AC 2011-1068: SIMULATED MOVING BED REACTORS - AN INSTRUCTIONAL MODULE FOR INCORPORATION OF PROCESS INTENSIFICATION CONCEPTS INTO THE SENIOR REACTOR DESIGN COURSE

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Simulated Moving Bed Reactors - An Instructional Module for Incorporation of Process Intensification Concepts into the Senior Reactor Design Course

Abstract

The combination of reaction and separation in a single process unit is one of the basic tenets of process intensification. With this coupling, constraints arising from thermodynamic equilibrium may be avoided and the combined process may be more efficient as well as more economical in terms of capital expenditures as well as operating costs. With rising energy prices and the need for the chemical industry to remain globally competitive, consideration of process alternatives including these hybrid processes will be required of practicing chemical engineers in the coming years.

Due to the compartmentalized mode of instruction in most chemical engineering departments, separations and reactor design are typically taught in different courses. As a result, hybrid processes combining reaction and separation are generally relegated to coverage during the senior year, either in a capstone design course or in a reactor design course. Fogler[1] examined membrane reactors as well as reactive distillation in his text, Elements of Chemical Reaction Engineering, and has developed web modules for instruction on these topics. The availability of the instructional content in the text as well as the web modules provide other instructors with tools that can be easily incorporated into their courses.

The simulated moving bed reactor (SMBR) exemplifies process intensification through the coupling of separation and reaction. The separation process is adsorption, with separation accomplished using a solid phase adsorbent that has an affinity for one or more reaction products. As the reaction proceeds in the SMBR, products are removed from the reaction phase, and in the case of an equilibrium-limited reaction, this allows the reaction to proceed and achieve greater conversion. The simulated moving bed (SMB) technology for separation has been successfully employed commercially since the 1960s by UOP.[2] Use of SMB as a platform for coupling reaction with separation is relatively recent.[3-5] This module provides instruction on the basic configuration of a simulated moving bed reactor, constraints/limitations on its use, and also contains an overview of representative technology applications. Through comparison of process variables such as relative affinity of the adsorbent for reactants/products, process flow rates, reactor temperature, and feed stoichiometry, students gain insight into the impact of these variables on SMBR performance compared to a conventional packed bed reactor.

Introduction

The simulated moving bed was first developed as a separations process to mitigate difficulties with transport of a solid phase encountered in traditional moving bed technology. In a true moving bed, the solid phase is circulated countercurrently to the liquid phase, with separation accomplished. Moving a solid phase is difficult to implement. Disadvantages of the moving bed technology include solid particle attrition and limited liquid velocity to avoid fluidization of the solid particles.[6] By allowing the solid phase adsorbent to remain stationary and by switching process streams along a sequence of adsorbent beds, the desired separation can be accomplished while also eliminating the difficulties associated with moving a solid phase. The first implementation of the simulated moving bed was in the Sorbex technology by UOP.[7] UOP offers a suite of processes that utilize this technology for separation for isomer recovery at high purity, including the Parex process for separating p-xylene from a C8 isomers mixture, the Ebex process for separating ethylbenzene from a C8 isomers mixture, and the Olex process for separating olefins and paraffins.[7] These processes differ in the adsorbent employed to facilitate the desired separation. The technology has also been employed in the food industry, the fine chemical industry, and the pharmaceutical industry.

The coupling of reaction with the simulated moving bed separation process allows for significant advantages for many reactive systems. In the case of equilibrium-limited reactions such as esterifications and isomerizations, removal of one or more reaction products allows for the equilibrium conversion limit to be surpassed.[8] Additionally, this technology may also provide advantages for reactions that involve temperature-sensitive compounds (pharmaceuticals and/or natural products) or complex molecules that are difficult to evaporate. One of the challenges for this coupling of reaction and separation is identification of catalysts and adsorbent materials that offer the necessary performance in terms of high yields and selectivities under the same process conditions.[9]

Module Structure

The instructional module is comprised of a number of sections, each designed to provide exposure to one or more components of the simulated moving bed reaction technology. It is assumed that this module is stand-alone, therefore containing all necessary background and information for instruction. The sections of the module include:

