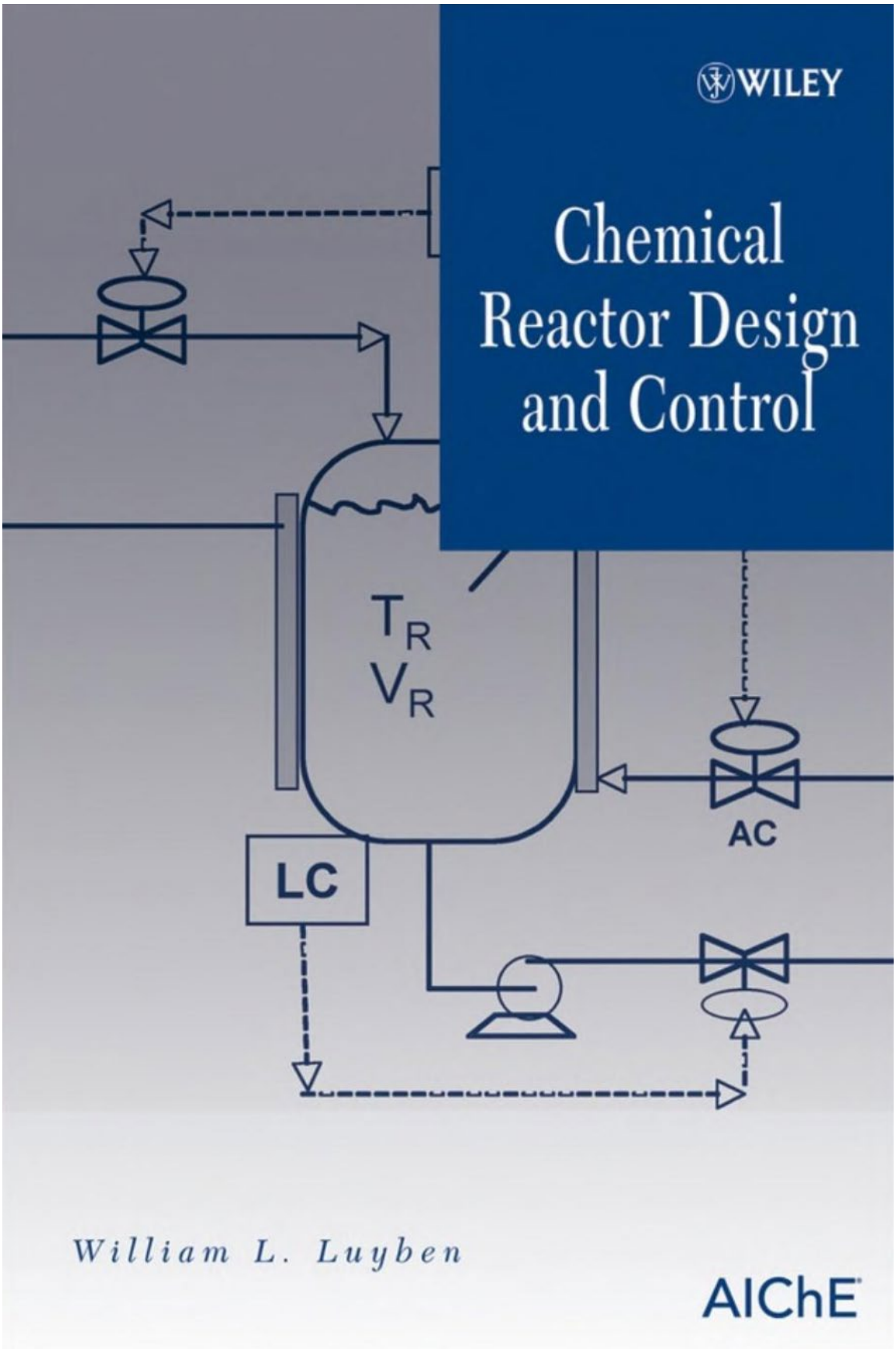

Petitioner's Exhibit 1012
Clean Chemistry v. EnviroTech
IPR2025-01472 – Page 001

CHEMICAL REACTOR DESIGN AND CONTROL

WILLIAM L. LUYBEN
Lehigh University

AIChE®

WILEY-INTERSCIENCE
A JOHN WILEY & SONS, INC., PUBLICATION

Petitioner's Exhibit 1012
Clean Chemistry v. EnviroTech
IPR2025-01472 – Page 002

Copyright © 2007 by John Wiley & Sons, Inc. All rights reserved.

