Enhancing Core Chemical Engineering Courses with Computationally-Intense Course Modules

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This paper presents two new course modules that have been developed for junior-level Chemical Engineering core courses: Chemical Reaction Engineering and Chemical Engineering Thermodynamics II. As currently offered at Rowan University, both of these courses integrate simulation and computer lab activities in which students devise models of key physical systems, and then interrogate the models to study cause-and-effect in these physical systems. These computer labs are an integral part of both courses, but the scope (one 160-minute period) limits the complexity of the models that can be used, if the students are required to build the model themselves. In the course modules described here, students will study two physical systems that are significant in chemical engineering by making use of more complex models that have already been built. The modules were developed during the 2016/2017 academic year and are being implemented in classes for the first time during the Spring 2018 semester. Assessment results are therefore not available at time of writing but will be presented at the conference in June 2018.

Introduction

This paper describes new course modules that have been developed for the Chemical Engineering core courses Chemical Reaction Engineering and Chemical Engineering Thermodynamics II. At Rowan University, Chemical Reaction Engineering is a required 4-credit course that meets three times a week; two 75-minute single periods and a 160-minute double period. Chemical Engineering Thermodynamics II is a required 3-credit course that meets for one 75-minute single period and one 160-minute double period. The double periods in both courses are typically devoted to computer laboratories.

Computer labs in both courses fall into two general categories: activities in which students use ASPEN process simulation software to model a system, and activities in which students build their own models of a system from fundamental equations. The use of commercial simulation software such as ASPEN in the chemical engineering curriculum has been mainstream for many years, and there is a body of work in the literature on pedagogically sound strategies for using simulation [1,2]. One compelling feature of process simulation software is that, once the model is complete, users can change a single parameter, re-run the simulation, and immediately see the effect of the change on the process outcomes. In this way, process simulation software can be used to support an inductive exploration of the cause-and-effect relationships in the physical process being modeled. However, one possible pedagogical challenge associated with process simulation is that the software can act as a "black box;" students can see the output but the underlying model equations and modeling assumptions are not always readily apparent to the user. This danger is addressed when students build their own models of physical systems, but the 160 minute time frame limits the complexity of the model that can be employed.

The two modules described in this paper are intended to combine the best attributes of the two types of computer lab described above. Students will go through the thought process associated with identifying relevant physical principles and writing the key model equations, but are not then required to implement and solve the equations themselves. Instead, they will, at this point, be presented with a complete, working model. The two models were developed during the Spring of 2017 by chemical engineering juniors and seniors as an Engineering Clinic project. One is implemented in POLYMATH and the other in Microsoft EXCEL. These are the same tools students are accustomed to using when building their own models, and the model equations are readily accessible to the user in each. Students can then progress to exploring cause-and-effect as they do in the ASPEN labs.

The next two sections give specifics concerning the two modules.

Chemical Reaction Engineering Module

A foundational concept in reaction engineering is the use of mole balance equations to model the relationship between extent of chemical reactions and an independent variable such as reactor volume or reaction time. For several standard types of reactor (e.g., plug flow, batch, semi-batch) the mole balances are ordinary differential equations; one equation for each chemical compound present in the system. POLYMATH software is commonly used for solution of the ODEs [3]. The Folger textbook [4], which has been used at Rowan University for the last several years, integrates POLYMATH programs and results generated from POLYMATH in both the solution manual and examples within the text itself. However, the number of simultaneous ODEs is typically 5 or fewer in textbook examples and homework problems.

The Chemical Reaction Engineering module, which is expected to occupy one double-period, involves the thermal cracking of propane. Thermal cracking proceeds by free-radical reaction mechanisms and the number of individual elementary reactions required for a mechanistic model is quite large. A published reaction mechanism for propane pyrolysis [5] was used as the basis for a POLYMATH model. The approach used in developing this model consists of writing an ODE for each chemical species (including stable compounds and free radicals) that is present in the system. This process is conceptually no different from that employed throughout the Fogler text. However, the reaction mechanism is large and complex enough that it takes several hours to run a single simulation on a conventional laptop such as owned by the typical engineering student. Consequently, while students in the introductory course should be capable of writing and understanding the individual model equations, having students run the model themselves is impractical in a classroom or lab setting. However, a number of these long simulations, representing a range of operating conditions (various temperatures, various pressures etc.), have already been completed by the 2017 Engineering Clinic team, and the results are available in both figure and table formats.

