AC 2010-1882: ENGINEERING FUTURE CHEMICAL ENGINEERS: INCORPORATION OF PROCESS INTENSIFICATION CONCEPTS INTO THE UNDERGRADUATE CURRICULUM

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Engineering Future Chemical Engineers: Incorporation of Process Intensification Concepts into the Undergraduate Curriculum.

ABSTRACT

Process intensification (PI) encompasses a broad spectrum of activities focused on identifying fundamental limitations in a chemical production route, and developing or combining processes to minimize resource utilization and optimize product quality. Such activities are essential to industrial competitiveness as they can enhance safety, increase operating efficiency, lower energy usage, reduce capital costs, and/or reduce waste emissions and process hazards. Improving processes using PI concepts requires engineers to integrate many fundamental concepts and goes beyond traditional unit operations. Engineers are often taught how to synthesize a process by linking together standard unit operations, but are frequently not trained to synthesize processes through linking together fundamental concepts in new ways for novel and efficient process designs. This project seeks to correct this deficiency through the development of instructional modules for use in existing courses.

Four core chemical engineering courses are targeted: fluid flow operations, heat transfer operations, mass transfer operations, and chemical reactor design. Over the three-year CCLI project, activities/modules will be developed and incorporated into each of these courses, with each activity/module focusing on a particular element from the process intensification spectrum and designed to also enhance vertical concept integration. This poster presentation will focus on the activities and modules developed in Year 1.

INTRODUCTION AND BACKGROUND

The chemical industry faces numerous challenges in the coming years due to decreasing availability of raw material and energy resources. Thus, existing processes must operate in an efficient manner, with maximum yield of products from a fixed feedstock. Development and design of new chemical processes requires chemical engineers to sequence production steps to accomplish the necessary transformative steps taking the feed material and converting it in to a product or products with acceptable market value. The manner in which the conversion is accomplished may vary slightly from company to company; however, the traditional approach has been to sequence single-purpose unit operations to accomplish the conversion. This has been a very successful strategy in the past, and has been the model for instruction of chemical engineering design education.

In recent years, a paradigm has begun to emerge in the industry, whereby two or more steps in the production sequence are combined to yield a more energy efficient or more environmentally friendly process to accomplish multiple steps simultaneously. The reduced energy footprint is often accompanied by a decrease in capital cost, as these multiple steps are accomplished in a single piece of equipment.

The need to align chemical engineering design education with this new paradigm is essential for the U.S. chemical industry to remain competitive in the coming decades. However, the premise of the project investigators is that process intensification education and activities cannot simply be considered in the final stages of design, and not only in an upper level elective course, but must permeate throughout the undergraduate chemical engineering curriculum. Thus, instructional materials are being developed for a sequence of four core chemical engineering undergraduate courses. Typically, these courses are taken prior to the student enrolling in the senior design course (or courses). The four core courses that are targeted are: 1) fluid flow operations; 2) heat transfer operations; 3) mass transfer operations; and 4) reactor design. The first three of these courses are typically grouped as the ‘unit operations’ courses and are taught at the sophomore and junior levels. The last course may be taken prior to the senior year design courses, or during the first semester of the senior year simultaneously with the first course in the design sequence.

Process Intensification

Process intensification was identified by the NSF as early as 1993 as a specific area in which research endeavors should be concentrated to meet the needs of the chemical industry [1]; in excess of 75 archival articles were published on process intensification topics in 2009 [2]. Benefits of process intensification activities include [3,4]: 1) novel or enhanced products; 2) improved chemistry; 3) enhanced safety; 4) improved processing; 5) energy and environmental benefits; 6) capital cost reduction; and 7) low inventories. Key to the endeavor is an ability to identify the limitation(s) in a process, and knowledge of mechanisms that may be employed to eliminate them. One of the barriers identified by Tsouris and Porcelli [3,4] as well as Stankiewicz and Moulijn [5] is the sequential, unit operations-oriented approach typically used in undergraduate chemical engineering education. Much of the activity in the process intensification area has been in the European community [4]. Interestingly, the University of Newcastle on Tyne in the UK has established a graduate curriculum in chemical engineering focused on “intensified processing” [6]). Recently, it has been suggested that Chemical Engineering Education (ChE Ed) should include aspects of integrated concepts at the undergraduate level [7,8]. Also posed by these proponents is the question “Should ChE Ed include new disciplines such as … process intensification and miniaturization technology?” In the United States, the process intensification discussion is still primarily conducted in industry and by academic research teams [4]; to the knowledge of the project team, incorporation of process intensification at the undergraduate level has not been explored to date.

