A STUDENT-LED APPROACH TO INTEGRATE ASPEN PLUS® IN THE CHEMICAL ENGINEERING CURRICULUM AT THE UNIVERSITY OF KANSAS

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INTRODUCTION

Simulations and modeling software are increasingly used today for process design applications. This is especially true in the chemical engineering field when reaction chemistry, thermodynamics, and fluid mechanics are often required to construct chemical processes and manufacturing plants. Chemical engineering departments have incorporated ASPEN Plus® process modeling into many undergraduate curriculums so that students are better prepared to use such tools after graduation in an industrial setting.[1-6]

The Chemical and Petroleum Engineering Department (C&PE) at the University of Kansas (KU) has introduced the use of ASPEN Plus® version 10 (hereafter referred to as ASPEN) into the chemical engineering undergraduate curriculum from freshmen to senior years. While common pedagogical methods to teach ASPEN refer to lessons from a professor, the approach at KU also includes a student-led method in collaboration with a faculty advisor.[1,2,5] The first author, a 2020 BS chemical engineering graduate from KU, worked with a faculty advisor (second author) from his freshmen to senior years (2016-2020) to create ASPEN simulations for each of the courses he took throughout his undergraduate education. The authors chose to create example problems for each course that could first be worked by hand and then compared with simulations performed using ASPEN. The authors also felt that students learn best using a variety of delivery methods. Simulations were created, and both videos and handouts were prepared for in-class lectures.[7] The student author led the lectures as well as prepared homework problems and answer keys for the course graders.[8,9] The student's peers enjoyed the student-led learning experience, resulting in increased class participation and feedback.

This article presents the simulations that were created for integrating ASPEN into the chemical engineering courses at KU. Key principles used in each simulation will be highlighted with direct comparisons to the methods and content taught in the respective course. The student-led teaching experience with advisor guidance was extremely effective in teaching ASPEN and integrating the software throughout the KU chemical engineering curriculum from freshmen to senior year. Student feedback and supporting information is available upon request from Dr. Mark B. Shiflett at mark.b.shiflett@ku.edu. The videos are free and available at www.shiflettresearch.com and also through the YouTube channel Shiflett Lab Group at https://www.youtube.com/channel/UCPluIlsSMIkTE9UE3HHyD8g.

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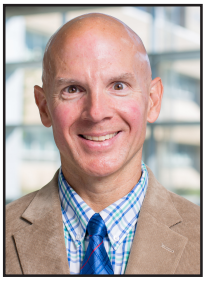

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ASPEN SIMULATIONS FOR UNDERGRADUATE COURSES AT KU

Material and Energy Balances: The Hydrogenation of Benzene to Cyclohexane

Instructional materials to introduce ASPEN for the Materials and Energy Balance course (C&PE 211) include a set of nine videos and nine accompanying written handouts. The cumulation of all these example videos results in the complete plant simulation for the hydrogenation of benzene to cyclohexane process. The goals for these video modules are to teach students the fundamental features of ASPEN, introduce new concepts that students are learning in the course as well as future courses, and help students understand that process simulators can analyze problems too complex to perform by hand calculations.

Each sequence consists of a video and handout. The first sequence (Chapter 1: Part 1) introduces how to set up a new simulation in ASPEN, how to input the chemical components of the hydrogenation process, the methods required for the simulation, and how to begin constructing the hydrogenation flowsheet. This simulation is also taught in person through a class lecture. Unit operations such as a pump, mixer, and heat exchanger are also introduced. The user can specify variables such as the mass flow of benzene through the pump, hydrogen feed impurity, and operating temperature and pressure in order to calculate the heat duty and outlet mass flow rate of products from the heat exchanger in the simulation. Determining the outlet stream compositions through mass balances and illustrating a process diagram are the first principles taught in C&PE 211 and are well supported through this first video module.

The second sequence (Chapter 1: Part 2) builds upon the hydrogenation flowsheet by introducing a reactor, cooler, and flash unit blocks. The hydrogenation of benzene to cyclohexane reaction is introduced when specifying the reactor. Utilizing fractional conversion in a reactor and chemical stoichiometry to determine outlet compositions are common exercises in C&PE 211. The heat duty produced by the reactor is also an output of the simulation.

The third sequence (Chapter 1: Part 3) introduces a splitter block, compressor block, purge stream, and recycle stream to the hydrogenation flowsheet. A recycle stream is necessary to limit the waste of hydrogen and cyclohexane, and the purge stream is used to prevent vapor buildup in the system. Material balances incorporating recycle and purge streams are concepts also taught in the course. In this chapter, features shown in ASPEN include changing unit sets and producing heat curves for heat exchangers. Specifically, a heat curve is produced, demonstrating the heat loss, temperature, and vapor pressure for the heat exchanger.

With the core structure of the hydrogenation simulation complete, the next few chapters of the cyclohexane process are devoted specifically to analytical techniques and unit blocks found in ASPEN. The fourth video of the hydrogenation series (Chapter 2) introduces how to set up and execute a sensitivity analysis block. This simulation demonstrates the sensitivity of the ratio of hydrogen to benzene in the 4-MIXHOT stream to changes in the temperature and molar flow rate of the inlet hydrogen stream (5-H2 as shown in Figure 1). First, the exercise shows the effect of ratio changes from 280 kmol/hr to 305 kmol/hr in the 5-H2 stream. Simultaneously with the range of mole flows of hydrogen, temperature is also varied from 47 °C to 49 °C. The results from this test can be calculated from material balance methods taught in the C&PE 211 course or intuitively deduced, that is, increasing hydrogen mole flow leads to a higher hydrogen to benzene ratio in the 4-MIXHOT stream, with temperature having no effect. The heat exchanger (Chapter 2) models the heat dissipated on the hot side as previously shown from the heat curve introduced in Chapter 1: Part 3. The next hydrogenation series tutorial (Chapter 3) introduces a heat exchanger (B10-HTEX) that measures the energy absorbed from the hot side by introducing a counterflow water stream, the "cold side." Chapter 3 also demonstrates how to replace the B5-COOL block with the HTEX heat exchanger, specify the parameters for the new heat exchanger, and observe the results of the HTEX cooling block. The inlet water temperature is specified at 27.0 °C, and with all variables kept constant, the observed outlet water temperature is 46.6 °C from the heat duty generated by the 6-ALL stream.

