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GUEST EDITORIAL

What's Your Legacy?



LISA G. BULLARD North Carolina State University

At a recent AIChE annual meeting, the incoming
division chair presented a recognition plaque to one of
the outgoing board members. Upon thanking the new
chair, the departing member joked, "One day my kids
are going to wonder what to do with all these things."
A chuckle went through the room; everyone knew
exactly what he meant. As the spouse of a colleague
once observed, we all have "I Love Me" walls at work
or at home on which we display our framed certificates
and plaques. The entrepreneurial academic culture is
individually focused on publications, grants, awards
for research and teaching, and "best paper" recogni-
tions. Faculty candidates are scrutinized based on their
number of thesis and post-doctoral papers. The rewardleadersh
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to offer the stant post-doctoral papers. The reward

for research and teaching, and "best paper" recognitions. Faculty candidates are scrutinized based on their number of thesis and post-doctoral papers. The reward system in academia doesn't help; it mainly reinforces those things that can be easily counted and displayed. Professors have been seduced by titles, awards, and indices away from what really matters—making a long-lasting impact on the lives of our students and colleagues.

At my (hopefully distant) retirement, either my family or I will load all the plaques and certificates on my office wall into a box, which will go in the attic and sometime later be discarded. At my retirement reception, when my colleagues and former students talk about me, I hope they will talk about my real legacy—the difference I made in the lives of my colleagues and students.

What will your colleagues and former students talk about at your retirement party? What would you like them to talk about?

Here are some examples of how to be intentional about your legacy and leave your imprint on the lives of others:

• Support younger colleagues at your institution and within your field. Serve as a teaching or research mentor, encourage them to apply for leadership positions that might stretch them, and nominate them for awards. Think about a role you're currently filling, such as a highly visible committee chair, that could provide an opportunity for a junior colleague to develop and grow.

- Invest in your students—not only the "stars," but also those who are struggling. Be especially aware of students who have missed class or are doing poorly; invite them to meet with you, express concern, and ask them what might be going on to affect their performance. Often you will find that your sincere interest causes them to open up about their situations, and you might then be able to offer helpful guidance.
- On your website and the bulletin board outside your office, look for ways to affirm the accomplishments of the graduate students and undergraduate researchers in your group.
- Take the time to write a personal note or email to colleagues who have received recognition.
- Stay in touch with former students and celebrate their accomplishments and important life events.
- Donate money to your department or university to support something that is important to you perhaps an endowed lectureship, an undergraduate scholarship, a graduate fellowship, or support of the AIChE student chapter.

There's nothing wrong with papers and awards and plaques—they recognize excellence and encourage contributions to our universities and our discipline. However, the real opportunity to make a lasting difference lies in your relationships, not your resume. While it may be difficult or impossible to quantify, your legacy is what will survive you when your plaques and papers are long forgotten. Instead of focusing exclusively on your next accolade, consider your legacy, and be proactive about making it what you would like it to be. □

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A COMPREHENSIVE REAL-WORLD DISTILLATION EXPERIMENT

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istillation is the major separation method in industry, and its analysis brings together many important chemical engineering principles: component balances, energy balances, heat transfer, and phase equilibrium. Distillation is a core subject in all chemical engineering educational programs. The basic concepts can be very effectively conveyed by simple graphical methods, particularly in binary systems where McCabe-Thiele diagrams clearly demonstrate the effects of number of stages, reflux ratio, relative volatility (pressure), and vapor-liquid phase nonideality. Many textbooks^[2-7] covering distillation principles have appeared since the 1950 pioneering book by Robinson and Gilliland.^[1]

The examples used in introductory courses usually make many simplifying assumptions in order to not cloud the fundamental concepts. These include theoretical trays, total condenser with saturated liquid reflux and distillate, partial reboiler, and a single feed stream (either saturated liquid or saturated vapor). Operating lines are represented as functions of the reflux ratio (reflux flow divided by distillate flow). University distillation experiments^[8–12] are usually small scale with glass components, which are not typical of industrial distillation systems.

The experimental distillation column in the Lehigh University Process Laboratory has some features that are more representative of actual industrial columns, and these features complicate the analysis.

For many years, our senior students have found that performing experiments and analyzing the performance of this column is a very effective way to extend the basic concepts and theory that they learned in their junior-year mass transfer course.

