“Real” Engineering for a multi-disciplinary 1st. year project/design course APSC100

The introduction of commercial FlowSheet simulators to freshmen students

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Abstract

Queen’s University has a common first year for engineering. A few years ago a project/design course was introduced, APSC100, which has been quite successful. It was predicated on the fact that students who are attracted to engineering are really excited about the possibility of “doing engineering” early in their student experience.

The design of Chemical processes is something that few if any first year students have any appreciation of. We are in the process of developing a project for APSC100 which will introduce the subject as well as have the students work with a commercial FlowSheet simulator. We believe that simulators “warts and all (1)” can be an excellent learning tool, and exposure to these programs is essential as they have become so much a part of today’s engineering career experience.

Commercial Flowsheet simulators continue to be a challenge for people with many years familiarity with these systems. There is however a potential for a great deal of learning about the “design process” by the use of these tools, provided these tools are presented in such a way as to be challenging but not intimidating.

The paper will describe the approach to developing the APSC100 module, the challenges faced and the anticipated solutions. One particular problem will be developing something that will interest a broad spectrum of students. It has been noted that “Chemistry” often seems to be a subject that is avoided by many. This module will hopefully demonstrate the fact that “Chemistry” is one of the basic sciences and how it is the basis for much of the product of the modern world.

Since this is a “work-in-progress” we anticipate and welcome suggestions as to how to present a successful module to our students.

Introduction

Queen's Faculty of Applied Science has a common first year. Several years ago the faculty introduced a first year course that gave the students the opportunity to work in teams on various projects that required in many instances laboratory investigations, and hopefully some consideration of design. This has been quite successful; as most students enter Queen's engineering programs to be engineers. The initial exposure of the students to engineering projects as a replacement for the previous interminable labs meets this need.

The design of chemical processes has traditionally been a key role of chemical engineers. Although Chemical Engineers find career opportunities in a broad array of fields, we felt it important to introduce the concept of the design process as it applies to chemical plant process design to incoming engineering students.

Since Process Flowsheet Simulators have become an essential component of process design we have endeavored to introduce this concept as well.

Rationale

Recently Dr. Tom Brzustowski the President of NSERC addressed the Annual General Meeting of Professional Engineers Ontario. In this talk the distinction between, Science, Engineering, Technology and Design was clearly spelled out as follows

Science: the social system for generating knowledge that involves three sequential and interrelated activities:

- **Research** conducted according to a prescribed method (the scientific method)
- **Processes for accepting (or not) the results of research as fact**
- **Predictions** based on facts

Engineering: the professional activity of creating artifacts and systems to meet people's material needs, with:

- **Design** as the central creative process
- **Scientific knowledge** and **economic considerations** as its essential inputs
- **Public safety** as its overriding responsibility

Technology: the *set of procedures and tools* that predictably and reproducibly produces a specified desired effect in the material world

The main form of creative intellectual activity in science is research

It is both research and design in engineering

*The context for creative intellectual activity in science is an **experiment**, and in engineering it is most often a **project**.*

The basic rationale of introducing the first year project course, APSC100 was to provide students entering engineering with an opportunity to be exposed to the **design process**, which we believe, is the quintessential aspect of engineering.

When dealing with Chemical process design, the first step has to be the basic reason for proceeding with the design. In the introduction to the students we will present the various reasons for beginning a process design. Fundamentally this is based on economics. A manufacturing enterprise may wish to expand throughput, new technology may offer a potential for cost reduction, or environmental compliance requires plant addition or modification. Entry into the marketplace with a new process is another case and in many instances expenditure is justified simply to maintain position. . There are four fundamental principles of Engineering Economics ⁽²⁾

- A nearby dollar is worth more than a distant dollar (time value of money)
- All that counts is the difference between alternatives
- Marginal revenue must exceed marginal cost
- Additional risk is not taken without the expected additional return

While it is recognized that we certainly cannot expect freshmen students to be able to grasp these concepts totally, it is important that they have some understanding as to why engineers carry out designs.

The Science of the project

While it is important that we recognize that we are dealing with engineering education as separate from a science education there are grey areas. As Dr. Tom Brzustowski pointed out the role of the scientist is to provide the data necessary for the engineer to carry out his or her design. To demonstrate this we propose to have the students

carry out some bench scale experiments to generate some important kinetic data for the process chosen.