In ASPEN a calculator block is another analytical tool that can conduct similar sensitivity analyses using computer statements such as FORTRAN. For the hydrogenation series, the calculator block is introduced by demonstrating how to

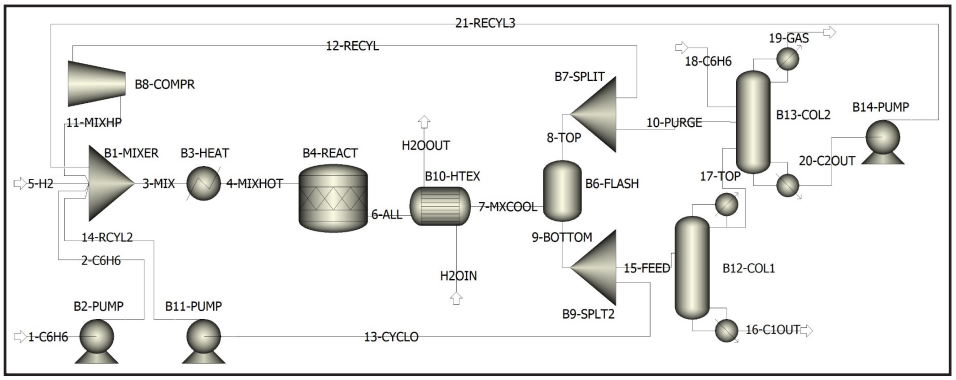


Figure 1. *Complete hydrogenation of benzene to cyclohexane ASPEN model.*

change the temperature of the B10-HTEX heat exchanger by varying the 5-H2 inlet stream temperature. This tutorial (Chapter 4) changes the 5-H2 inlet temperature from 50°C to 51°C, shows how to set up and specify a calculator block, and shows the FORTRAN statement to increase the B10-HTEX temperature to 52°C. A second example shows how to set up the hydrogen and benzene molar flows in the 4-MIXHOT stream, obtain their ratio, and compare the results with the sensitivity analysis from Chapter 2. Similar to the first exercise, the tutorial demonstrates how to create a new calculator block for this test, which parameters to specify, and how to create the variables to input as FORTRAN statements. Once the simulation is run, the results of the calculator block show the molar flow of the 4-MIXHOT stream. The ratio between these values is equivalent to the result obtained from the sensitivity analysis.

The seventh hydrogenation series tutorial (Chapter 5) is dedicated to simulating a DSTWU distillation, a simplified distillation design. Utilizing reflux ratios to determine output compositions of distillation columns is a key exercise performed in C&PE 211. These videos and handouts demonstrate how to create and specify a DSTWU distillation column that will be used to complete the hydrogenation simulation. The inlet stream of methanol, water, and phenol at mass fractions of 0.60, 0.39, and 0.01, respectively, enter the column at a flow rate of 4530 kg/hr and a temperature and pressure of 65 °C and 1.7 bar. The column's condenser and reboiler operate at 1.1 bar and 1.7 bar, respectively. With a recovery fraction of methanol in the distillate set to 0.99, the recovery fraction of water in the bottom stream is set to 0.01. The generated results for this simulation include outlet compositions of the distillate and bottom streams, as well as reflux ratios at different stages of distillation that will be used for the next distillation model of the hydrogenation series.

RadFrac distillation, a more rigorous distillation calculation model, is simulated for Chapter 6. The feed stream to the column is composed of methanol, water, and phenol with mass fraction compositions of 0.60, 0.39, and 0.01, respectively. The total mass flow rate to the column is 4530 kg/hr with an operating temperature and pressure of 65°C and 1.7 bar. The distillation column has 10 stages, a distillate flow rate of 2720 kg/hr, and a reflux ratio of 0.8. The feed stream enters above the sixth stage, and the condenser operates at 1.1 bar with a column pressure drop of 5.08 cm-water (2 inches-water). In addition to determining the compositions of the outlet streams and reflux ratio profile from the DSTWU model exercise, the results of the RadFrac simulation show the temperature and heat duty of the top condenser stage and bottom reboiler stage. In addition this chapter shows how to create a temperature profile as a function of stages for the RadFrac column. A design specification block is used to optimize the reflux ratio to 7.5 to achieve a mass fraction purity of 0.996 methanol in the distillate stream.

The final tutorial of the hydrogenation series (Chapter 7) completes the simulation by adding additional streams and blocks, new RadFrac distillation columns, and adjustments to the sensitivity analysis. A split block, B9-SPLT2, is introduced to the bottom of the B6-FLASH block to create an additional recycle stream with a pump that feeds into the B1-MIXER. Another outlet from the B9-SPLT2 block will feed into a series of RadFrac distillation columns, which create a third overall recycle stream (21-RCYL3) with a pump and outlet cyclohexane product stream (19-GAS) as shown in Figure 1. The inlet stream (18-C6H6) of the second RadFrac column (13-COL2) operates with a 500 kg/hr flowrate of pure benzene at 5 °C and 4 bar. The H2OIN stream for the B10-HTEX block operates with a 175,000 kg/hr flowrate of water at 30 °C and 4.5 bar and the RadFrac column specifications are the same as described in Chapter 6. Once the simulation is complete, 7.00 kg/hr of cyclohexane is produced from the 19-GAS stream.

Introduction to the Chemical Engineering Profession I: Distillation of Glycerol, Methanol, and Water

Freshman students entering the chemical engineering program at KU take Introduction to the Chemical Engineering Profession I (C&PE 111), a 1-credit hour course that exposes students to fundamental calculations in material and energy balances, career opportunities in chemical engineering, laboratory safety, engineering ethics, and technical writing. A new laboratory component was introduced in Fall 2019 where students get hands-on experience with lab-scale chemical engineering processes and unit operations to produce, purify, and test the quality of biodiesel. In this lab a byproduct of the biodiesel process is a glycerol solution that also contains methanol and water. While learning about basic distillation concepts in lecture, students learn to operate a fractional distillation column in the lab and distill a glycerol solution to recover methanol. Later, for a post-lab assignment, the students then simulate this experiment using ASPEN.