This paper describes the equipment, startup procedure, reconciliation of the raw data, energy balances around various sections of the column, calculation of tray efficiencies, and simulation of the column to compare theoretical predictions with experimental data.

Safety issues are fairly minimal in the experiment. Methanol is flammable but is mixed with water except in the reflux drum. An alarm is activated if the flowrate of cooling water to the condenser is too low. Another alarm is activated if the base pressure gets too high, indicating column flooding. An interlock shuts off the feed pump if the base level gets too high.



is also a part of AIChE at the national level and on the board of the local Delaware Vallev Section.

Christos Kazameas studied chemical engineering at Lehigh University. A New Jersey native, he now resides in Lewisburg, WV. Chris-



works at Merck and Co. doing process development work on vaccines and biologics. Kaitlin

tos is employed as a materials engineer for UTC

Aerospace Systems where his primarily focus is on elastomer compounding and development of aircraft de-icing systems.

William L. Luyben has taught at Lehigh for 47 years in the areas of process design and process control. He is the author of 14 books and more than 280 papers.

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PROCESS STUDIED

Figure 1 gives the flowsheet of the unit. The distillation column separates methanol-water at 1 atm pressure. It is 8 inches in diameter and has 14 trays with three Glitch V-1 ballast caps on each tray. Feed is pumped from a tank (crosssectional area = 3.57 ft²) through a control valve and into the tube side of a heat exchanger where it is heated by the overhead vapor from the column. This setup is sometimes called an "economizer." The feed is still subcooled when it is fed to one of three alternative trays (4, 6, or 8). Trays are numbered from the bottom.

Saturated steam at 35 psig flows through a control valve into the shell side of a vertical thermosiphon reboiler. Condensate leaves through a steam trap. The steam pressure in the shell of the reboiler is 5 psig. Vapor flows up through the column and enters the shell side of the feed preheater, which is a horizontal tube-in-shell heat exchanger. Any liquid that has condensed flows out the bottom of the shell side of the preheater into the reflux drum. Vapor leaves the top of the feed preheater and goes to the shell side of two more heat exchangers in series with cooling water flowing countercurrently through the tube side. The vapor is totally condensed and the liquid flows by gravity to the reflux drum. The shell side of the final condenser is vented to the atmosphere, so the pressure in the column is 1 atm and the reflux is subcooled.

Liquid from the reflux drum is pumped and split into a reflux stream and a distillate stream with control valves in both lines setting the flowrates of the two streams. Reflux is fed on Tray 14 at the top of the column. Distillate goes to a distillate tank (cross-sectional area = 1.24 ft^2).

The bottoms stream from the base of the column goes to a cooler and into a pump. The pump discharge goes through a control valve and into a bottoms tank (cross-sectional area = 1.24 ft²). Both the distillate and the bottoms tanks can be drained into the feed tank. These three tanks are used to determine flowrates by tank gauging during the run when steady-state conditions have been attained. All control valves are electronic and are manually positioned from five controller faceplates.

Instrumentation includes temperature measurements of all streams and on all trays. Base pressure, steam supply pressure, and steam pressure in the reboiler are measured. Level indicators and sight glasses are available on the reflux drum and the column base. Sight glasses are available on the feed, bottoms, and distillate tanks.

Liquid samples can be taken from the feed tank, from the line leaving the reflux drum, and from the base of the column. Hydrometers are used to measure the density, from which compositions can be calculated because of the significant difference in density between water (sp. gr = 1) and methanol (sp. gr. = 0.792).

STARTUP PROCEDURE

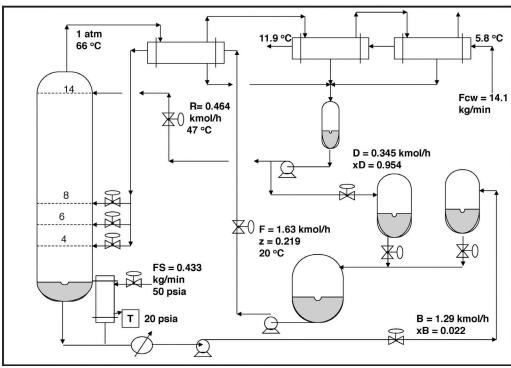
One of the most important educational features of the experiment is requiring the students to develop and perform a

> safe and rapid startup from a cold column initial condition. After electric power is turned on, the first step is to open the cooling water inlet valve and to guarantee by visual inspection that there is sufficient cooling water flowing to the two condensers at the top of the column.