We propose to use a well established manufacturing route to produce Methyl Isobutyl Ketone MIBK from Acetone the starting material. Although MIBK a very active chemical solvent,

has become a victim of the Rule 66 , volatile hydrocarbon legislation, it is still an excellent illustration of sequential chemical processes. The chemistry of the process is given below.

CRUDE DAA and WET MO PRODUCTION

BASIC REACTION

SIDE REACTIONS

SLIDE 6A

There are several interesting aspects concerning the process. Traditionally as shown above it was carried out in two steps. One of the more recent versions of the two step process used methanolic caustic as the catalyst. A process flowsheet is attached for the front-end of this process Figure 1.

Although this system has a great number of variables that can be manipulated , a real advantage for a "discovery" project, it is in our opinion necessary to limit these in order for first year students to have a learning experience that isn't overly intimidating. This is particularly the case since our APSC100 program is open to all of first year students, where only a few are interested in chemical engineering.

The methanolic caustic was an effective way to solubilize the necessary caustic NaOH which was the catalyst for the above process; however it introduced the additional reaction to form "Pentoxone". For the student project we intend to use a heterogenous catalyst, an ion-exchange resin catalyst. This should greatly simplify the project. It is also an opportunity to introduce the concept of novel advanced catalysis based on ion-exchange resins.

One issue that unfortunately does not get sufficient recognition in the undergraduate program is Environmental Health and Safety issues. This is one of the keys aspects of engineering as emphasized by Dr. Brzustowski. Having the students collect all the WYMYS sheets for all the

compounds expected in this system would be a most useful exercise. We recognize however that there is a limit to the amount of time that the students have available for this project. Gathering a lot of data would be an intimidating exercise for many, accordingly we intend to rely on an introduction to the project conducted by the faculty advisor as well as providing a manual that will include much of the background data such as the necessary WYMYS sheets.

Mesityl Oxide is a particularly noxious compound. Although the amounts that we will be dealing with under closely controlled conditions in appropriate fume hoods will not present a risk to anyone, it will be quite instructive for the students to appreciate that chemical engineers routinely must deal with chemicals that are dangerous unless carefully controlled.

As part of the design process we expect the students to carry out some experiments to gather reaction data that can be appropriately regressed to provide kinetic constants for the reactor module available in the simulator. This will also introduce the students to bench scale reactor experiments and analysis by Gas Liquid Chromatography. GLC analysis is a “work-horse” of chemical analysis and an introduction to it should be most useful. Fortunately the compounds present in the reaction product are quite readily separated and analysis should be quite straightforward.

The Engineering Design Step

The next step in the process is to have the students introduce their kinetic constants into the flowsheet simulator in order to model the reactor. We have a significant amount of kinetic data from literature sources;^(3,4,5,6) however it will be interesting to see how the student data compares with this data. Before we introduce the students to the commercial flowsheet simulator we will provide them with a block flow diagram of the overall process as well as an Excel overall material balance with all recycles accounted for.

The particular simulator that we have chosen for this work is PRO/II™ a product of Simulation Sciences. Although these simulators are a very powerful design tool, they require a considerable amount of experience in order to use them effectively. In our experience the greatest risk associated with these simulators is that while extremely powerful they are exceptionally prone to

GIGO. There is simply no substitute for experience when interpreting the output.

Originally we had hoped to develop a simple “LEGO BLOCK” approach to process design however upon considerable reflection we came to the conclusion that we would be further ahead using a commercial flowsheet simulator. These are more or less a “LEGO BLOCK” approach although much more sophisticated than we require for our purposes. Accordingly we must develop a system where the simulator can be adapted to the level of first year students. It has been most beneficial to have a student involved in the development of this project. The student is a second year student so that his experience with APSC100 is relatively fresh in his mind

It is not our intention to use the simulator as an actual design tool, rather as an illustration of the design process. In order to do this we must prepare a much simplified user manual that instructs the students as to how they can access the simulator and the various steps required in order to develop a simple reactor module. This will be included with the overall data manual for the project.