Published by John Wiley & Sons, Inc., Hoboken, New Jersey
Published simultaneously in Canada.

No part of this publication may be reproduced, stored in a retrieval system, or transmitted in any form or by any means, electronic, mechanical, photocopying, recording, scanning, or otherwise, except as permitted under Section 107 or 108 of the 1976 United States Copyright Act, without either the prior written permission of the Publisher, or authorization through payment of the appropriate per-copy fee to the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923, 978-750-8400, fax 978-750-4470, or on the web at www.copyright.com. Requests to the Publisher for permission should be addressed to the Permissions Department, John Wiley & Sons, Inc., 111 River Street, Hoboken, NJ 07030, 201-748-6011, fax 201-748-6008, or online at http://www.wiley.com/go/permission.

Limit of Liability/Disclaimer of Warranty: While the publisher and author have used their best efforts in preparing this book, they make no representations or warranties with respect to the accuracy or completeness of the contents of this book and specifically disclaim any implied warranties of merchantability or fitness for a particular purpose. No warranty may be created or extended by sales representatives or written sales materials. The advice and strategies contained herein may not be suitable for your situation. You should consult with a professional where appropriate. Neither the publisher nor author shall be liable for any loss of profit or any other commercial damages, including but not limited to special, incidental, consequential, or other damages.

For general information on our other products and services or for technical support, please contact our Customer Care Department within the United States at 877-762-2974, outside the United States at 317-572-3993 or fax 317-572-4002.

Wiley also publishes its books in a variety of electronic formats. Some content that appears in print may not be available in electronic formats. For more information about Wiley products, visit our web site at www.wiley.com.

Wiley Bicentennial Logo: Richard J. Pacifico.

Library of Congress Cataloging-in-Publication Data:

Luyben, William L.
Chemical reactor design and control/William L. Luyben.
p. cm.
Includes index.
ISBN 978-0-470-09770-0 (cloth)
1. Chemical reactors—Design and construction. I. Title.
TP157.L89 2007
600'.2832--dc22 2006036208

Printed in the United States of America

10 9 8 7 6 5 4 3 2 1

Petitioner's Exhibit 1012
Clean Chemistry v. EnviroTech
IPR2025-01472 – Page 003

PREFACE

Chemical reactors are unquestionably the most vital parts of many chemical, biochemical, polymer, and petroleum processes because they transform raw materials into valuable chemicals. A vast variety of useful and essential products are generated via reactions that convert reactants into products. Much of modern society is based on the safe, economic, and consistent operation of chemical reactors.

In the petroleum industry, for example, a significant fraction of our transportation fuel (gasoline, diesel, and jet fuel) is produced within process units of a petroleum refinery that involve reactions. Reforming reactions are used to convert cyclical saturated naphthenes into aromatics, which have higher octane numbers. Light C4 hydrocarbons are alkylated to form high-octane C8 material for blending into gasoline. Heavy (longer-chain) hydrocarbons are converted by catalytic or thermal cracking into lighter (shorter-chain) components that can be used to produce all kinds of products. The unsaturated olefins that are used in many polymerization processes (ethylene and propylene) are generated in these reactors. The polluting sulfur components in many petroleum products are removed by reacting them with hydrogen.

The chemical and materials industries use reactors in almost all plants to convert basic raw materials into products. Many of the materials that are used for clothing, housing, automobiles, appliances, construction, electronics, and healthcare come from processes that utilize reactors. Reactors are important even in the food and beverage industries, where farm products are processed. The production of ammonia fertilizer to grow our food uses chemical reactors that consume hydrogen and nitrogen. The pesticides and herbicides we use on crop fields and orchards aid in the advances of modern agriculture. Some of the drugs that form the basis of modern medicine are produced by fermentation reactors. It should be clear in any reasonable analysis that our modern society, for better or worse, makes extensive use of chemical reactors.