- Introduction to Adsorption
- Coupling of Reaction with Separation
  - Background
  - Advantages for equilibrium-limited reactions
- Moving Bed Technology
  - Basic configuration
  - Disadvantages of moving beds
- Simulated Moving Bed (SMB) Technology
  - Basic configuration
  - Advantages of SMB
- Simulated Moving Bed Reactors (SMBR)
  - Basic configuration
  - Constraints/limitations
  - Process variables
- Applications of SMBR in Industry

Introduction to Adsorption

The topic of adsorption is covered currently in the Mass Transfer Operations course and discussed extensively in the text.[10] This segment of the instructional module covers basic theory of adsorption, commonly used adsorbents, as well as typical configurations of adsorbent beds. This section is designed as a review for the students.

Coupling of Reaction with Separation

One of the tenets of process intensification is the combining of process steps to achieve superior performance compared to when the processing steps are accomplished individually. The advantages of combining reaction with separation are detailed. In addition to the advantages associated with equilibrium-limited reactions, combining reaction with separation provides for the use of smaller equipment, reduction in required piping, smaller inventory, and lower energy consumption. Reduced operating costs may also be achieved in downstream separation equipment. To achieve these benefits, however, process conditions for optimal separation and optimal reaction must overlap. Select screen shots from this section are shown in Figure 1.