One of the 50-minute lecture periods is devoted to teaching the students via video and handout how to simulate a distillation column using ASPEN. Although devoted to C&PE 211, the DSTWU module (Chapter 5) of the hydrogenation series is used to teach C&PE 111 students how to simulate a simple distillation column. The students are also given a handout to fill in information taught in class during the lecture. The first ASPEN assignment simulates a continuous distillation of glycerol solution to separate methanol and water. Students use data measured in lab to create the simulation using the DSTWU model with the NRTL-RK method. Although some of these concepts, such as the NRTL solution model and the RK equation of state (EoS), are new to the students, there is an important connection that can be made to future classes the students will take, such as thermodynamics. The students appreciate getting a view of what is to come; there-

fore, introducing some of these topics early led to questions and good discussions with the students about future course topics. A glycerol solution flow rate of 0.045 kg/hr, feed mass fraction of 0.3, 0.05, and 0.65 for methanol, water, and glycerol, respectively, and a 0.93 mole fraction recovery of methanol were specified to simulate the experimental results obtained in the lab.

Students compare their experimental recovery of methanol measured in lab with their ASPEN model results. With a feed mass flow rate of 0.045 kg/hr, 0.013 kg/hr of methanol was recovered in the distillate from ASPEN, which is approximately the amount students found experimentally if they ran a continuous process. The distillate and bottom stream temperatures from ASPEN were 64.58 °C and 124.72 °C, respectively, which agrees well with temperatures measured by students using the fractional distillation setup in the lab. Demonstrating how ASPEN simulations can accurately predict experimental results helps reinforce to students the benefits of process simulation software and modeling in the chemical engineering profession.

Thermodynamics I: Adiabatic Turbine & Rankine Power Generation Cycle

Two sets of videos with accompanying written handouts and lecture tutorials were created for the Thermodynamics I (C&PE 221) course. The tutorials draw inspiration from Prof. Stan Sandler's textbook that is used for the course.[10] Prof. Sandler has been using software such as MathCad and ASPEN for over 20 years when teaching thermodynamics and has written a book with step-by-step instructions on teaching ASPEN in thermodynamics instruction.[11]

The first ASPEN tutorial demonstrates how to construct an adiabatic turbine (Figure 2) using the following problem:

> *An adiabatic turbine expands steam from 500 °C and 3.5 MPa to 200 °C and 0.3 MPa. If the turbine generates 750 kW, what is the flow rate of steam through the turbine?*

This example was chosen so students early in the course can (1) practice solving it using material and energy balances, (2) prepare assumptions for the problem, (3) understand the topic of isentropic efficiency, and (4) conceptualize the unit operation, which provides the students a better understanding of how the adiabatic turbine will be constructed in ASPEN.

The adiabatic turbine example was introduced to the class during a 50-minute lecture period, and a graduate teaching assistant demonstrated how to solve the problem by using material and energy balances and physical properties of steam. Once the principles for the problem are demonstrated in class, the same problem is simulated in ASPEN for the students. This includes setting up the simulation physical properties and methods, creating the structure of the turbine (Figure 2), specifying input variables, and analyzing the results. This simulation is run with a steam flow rate of 1 kg/hr through the turbine as shown in Table 1. The power generated (750 kW provided in the problem statement) divided by the calculated horsepower (-0.1627 kW of work produced per 1 kg/hr of steam) shown in Table 1 results in the answer of 4,609 kg/hr of steam through the turbine.

The student's proficiency with ASPEN is also tested using the following homework problem:

> *An adiabatic turbine operates at an isentropic efficiency of 0.6 inputs steam at 500 °C and 3 MPa. With an outlet pressure of 500 kPa, determine the actual power generated and actual exit temperature of the outlet stream if 50 kg/hr of steam flows through the turbine. Verify your answers by also simulating this problem using ASPEN Plus.*

In addition to the principles taught in lecture for the adiabatic turbine example, an entropy balance must be performed in the student's ASPEN homework assignment.

Later in the course lecture, practical applications of material, energy, and entropy balances are demonstrated through power and refrigeration cycles. Thus, building on concepts of the adiabatic turbine, a Rankine power generation cycle example is introduced to apply the content of this section of the course in ASPEN (Figure 2). Specifically, the second ASPEN tutorial demonstrates how to construct a Rankine power generation cycle using the following problem:

> *A Rankine power generation cycle using steam operates at a temperature of 100 °C in the condenser, a pressure of 3.0 MPa in the evaporator, and a maximum temperature of 600 °C. Assuming the pump and turbine operate reversibly, determine the heat required and the amount of work produced by this cycle.*

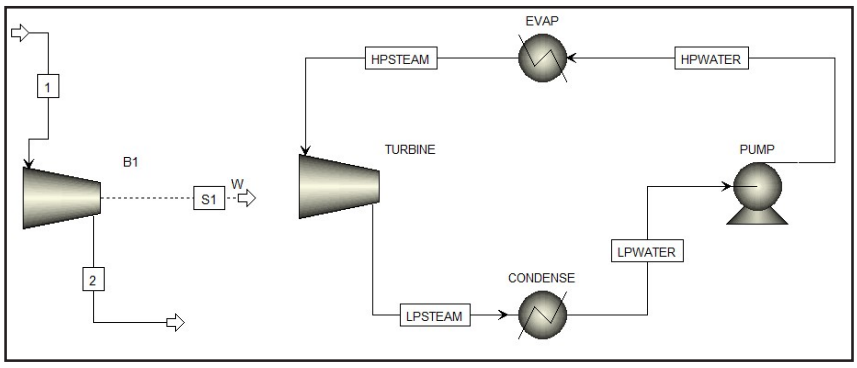


Figure 2. *Turbine (left) and Rankine power generation cycle (right) simulated in ASPEN.*

In similar fashion to the adiabatic turbine, this simulation provides students with a practical and visual understanding of the functionality of a Rankine power generation cycle and each of its components. More complex solutions unable to be completed manually can be shown to be easily computed using ASPEN.