Since the reaction results in low conversion there is a recycle column following the reactor. Since the simulation of distillation columns is one of the more difficult aspect of process simulation we propose to supply the students with a module that has been optimized for the recycle column. At this point we really can't see any justification to proceed further in the design of the unit. We must appreciate that the main purpose of this exercise is to introduce students to concepts, not to develop design engineers.

One additional important issue is the vast amount of thermodynamic and transfer property data that is required for a process simulation. The students will be made aware of the enormous amount of data that is available and how it should be used.

Process Economics

One of the most important aspects of process design is the economics of the process. We hope to introduce the concept of feed cost, product values as well as the cost of manufacture. This is an important concept as the operation of a two step process is dependant on the various values for the products. DiAcetone Alcohol has a value as a feedstock for the manufacture of Hexylene Glycol (hydrogenated DAA), a compound used

extensively in brake fluids and hydraulic fluids. MIBK has a value as a very active solvent although due to recent regulation it is being phased out of many applications.

We propose to supply the students with an Excel spreadsheet where they can input various values such as feedstock costs and utilities costs in order to generate a cost of manufacture. All the relevant data will be provided in the manual, with reference to the sources of information.

One example is that we so often see students using values for commodity chemicals such as Acetone derived from a laboratory supply house rather than the commodity bulk values.

Path Forward

There have been many variations on the process scheme for the manufacture of MIBK so there is ample opportunity to modify the contents of the particular project for future years. For example there has been a considerable amount of work on proposals for a “catalytic distillation” process^(3,4,5,6) which uses the principle of process compression in order to reduce the number of discrete unit operations in any process. This will allow us to continue to modify and develop the project course based on the previous year’s work.

Our current plans are to develop the project over the summer and then have a fourth year laboratory project team pilot the project in order to work out any bugs and also assess the feasibility of the overall project as a first year exercise that while challenging will also be rewarding for the student participants.

References

- [1] Simulators Stimulate Students, Philip Wankat and Frank Oreovicz, ASEE Prism January 2004.
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- [4] The Production of Diacetone Alcohol with Catalytic Distillation, Part II: A rate-based catalytic distillation model for the reaction zone, G.G. Podrebarac, F.t.T. Ng and G.L. Rempel.
- [5] The Production of Diacetone Alcohol with Catalytic Distillation, Part 1: Catalytic distillation experiments, G.G. Podrebarac, F.T.T. Ng and G.L. Rempel.
- [6] One-step Methyl Isobutyl Ketone Synthesis from Acetone and Hydrogen using Amberlyst CH28, W. Nicol, E. du Toit.

Figure 1

<u>X-1833</u>	<u>X-1832</u>	<u>X-1834</u>	<u>V-1834 to V-1837</u>	<u>X-1846</u>	<u>D-1846</u>	<u>X-1848</u>	<u>D-1847</u>	<u>X-1850</u>	<u>V-1847</u>
FEED PREHEATER	PIPE REACTOR	CHILLER	TIME TANKS	NO. 1 COLUMN PREHEATER	NO. 1 DISTILLATION COLUMN	NO. 1 COLUMN CONDENSER	NO. 2 DISTILLATION COLUMN	NO. 2 COLUMN CONDENSER	ACCUMULATOR
104 Ft./2	425 Ft. 6/8" SCH. 40 PIPE	624 Ft./2	3'-0" X 22' - 0"	735 Ft./2	5'-0" X 86' - 6"	2146 Ft./2	4'-6" X 86' - 0"	1400 Ft./2	3'-0" X 15' - 0"
					50 VALVE TRAYS		50 VALVE TRAYS		
<u>X-1831</u>	<u>T-1831</u>		<u>V-1838/V-1839</u>	<u>X-1847</u>		<u>V-1846</u>	<u>X-1849</u>	<u>X-1851</u>	<u>V-1848</u>
FEED/PRODUCT EXCHANGE	RECYCLE ACETONE TANK		ION EXCHANGER	NO. 1 COLUMN REBOILER		ACCUMULATOR	NO. 2 COLUMN REBOILER	NO. 2 COLUMN SUBCOOLER	PHASE SEPARATOR
424 Ft./2	15' - 0" X 18' - 0"		22 Ft./3 RESIN EACH	650 Ft./2		4'-0" X 15' - 0"	389 Ft./2	107 Ft./2	5' - 0" X 11' - 0"

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