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Book review

CHEMICAL REACTOR DESIGN AND CONTROL

William L. Luyben

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The book *Chemical Reactor Design and Control* is based on the experience of author William L. Luyben, who is a professor of chemical engineering at Lehigh University, and who has also gained rich experience as an engineer with Exxon and DuPont. The great variety of chemical reactions leads to a great variety of chemical reactors with various configurations, operating conditions, sizes.

As a result of this, the book offers along 8 chapters a wide spectrum of information concerning reactor basics, as well as design and control of CSTR, tubular and batch reactors. Several types of heat transfer to or from the reactor vessel are presented.

Chapter 1, *Reactor Basics*, reviews some aspects concerning the fundamentals of kinetics and reaction equilibrium (power-law kinetics, heterogeneous reaction kinetics, biochemical reaction kinetics), together with the effects of temperature on rate and equilibruim for different types of reactions, particularized through several examples.

Multiple reactions are also discussed, given that they have a major impact on the design of the entire process. In order to supress undesirable side-reactions, it is often necessary to operate the reactor with a low concentration of one of the reactants and an excess of other reactants which have to be recovered in a separation section and then recycled back to the reaction section. Parallel reactions, series reactions are analyzed briefly, in order to allow further discussions on the possibilities to determine the kinetic parameters of the chemical reactions.

The classical types of reactors are discussed in a qualitative way, pointing out the features of a batch, continuous stirred-tank reactor (CSTR) and plug-flow reactor (PFR), as idealizations of real industrial reactors.

An important feature highlighted in this chapter is the that batch and CSTR reactors can be cooled or heated in a variety of ways, which accounts in part for their superior controllability compared to tubular reactors. Many tubular reactors are operated adiabatically, because of the problems in providing heat transfer. The author also writes about one of the most challenging aspects of chemical engineering: the problem of scaling up a process unit from a small laboratory or pilot plant to a large commercial size, the reactors being one of the more difficult systems to deal with.

Chapter 2, *Steady-state Design of CSTR Systems* studies the steady-state design of perfectly mixed continuously operating liquid-phase reactors, which can provide valuable information which gives reasonably reliable indications of how effectively the reactor can be dynamically controlled. The contents of the chapter include analyses of several important types of reactions and the equations describing each of these systems.

Matlab programs are used for hypothetical chemical examples, while the commercial software Aspen Plus is used for real chemical examples. The following types of reactions are analyzed: irreversible, single reactant; irreversible, two reactants; reversible exothermic reactions; consecutive reactions; simultaneous reactions, in a single unit or multiple CSTRs (multiple isothermal CSTRs in series with single reactions; multiple CSTRs in series with different temperatures; multiple CSRTs in parallel; multiple CSTRs with reversible exothermic reactions).

Chapter 3, *Control of CSTR Systems*, deals with steady-state designs of a vareity of CSTR systems previously discussed in Chapter 2, but with additionally including their dyanmics and control. There are quantitatively explored the effects of reaction types, kinetics, design parameters and heat removal schemes on system controllability. The first studied system is a CSTR with jacket cooling where a first-order irreversible reaction takes place. A non-linear dynamic model of the reactor jacket, with four non-linear ordinary differential equations is examined.

Also, the effects of various parameters on a linearized version of the system equations are investigated. The linear model allows the use of all the linear analysis tools available to the process control engineering. In order to demonstrate the superior dynamic controllability of high-conversion and low-temperature designs, the non-linear differential equations are numerically integrated. Disturbances in feed flow rate temperature controller set point, and overall heat transfer coefficient are made, and the peak deviations in reactor temperature are compared.

Moreover, the dynamics and control of the previously studied reactor column are investigated using a non-linear dynamic model of reactor and column. Besides, the steady-state design of an auto-refrigerated reactor system and dynamics and control of this process are considered.

The use of feed manipulation for reactor temperature control is considered a control scheme which has the potential to achieve the highest possible production rate. The simulation of CSTRs is carried out with the aid of ASPEN dynamic simulation.

