USER FRIENDLY MODULES FOR MULTIPHASE REACTORS MODELING

I-34. Developing User Friendly Modules for Modeling Multiphase Reactors

A. Problem Definition

Multiphase reactors are commonly employed in a variety of process industries. The reactor acts as the heart of a chemical process. Therefore, it is of utmost importance to understand and apply the key fundamental multiscale concepts in the selection, scale-up and proper design of chemical reactors to maximize process efficiency. Educational user-friendly software-based simulation packages that can be used by engineers, operators and students are important tools for illustrating and implementing the key concepts in reactor design and operation.

B. Objectives

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

C. Accomplishments and Current Work

Trickle-bed reactors are multiphase reactors that are commonly used in the petroleum and chemical industry. In this project, a user-friendly simulation package for trickle-bed reactors has been developed. The simulation package covers the key factors used in reactor design. The simulation platforms are designed for Windows using Excel Visual Basic (for the user interface) and Fortran (for the simulator). Several parameters that are needed in the reactor design calculations including reactor, operating and catalyst parameters are to be entered by the user. Figure 1 shows an example the individual entry parameters for the reactor and the catalyst. Once all the needed parameters are specified, the user can then execute the Fortran code to obtain the results. After the execution of the Fortran code, the user can view the results in a separate Excel file. Since this module is for educational purposes, a detailed explanation of the parameters is also provided.

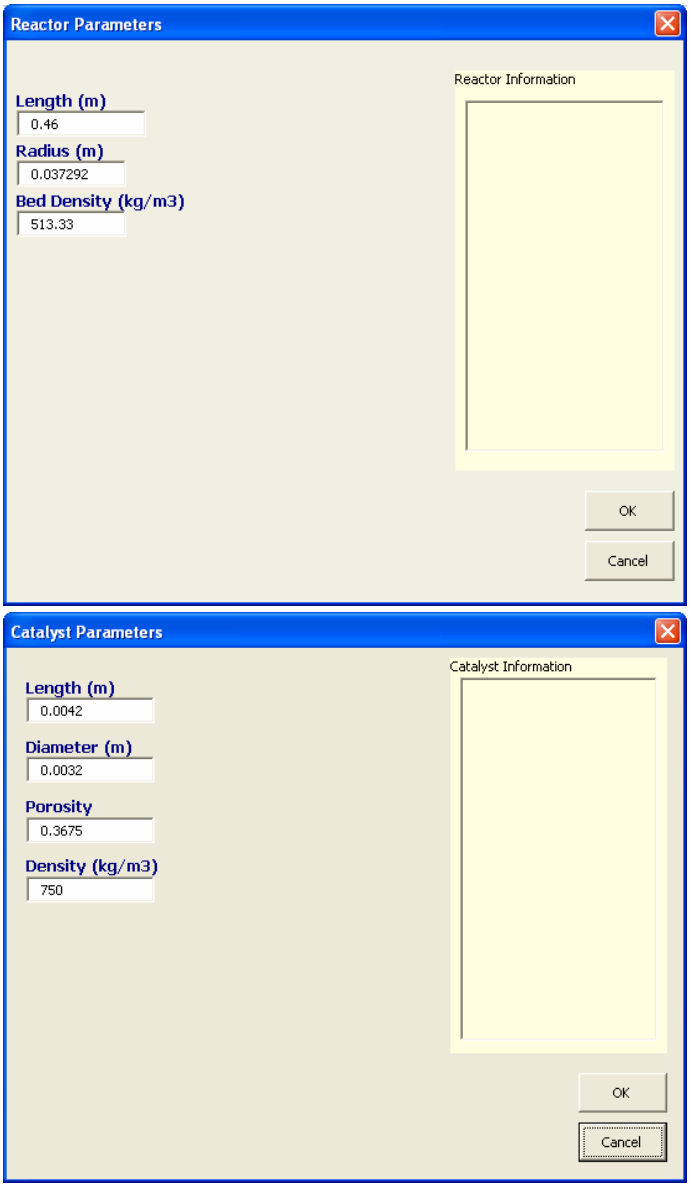

Figure 1: Individual parameters needed for reactor design. (a) Reactor parameters (b) Catalyst parameters

D. Future Work and Milestones

The simulation package is right now written for phenol oxidation in TBR. The objective is to develop the simulation package to cover different chemical processes in a TBR by Fall 2006.

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E. Acknowledgements

We would like to thank CEBC and CREL for their support that allowed us to develop the simulation package.

III-1. WASHINGTON UNIVERSITY REACTOR AND PLANT PROCESS CONTROL (Gregory K. McMillan, Retired Solutia Senior Fellow)

A HYSYS plant dynamic model of the reactor and control system has been installed and is available for simulation of desired processes. Automated Pseudo Random Binary Sequence (PRBS) tests are conducted to determine the dynamic relationships between key measurements and model parameters such as heat transfer and reaction rate coefficients. The experimental models from the PRBS tests are used by a Model Predictive Controller to adapt HYSIS model parameters so that HYSYS model outputs match plant data. The adapted dynamic HYSYS model becomes part of a virtual plant that has a complete working copy of the basic control system. Built-in tools in the virtual plant for automatic controller tuning and performance monitoring are then used to benchmark and improve the performance of the basic control system. Once this foundation is set, advanced control tools for property estimators and model predictive control are prototyped and layered on top. Equations are developed to calculate the benefits online for improvements made for reactor control. The HYSYS model is also used for Real Time Optimization. The result is a live “before” and “after” evaluation of basic and advanced control systems for various conditions and objectives.

Additional improvements to our virtual and actual control laboratory via introduction of Emerson Delta-V Pro systems will soon be described to interested sponsors.