Many types of reactions exist. This results in chemical reactors with a wide variety of configurations, operating conditions, and sizes. We encounter reactions that occur in solely the liquid or the vapor phase. Many reactions require catalysts (homogeneous if

Petitioner's Exhibit 1012
Clean Chemistry v. EnviroTech
IPR2025-01472 – Page 004

the catalyst is the same phase as the reactants or heterogeneous if the catalyst has a different phase). Catalysts and the thermodynamic properties of reactants and products can lead to multiphase reactors (some of which can involve vapor, multiple liquids, and solid phases). Reactions can be exothermic (producing heat) or endothermic (absorbing heat). An example of the first is the nitration of toluene to form TNT. A very important example of the second is steam–methane reforming to produce synthesis gas.

Reactors can operate at low temperature (e.g., C4 sulfuric acid alkylation reactors run at 10°C) and at high temperatures (hydrodealkylation of toluene reactors run at 600°C). Some reactors operate in a batch or fed-batch mode, others in a continuous mode, and still others in a periodic mode. Beer fermentation is conducted in batch reactors. Ammonia is produced in a continuous vapor-phase reactor with a solid "promoted" iron catalyst.

The three classical generic chemical reactors are the batch reactor, the continuous stirred-tank reactor (CSTR), and the plug flow tubular reactor (PFR). Each of these reactor types has its own unique characteristics, advantages, and disadvantages. As the name implies, the *batch reactor* is a vessel in which the reactants are initially charged and the reactions proceed with time. During parts of the batch cycle, the reactor contents can be heated or cooled to achieve some desired temperature–time trajectory. If some of the reactant is fed into the vessel during the batch cycle, it is called a "fed-batch reactor." Emulsion polymerization is an important example. The reactions conducted in batch reactors are almost always liquid-phase and typically involve slow reactions that would require large residence times (large vessels) if operated continuously. Batch reactors are also used for small-volume products in which there is little economic incentive to go to continuous operation. In some systems batch reactors can provide final product properties that cannot be achieved in continuous reactors, such as molecular weight distribution or viscosity. Higher conversion can be achieved by increasing batch time. Perfect mixing of the liquid in the reactor is usually assumed, so the modeling of a batch reactor involves ordinary differential equations. The control of a batch reactor is a "servo" problem, in which the temperature and/or concentration profiles follow some desired trajectory with time.

The CSTR reactor is usually used for liquid-phase or multiphase reactions that have fairly high reaction rates. Reactant streams are continuously fed into the vessel, and product streams are withdrawn. Cooling or heating is achieved by a number of different mechanisms. The two most common involve the use of a jacket surrounding the vessel or an internal coil. If high conversion is required, a single CSTR must be quite large unless reaction rates are very fast. Therefore, several CSTRs in series are sometimes used to reduce total reactor volume for a given conversion. Perfect mixing of the liquid in the reactor is usually assumed, so the modeling of a CSTR involves ordinary differential equations. The control of a CSTR or a series of CSTRs is often a "regulator" problem, in which the temperature(s) and/or concentration(s) are held at the desired values in the face of disturbances. Of course, some continuous processes produce different grades of products at different times, so the transition from one mode of operation to another is a servo problem.

The PFR tubular reactor is used for both liquid and gas phases. The reactor is a long vessel with feed entering at one end and product leaving at the other end. In some applications the vessel is packed with a solid catalyst. Some tubular reactors run adiabatically (i.e., with no heat transferred externally down the length of the vessel). The heat generated or consumed by the reaction increases or decreases the temperature of the process

Petitioner's Exhibit 1012
Clean Chemistry v. EnviroTech
IPR2025-01472 – Page 005

material as it flows down the reactor. If the reaction is exothermic, the adiabatic temperature rise may produce an exit temperature that exceeds some safety limitation. It may also yield a low reaction equilibrium constant that limits conversion. If the reaction is endothermic, the adiabatic temperature change may produce reactor temperatures so low that the resulting small chemical reaction rate limits conversion.