Chapter 4, *Control of Batch Reactors*, analyzes the batch chemical reactor, widely used by chemists in laboratory studies of the chemistry of various systems. The surface to volume area is very large, thus heat transfer is very good. At the beginning of the chemical industry, most commercial reactors were batch, as simply large versions of the chemists' laboratory apparatus. Because batch reactors have very important inherent kinetic advantages for some reaction systems, they continue to be fairly widely used, even when production rates are high (polymerization, fermentation). Batch reactors are also frequently used in situations where production rates are low, such as specialty chemicals, because they are quite flexible and can be used to produce a number of different products under a variety of conditions in the same vessel. The design and control problems for batch reactors are more difficult than for CSTRs, because of the time-varying nature of the batch process. The typical design problem is to be given a desired annual production rate. The system is non-linear and the control system must be capable of handling this non-linearity. The optimal operation of a batch reactor is with irreversible single-reactant reactions. The temperature could be increased to its maximum value as quickly as possible, which can give the maximum reaction rate and therefore the shortest batch time.

Batch reactors with two reactants can operate quite similarly to the previous case. If consecutive reactions are conducted in a batch reactor, the optimization of the process aims at finding the optimal time to stop the batch, and determining the optimal temperature.

The simulation of this type of reactor is also performed using ASPEN Plus. Some examples of simulation are provided: ethanol batch fermentor, fed batch hydrogenation reactor, batch tetramethyl led reactor, fed batch reactor with multiple reactions.

Chapter 5, *Steady-State Design of Tubular Reactor Systems* discusses about the tubular or plug flow reactor, which is characterized by the change of variables with axial and radial position. The fundamental differences between CSTRs and tubular reactors are highlighted, and include: the variation in properties with axial position down the length of the reactor; the dynamic response to disturbances or changes in manipulated variables, i.e. while in a perfectly mixed CSTR, a change in an input variable has an immediate effect on variables in the reactor, in a tubular one it takes time for the disturbance to work its way through the reactor to the exit; it is mechanically very difficult to achieve independent heat transfer at various axial positions, because the only two variables which can be manipulated are the flow rate of the medium and its inlet temperature; the feed temperature is a very important design and control variable, unlike the CSTR, where the feed temperature has little effect; unlike the CSTR, which has essentially no pressure drop, a tubular reactor can have a very substantial pressure drop, which can be important in the gas phase systems with gas recycle.

Several types of tubular reactor systems are analyzed: adiabatic plug flow reactor (PFR), such as single adiabatic tubular reactor systems with gas recycle, multiple adiabatic tubular reactor with interstage cooling, multiple adibatic tubular reactor with cold-shot cooling, cooled reactor systems non-adiabatic PFR.

Chapter 6, *Control of Tubular Reactor Systems*, investigates the dynamic controllability of PFR. Four flowsheets are provided along with stream conditions and equipment sizes. The reactor is modeled by three partial differential equations: component balances for two components (A and B), and an energy balance. The dynamics of the momentum balance in the reactor are neglected, because they are much faster than the composition and temperature dynamics. The mass flow through the reactor is assumed to be constant. Results are presented for single-stage adiabatic reactor systems, multi-stage adiabatic reactor systems with interstage cooling, multi-stage adiabatic reactor system with cold-shot cooling, cooled reactor systems, cooled reactors with hot reaction.

Additionally, an ASPEN dynamic simulation is performed. Also, a very important industrial process for the production of methanol for synthesis gas is given as an example of ASPEN dynsmics simulation of tubular reactor systems.

Chapter 7, *Heat Exchanger/Reactor Systems*, considers the Feed-effluent heat exchangers (FEHE) system in detail, in order to illustrate the inherent dynamic problems with using reactor effluent for pre-heating the feed, despite its steady-state economic advantages.

Two alternative structures for feed pre-heating are discussed. Both use a feed effluent heat exchanger, but one also uses a furnace.

Dynamic controllability favors the use of both a heat exchanger and a furnace. A very effective dynamic control could be provided using a completely independent pre-heating and cooling system on the reactor feed and effluent streams. Unfortunately, this arragement could be unfeasible because of high energy consumption. All these conclusions are drawn after having studied several aspects, such as: steady state design of the process, linear analysis, non-linear simulation, hot reactions.

Chapter 8, *Control of Special Types of Industrial Reactors*, analyzes several industrially important reactors, which have non-ideal behavior, but operate in steady-state mode. The analysis is targeted toward fluidized catalytic crackers, gasifiers, fired furnaces, kilns, driers, pulp digesters, polymerization reactors, biochemical reactors, slurry reactors, micro-scale reactors.

Because chemical reactors transform raw material into valuable chemicals, they are the most important part of many chemical, biochemical, polymer and petroleum processes. They can operate at low or high temperatures, in batch, fed batch or continuous mode. The book could be very useful to specialists in the field of chemical engineering, professionals who work with chemical reactors and students in training in reactor design, process control and plant design.

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