In addition, a graduate teaching assistant illustrates this cycle in class on a temperature-entropy (T-s) diagram for steam and highlights the isobaric and isentropic components of the process, as well as how to obtain enthalpy values to manually solve for how much heat is required and how much work is produced. Next, the cycle is constructed and simulated using ASPEN, and a written handout and video module are provided to students to construct the Rankine power generation cycle.

A second ASPEN based homework assignment is given to the students to complete:

> *A Rankine power generation cycle using steam operates at a temperature of 300 °C in the condenser, a pressure of 15.0 MPa in the evaporator, and a maximum temperature of 550 °C. Assuming the pump and turbine operate reversibly, determine:*
>
> *a) The required work for the pump*
> *b) The heat required for the evaporator*
> *c) The work produced by the turbine*
> *d) The heat produced by the condenser*

This assignment builds on principles taught during the in-class lecture but requires the students to perform material, energy, and entropy balances on each component of the power generation cycle to understand each stage of the process. Written solutions, ASPEN results (Table 1), and a hand-drawn visualization of this cycle on a T-s diagram must also be submitted.

Thermodynamics II: Binary Phase Diagrams

ASPEN is used in the Thermodynamics II course (C&PE 512) to demonstrate different EoS (e.g. Redlich-Kwong and Peng-Robinson) and activity coefficient (e.g. NRTL, Margules, and Wilson) models for describing phase behavior of multi-component mixtures. Applications of Raoult's law and ideal mixtures are taught in class, while more complex models used to characterize non-ideal mixtures can be simulated using ASPEN. Students gain a visual representation of using activity coefficient and empirical-based predictions of phase equilibria that are not limited by computation or complexity, a key benefit in using simulation programs such as ASPEN.

To introduce ASPEN in this course, a video module and supplemental written handout are used to perform the following simulation:[10]

> *Create P-x diagrams for a benzene-ethanol system at 45 º C using the UNIFAC model and assuming the mixture is ideal.*

TABLE 1
ASPEN Plus® V10 simulation results for C&PE 221.

Exercise	Component	Net work required [kW]	Net duty [kJ/hr]	Efficiency	Outlet pressure [bar]	Outlet temperature [°C]	Isentropic outlet temperature [°C]
In-class Adiabatic Turbine	Turbine	-0.16		0.89	3	200.00	166.29
In-class Rankine Power Generation Cycle	Evaporator		3260.64		30	600	
	Turbine	-0.26		1	1.014	129.69	129.69
Homework Assignment Rankine Power Generation Cycle	Pump	0.003		1	150	302.85	
	Evaporator		2096.37		150	550	
	Turbine	-0.05		1	85.81	451.91	451.91
	Condenser		-1924.5		85.81	300	

The pressure-composition (P-x) diagram for both methods is shown in Figure 3. The P-x diagram generated through ASPEN using the ideal mixture method closely matches a P-x diagram created by hand calculating the values and plotting them. Using ASPEN to assist in simulating the UNIFAC model, the generated P-x diagram provides the correct representation for the pressure versus composition behavior of the binary mixture with a well-defined azeotrope.

Momentum Transfer: Applications of Bernoulli's Equation

Key relationships and phenomena of fluid flowing through pipes are illustrated by Bernoulli's equation or variations of Navier-Stokes equations. Thus, an introduction to ASPEN for the Momentum Transfer course (C&PE 511) is illustrated by simulating the observations and relationships governed by these equations in the following exercise:[12]

Create a simulation of water flowing through a carbon-steel 3-inch schedule 40 pipe that is 30 feet long. Calculate the pressure difference in the pipe by changing the elevation to 10 feet, nominal-diameter to 6 inches, and length to 60 feet, individually.

An example flowsheet of the simulation is shown in Figure 4. A video module and accompanying written handout teach students how to construct the simulation. This simulation has each pipe inlet operating at a temperature of 93.33 °C (200 °F), a pressure of 690 kPa (100 psia), and a water flowrate of 10,000 kg/hr. The base pipe is specified to be a 9.14-meter (30 feet) long, 76.2-millimeter (3-inch) diameter carbon-steel schedule 40 pipe with default roughness and erosional velocity coefficient values found in ASPEN. A "10-foot (10FT)" long pipe has the same specifications as the base pipe, with an elevation of 3.048 meters (10 feet). In addition, a "6-inch (6IN)" diameter (0.15 meters) pipe has the same specifications as the base pipe. The final "60-foot (60FT)" pipe has the same specifications as the base pipe, with a pipe length of 18.28 meters (60 feet). Simulating all four pipes simultaneously illustrates the relationship each variable (elevation, diameter, and length) has on pressure drop.

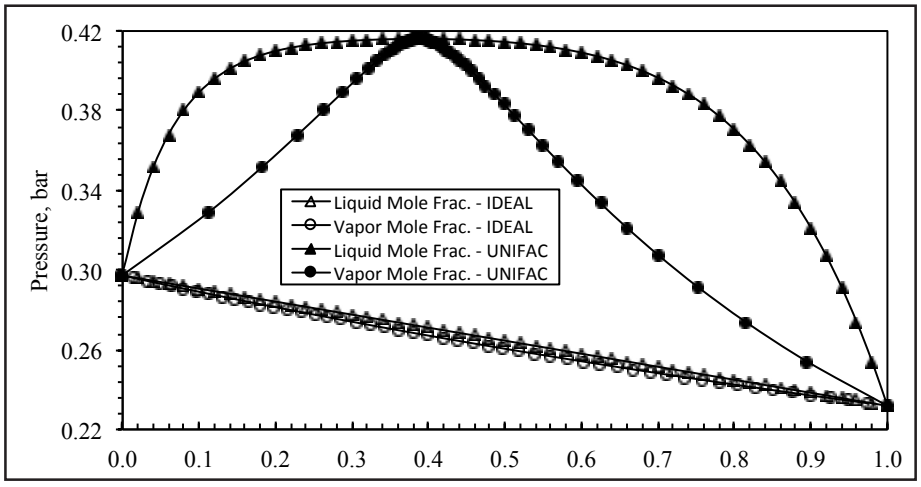


Figure 3. *P-x diagram of benzene-ethanol system at 45 °C simulated in ASPEN using IDEAL and UNIFAC Models.*