In these cases, some type of heat transfer to or from the reactor vessel may be required. The reactor vessel can be constructed like a tube-in-shell heat exchanger. The process fluid flows inside the tubes, which may contain catalyst, and the heating/cooling medium is on the shell side. Variables in a PFR change with both axial position and time, so the modeling of a tubular reactor involves partial differential equations. The control of a PFR can be quite challenging because of the distributed nature of the process (i.e., changes in temperature and composition variables with length and sometime radial position). Tubular reactor control is usually a regulator problem, but grade transitions can lead to servo problems in some processes.

The area of reactor design has been widely studied, and there are many excellent textbooks that cover this subject. Most of the emphasis in these books is on steady-state operation. Dynamics are also considered, but mostly from the mathematical standpoint (openloop instability, multiple steady states, and bifurcation analysis). The subject of developing effective stable closedloop control systems for chemical reactors is treated only very lightly in these textbooks. The important practical issues involved in providing reactor control systems that achieve safe, economic, and consistent operation of these complex units are seldom understood by both students and practicing chemical engineers.

The safety issue is an overriding concern in reactor design and control. The US Chemical Safety Board (CSB) published a report in 2002 in which they listed 167 serious incidents involving uncontrolled chemical reactivity between 1980 and 2001. There were 108 fatalities as a result of 48 of these incidents. The CSB has a number of reports on these and more recent incidents that should be required reading for anyone involved in reactor design and control. In 2003 the American Institute of Chemical Engineers published *Essential Practices for Managing Chemical Reactivity Hazard*, which is well worth reading.

There are hundreds of papers dealing with the control of a wide variety of chemical reactors. However, there is no textbook that pulls the scattered material together in a cohesive way. One major reason for this is the very wide variety in types of chemistry and products, which results in a vast number of different chemical reactor configurations. It would be impossible to discuss the control of the myriad of reactor types found in the entire spectrum of industry. This book attempts to discuss the design and control of some of the more important generic chemical reactors.

The development of stable and practical reactors and effective control systems for the three types of classical reactors are covered. Notice that "reactors" are included, not just control schemes. Underlying the material and approaches in this book is my basic philosophy (theology) that the design of the process and the process equipment has a much greater effect on the successful control of a reactor than do the controllers that are hung on the process or the algorithms that are used in these controllers. This does not imply that the use of models is unimportant in reactor control, since in a number of important cases they are essential for achieving the desired product properties.

The basic message is that the essential problem in reactor control is temperature control. Temperature is a dominant variable and must be effectively controlled to achieve the desired compositions, conversions, and yields in the safe, economic, and

Petitioner's Exhibit 1012
Clean Chemistry v. EnviroTech
IPR2025-01472 – Page 006

consistent operation of chemical reactors. In many types of reactors, this is achieved by providing plenty of heat transfer area and cooling or heating medium so that dynamic disturbances can be handled. Once temperature control has been achieved, providing base-level stable operation, additional objectives for the control system can be specified. These can be physical property specifications (density, viscosity, molecular weight distribution, etc.) or economic objectives (conversion, yield, selectivity, etc.).

The scope of this book, like that of all books, is limited by the experience of the author. It would be impossible to discuss all possible types of chemical reactors and presumptuous to include material on reactors with which I have little or no familiarity. Despite its limitations, I hope the readers find this book interesting and useful in providing some guidance for handling the challenging and very vital problems of chemical reactor control.

The many helpful comments and suggestions of Michael L. Luyben are gratefully acknowledged.

WILLIAM L. LUYBEN

Petitioner's Exhibit 1012
Clean Chemistry v. EnviroTech
IPR2025-01472 – Page 007

1.3 DETERMINING KINETIC PARAMETERS

The many preexponential factors, activation energies and reaction order parameters required to describe the kinetics of chemical reactors must be determined, usually from laboratory, pilot plant, or plant experimental data. Ideally, the chemist or biologist has made extensive experiments in the laboratory at different temperatures, residence times and reactant concentrations. From these data, parameters can be estimated using a variety of mathematical methods. Some of these methods are quite simple. Others involve elegant statistical methods to attack this nonlinear optimization problem. A discussion of these methods is beyond the scope of this book. The reader is referred to the textbooks previously mentioned.