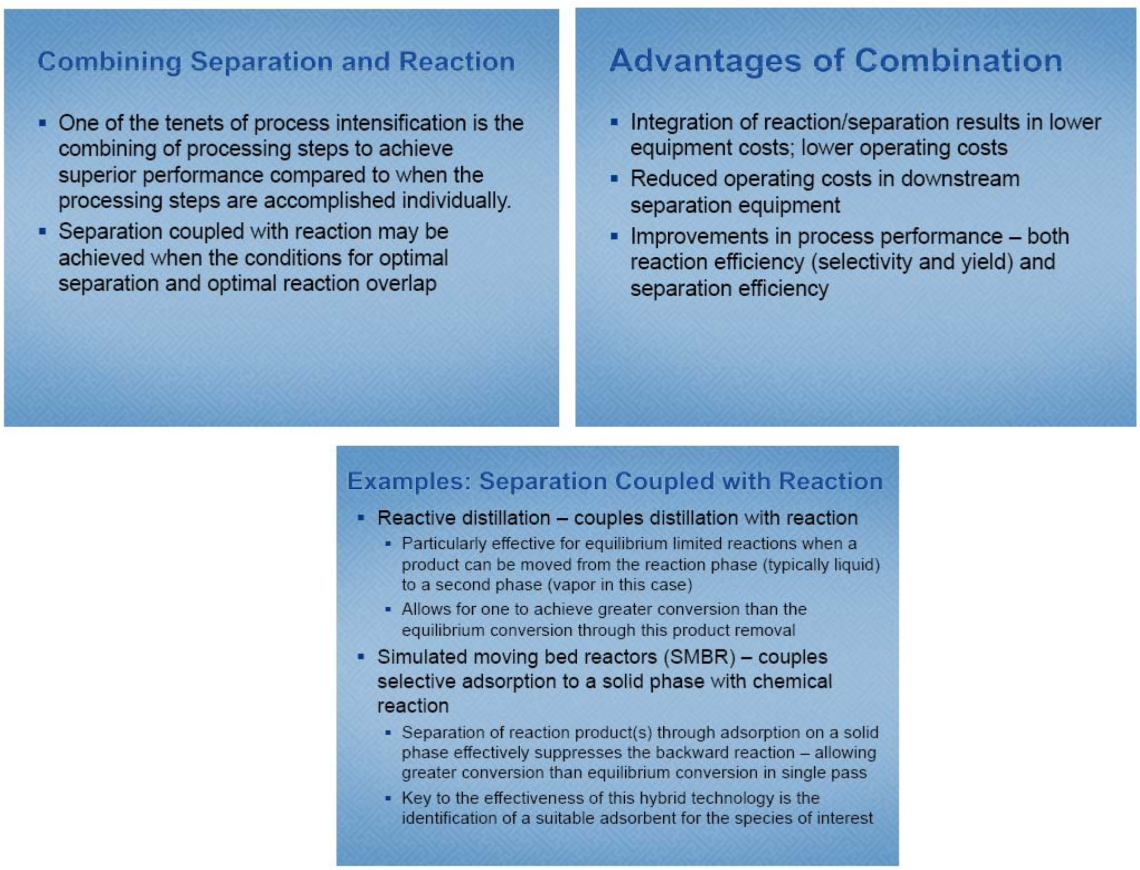

Figure 1. Combining Separation with Reaction Module Content.

Moving Bed Technology

An introduction to moving bed technology is provided. The basic configuration of a moving bed process is shown, along with the flow paths of the liquid and solid phases. The majority of instruction in undergraduate chemical engineering is focused on transport of liquids through piping and delivery systems; thus, the challenges of moving a bed of solid particles are delineated. These challenges include particle attrition as well as limitations on liquid phase velocity to avoid fluidization of the solid particles. Select screen shots from this section are shown in Figure 2.

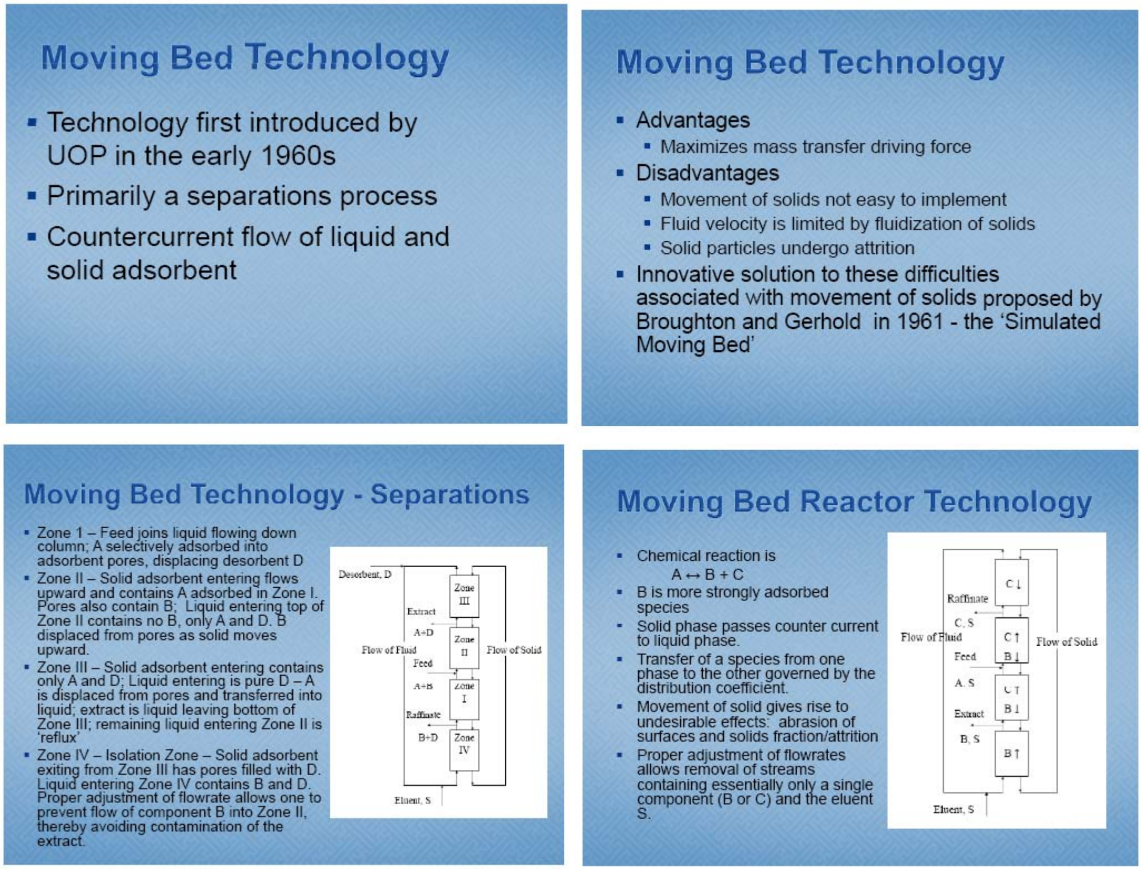

Figure 2. Moving Bed Technology Module Content.

