Summary: From beginning to end, and beyond

The progression through the course has followed a fairly typical reactor selection and design procedure The procedure started with the assembly of the thermodynamic and physical property information needed for the reaction system. Then the reaction equilibria were examined. If the equilibrium constraint is significant, an equilibrium curve was developed and adiabatic operation with multiple beds was examined. Reaction rate contours were also plotted, showing a desirable temperature for tubular reactor operation. Even if equilibrium is significant, the reactor must also be sized, which requires a kinetic model. Thus, kinetic models were discussed next, resulting in the recommendation for developing the kinetic model in a Berty type reactor using the commercial catalyst.

With the kinetic model, a pseudohomogeneous temperature model was used to examine an adiabatic bed for a gas system. A preferred approach would be to use the universal fixed bed model in adiabatic mode. This model calculates both the fluid and the catalyst temperature. If the heat of reaction is too high, the adiabatic bed will have an extreme temperature rise near the exit. This led to the tubular reactor mode in the universal fixed bed model. Continuing with the gas reaction system, a dynamic model was used to explore startup and sensitivity to changes in feed temperature.

For the liquid system, a steady state CSTR model examined optimal operation and exposed the multiple solution problem. A dynamic model of the CSTR showed the desired operating condition could be reached, but the inclusion of inerts was recommended to avoid the huge changes in temperature that would result if operation variations caused the temperature to jump to another steady state. An adiabatic reactor for this reaction system was examined and it too showed extreme sensitivity to temperature. Although not examined in the book, a cooled tubular reactor is a possible choice for this system if the use of inerts in the CSTR or fixed bed is too expensive.

The end of this course is just the beginning for you, the reader. If you have Mathcad, you now have templates for all of these models plus a start at integrating the models into a design procedure. Change the data and you have a new model/design. If you do not wish to use Mathcad, the model equations may be converted to other languages. For all members of the process development team, the Scale Down approach to process development was presented. Aside from the scaling issues involved in this method, the key feature was early identification of the economical commercial design. With the economic justification for target conversion and selectivity, the reactor design engineer could make design decisions without having to calculate economics, or guess at the optimum. The catalyst developer and reactor engineer also could determine if the catalyst needs improvement. And, with an understanding of scaling relationships and a reactor model, the pilot plant can be designed to maximize the likelihood of success at the commercial stage.

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