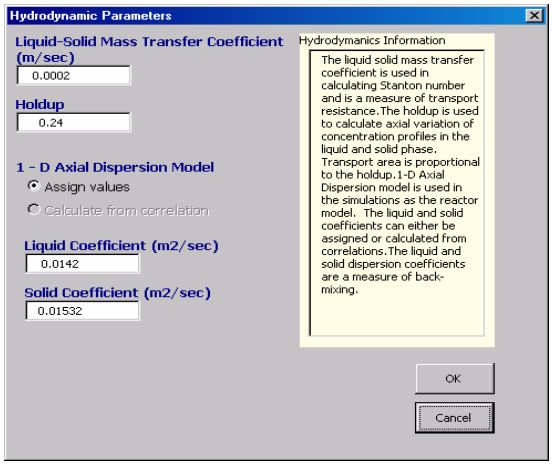

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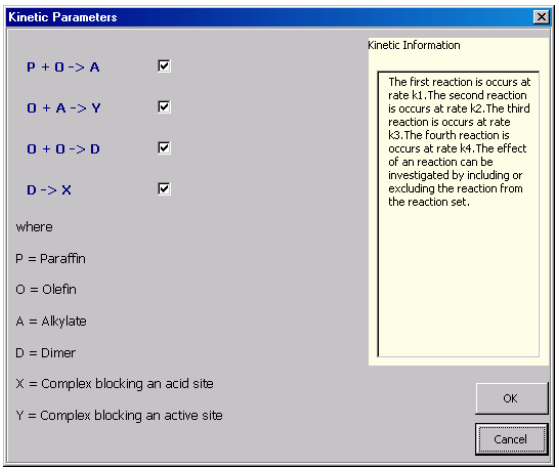
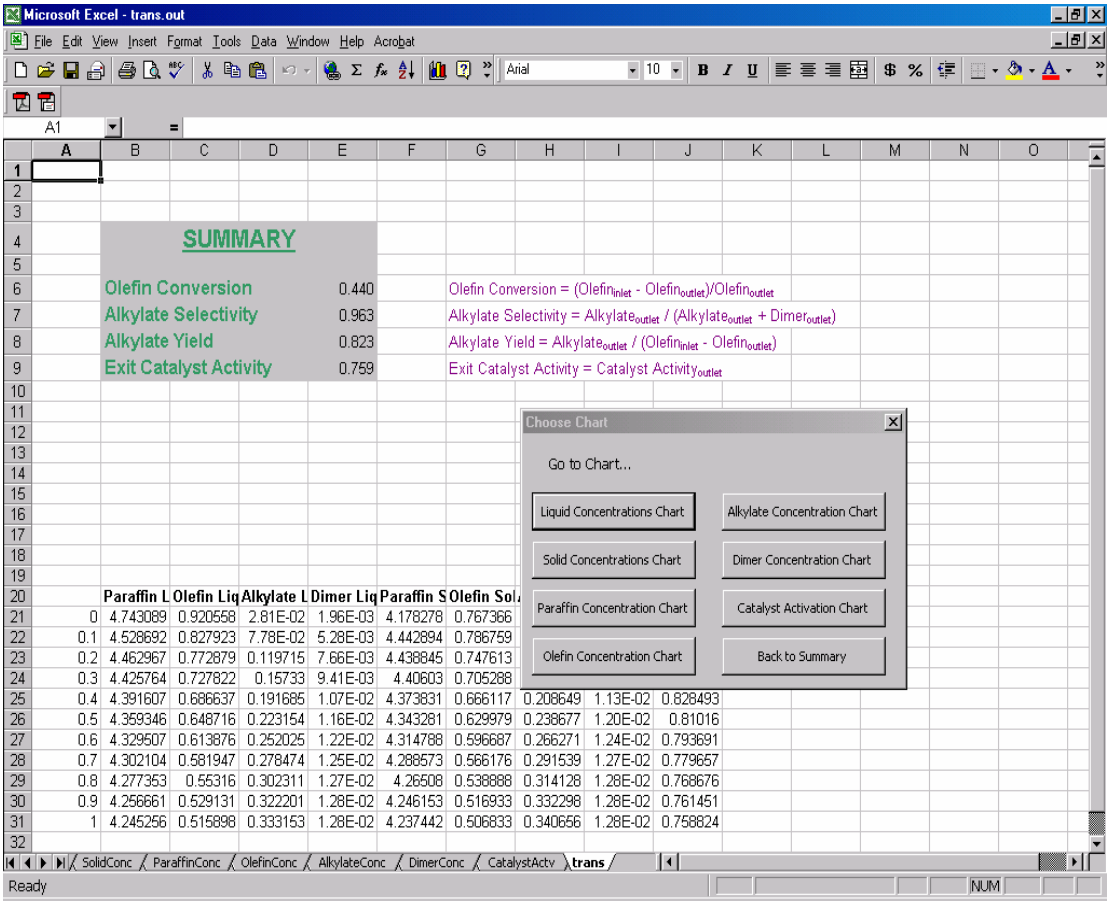
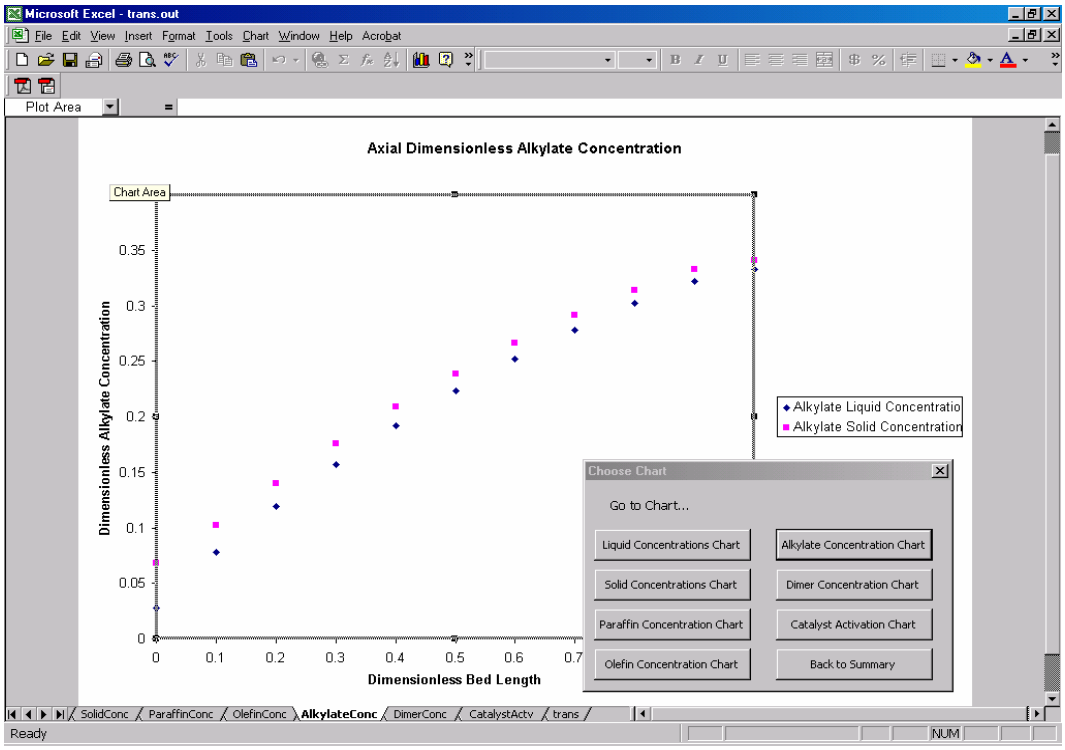


(e)

Figure 2. Individual parameters needed for reactor design. (a) Reactor parameters (b) Operating parameters (c) Catalyst parameters (d) Hydrodynamic parameters (e) Kinetic parameters.



(a)



(b)

Figure 3. Excel Results. (a) The summary is provided with charts. (b) Axial dimensionless alkylate concentration vs. dimensionless bed length chart.

D. Future Work

1. The software will be developed further to include different reactor types and processes.
2. The software will also be made available to CREL sponsors.

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