Simulated Moving Bed (SMB) Technology

The introduction of static beds for adsorption coupled with cyclic switching of the liquid phase process inlet and transfer streams, first developed by Broughton and Gerhold,[11] resulted in an approach, the SMB process, that overcame many of the difficulties associated with solid phase transport in the traditional moving bed technology. An overview of the simulated moving bed technology is provided along with process schematics for each stage of the separation process. A screen shot from this section is shown in Figure 3.

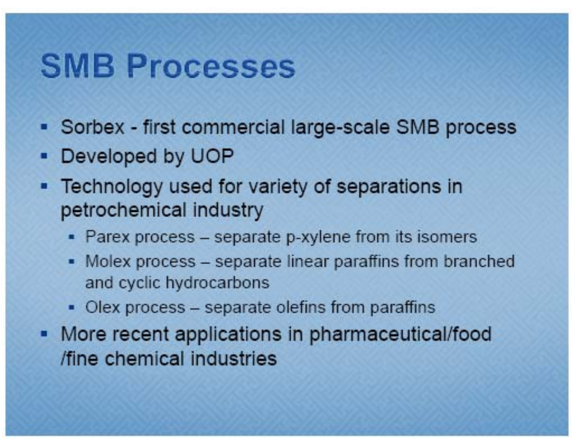

Figure 3. Simulated Moving Bed Module Content.

Simulated Moving Bed Reactors (SMBR)

The basic configuration of a simulated moving bed reactor is detailed. The operation of the process, typically configured as a series of adsorbent beds connected in a closed loop and separated by valves, is discussed. The solid phase remains stationary, with the countercurrent movement of phases accomplished through shifting the fluid inlets/outlets in the direction of flow. Each adsorbent bed passes through the same sequence of steps. Typically, four beds are employed. Select screen shots from this section are shown in Figure 4.

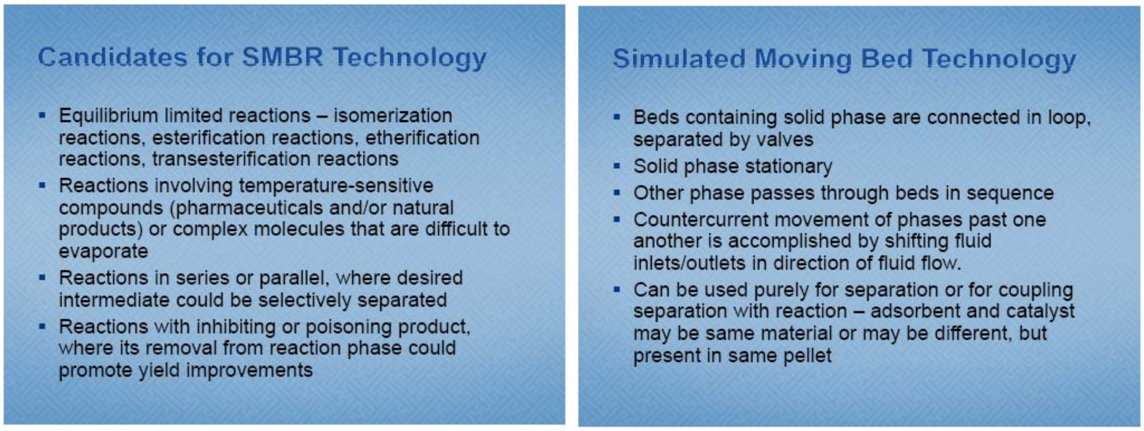

Figure 4. Simulated Moving Bed Reactors Module Content.