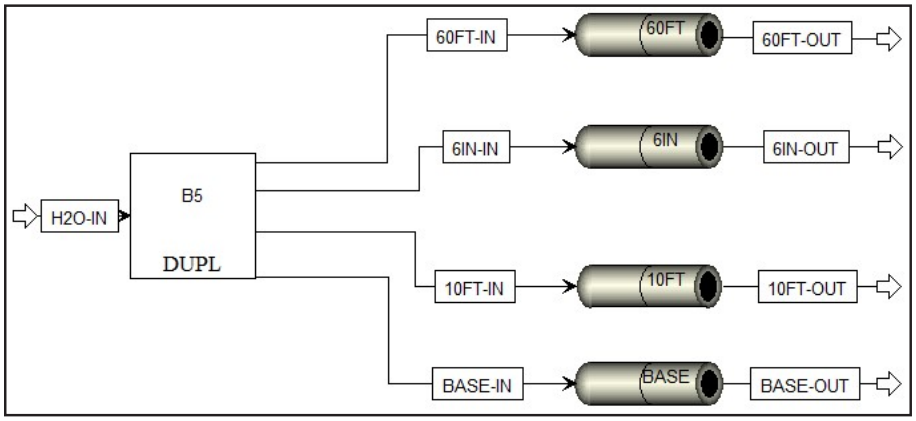


Figure 4. *Flowsheet of the ASPEN simulation designed for C&PE 511.*

In addition to introducing pipes in ASPEN, the learning goals of this simulation are to describe both the quantitative and qualitative results of principles taught in class. For example, the decrease in pressure at the outlet of the base pipe is a result of frictional losses as water flows through the 9.14-meter (30-foot) pipe as shown in Table 2. In comparison the expected pressure drop with an elevation of 3.048 meters (10FT) is greater than the base pipe pressure loss due to additional potential energy of the elevated pipe. The increase in nominal pipe diameter to 0.15 meters (6IN) leads to the expected increase in the outlet pressure with respect to the base pipe case due to the decrease in kinetic energy losses. In contrast to the base pipe, the outlet pressure is lower in the 18.28-meter (60FT) long pipe, which is a result of increased frictional losses along the length of the longer pipe.

TABLE 2 Inlet and Outlet Pressures for pipes using ASPEN simulation in C&PE 511.							
BASE-IN	BASE-OUT	10FT-IN	10FT-OUT	6IN-IN	6IN-OUT	60FT-IN	60FT-OUT
690 kPa	689 kPa	690 kPa	660 kPa	100 psia	690 kPa	690 kPa	689 kPa
(100 psia)	(99.94 psia)	(100 psia)	(95.77 psia)	(100 psia)	(99.99 psia)	(100 psia)	99.88 psia)

Economic Appraisal of Chemical & Petroleum Projects: Aspen Process Economic Analyzer

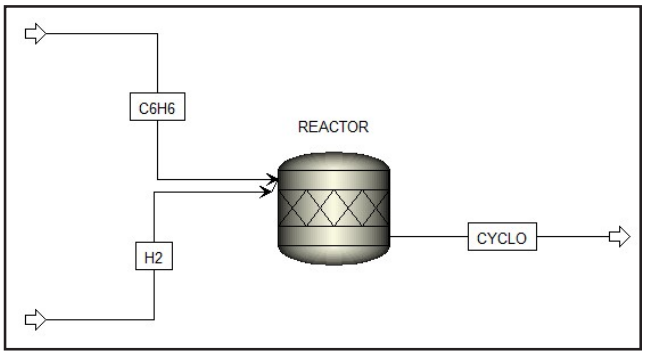
The Economic Appraisal course (C&PE 522) introduces economic evaluation methods, risk, and ethics. Economic factors important in the development of the chemical or petroleum enterprise are discussed using project development examples. One of the main engineering applications of the course is determining a project's Minimum Acceptable Rate of Return (MARR). Common factors to consider for these applications are loan payments over time, depreciation, and taxable income. To introduce ASPEN, an economic analysis is conducted to determine whether a hypothetical project that is simulated in ASPEN should be approved for construction. For example, the following hydrogenation project is provided to the class:

> *Two inlet streams, one with 300.3 kmol/hr of pure hydrogen and the second with 7105 kg/hr of pure benzene, operate at 25 °C and atmospheric pressure. The streams enter a stoichiometric reactor operating at 100 °C and 5 atm, where 99.8% of the benzene is converted to cyclohexane. Cyclohexane, measured in ktonne/year, is obtained from the single outlet stream from the reactor.*

Once this project has been simulated (Figure 5), the Aspen Process Economic Analyzer (APEA) is used to estimate the capital and operating costs. This feature of ASPEN provides estimates for the hydrogenation project, specifying the initial start-up costs and yearly recurring costs to create cyclohexane (Figure 5). Using these cost values, the second section of the written handout provides the financial parameters to determine the feasibility of the project:

> *Assuming negligible inflation over the 8-year life of this production, the initial and reoccurring costs of this process are obtained from the Aspen Process Economic Analyzer. The total initial costs of the operation will be borrowed from the bank. This loan will be paid back in seven equal annual payments, where the interest rate on the loan is a flat 7% per year. This unit will be classified as a 7-year Modified Accelerated Cost Recovery System (MACRS) depreciation property with no salvage value at the end of the 7 years. With the current market for cyclohexane being ~$2000/tonne ($2/kg), this operation will generate income based on how much cyclohexane is produced per year. The current income tax rate is 25%, and this operation will have a MARR of 15%. Should the team carry out this operation?*

Using evaluation methods from lecture, the cumulative present worth of the hydrogenation project is substantially greater than zero at a MARR of 15% as shown in Table 3, so this project is financially profitable and should be approved for construction. The ASPEN hydrogenation model simulates that cyclohexane is produced at a rate of 66.9 ktonne/year, generating $133,940,400/year in revenue for its 8-year lifespan, assuming a constant market price of $2/kg ($2000/tonne) for cyclohexane. The total capital, equipment, and installation costs from the APEA (Figure 5) will be financed by a loan from the bank equaling $2,249,070 paid in yearly