The module that was developed involves:

(1) Having students model propane pyrolysis using a simplified approach, the pseudo-steady state hypothesis (PSSH), which is covered in Chapter 9 of the Fogler text.

(2) Presenting the students with experimental results that well match the results of the PSSH model, and other experimental results which the PSSH model is incapable of explaining.
(3) Discussing the assumptions behind the PSSH model and how these relate to the physical situations in the experiments, and also exploring how to develop a more rigorous model.
(4) Sharing the results of the already-completed simulations, challenging students to explain the cause-effect relationships revealed by these results, and to explain why the results are in some cases substantially identical to the PSSH results and in other cases fundamentally different.

The student deliverable will be a 2-3 page write-up of the results and answers, due one week after the double period in which the work is completed.

Chemical Engineering Thermodynamics II Module

The Thermodynamics II module, which will also be integrated into the course as a computer laboratory, involves modeling of vapor-liquid equilibrium. A major learning objective of the course is students learning to apply and use models such as the Wilson model to vapor-liquid equilibrium systems. One type of textbook example problem involves presenting students with a data set (e.g., data at a single temperature and multiple pressures) such as that shown in Figure 1, and challenging students to produce the "best-fit" parameters that maximize agreement between the data and the model, the results of which are also illustrated in Figure 1. In the class as taught in recent offerings (through Spring 2017), problems like this were integrated as examples in lecture and assigned as homework problems. In such problems, either temperature or pressure was held constant.

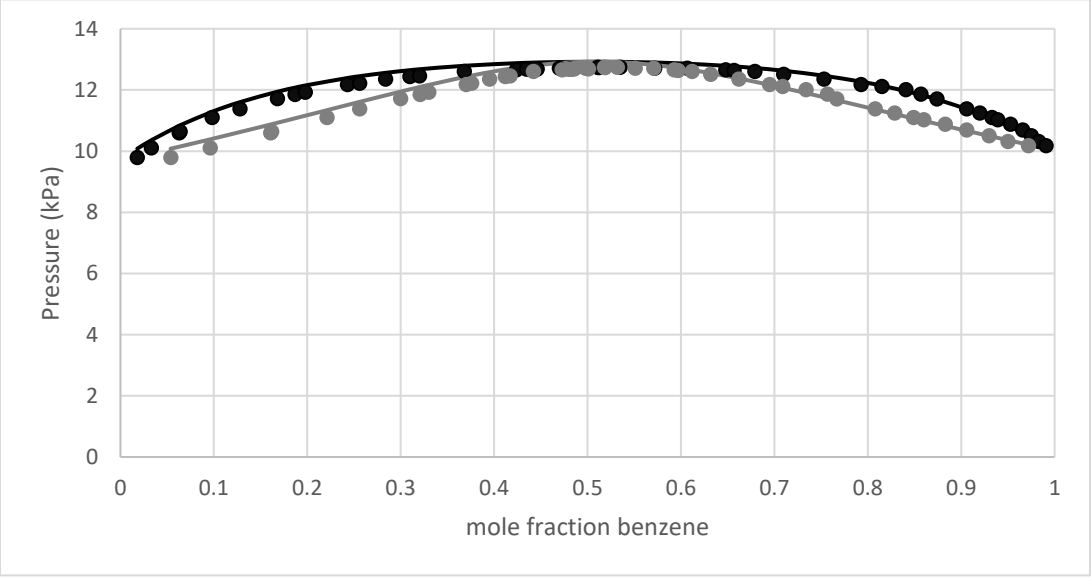

Figure 1: P-x-y diagram for benzene and acetonitrile at T=25 °C. Symbols represent data obtained from [6] and lines represent results obtained from the Wilson model. Black represents saturated liquid and grey represents saturated vapor.

What the new module does is extend this process to a much larger data set (including varying both temperature and pressure). As in the Chemical Reaction Engineering module, a model has already been constructed using Microsoft EXCEL and students will be able to interrogate it, seeing results in both tabular and graphical form and examining the effect of changing parameters.