> The feed pump is started and the feed control valve is opened to bring liquid into the base of the column. The feed pump is shut off and the feed valve closed when the liquid level in the column base is about 80% full as indicated by both the sight glass and the level transmitter. Then steam is slowly introduced into the shell side of the reboiler. It takes about 15 minutes to heat up the liquid in the column

66 °C 14 $F_{CW} = 14.1$ R= 0.464 kg/min kmol/h 47 °C D = 0.345 kmol/h xD = 0.954R 8 6 🗶) F = 1.63 kmol/h 4 z = 0.21920 °C FS = 0.433 kg/min 50 psia B = 1.29 kmol/hт 20 psia Q xB = 0.022Q Figure 1. Flowsheet and experimental conditions.

Chemical Engineering Education



base, at which point vapor begins to flow up the column. The rising hot vapor heats the metal of the trays and the vessel wall. The temperature on Tray 1 increases, then Tray 2, and so forth up the column. It takes about 10 more minutes for the hot vapor to work its way up to Tray 14.

When vapor starts to come overhead, the liquid level in the reflux drum begins to rise. When the drum is about 25% full, the overhead pump is started and the reflux valve is opened. The distillate valve is completely closed. The position of the reflux valve is adjusted to maintain a constant liquid level in the reflux drum.

Thus the initial part of the startup is putting the column on total reflux. The flowrates of the feed, distillate, and bottoms streams are all zero. The steam valve is in a fixed position and the reflux valve is controlling reflux drum level. The base level is uncontrolled, but there must be adequate liquid in the base. Material from the initial quantity charged to the column base goes to build liquid inventory on all the trays and in the reflux drum. If the base level gets too low during the startup, more feed is introduced.

Once reflux starts flowing down the column and contacting the rising vapor, fractionation begins. We will analyze the total reflux operating conditions in a later section of this paper. First we will examine normal steady-state operation with feed and product streams.

NORMAL FEED RUN

The transition from total reflux to feed operations is achieved by starting the feed pump and opening the feed valve to about 40%. The steam valve is set at about 50%. The distillate valve is opened to about 15% and a level controller is put on automatic to adjust the distillate valve to maintain the liquid level in the reflux drum. The bottoms pump is started and the bottoms valve is opened to about 25%. A second level controller is put on automatic to adjust the bottoms valve to maintain the liquid level in the base of the column.

Raw data

It takes about 45 minutes for the column to come to a steady-state condition as indicated by constant temperatures and levels. During this period the bottoms and distillate tanks are draining back into the feed tank. When the valves in the exit lines of these product tanks are closed, the level in the feed tank falls and the levels in the product tanks climb. Recording level changes over a period of time gives flowrate information for feed F, distillate D, and bottoms B. This "tank gauging" procedure is what would often be done in industry using feed and product tank level changes over a prolonged test period. Cooling water and steam condensate flowrates are determined by the "bucket and stopwatch" method (ice is used in the bucket to catch the hot steam condensate).

Liquid samples are taken of the feed, reflux (distillate), and

bottoms in a graduated cylinder, and hydrometers are used to find densities, from which compositions can be calculated. Temperatures of all streams and on all trays are recorded. Table 1 gives some of the important raw data from a typical run.

The flowrate of the reflux cannot be determined during the run, but it can be obtained after the column has been shut down. Liquid is retained in the reflux drum. The overhead pump is started and the reflux valve is set in the same position that it was during the run. Nothing is entering the reflux drum, so the drop in level with time gives the reflux flowrate that we had during the run.

Data reconciliation

A major educational feature of the experiment is exposing the students to real data with its inherent inaccuracies. Flow and composition measurements are imprecise in an industrial environment. Material balance calculations show that "In" is not equal to "Out" in terms of both mass (and molar flowrates in this non-reactive process where moles are conserved) and components. The students are forced to develop a rational data reconciliation procedure to make the total molar and component balances perfect before getting into further analysis to generate McCabe-Thiele diagrams, determine tray efficiencies, and check energy balances.