Enabled by **Aspen Process Economic Analyzer (APEA)**

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Summary | Utilities | Unit operation | Equipment | Agitated reactor

Total Capital Cost [USD]	1,958,570
Total Operating Cost [USD/Year]	1,303,330
Total Raw Materials Cost [USD/Year]	0
Total Product Sales [USD/Year]	0
Total Utilities Cost [USD/Year]	43,146.5
Desired Rate of Return [Percent/Year]	20
P.O. Period [Year]	0
Equipment Cost [USD]	75,100
Total Installed Cost [USD]	215,400

***Figure 5**. Hydrogenation flowsheet for C&PE 522 simulation with Aspen Process Economic Analyzer results.*

increments, which includes the loan payment principal and the 7% loan payment interest. With total operational and utilities costs from the APEA per year being $1,346,476 (Figure 5), the Cash Flow Before Taxes (CFBT) for the project is computed from the income, operating costs, amount remaining on the loan, equipment cost, and salvage values each year as shown in Table 3. MACRS depreciation factors[13] are multiplied by the initial loan amount to estimate the depreciation of the project over its 8-year lifespan. The taxable income each year is computed from the difference between the income, operating costs, depreciation, loan interest payments, and adding any salvage value as shown in Table 3. These yearly amounts are taxed at the specified 25% and subtracted from CFBT to get Cash Flow After Taxes (CFAT) for the project. These cashflow values are evaluated at both the present time and year zero and are summed to determine the net worth of the project over its 8-year lifespan.

Chemical Engineering Kinetics & Reactor Design: PFR Reactor Simulation

ASPEN simulations are ideal for designing and optimizing reactors. A number of exercises were chosen to integrate ASPEN into the Kinetics and Reactor Design course (C&PE 524). Specific exercises that can be performed by hand involve determining reaction orders, kinetic rate constants, and activation energies from empirical data. Applications for reactor design include calculating the reactor volume to achieve a specified fractional conversion, inlet and outlet compositions, and temperature or heat generation from a reactor. A video module and written handout were developed to introduce ASPEN using the following exercise:[14]

> *8000 kg of acetone per hour is fed into a PFR reactor for the vapor-phase cracking of acetone to ketene and methane. The inlet temperature is 1000 K, the pressure is 1.5 atm, and the reactor*

TABLE 3
Present worth analysis of the Hydrogenation Project at 15% MARR and effective interest rate at 7%, considering loan payments, depreciation, and taxes.

Year	Income	Operating Costs	Depreciation Factor	Depreciation	Loan Remaining	Loan Payment Interest	Loan Payment Interest	Loan Payment Principal
0					$ 2,249,070			
1	$ 133,940,400	$ 1,346,477	0.1429	$ 321,392	$ 1,989,183	$ 417,322	$ 157,435	$ 259,887
2	$ 133,940,400	$ 1,346,477	0.2449	$ 550,797	$ 1,711,103	$ 417,322	$ 139,243	$ 278,079
3	$ 133,940,400	$ 1,346,477	0.1749	$ 393,362	$ 1,413,558	$ 417,322	$ 119,777	$ 297,545
4	$ 133,940,400	$ 1,346,477	0.1249	$ 280,909	$ 1,095,185	$ 417,322	$ 98,949	$ 318,373
5	$ 133,940,400	$ 1,346,477	0.0893	$ 200,842	$ 754,526	$ 417,322	$ 76,663	$ 340,659
6	$ 133,940,400	$ 1,346,477	0.0892	$ 200,617	$ 390,021	$ 417,322	$ 52,817	$ 364,505
7	$ 133,940,400	$ 1,346,477	0.0893	$ 200,842	$ -	$ 417,322	$ 27,301	$ 390,021
8	$ 133,940,400	$ 1,346,477	0.0446	$ 100,309				

Year	Equipment Cost	Salvage	CFBT	Taxable Income	Tax @ 25%	CFAT	Present Worth@15%	
0	$ 2,249,070		$ (2,249,070)			$ (2,249,070)	$ (2,249,070)	**This project should be approved since cumulative present worth at MARR is greater than zero.**
1			$ 132,176,601	$ 132,115,097	$ 33,028,774	$ 99,147,827	$ 86,215,502	
2			$ 132,176,601	$ 131,903,883	$ 32,975,971	$ 99,200,630	$ 75,009,929	
3			$ 132,176,601	$ 132,080,784	$ 33,020,196	$ 99,156,405	$ 65,196,946	
4			$ 132,176,601	$ 132,214,066	$ 33,053,516	$ 99,123,085	$ 56,673,946	
5			$ 132,176,601	$ 132,316,419	$ 33,079,105	$ 99,097,497	$ 49,268,970	
6			$ 132,176,601	$ 132,340,490	$ 33,085,122	$ 99,091,479	$ 42,839,981	
7			$ 132,176,601	$ 132,365,780	$ 33,091,445	$ 99,085,156	$ 37,249,780	
8		$ -	$ 132,593,924	$ 132,493,615	$ 33,123,404	$ 99,470,520	$ 32,517,089	
						Σ =	**$442,723,073**	

runs adiabatically. What is the volume required to achieve 15% conversion of acetone, if the following reaction happens first-order with respect to acetone?

The chemical reaction and the reaction rate constant can be expressed by:

$$CH_3COCH_3 \rightarrow CH_2CO + CH_4 \quad (1)$$

$$k(s^{-1}) = 8.2 \times 10^{14}[284{,}507.816\ (J/mol)/RT] \quad (2)$$

Using the unique SYSOP0 property method in ASPEN, the vapor and liquid phases in this simulation are run assuming ideal behavior, a common assumption used for in-class exercises. Students then construct a simple plug flow reactor (PFR) flowsheet with inlet stream process conditions as stated in the exercise. Using principles taught in previous simulations, the decomposition reaction of acetone from Eq. 1 is specified in ASPEN. The pre-exponential factor and activation energy of the Arrhenius equation are introduced to specify the kinetics of the reaction in the ASPEN simulation (Eq. 2). Students can evaluate the diameter and length of the PFR to achieve the desired fractional conversion. For this example, the diameter of the PFR is 1 meter with a length of 3.2 meters, creating a volume of 2.513 m^3. This reactor design creates 20.717 kmol/hr of ketene and methane, which meets the 15% fractional conversion of acetone.