In many practical applications, the engineer often has only plant performance data to use to backcalculate kinetic parameters. Data of this type are seldom extensive enough to permit precise calculation of all parameters since the plant normally operates in a fairly narrow window of operating conditions. However, useful simplified kinetics and parameters can often be determined that describe the major kinetics inside this region. Extrapolation outside the region from which the data has been obtained is very risky.

1.4 TYPES AND FUNDAMENTAL PROPERTIES OF REACTORS

In this section we discuss in a qualitative way the *classical* types of reactors: batch, continuous stirred-tank reactor (CSTR), and plug flow reactor (PFR). Our purpose is to point out the features of each that impact the ease or difficulty of their temperature control.

These classical reactors are idealizations of real industrial reactors. Perfect mixing is assumed in classical batch and CSTR reactors, but mixing is never perfect in an agitated vessel, no matter how intense the mixing. No axial mixing and no radial gradients (plug flow) are assumed in the classical PFR tubular reactor, but the flow patterns in a real tubular reactor are never without some axial mixing and differences in flow velocities and properties at different radial positions. However, the classical idealizations are usually close enough to reality so that they can be used for studying both steady-state design and the dynamic control of chemical reactors.

1.4.1 Continuous Stirred-Tank Reactor

Figure 1.8 shows a vessel with an agitator for mixing, a jacket that surrounds the vessel for heating or cooling, feedlines entering the vessel and a liquid product stream exiting from the bottom. The liquid in the reactor is assumed to be perfectly mixed, that is, with no radial, axial, or angular gradients in properties (temperature and composition). The product stream has a composition and a temperature that are exactly the same as the contents of the liquid throughout the vessel. This is always true, both under steady-state conditions and dynamically at any point in time.

This characteristic of a CSTR immediately generates an inherent weakness of the CSTR type of reactor, that is, the concentration of reactant in the vessel is the same as the concentration of reactant in the product. The concentration of reactant is inversely related to conversion.

Petitioner's Exhibit 1012
Clean Chemistry v. EnviroTech
IPR2025-01472 – Page 008

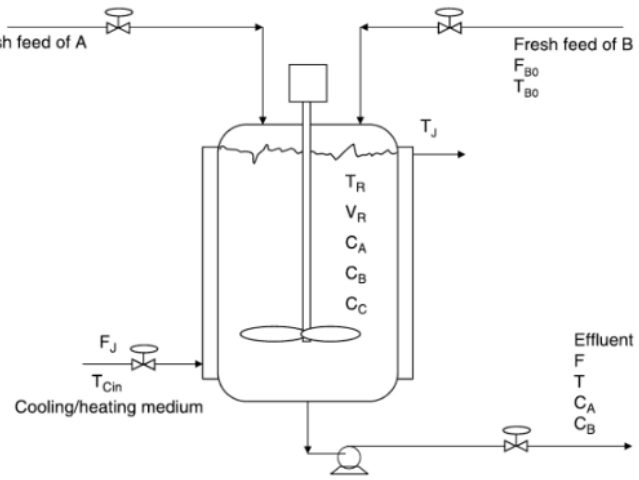

Figure 1.8 CSTR with jacket.

Fractional conversion χ defined as

$$\chi = \frac{C_{A0} - C_A}{C_{A0}} \tag{1.47}$$

If a high conversion is desired, the reactant concentration must be small. But the reaction rate depends directly on the reactant concentration. It also depends on the reactor volume. So, if a high conversion desired, the reactor must be large to compensate for the small reactant concentration. Thus a single CSTR is seldom used if high conversion is desired. Of course, using several CSTRs in series is one way to reduce the total reactor volume because only the last vessel will have the small reactant concentration.