Applications of SMBR in Industry

In recent years, a number of applications of this technology have been identified and examined; a summary is shown in Table I. Currently incorporated in the instructional module is a detailed examination of p-xylene production via conventional processing and via SMBR technology. Efforts will continue to integrate additional SMBR application notes comparing conventional processing and SMBR technology for each of the applications identified in Table I. Select screen shots from this section are shown in Figure 5.

Table I. SMBR Applications.

Petrochemical Industry	Food Industry
p-Xylene production	Isomerization of glucose
Esterification of acrylic acid with methanol	Inversion of sucrose
Diethylacetal synthesis from ethanol and acetaldehyde	Synthesis of dextran from sucrose
Synthesis of MTBE from TBA and methanol	Production of lactosucrose from sucrose and lactose
Esterification of acetic acid with methanol or ethanol	Saccharification of modified starch
Synthesis of bisphenol A from acetone and phenol	Hydrolysis of lactose
Hydrogenation of 1,3,5-trimethylbenzene	
Isomerization of 2-methylpentane to 2-2 dimethyl butane	

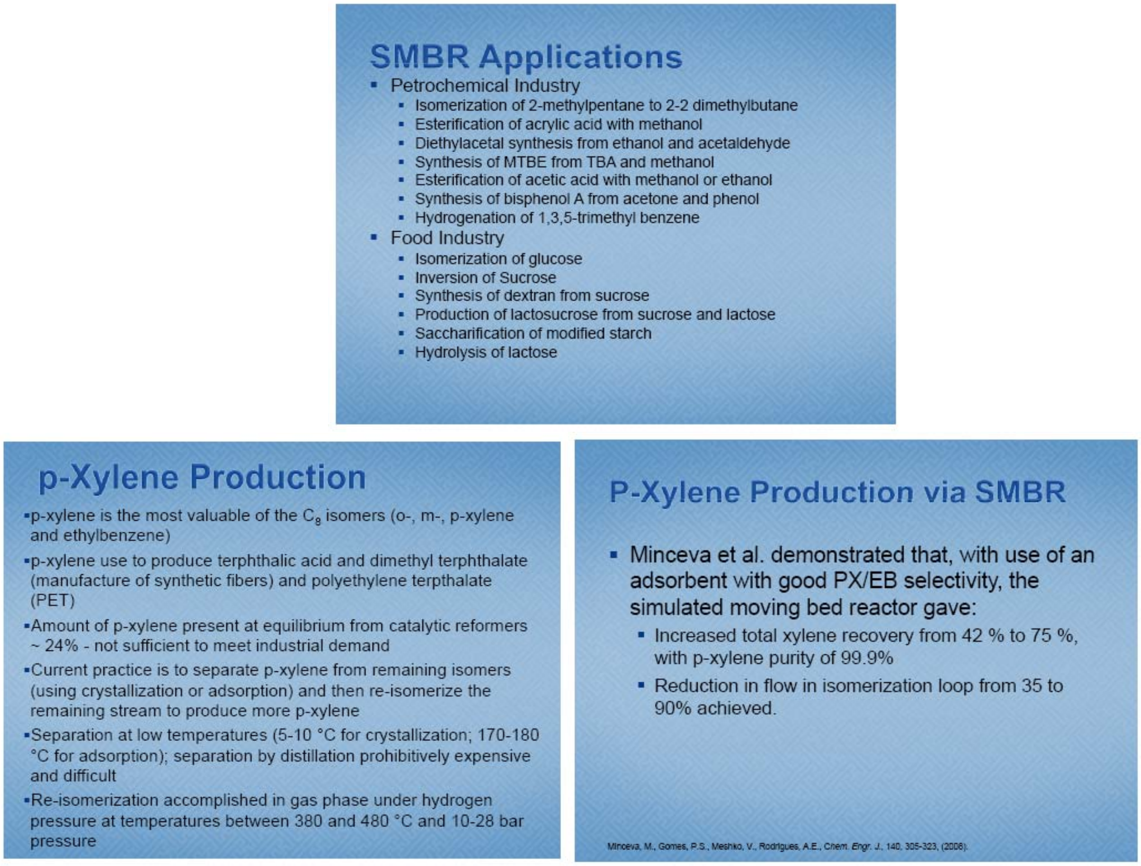

Figure 5. Simulated Moving Bed Reactor Module Content.