Heat & Mass Transfer: HXFlux Block

In the Heat and Mass Transfer course (C&PE 525), engineering applications are created to reinforce solutions to heat and mass transfer problems. These include Fick's law of diffusion and Fourier's law of heat conduction, chart-based and correlation-based methods for convective transfer, or a combination of heat conduction and heat convection or mass flux and free convection. Drawing from these applications, a heat exchanger simulation for this course utilizes Eq. 3 and Eq. 4 to solve for inlet and outlet stream temperatures, overall heat transfer coefficient (U), heat duty (Q), and heat transfer area (Ar). ΔT_A is the difference between the inlet hot stream temperature and outlet cold stream temperature, and ΔT_B is the difference between the outlet hot stream temperature and inlet cold stream temperature.

$$LMTD = \frac{\Delta T_A - \Delta T_B}{\ln\left(\frac{\Delta T_A}{\Delta T_B}\right)} \quad (3)$$

$$Q = U \times Ar \times LMTD \quad (4)$$

The following problem was created in a video and handout to demonstrate how to construct the heat exchanger and observe the simulated process variables:

> *A counterflow heat exchanger is used to cool down a hot stream of water from 75 °C to 50 °C. The heat transfer area is 20 m^2, and the heat duty for the heat exchanger is 200 Joules/second (J/s). If the cold counterflow inlet stream enters at 20°C and leaves at 66.9 °C, what is the overall heat transfer coefficient?*

The simulation heat exchanger is a HXFlux block that is used to perform convective heat transfer calculations between a heat source and heat sink. The HXFlux block uses the logarithmic mean temperature difference (LMTD) (Eq. 3) in the basic relationship of convective heat transfer to determine heat flow in a heat exchanger (Eq. 4). Using Eq. 4, the HXFlux block solves for the overall heat transfer coefficient as the unknown variable, which is 0.598 J/s·m^2·K (Table 4).

TABLE 4
HXFlux Block results.

Inlet hot stream temperature	75 °C
Inlet cold stream temperature	20 °C
Outlet hot stream temperature	50 °C
Outlet cold stream temperature	66.9 °C
Log-Mean temperature difference	16.726 °C
LMTD correction Factor	1
Over-all heat transfer coefficient	0.598 $J \cdot sec^{-1} \cdot m^{-2} \cdot K^{-1}$
Heat transfer area	20 m^2
Heat duty used	200 $J \cdot sec^{-1}$

RESULTS AND STUDENT FEEDBACK OF ASPEN INTEGRATION

Chemical Engineering Thermodynamics I

To assess the teaching, learning, and incorporation of ASPEN in Chemical Engineering Thermodynamics I (C&PE 221), student surveys were given after each homework assignment that used ASPEN. After the adiabatic turbine lecture and homework assignment, 69 students (78% of the class) responded that over 90% had little to no prior experience working with ASPEN before taking C&PE 221, as shown in Figure 6A. Another survey was conducted after the Rankine power generation cycle lecture and homework assignment. Eighty students (90% of the class) reported having a skill level of 2.63 (where 1 is not skilled and 5 is skilled) in using ASPEN as shown in Figure 6A. In addition, after the first homework assignment, over 85% of the responding students responded with ≥3 (3.49 average) on how effectively ASPEN enhances classroom learning on a scale of 1 (not effective) to 5 (effec-

tive) as shown in Figure 6B. The students again were asked how effectively utilizing ASPEN enhances classroom learning after the second homework assignment, with a slightly higher average score of 3.58 as shown in Figure 6B. Choosing all that applied, the videos posted on Blackboard®option were selected by 64% of the participants as one of the most popular formats for learning how to use ASPEN, followed by handouts posted on Blackboard (58%), the in-class lectures on ASPEN (45%), and self-learning (38%) as shown in Figure 6C. Students who preferred the videos commented on the ease of following along with the instruction (seeing someone actually doing the simulation live versus snapshots in a handout), having the ability to rewind the video to watch again, and being able to work at their own pace to create the simulation. To evaluate the helpfulness of solutions worked out by hand versus using ASPEN, the average score for solving the adiabatic turbine example by hand during a lecture was 3.64 (1 = not helpful; 5 = helpful) compared to using ASPEN with a higher average score of 3.75.

Based on individual comments, students thought the lectures, handouts, and videos prepared by the authors were all beneficial, as they were organized and targeted to specific concepts taught and tested in class. Engagement from students stemmed from seeing similar content they learned in class be applied in a different way through ASPEN, as it provided more practice solving problems and reinforced underlying concepts in a visual manner. Professors commented that the student-led teaching of ASPEN was beneficial for them too,