The incorporation of process intensification across the curriculum requires a critical examination of traditional topics currently taught in each course, and identification of appropriate topics that may allow expansion of existing instruction to concepts directly related to the tenants of process intensification. Integration of concepts from one course to subsequent courses is also an essential component of this incorporation process. The ability of students to successfully perform this integration has been a recent interest of the project team [9]. Further, it is believed that the development of process intensification modules would significantly impact academia and the diverse industries relying on chemical engineers because students trained to be versatile thinkers are more likely to conceive novel, more efficient production routes leading to innovative processes with respect to energy and material efficiencies.

U.S. Educational Needs

Chemical engineering departments in the U.S. cannot afford to be complacent about ChE Ed given the need for global competitiveness. A CCR/NSF Discipline Wide Curriculum Workshops panel was convened to determine what chemical engineering curricular changes are necessary to keep the U.S. competitive [10]. The panel concluded "the curriculum should integrate all organizing principles and basic supportive sciences throughout the educational sequence", that "all organizing principles should be operative in the curriculum throughout the sequence", and that "the curriculum should be consistently infused with relevant and demonstrative laboratory experiences." There is a critical need for chemical engineers to be conversant in synthesizing and optimizing unit operations. The new process intensification examples require the integration of concepts across four core courses, reinforce these concepts throughout the curriculum, and provide examples of how the combination of basic principles from different unit processes are required to solve real problems.

PROJECT ACTIVITIES

An overarching structure to the development of instructional modules has been developed. A minimum of three modules for each of the four core courses will be developed over the three year project. Table 1 summarizes the concepts that will be targeted over the project lifetime.

The instructional materials in development focus on concepts critical to process intensification, with an emphasis on both cross-fertilization and vertical integration. For example, in Year 1, instructional materials for the mass transfer operations course focus reactive distillation, an intensified process where reaction and separation are carried out simultaneously in an integrated reactor/column. To build on this coupling of separation and reaction, Year 2 instructional materials for the reactor design course focus on SMBR technology (simulated moving bed reactor), which combines reaction with adsorption. Thus, the concept of coupling reaction and separation is reinforced through these activities.

Year 1 Activities

Both fluid flow operations and reactor design courses were taught during the Fall 2009 semester. Heat transfer operations and mass transfer operations are being taught during the Spring 2010 semester. A total of 52 students completed the fluid flow operations course, while 41 students completed the reactor design course. As this is the first year for single semester offerings of the unit operations courses in the CHE department, enrollment in the heat transfer operations and mass transfer operations courses during Spring 2010 is higher, standing at approximately 60 in each course.

In addition to the module development and activities planned as part of the CCLI project, one additional activity was undertaken during the Fall 2009 semester. In the freshman seminar offered to chemical engineers, an introduction to process intensification was provided, after limited discussion of the unit operations approach to chemical engineering education. The developed Powerpoint presentation will be made available to chemical engineering educators interested in adapting it to their programs. Additionally, a survey of chemical engineering education efforts as they pertain to process intensification is in development.

Fluid Flow Operations

The module implemented in the Fall 2009 offering of Fluid Flow Operations was on the Bernoulli's Equation (BE), Mechanical Energy Balance (MEB), and Reynolds Number (N_{Re}). The specific objectives of this module were to: 1) demonstrate knowledge of the physical meaning of each term in the standard and expanded forms of the Bernoulli equation (Mechanical Energy Balance); 2) investigate the relative magnitude of individual terms in the Bernoulli Equation and the physical interpretation of each; and 3) evaluate Reynolds number to demonstrate the importance of length scales on fluid mechanics.

<u>Activity #1: Tank and Pipe Flow Laboratory (optional assignment)</u>

The students were exposed to a tank/piping system through an experimental laboratory. In order to approximate hydrostatic equilibrium, the tank level was maintained at approximately the same level throughout the experiment. Specific elements of the module included: 1) comparison of internal flows with varying tube diameter, pressure drop, velocity, and volumetric flow rates. Each team of students participated in collecting time and collected water volume from three different systems, each with a different discharge pipe diameter. The students calculated their experimental volumetric flow rates and then compared their results to the values given by the Bernoulli equation. Experimental error, statistical t-tests, and entrance effects on frictional losses were discussed in context of these results. To further reinforce important aspects of these elements, student teams used MS Excel™ to prepare a spreadsheet that allowed them to quickly compare calculated Reynolds numbers, pressure drops, and velocities (average and maximum) and visualize changes in velocity profiles when the hydrostatic pressure, entrance effects, and fluid properties were varied.