We will develop detailed steady-state and dynamic mathematical models of CSTRs in Chapters 2 and 3 with several types of reactions and quantitatively explore the effect of kinetic and design parameters on controllability. For the moment, let us just make some qualitative observations. There are several features of a CSTR that impact controllability:

1. A variety of methods and configurations can be used for heat transfer. These are described in Section 1.5. Since heat transfer is one of the key issues in reactor control, the CSTR is usually more easily controlled than a tubular reactor. It is physically difficult to adjust the heat removal down the length of a tubular reactor.
2. The temperature of the feed has some effect on controllability, but it is much less important in a CSTR than in a tubular reactor, as discussed in Section 1.4.3. If heat is being removed from the reactor, a feed that is at a lower temperature than the temperature in the reactor will reduce the heat transfer requirements.
3. Conversion is the fraction of a reactant that is fed to the reactor that reacts in the reactor. The level of conversion in a CSTR has a very significant impact on its stability and controllability. This is discussed in detail in Chapter 2. A high conversion means a small reactant concentration in the reactor vessel, so there is little "fuel"

Petitioner's Exhibit 1012
Clean Chemistry v. EnviroTech
IPR2025-01472 – Page 009

available to permit a reactor runaway. On the other hand, a low conversion means that there is plenty of reactant available to react. If the reaction is exothermic and irreversible, a reactor temperature runaway can more easily occur in a CSTR operating with low reactant conversion than in one operating with high reactant conversion. In addition to affecting reactant concentration, the design conversion affects reactor size. Low conversion means a smaller reactor. This small reactor has less heat transfer area if an external jacket or an internal coil is used, which has a negative impact on controllability.

1.4.2 Batch Reactor

The classical batch reactor is a perfectly mixed vessel in which reactants are converted to products during the course of a batch cycle. All variables change dynamically with time. The reactants are charged into the vessel. Heat and/or catalyst is added to initiate reaction. Reactant concentrations decrease and product concentrations increase with time. Temperature or pressure is controlled according to some desired time trajectory. Batch time is also a design and operating variable, which has a strong impact on productivity.

Temperature profiles are established so that conversion and yield objectives are achieved while not exceeding heat transfer capacity limitations. These optimum temperature profiles depend on the chemistry. For example, if the reaction is reversible and exothermic, the temperature profile may ramp up to a high temperature to get the reactions going and then drop off with time to avoid the decrease in the chemical equilibrium constant at high temperature. If the reaction is reversible and endothermic, the temperature profile would rise to the highest possible temperature as quickly as possible because the chemical equilibrium constant increases with temperature.

If all the reactants are charged to the reactor, the reactant concentrations are initially large, which means that the reaction rate is high and the heat transfer load is high at the beginning of the batch cycle unless the temperature is kept low. The initial high reactant concentration problem can be avoided by using a "fed-batch reactor." Some material is initially charged to the reactor, but most of the reactant is fed during the course of the batch cycle. This causes the volume of the liquid in the reactor to increase with time, so volume as well as compositions and temperatures are all time-varying.

Several special features of a batch reactor impact control:

1. The process is inherently time-varying. There is no steady state. This causes process parameters to change with time, which means that controller parameters may have to change with time. Control strategies such as "gain scheduling" (changing controller gain and integral time) are frequently required in batch reactor control.
2. Rigorous nonlinear models must be used in analyzing batch reactors because of the changing process parameters. Continuous reactors operate around some steady-state level, so linear models are sometime adequate for establishing controller tuning constants.
3. Selecting the best time–temperature trajectory is a challenging dynamic optimization problem with constraints. There are rigorous nonlinear programming approaches to this problem, but there are also some more simple and practical methods that can be employed, as discussed in Chapter 4.
4. All the heat transfer configurations used on CSTRs can be applied to batch reactors.

Petitioner's Exhibit 1012
Clean Chemistry v. EnviroTech
IPR2025-01472 – Page 010

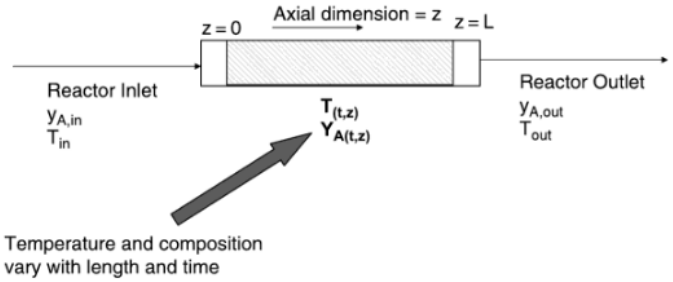

Figure 1.9 Adiabatic tubular reactor.