The data given in Table 1 are used to calculate molar compositions and molar flowrates. The first and second columns in

TABLE 1Raw data from feed run				
	sp. gr.	Flowrate		
Feed	0.927	677 cm ³ /min		
Distillate	0.797	226 cm ³ /min		
Bottoms	0.992	396 cm ³ /min		
Reflux	0.797	304 cm ³ /min		
Steam		0.433 kg/min		
CW		14.1 kg/min		
	Temperatures (°C)			
Feed Tank	20			
Feed to Column	63			
CW Into Condenser	5.8			
CW Out Condenser	11.9			
Reflux Drum	47			
Tray 1	89			
Tray 14	66			

The specific gravity of methanol is 0.7815 and that of water is 1. The molecular weights are 32 and 18, respectively.

One possible data reconciliation procedure is to assume that the flowrates of the distillate and **bottoms** are correct and that the feed flowrate is the sum of the two product flowrates. This makes the total molar balance perfect.

TABLE 2 Calculated and adjusted results						
Calculated MolarCalculated MoleAdjusted MolarAdjusted MoleFlowrate (kmol/h)Fraction MethanolFlowrate (kmol/h)Fraction Methanol						
Feed	2.056	0.2322	1.631	0.2191		
Distillate	0.345	0.954	0.345	0.954		
Bottoms	1.286	0.022	1.286	0.022		
Reflux	0.464	0.954	0.464	0.954		

Table 2 give the calculated molar flowrates of the feed F, bottoms B, the distillate D, and the reflux R, together with the molar compositions of these streams (z, x_{p} , and x_{p}). Ideal mixing of methanol and water is assumed.

Adding D and B gives 1.621 kmol/h, which is not equal to F (2.056 kmol/h). Do we have a leak in the equipment? No, the flow measurements are not precise. In addition, the feed tank has an internal heat exchanger of unknown size, which occupies a portion of the cross-sectional area. So the tank gauging of the feed would be expected to give calculated flowrates that are too high.

Therefore one possible data reconciliation procedure is to assume that the flowrates of the distillate and bottoms are correct and that the feed flowrate is the sum of the two product flowrates. This makes the total molar balance perfect. The adjusted feed flowrate is Fadj.

To make the methanol component balance perfect, the feed composition z is back calculated assuming the distillate and bottoms compositions and flowrates are correct. The adjusted feed composition is zadj.

Fadj = D + B = 0.345 + 1.286 = 1.631 kmol/h
zadj =
$$\frac{Dx_{\rm D} + Bx_{\rm B}}{Fadj} = \frac{(0.345)(0.954) + (1.286)(0.022)}{1.631} = 0.2191$$
 (1)

The experimental value of z is 0.232, and the adjusted zadj is 0.219, so there is only a minor adjustment. The last two columns in Table 2 give the flowrates and compositions used in the subsequent analysis.

McCabe-Thiele diagram

Figure 2 gives the McCabe-Thiele diagram using a rectifying operating line (ROL) with a slope that considers the effect of subcooled reflux. The slope of an operating line in any section of the column is the ratio of the liquid to vapor flowrates in that section. The flowrate of the subcooled reflux is 0.464 kmol/h and its composition is 0.954 mole fraction methanol. It is not at its bubblepoint temperature but is subcooled at 46.9 °C while the temperature on Tray 14 is 66.3 °C. An energy balance is used to calculate the internal liquid flowrate LR in the rectifying section of the column.

$$LR = R \left[1 + \frac{C_{p} (T14 - TR)}{\Delta H_{v}} \right]$$

= (0.464 kmol/hr) $\left[1 + \frac{(80.8 \text{ kJ/kmol-K})(66.3 - 46.9)}{36,200 \text{ kJ/kmol}} \right] = 0.484 \text{ kmol/hr}$ (2)
$$LR/VR = \frac{LR}{LR + D} = \frac{0.484}{0.484 + 0.345} = 0.584$$

Liquid heat capacity is calculated using the molar composition and the component liquid molar heat capacities (methanol = $81.03 \text{ kJ kmol}^{-1} \text{ K}^{-1}$ and water = $74.93 \text{ kJ kmol}^{-1} \text{ K}^{-1}$). Heat of vaporization is calculated using molar composition and component heats of vaporization (methanol = 36,000 kJ/kmol and water = 40,860 kJ/kmol). In later calculations of enthalpy, vapor molar heat capacities are used (methanol = $49.28 \text{ kJ kmol}^{-1} \text{ K}^{-1}$ and water = $36.0 \text{ kJ kmol}^{-1} \text{ K}^{-1}$).