Even though this laboratory was optional (held outside of the assigned class time), 100% of the students participated in this optional laboratory assignment. Their work was very useful in demonstrating the Bernoulli equation, design impacts on the loss term, experimental error, and the importance of each group member's efforts to the project's success. The student feedback on both their interest in a hands-on activity and their self-perceived learning from this activity were both very high, as assessed by an in-class survey. Time did not allow for the analytical and experimental results to be compared to computation solutions. But a CFD module and discussion of computational solution methodologies will be added the next time this course is taught.

<u>Activity #2: Comparison of Approaches: Shell Balances, Equations of Continuity & Motion, and Bernoulli Equation/Mechanical Energy Balance</u>

This assignment involved conceptual understanding of velocity profiles, momentum, average velocity, volumetric flow rates, surface force, etc. and was combined with a comparison of different methods for obtaining these expressions for horizontal pipe flow, a film flowing down an inclined plane, and a vertical pipe. The students were first instructed in depth on the Bernoulli Equation and the Mechanical Energy Balance and the physical meaning and origins of the mathematical form for each term. Once an understanding of the Bernoulli Equation and the Mechanical Energy Balance had been demonstrated, the students were introduced to the shell balance development method, including the derivation of a differential equation to describe the system and the mathematical solution using boundary conditions. They were also introduced to the Equation of Continuity and Equations of Motion, in 3-D form for rectilinear, cylindrical, and spherical coordinate systems. The physical meanings of each term were discussed and a methodology was given for the elimination of terms based on an understanding of 'givens' and appropriate assumptions for particular systems. The students were asked to complete several assignments using these different methods to demonstrate their ability to understand and use all three methods.

This exercise required a somewhat higher level of conceptual understanding of fluid mechanics than might be traditionally required in a sophomore-level fluids course. However, these different methods and the physical interpretation and mathematical representation of fluid mechanics are very important for the students as they examine relative magnitudes (and so resistance to momentum transport) and physical interpretation of mathematical terms in any equation. The students seemed to conceptually have the most difficulty with the shell balance method. Defining the 'shell' presented difficulty, but was overcome in many students through the repeated exposure (practice) with this method and objects brought into class to represent 'layers' of fluid in different geometries.

Heat Transfer Operations

During the Spring 2010 semester, project activities will focus on heat transfer in small volumes and microchannels. These activities will build on the fluid flow knowledge gained by students during the Fall 2009 semester. In the heat transfer operations course, extensive coverage of conduction is provided. Students are exposed to conduction in ideal geometries (flat slab, cylindrical pipe), as well as conduction through many layers of materials (wall insulated, insulated pipes, jacketed reactors), all of which are macro-scale. To help enhance the necessary fundamental understanding of conduction, while simultaneously alerting students to subject overlap, in-class and homework activities will focus on heat transfer in small volumes of fluids. Small volume systems will become more prevalent in process intensification as more is done with less volume and in new geometries. Typical applications of these fundamental phenomena are found in microdevices and microreactors as well as in the intensified absorption cycle air conditioner [32, 54] where heat transfer in thin films is exploited.

Mass Transfer Operations

Tennessee Eastman successfully commercialized reactive distillation in its methyl acetate process [55, 56]. UOP developed the 'Ethermax' technology in the early 90s where ethers (methyl *tert*-butyl ether, *tert*-amyl methyl ether) were produced by the reactive distillation of methanol and isobutylene/isoamylene feedstocks [56]. These commercial successes provide an excellent starting point for the discussion of the advantages of this coupling of processes for intensification. For successful implementation of reactive distillation, phase equilibria and reaction kinetics must both be favorable over an overlapping temperature range. A discussion of the key elements of the reactive distillation process is contained in the currently used text. Because students enrolled in this class will not take reactor design until the following semester, only qualitative discussion will be included and will focus on the elimination of the reactor through incorporation of a reactive section in the distillation tower. Since MSU students use the process simulator ChemCAD in their courses, an existing ChemCAD example will be used for instruction. A new ChemCAD example problem will be developed for use as a homework exercise.

Reactor Design

In the chemical reactor design, plug flow reactors are examined in detail. Under this project, the expansion of a jacketed plug flow reactor to examine coupling two reactions via heat exchange was examined during the fall semester. One of the tenets of process intensification is the more efficient use of energy combined with coupling of process units to yield a smaller equipment footprint. The coupling of an endothermic reaction on the tube side of a jacketed plug flow reactor with an exothermic reaction in the jacket provides for such an efficient use of energy. Additionally, the use of a membrane reactor with the transfer of a product/reactant across the membrane provides additional opportunities for process intensification.