Mathematical models of batch reactors and control strategies are developed in Chapter 4. Both classical batch and fed-batch reactors are discussed using numerical examples.

1.4.3 Tubular Plug Flow Reactor

Figure 1.9 gives a sketch of a typical adiabatic tubular reactor. The major distinguishing characteristic of tubular reactors is their distributed-parameter nature, that is, variables change with physical dimensions as well as with time. The classical plug flow reactor assumes that the reactor vessel is cylindrical, that fluid flows down the length of the reactor with a flat velocity profile, that no axial mixing occurs, and that no radial gradients exist in temperature or compositions.

The tubular reactor can be an empty vessel if no catalyst is used. If a solid catalyst is required, the vessel is packed with catalyst, either in a bed or inside tubes. The dynamic behavior of the reactor is significantly affected by the presence of catalyst in the reactor because the thermal capacitance of the catalyst is usually greater than that of the process fluid, particularly if the system is gas-phase. The temperatures of both the process fluid and the catalyst change with time. Of course, under steady-state conditions, the two temperatures are equal at any axial position.

There are several modes of operation of tubular reactors:

1. *Adiabatic*. There is no heat transfer to or from the reactor. Temperature and compositions change with length. Since there is no heat transfer, there are no radial gradients in temperature. The adiabatic temperature change depends on the per-pass conversion in the reactor and the amount of material fed to the reactor and its heat capacity. The adiabatic temperature change is small if conversion is low. If the feed contains materials (inerts or product components) that do not reactant, this material can serve as a "heat sink" to reduce the adiabatic temperature change. The sensible heat of this material can soak up some of the heat of reaction. Of course, this nonreacting material usually has to be recovered and recycled, so this mode of operation increases the capital and energy costs of the separation section of the plant.

2. *With Heat Transfer*. The tubular reactor is constructed in a similar way as a tube-in-shell heat exchanger or a fired furnace. Process fluid flows inside the tubes and is cooled or heated by the heat transfer medium within the shell. Radial temperature gradients are inherent in tubular reactors with heat transfer, so the plug flow assumption

Petitioner's Exhibit 1012
Clean Chemistry v. EnviroTech
IPR2025-01472 – Page 011

is less accurate. These radial gradients depend strongly on tube diameter and fluid properties and fluid velocities. The larger the tubes, the larger the radial temperature gradients. One standard reactor design and development procedure is to study the system and/or catalyst in a single tube in the laboratory or pilot plant and then use multiple tubes of the same diameter in parallel in the plant reactor. The furnace or reactor used in steam–methane reforming to produce synthesis gas (a mixture of hydrogen, carbon monoxide, and carbon dioxide) is an important example. The furnace has multiple parallel tubes that are heated by burning fuel to provide the required heat to drive the endothermic reactions at a high temperature level. The problem of flow maldistribution among a large number of parallel tubes presents further potential complications.

3. *Adiabatic with Intermediate Heat Transfer*. Many tubular reactor systems use a series of adiabatic reactors with heating or cooling between the reactor vessels. For example, naphtha reforming has endothermic reactions of removing hydrogen from saturated cyclical naphthene hydrocarbons to form aromatics. The process has multiple adiabatic reactors with fired furnaces between the reactors to heat the material back up to the required reactor inlet temperature.

4. *Adiabatic with "Cold-Shot Cooling."* Some exothermic reactions are conducted in vessels with multiple beds of catalyst, which operate adiabatically (temperature increases through the bed). At the exit of each bed, a cold stream is mixed with the hot stream leaving the bed to bring the temperature back down to the desire inlet temperature for the downstream bed. This cold stream is typically some of the feedstream that has been bypassed around the reactor feed preheating system.

All of these alternatives are discussed in Chapter 5.