Incorporation of Module into Chemical Reactor Design Course

This module is intended to be incorporated into a senior-level Chemical Reactor Design course. In this initial implementation, the module was used in a single lecture session, with the professor providing instruction. To allow for incorporation of the module as a lecture during this first offering, instruction on simulation of chemical reactors using Chemcad was transferred from the lecture to a self-paced instructional activity performed by students outside of class, with submitted simulations to verify completion of the simulation module. As development continues on the Simulated Moving Bed Reactor module, it will be used by students outside of class in a self-paced interactive instructional mode, developed using Adobe Authorware.® Each segment of the module will incorporate an evaluation of student understanding through use of multiple choice/fill in the blank questions. Performance on these evaluations will be captured using a score that may be submitted for credit. This coming semester (Fall 2011), the module will be deployed as a self-paced instructional unit with assessment of student performance using the myCourses platform. Plans are to provide the refined module to other educators wishing to incorporate the content into their courses. The modular format allows the content to be readily incorporated into a variety of courses in the chemical engineering curriculum in addition to chemical reactor design, including process or plant design, advanced separations, or an elective focused on process intensification.

Assessment

This module was first used during the Fall 2010 semester with the senior Chemical Reactor Design course. A pre- and post-module survey was conducted to gather baseline data of student knowledge (Table II). 49 students participated in the activity. The responses were grouped according to a single correct response on three questions (questions 1-3, score right or wrong; e.g., range 0 to 3) and a multiple-choice question (question 4, scored 1 for each correct selection, e.g., 0 to 3). A paired sample t test was calculated to determine differences pre to post. Students scored significantly better, $t(48) = -8.01$, $p < 0.000$ and $t(48) = -12.95$, $p < 0.000$, respectively, on the post lecture than they did at pre lecture. Table III provides a summary of assessment results.

Table II. Process Intensification Pre/Post Survey of Student Knowledge

1. In Moving Bed Technology:
   a. the solid phase is stationary and the liquid phase moves
   b. both solid phase and liquid phase move
   c. the liquid phase is stationary and the solid phase moves

2. In Simulated Moving Bed Technology:
   a. the solid phase is stationary and the liquid phase moves
   b. both solid phase and liquid phase move
   c. the liquid phase is stationary and the solid phase moves

3. Moving Bed Reactor Technology and Simulated Moving Bed Reactor Technology both combine reaction with:
   a. distillation
   b. extraction
   c. adsorption
   d. absorption

4. Advantages of combining reaction with separation include which of the following:
   a. lower operating costs
   b. lower capital equipment costs
   c. improved process performance

Table III. Comparison of Pre and Post-Survey on Simulated Moving Bed Reactor Module.

	Paired Differences					t	df	Sig. (2-tailed)
	Mean	Std. Dev.	Std. Error Mean	95% Confidence Interval of the Difference: Lower	Upper			
Single Answer Questions Pre	1.35	.72	.20	-1.48	-.89	-8.01	48	0.000
Single Answer Questions Post	2.53	.84						
Multiple Answer Questions Pre	1.18	.86	.16	-1.89	-1.38	-12.95	48	0.000
Multiple Answer Questions Post	2.81	.39						

Summary

An instructional module on simulated moving bed reactors is in development. Used for the first time during the Fall 2010 semester in a senior Chemical Reactor Design course, this module provided exposure of seniors to one of the basic tenets of process intensification through the SMBR technology, where separation and reaction are combined to achieve enhanced performance. Refinement of the module will continue with additional applications incorporated and assessment of student learning to enhance exposure to the subject.

Acknowledgement

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