During the Fall 2009 semester, one module was developed and used in the Chemical Reactor Design course. This module focused on the coupling of endothermic and exothermic chemical reactions. Students in this course had not been exposed to the concepts of process intensification in earlier chemical engineering courses; thus, a general introduction to process intensification was also provided, so that they would have an understanding of why it might be desirable to carry out multiple processes/process steps in a single piece of equipment. This general introduction was also used in a discussion of chemical engineering education during the seminar offered to chemical engineering freshmen.

The topic of membrane reactors was already an element of instruction in the reactor design course. Thus, this provided an excellent platform from which to introduce the coupling of reactions. In examining membrane reactors, equilibrium limited reactions provide the foundation for examining how the removal of a reaction product allows for one to achieve a conversion greater than the equilibrium conversion at a given temperature. Dehydrogenation reactions often fall into this category. The coupling of hydrogenation/dehydrogenation reactions was explored in the module. Examination of this couple provides for one to examine whether the advantages come from energy exchange only, mass exchange only, or exchange of both mass and energy. Additionally, the influence of relative concentrations, their impact of reaction rates, and mode of operation (cocurrent versus countercurrent) were also explored. This module was developed as a presentation. Current efforts are focused on using the Authorware (Adobe Systems) software to allow the module to be fully interactive, and self-contained.

Work has also begun on the module for year 2. This module is focused on simulated moving bed reactor (SMBR) technology, where chemical reaction is coupled with adsorption in a single operation.

SUMMARY

Integration of key concepts related to process intensification across multiple core chemical engineering courses provides the opportunity for students to become both familiar with the tenets of process intensification as well as be equipped to examine intensified process alternatives during the senior design courses. As students progress through the four course sequence, it is expected that their foundation will become stronger in these tenets and they will be better equipped to face the challenges that will be present when they graduate and enter the chemical engineering workforce. Assessment of student learning and module effectiveness is currently underway.

ACKNOWLEDGEMENT

This work is funded through the National Science Foundation Course, Curricula and Laboratory Improvement (CCLI) program under grant DUE-0837409.

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Table 1. Summary of Topics to be Enhanced by Incorporation of Process Intensification

Course	Topic	Vertical Integration	Modules (in-class and homework)	References
Fluid Flow Operations	Bernoulli Equation/ Reynolds Number	Heat Transfer Mass Transfer Reactor Design	Flow regimes & impact on (h) Micro-channel flows Vary fluid properties & flow geometries	[11] [12-14]
	Mixing	Heat Transfer Mass Transfer Reactor Design	Roughened/machined surfaces; Baffles; Static mixer-reactor (SMR); Oscillatory flow mixing; Flow regimes	[15 16 [17-19] [20]
	Centrifugal Field	Heat Transfer Mass Transfer Reactor Design	Spinning disk reactor (SDR) HiGEE separator	[21-24]
Heat Transfer Operations	Conduction	Reactors All, scale considerations	Conduction in an unstirred reaction vessel HT in small volumes & microfilms	[11] [12, 13, 25-29]
	Convection	Fluid Flow Fluid Flow, Reactors Mass Transfer	Oscillatory flow mixing Convection/reaction in jacketed laminar flow pipe HT on a distillation column stage	[19, 30-35] [11] [36]
	Heat Exchangers	Fluid Flow Fluid Flow, Mass Transfer	Thin film heat exchangers (conduction path reduction) Spinning disc for gas/liquid heat exchanger	[16, 21, 37-39] [40-42]
Mass Transfer Operations	Reactive Distillation	Reactor Design	Reactive distillation	[36]
	Column Internals/Configuration	Fluid Flow Heat Transfer	High capacity structured packings Thermal coupling and column configuration	[43, 44] [45, 46]
	Hybrid Separations	Heat Transfer	Extractive distillation for azeotropes	[47]
Chemical Reactor Design	Consecutive/parallel reactions	Fluid Flow Mass Transfer	Coupling of consecutive and/or parallel reactions in membrane reactor; compare with conventional packed bed reactor	[48, 49]
	Simulated moving bed reactor	Fluid Flow Heat Transfer Mass Transfer	Adsorption and reaction are coupled; comparison with conventional two-step sequence	[50-52]
	Novel reactors	Fluid Flow Heat Transfer Mass Transfer	Cavitational reactor; uses ultrasound to enhance mass transfer Spinning disk reactor; uses centrifugal field to minimize mass/heat transfer limitations	[53] [41]