Advanced Chemical Reactor Modeling (with Mathcad®)
Single Phase Fluid

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Preface

This course was written to demonstrate reactor models for industrial use, primarily for conceptual design. I, like most graduates, received a sound introduction to reactor modeling as both an undergraduate and as a post graduate. However, when faced with an industrial reaction system involving many species and several reactions taking place in a heated, tubular reactor, I soon realized that my introduction to reactor design was just that...only an introduction. I then "discovered" the advantages of (1) vector/matrix methods using the stoichiometric matrix and (2) the use of mass fractions for state variables instead of the more common choices. And, after studying numerous numerical analysis books, I finally chose a numerical method for the tubular reactor model.

The stoichiometric matrix and the use of mass fractions as state variables are not new concepts, but most textbooks on reactor design and modeling do not emphasize their advantages. Instead, many textbooks, even those advertised as advanced, continue to use named concentrations in their examples instead of using vectors and vector functions. Also, the textbooks often show models using a variety of dependent variables, including molar fluxes, molar concentrations, mole fractions, extents of reactions, and mass fractions. In this book, all models use mass fractions. That allows the engineer to supply just one function for the reaction rate expressions. This unified approach makes it easy for the design engineer to explore different reactor types.

A reactor design textbook has a lot of material to cover and therefore the numerical methods needed to solve the reactor models are usually not included. In recent years, the authors of reactor design texts probably assume that the reader will use a "canned" integration routine. That works well for the adiabatic fixed bed reactor and for a dynamic continuous stirred tank reactor (CSTR). I have included examples of models for those reactors using a Mathcad integration routine. Canned routines are not easy to find for solving systems of partial differential equations (PDEs) written in vector notation, and with nonlinear constraints. An orthogonal collocation method is used for the steady state PDE models in this course. For the dynamic PDE models, the hopscotch method is used. The models in the course can be written in a language other than Mathcad if the reader wishes. The main requirement is a robust root finding routine.

This course is not intended to be a complete reactor design reference. There are several books [e.g. Rase (1977 and 1990), Froment and Bischoff (1990), and Rose (1981)] that superbly cover most of the issues needed regarding reactor design. The worksheets in this book, however, do show how the models can be used in the reactor selection process. These worksheets, which require very little changes to examine a new reaction system, can serve as templates for both the execution and documentation of the reactor selection process.

I am indebted to the professors that provided my introduction to reactor modeling. I hope they, and you, find this monograph on reactor modeling in an industrial environment worthy of their legacy.

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