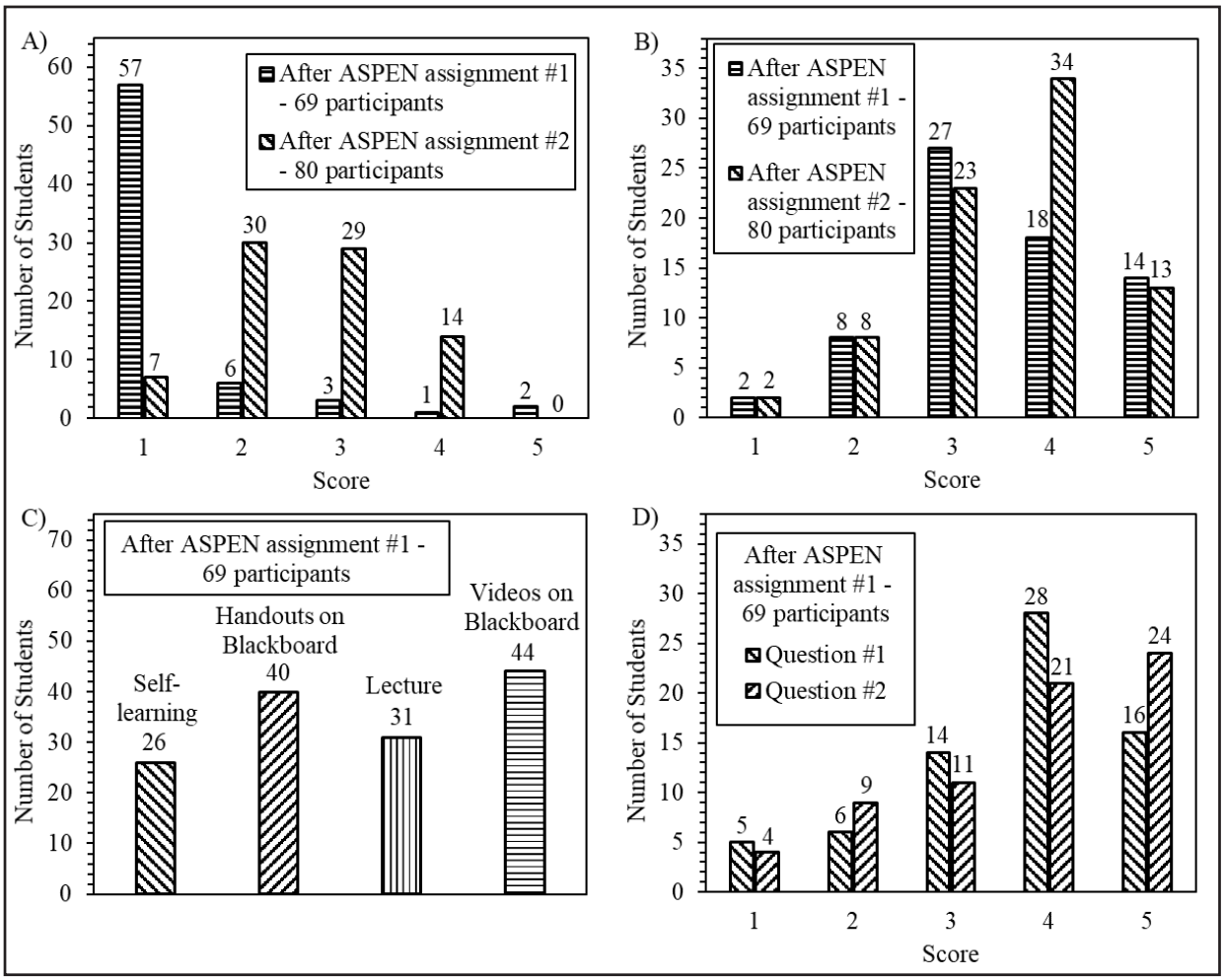

Figure 6. *Student survey responses after incorporating ASPEN in C&PE 221. After ASPEN assignment #1, students were asked* ***A)*** *how experienced were you in Aspen Plus before C&PE 211 and after ASPEN assignment #2, students were asked the same question from a score of 1 (not experienced) to 5 (experienced);* ***B)*** *how effective does the utilization of Aspen Plus enhance classroom learning after assignment #1 and #2 from 1 (not effective) to 5 (effective);* ***C)*** *which format(s) were best for learning how to create ASPEN simulations;* ***D)*** *Question #1: how helpful was doing the in-class problem by hand in understanding how to solve it in ASPEN and Question #2: how helpful was simulating the in-class problem in ASPEN for completing the homework assignment from 1 (not helpful) to 5 (helpful).*

as it offered an application-based exercise for students without committing additional time to prepare lessons, homework assignments, and videos. Learning how to use ASPEN is also believed to be beneficial for potential employment opportunities for the students, and 87% of the respondents of the second survey were interested in seeing more ASPEN modules (particularly videos) implemented in their future chemical engineering courses or a course specifically focused on ASPEN programming.

CONCLUSIONS

The KU C&PE department has incorporated Aspen Plus into the undergraduate chemical engineering curriculum using a student-led approach. Simulations have been prepared for each chemical engineering course taught from freshman to senior level classes. The simulations, along with videos, handouts, and in-class lectures, teach students how to create ASPEN simulations and reinforce fundamental concepts taught in class. The simulations and videos were created by an undergraduate senior in chemical engineering (Shao) with guidance from his advisor (Shiflett) to teach students how to use ASPEN throughout their chemical engineering courses. Data collected from this work showed that students gained increased skill in using ASPEN and indicated that learning through these student-created modules enhanced classroom learning.

Aspen Plus simulations created for each course in the KU chemical engineering curriculum incorporate fundamental concepts covered in the classroom. By doing so, students have a new means to apply and visualize content taught in each class. Student feedback supports these ideas, and the students' personal responses expressed interest in simulation learning for its potential career benefit. The videos, handouts, and lectures to teach ASPEN were effective, with the video format being highly favored due to ease of use and flexible instruction. The authors plan to create new ASPEN videos and make the material freely available via the website www.shiflettresearch.com.

ACKNOWLEDGMENTS

The authors gratefully acknowledge the donation made by Vance V. Kershner for supporting this effort. The authors would like to also acknowledge Alejandra Rocha Doresky and Dr. Sheng-Lung Lien for helping create the adiabatic turbine and hydrogenation of benzene to cyclohexane simulations, respectively. Emily Bruggeman and Tanisha Kaur are gratefully acknowledged for creating the voice-overs for the ASPEN videos. Additional thanks go to Dr. Prajna Dhar (C&PE 211), Dr. Arghya Paul (C&PE 221), Dr. Susan Williams (C&PE 111), and Dr. Aaron Scurto (C&PE 512) for providing class time to the authors to present and lecture about ASPEN simulations. The authors also acknowledge graduate teaching assistant Ankit Verma for assisting with developing ASPEN lectures and helping students learn how to use ASPEN outside of the classroom. Finally, Dr. Shiflett acknowledges Katherine Roop who worked with him at the University of Delaware to create the first ASPEN videos that served as a guide for this work.

FUNDING AND CONFLICT OF INTEREST STATEMENT

This work was supported by a financial gift from Vance V. Kershner (President & CEO, LabWare, Inc., Wilmington, Delaware).

No potential competing interest was reported by the authors.

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