AC 2012-3672: NOVEL CHEMICAL REACTORS IN THE CURRICULUM: AN INSTRUCTIONAL MODULE

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Novel Chemical Reactors in the CHE Curriculum: An Instructional Module

Abstract

For the production of fine chemicals and pharmaceuticals, chemical reactions are often carried out in batch rather than continuous mode. Novel alternatives are the spinning disk reactor [1] and the rotating packed bed reactor [2]. These reactors utilize high gravity to enhance mass transfer in the reactor, leading to significant performance improvements over batch reactors. This module will provide instruction on the phenomena exploited to achieve the improvements in the reactor and its basic configuration. An overview of technology applications and commercial use will be provided. Examination of reaction system yields/selectivity for the alternative reactors will be compared to performance data for conventional reactors. The module is designed for use in the traditional undergraduate reactor design course and could be incorporated into the course as a single lecture or as a homework exercise.

Introduction

In a typical undergraduate chemical reactor design course, students learn the fundamentals of designing continuous stirred tank reactors, plug flow reactors and packed bed reactors. Various other reactor configurations (trickle bed reactor, straight-through transport reactor, falling film reactor) are used in industry, but may only be casually mentioned in the undergraduate course. Novel reactor configurations may be required for an industrial application for different reasons, including elimination/reduction of mass transfer resistances.

Key Elements and Structure of Instructional Module

The instructional module is divided into sections, which are designed to complement one another, yet stand independently.

- Introduction to Novel Reactors
- Kinetic versus Mass Transfer Control in Reactors
- High Gravity Environment (Higee)
- Configuration/Operation of Spinning Disk Reactor (SDR)
- Configuration/Operation of Rotating Packed Bed (RPB) Reactor
- Case Studies/Applications
  - CO_2 Absorption/Desorption in RPB
  - Esterification of Free Fatty Acids in RPB
  - SDR Technology for Pharmaceutical Manufacturing
- Summary

Introduction to Novel Reactors

The use of different types of reactors to overcome limitations imposed by conventional configurations is presented. The limitations of conventional batch reactors, CSTRs, PFRs and PBRs with respect to heterogeneous systems are discussed. The concept of using other fundamental phenomena such as the centrifugal field to overcome limitations is discussed.

Kinetic versus Mass Transfer Control in Reactors

This topic is typically covered at the end of the semester in the undergraduate chemical reactor design course at Mississippi State University. A brief introduction to catalytic processes with the sequential steps associated with migration of reactants from the fluid bulk to the catalyst surface, adsorption/reaction/desorption of species on/from the surface, and migration of products from the catalyst surface into the fluid bulk is typically the starting point in the lecture. Very little time is available during the regular lecture to cover these concepts and their implications. Thus, the concepts of kinetic control versus mass transfer control must be well described in this instructional module. How one experimentally determines the operating regime is presented, as are typical data from such an experiment, so that students have a visualization of what is happening in each control regime.

High Gravity Environment (Higee)

The innovation of the Higee environment [3] back in the late 1970s allowed the development of processes that exploited the action of a centrifugal field to enhance mass transfer and heat transfer, leading to increased process efficiency and enhanced control of temperature. The coordinate system for rotating systems is reviewed. The action of a centrifugal field on a thin film of liquid on a surface is examined. The action of the centrifugal field on the flow of liquid through a porous medium that is rotating is examined. The impact of the speed of rotation on the thickness of fluid boundary layers is revisited (this is covered during an earlier fluids course). The reduced residence times arising from the use of a high gravity environment may also give rise to benefits with respect to materials of construction, as it may be possible to use less exotic materials of construction for a particular application due to the reduced time of contact between process fluids and vessel walls.

Configuration/Operation of Spinning Disk Reactor (SDR)

A schematic of the basic configuration of a spinning disk reactor is presented. Special attention is given to the entry/exit of the process/reacting fluid to the reactor and how the fluid is channeled as it passes through the reactor. ` The impact of speed of rotation on residence time, as well as on heat and mass transfer resistances, is discussed.

Configuration/Operation of Rotating Packed Bed (RPB) Reactor

A schematic of the basic configuration of a rotating packed bed reactor is presented. The moving of the fluid around the solid catalyst is examined, with attention given to the liquid boundary layer and how this changes with speed of rotation.

Case Studies/Applications

1. CO_2 Absorption/Desorption in RPB [3].

In reactive gas absorption, the solute (CO_2) undergoes reaction once it has solubilized into the solvent (aqueous monoethanolmine). Thus, the reaction is controlled by the rate at which the CO_2 is solubilized, which is in turn influenced by the interfacial area available between the gas

phase and the solvent phase. Performance in the rotating packed bed is compared to that of a conventional absorber. The effects of rotation speed as well as solvent concentration are presented.

2. Esterification of Free Fatty Acids in RPB [4].

In the production of biodiesel, the free fatty acids may be problematic if alkaline transesterification reactions are desired. The free fatty acid concentration must be reduced to tolerable levels in order for alkaline transesterification reactions to be used. Thus, esterification of the free fatty acids is performed via a pretreatment process. The case study of continuous flow esterification of free fatty acids is presented based on research performed by Chen et al. [4]. This example of the rotating packed bed reactor showed that the reaction could be performed in a continuous fashion with high conversion of free fatty acids. The effects of molar ratio of the feed, temperature, and rotational speed of the PBR are considered.

3. SDR Technology for Pharmaceutical Manufacturing [1].

In the manufacture of pharmaceuticals, stirred vessels are often used in batch mode. The scaleup of these processes is problematic, as it is difficult to ensure geometric and hydraulic similarity as the stirred vessel increases in size. Use of the spinning disk reactor (SDR) for continuous manufacture of pharmaceuticals is presented as a case study. Reactions known to be mass transfer limited were examined in the SDR by Oxley et al. [1]. The performance of the SDR to conventional batch processing is compared.

Summary

The benefits of using a centrifugal field in terms of enhancement of heat and mass transfer are reviewed for each of the case studies. This module builds on companion modules examining centrifugal fields and their impact on fluid boundary layers/velocity profiles and heat transfer resistances.

Implementation

The module was used during the Fall 2012 semester. The module is designed to be used in a stand-alone format (currently Powerpoint slides), structured for use as a single lecture in the required chemical reactor design course. However, it could also be used as a supplement to traditional course material and assigned as a homework exercise; current efforts are focused on developing a multiple choice quiz to accompany the module that could be used to assess student mastery of concepts. During this coming summer, the module will be transferred to the Authorware platform for dissemination.

The topics covered in the module are best introduced once the students have exposure to nonisothermal reactor operating modes and to catalytic processes, including the multi-step sequence involved in reactants migrating to the catalytic surface, surface adsorption, surface reaction, desorption from the surface, and products migrating away from the catalytic surface. The text used in the course is Fogler's Elements of Chemical Reaction Engineering. With this

text and with the structure used in our undergraduate course, placement of this module in the course was necessarily during the last two weeks of the semester after Chapters 8 and 10 of the text are covered.

Conclusion

The development of an instruction module featuring novel reactors is discussed. Exposure to novel reactors at the undergraduate level is beneficial as graduates will then be familiar with both conventional reactors as well as those novel reactors that may be needed to achieve enhanced heat and mass transfer for particular reactions.

Acknowledgements

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