The control of tubular reactors is probably the most difficult of all reactor systems. The reasons for this difficulty and the special features of tubular reactors are summarized below:

1. The distributed nature of the process leads to complex dynamic responses in which axial changes in variables can sometimes result in counter-intuitive dynamic behavior. One example of this is the "wrongway" response that occurs in some adiabatic packed-bed tubular reactors. A decrease in the reactor inlet temperature will eventually result in a lower reactor exit temperature. But there may be a transient *increase* in the exit temperature. This is caused by the colder feed decreasing the temperature in the front end of the reactor. The lower reaction rate consumes less reactant, so the reactant concentration increases at locations further down the reactor. The solid catalyst packing is still hotter at this location because of its thermal capacitance. So the combination of higher reactant concentration and higher temperature causes a rapid reaction rate at locations further down the length of the reactor, which raises the temperature above the normal steady-state value that will eventually be established.

2. Temperature and composition transients move in waves down the length of the reactor, and this can lead to limit cycles when the reactor is part of a complete plant with feed preheating and recycle streams.

3. Tubular reactors often have high-temperature limitations because of the occurrence of undesirable reactions, catalyst degradation, or materials of construction. This means that the maximum temperature anywhere in the reactor cannot exceed this limit. An exothermic reaction in an adiabatic reactor produces a maximum temperature at the exit under steady-state conditions. An exothermic reaction in a cooled reactor can

Petitioner's Exhibit 1012
Clean Chemistry v. EnviroTech
IPR2025-01472 – Page 012

have the maximum temperature at some intermediate axial position or at the end. Both the magnitude and the location of the "peak" temperature vary with the design of the system and the age of the catalyst. They also vary with the operation of the system as disturbances occur. Controlling this peak temperature requires that multiple temperature measurements must be used down the length of the reactor for its detection.

4. Feed temperature is a very important design parameter in tubular reactors. A low feed temperature results in low reaction rates. So a long reactor is required to achieve the desired level of conversion. A high feed temperature results in a high exit temperature. If the reaction is exothermic and if there is a maximum temperature limitation, the per-pass conversion may have to be reduced or more "heat sink" material may have to be fed to lower the temperature rise. This usually means higher recycle flowrates with the associated higher capital and energy costs of the downstream separation system.

5. In cooled or heated tubular reactors the heat transfer options are limited. It is mechanically very difficult to change the temperature of the cooling or heating medium with axial position. The usual configuration is an essentially constant temperature of the heat transfer medium down the length of the reactor. In systems requiring cooling at fairly high temperatures, steam is generated on the shell side of the reactor to remove heat. The steam temperature is the same at any axial position. In systems requiring heating, burning fuel or condensing high-pressure steam is used at an essentially constant temperature at any axial position. If a heat transfer medium is used that does change in temperature down the length of the reactor, the available design parameters are the direction of flow (co-current or countercurrent flow of the cooling medium with respect to the direction of the process flow), the inlet temperature of the heat transfer medium and its flowrate. All of these must be balanced so that the desired temperatures and conversions are achieved. In systems requiring cooling at very high temperatures, molten salt is sometimes used as the heat removal medium.

The need to reduce energy consumption and reuse the exothermic heat of reaction so that we achieve a certain inlet temperature in a tubular reactor often leads to the use of a feed-effluent heat exchanger (FEHE). This can create some challenging control problems. Consider an exothermic reaction occurring in an adiabatic tubular reactor that has an inlet temperature of 450 K and an exit temperature of 500 K. One inefficient way to achieve the inlet temperature is to use a hot utility (steam or combustion of fuel) to heat up the cold feed. Energy can be saved by using the hotter reactor effluent stream in a FEHE. We study the dynamic problems that occur in reactor–FEHE systems like this in Chapter 4 and show that the positive feedback of energy can produce an openloop unstable process. The system can be made closedloop-stable by the use of an inlet temperature controller that bypasses cold material around the heat exchanger and mixes it with the heated stream to achieve the desired inlet reactor temperature. Chapter 7 contains a quantitative discussion of the interesting steady-state and dynamic tradeoff between energy and controllability in this type of system.

1.5 HEAT TRANSFER IN REACTORS

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. Figure 1.10*a*–1.10*f* show several of these alternatives.

Petitioner's Exhibit 1012
Clean Chemistry v. EnviroTech
IPR2025-01472 – Page 013