The specific physical system examined is mixtures of butanol and cyclohexane. The data was obtained from the Dortmund Data Bank, accessible at (http://www.ddbst.com/en/EED/VLE/VLE%201-Butanol%3BCyclohexane.php), and the Data Bank attributes [7] and [8] as the original sources. An example result is shown in Table 1. The Wilson model, when applied to a binary mixture of compounds, involves two adjustable parameters called $\acute{\alpha}_{12}$ and $\acute{\alpha}_{21}$ that are assumed to be characteristic of that pair of compounds and constant with respect to temperature and pressure. However, it is important to stress that Wilson is a semi-empirical model. Many quantities that are used importantly in Thermodynamics are fundamental state properties like enthalpy, entropy and internal energy that have unique, measurable values. Students do not always appreciate that the adjustable parameters in a semi-empirical model do not fall into this category. The results in Table 1 are intended to challenge possible student misconceptions regarding the uniqueness of "best fit" parameters.

Additional uses of the larger data set include:

(1) Illustrating the difference in accuracy that is expected when using a correlative model to interpolate vs. using it to extrapolate.
(2) Allowing students to quantify "agreement" between data and model for different values of $\acute{\alpha}_{12}$ and $\acute{\alpha}_{21,}$ illustrating how training a model using larger data sets at multiple conditions produces a model that is more robust and more broadly applicable.

Table 1: Best fit parameters determined when applying the Wilson model to different data sets for vapor-liquid equilibrium mixtures of butanol (1) and cyclohexane (2).

Data Set	$\acute{\alpha}_{12}$ (J/molK)	$\acute{\alpha}_{21}$ (J/molK)
T=50 °C only	282.5	9803
T=70 °C only	372.3	8360
T=110 °C only	125.9	4827
All data at all temperatures	506.2	6024

Here again, the activity is intended as a computer lab and the student deliverable will be a write-up due one week after the double period in which the activity is completed.

Assessment

Building models and interpreting model results are fundamental aspects of engineering practice. The two modules presented here are intended to allow students to delve deeper into the challenges associated with modeling two important and complex physical systems, without dedicating the class time that would be required for students to build and run the model

themselves. A goal of these modules is to heighten students' awareness of some of the key aspects of using models, such as recognizing limitations and the significance of assumptions, appreciating the distinctions between correlative and predictive models and between theoretical and empirical models, etc. Exams in Chemical Reaction Engineering and Chemical Engineering Thermodynamics II have routinely included problems that tested the students' facility at making logical model-building decisions and interpreting results. An example from Chemical Engineering Thermodynamics II is shown here:

> This problem concerns vapor-liquid equilibrium for a pair of compounds, identified as 1 and 2:
>
> You have five known VLE data points at 325 K. Your task is to generate the Pxy diagram describing all VLE mixtures of these compounds at 325 K, using phi-phi modeling and the Peng-Robinson equation.
>
> A) If the value of the binary interaction parameter is k_{12}=0.1, determine the values of the Peng-Robinson parameters a_m and b_m that you would use to model a vapor phase mixture composed of 65 mol% component 1.
> B) The table below shows the five data points, and corresponding predictions from the Peng-Robinson equation of state made using the binary interaction parameters k_{12}=0.1 and k_{12}=0.3. If your ONLY options were to use either k_{12}=0.1 or k_{12}=0.3, which would you pick? Indicate clearly the criterion you as using for determining which is "better".

Actual Experimental Data			P-R, with k_{12}=0.1			P-R, with k_{12}=0.3		
x_1	y_1	P (bar)	x_1	y_1	P (bar)	x_1	y_1	P (bar)
0.1	0.16	8.3	0.1	0.14	8.3	0.1	0.16	8.1
0.3	0.48	9.0	0.3	0.46	9.0	0.3	0.48	8.8
0.5	0.66	10.1	0.5	0.65	10.2	0.5	0.65	9.9
0.7	0.81	11.5	0.7	0.79	11.5	0.7	0.80	11.3
0.9	0.91	13.0	0.9	0.88	13.0	0.9	0.91	12.8

The authors will assess the effect of integrating the two modules into Chemical Reaction Engineering and Chemical Engineering Thermodynamics II by examining whether student performance on such problems improved in Spring 2018 compared to previous offerings of the courses that had the same instructional objectives but did not use the computationally-intensive modules. In addition student opinion will be solicited through questions integrated into the year-end course and teacher evaluation. These results are not available at time of writing but will be presented at the conference in June 2018.

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