Chapter 1. Introduction

1.1 Objectives:

1. Provide the equations needed to model the common reactor types for a single phase fluid, including non-adiabatic tubular reactors.
2. Provide examples of the program structure and numerical methods needed to solve the model equations.
3. Provide a practical framework for developing a commercial reactor design based on laboratory and pilot plant experimental programs.

The focus of this course is on the modeling of reactors for design. This course may be used as a supplement for a graduate level course in advanced reactor design. Recent graduates working in industry may also discover that their reactor modeling needs go beyond the introductory course they took as an undergraduate. This course is designed for their self study.

There are several books that address advanced reactor modeling and design. The author believes that the approach presented in this course is unique in several ways. The remainder of this introduction addresses both the uniqueness and the questions the reader may have regarding the course.

1.2 Questions regarding the book

How is this course different from most reactor engineering books?

A 1: The mathematical structure and programming methods will encourage model reuse.

Introductory reactor books deal with simple reaction systems, so the examples, including program codes, invariably are specific to one problem. In those books, the variables (concentrations, heats of reaction, heat capacities) are all uniquely named (e.g. C_A, Cp_A). The stoichiometric coefficients of each species appear explicitly in the equations instead of using a stoichiometric matrix. Solving a design with a different reaction system would require a complete re-write of the program. The methods used in introductory books are convenient for illustration, but they do not demonstrate the programming practices needed by the industrial reactor design engineer.

In this book, all programs are written in a more generic manner, using vectors, matrices, and linear algebra. Thus, a well validated and proven program can easily be modified and reused for other designs. The minimal knowledge of linear algebra needed will be covered in Appendix 2.

A 2: This course does not cover the development of reaction mechanisms.

Often the reaction mechanism has been determined by the catalyst developer before the reactor engineer becomes involved. If needed, the reader may consult other texts.

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A 3: Multiple reactions will be the norm.

Multiple reactions commonly occur in industrial reactors, particularly in the petroleum and biochemical industry. A systematic method of modeling these systems will be provided.

A 5: All reactor models that include differential equations will be developed using mass fractions.

The advantages of mass fractions over concentrations, mole fractions, molar fluxes, and extents of reaction will be presented. However, extents of reaction are convenient for equilibrium models, particularly for single reaction systems, as demonstrated in Example 3.

A 6: Molar change in the reactor will be followed using molecular weight and density.

Many texts use extents of reaction to follow molar change and its effect on gas velocity. The approach used in this course eliminates the need for extents of reaction in non-equilbrium models. The approach is valid for single and multiple reactions and all types of reactors, including reactors with side feeds or effluents and for both steady state and dynamic models. This approach provides a more unified basis for the model equations for the various reactor types.

A 7: Effectiveness factors will not be used in the models.

An alternative approach will be recommended for developing kinetic models without effectiveness factors. If effectiveness factors have been determined by the modeler, they may be easily incorporated in the models.

A 8: Tubular reactors will be covered in more detail than in introductory books.

The need for using two dimensional (2D) models instead of one dimensional (1D) models for tubular reactors will be justified by example. A robust numerical integration method for up to 2D dynamic systems will be demonstrated. Recommendations for correlations for the transport parameters in the models are provided in the examples.

Is a Mathcad license required to follow the book?

No. All text and examples are provided in a .pdf format for those without a Mathcad license.

Is knowledge of the Mathcad language required to comprehend the book?

No. Mathcad uses very little syntax beyond normal mathematical symbols. Appendix 1 shows the syntax for readers without Mathcad. It also is a mini tutorial for those new to Mathcad. A few Mathcad routines are used, such as an integration routine. The arguments for those routines are described where used. Appendix 2 is provided for readers who desire a refresher or introduction to linear algebra.

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Can another programming language be used for the design models?

Yes. All of the recommended forms of the material and energy balances can be programmed in other computer languages. The languages that allow user defined functions will make the translation easier for some of the models.

Mathcad can make some tasks much easier than other programs. For example, the exploration of multiple steady states in a continuous stirred tank reactor (CSTR), the development of equilibrium curves, and the examination of staged reactors are easily accomplished using some Mathcad features. These features include the parametric solutions of systems of equations, optimization, and interactive, rapid 2D and 3D graphing methods. Mathcad also automatically performs unit conversions. If the models are to be converted to another language without unit handling capability, a consistent set of units should be chosen.

Can a process simulation program be used instead of the models in the examples?

Process simulation programs often have limited reactor modules with only ideal reactors, no 2D models. Also, Mathcad allows the engineer to integrate other calculations with the reactor model, such as the calculation of catalyst decay. The integration of the models with other calculations allows the design engineer to develop templates for routine workflow tasks.

The models developed in this course will be used along with process simulation programs during the development of a new process design. The integration of these programs will be discussed in Ch. 2.

Are CFD models included?

No. Computational fluid dynamics (CFD) programs are invaluable for problems where the geometry or dispersed phases make the flow "irregular" (i.e. not simple). For the types of problems considered in this book, CFD would be "overkill", and in most cases would not provide any additional information or accuracy. For example, CFD programs would require user input of the same dispersion parameters used in the models in the course because the fluid flow is normally not modeled at the catalyst particle level for a CFD reactor model. Even if modeling at the particle level were feasible, the stochastic nature of the particle shapes and orientation would probably not be easy to simulate so the results may not represent the real system well.

Another disadvantage of CFD programs is that they are difficult to integrate into other design calculations. The steady state models developed in the examples in this course are very fast, allowing quick case studies that can be integrated easily into a design workflow process.

In some cases, a CFD program may be useful. First, the CFD program may be used to determine the reactor geometry (reactor, spargers, inlet size and location, etc.) that produces the closest approach to ideal flow patterns (plug flow or well mixed). Second, the CFD program may be used to determine liquid and gas holdup in a gas/liquid system. This information could then be used in a non-CFD reactor model.

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Some CFD programs include reaction capability, but the implementation may not be what you expect or need. The CFD program may only allow a very limited number of options for the rate expressions. Also, the reactions may be allowed to take place in the fluid only, so the model must be pseudohomogeneous with respect to the catalyst and fluid temperatures.

1.3 More about this course.

The course is formatted for printing on 8.5" x 11" paper in landscape orientation with 0.5" margins. This orientation was chosen for two reasons. First, most readers will be using a computer rather than a printed copy of the book. The aspect ratio of most computer monitors is more compatible with landscape orientation than with portrait. Second, the added page width allows longer equations to be shown in the pdf version.

The examples are much more than numerical computations, they are an extension of the main text. Some examples include derivations not found in the main text. Most of the "how to" information is included in the examples. All but one of the examples appear in separate files. This separation eliminates complete recalculation of all of the examples in the main text. Also, the separation makes it easy to reuse the worksheets for your own application. The main text (i.e. this file), in addition to deriving the model equations, discusses the models in the context of design and their use in the progression through the development of a process.

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