A similar energy balance around the feed tray gives a q value of 1.035 because the subcooled feed temperature is 62.6 °C while the temperature on the feed tray (Tray 4) is 81.1 °C. Now the operating lines can be drawn.

A value for Murphree vapor-phase efficiency is guessed, and stages are stepped off between the stripping operating line (SOL) and a fraction of the vertical distance to the vapor-liquid equilibrium line, starting at the

bottoms composition x_B . The partial reboiler is assumed to be an equilibrium stage. Aspen NRTL physical properties are used to generate the VLE curve at 1 atm.

Unlike a design problem in which the optimum feed tray occurs at the intersection of the ROL and SOL, the analysis of an operating column has a fixed feed stage. So we must step back and forth between the SOL and the VLE curve until we reach Tray 4. Then we can step to the ROL.

By trial and error, an efficiency of 65 % was found to give a vapor composition leaving Tray 14 that is equal to the distillate composition $x_D = 0.954$. See Figure 2.

The experimental temperature profile (the circles) is shown in Figure 3 (following page). The solid line is the predicted temperature profile from a simulation discussed later in this paper.

Energy balances

Energy balances can be made around various sections of the column. The heat removed in the three overhead heat exchangers condenses and subcools the vapor leaving the top of the column. The flowrate of this vapor is the sum of the flowrates of the reflux and the distillate. The heat transferred into the cooling water in the condenser is:

QCW = FCW *
$$C_p$$
 (Tout – Tin)
= (14.1 kg/min) (4.163 kJ/kg – K) (11.92 – 5.85) (min/ 60 sec) = 5.94 kW (3)

Unlike a design problem in which the optimum feed tray occurs at the intersection of the ROL and SOL, the analysis of an operating column has a fixed feed stage. So we must step back and forth between the SOL and the VLE curve until we reach Tray 4. Then we can step to the ROL.

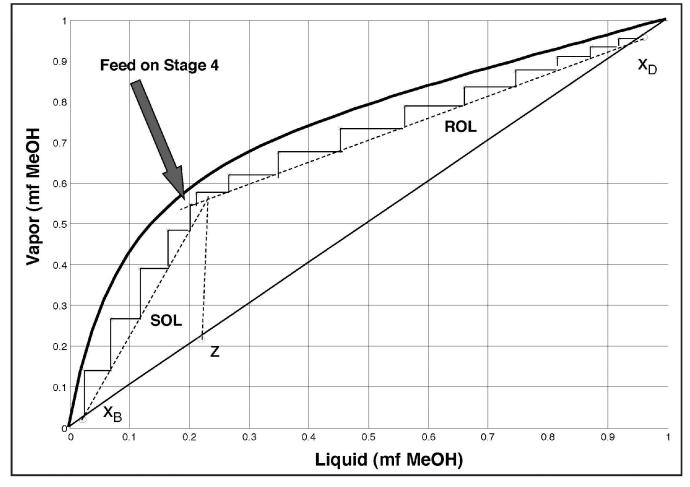


Figure 2. McCabe-Thiele diagram; feed run.

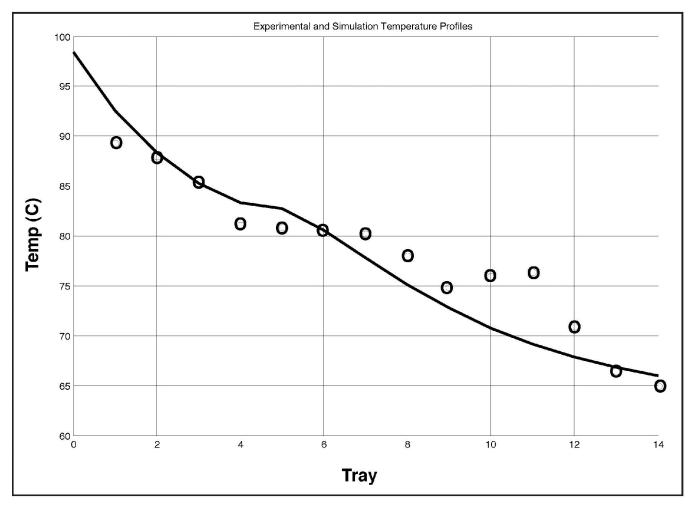


Figure 3. Temperature profiles; simulation and experimental diagram; total reflux.

The heat transferred into the feed in the preheater is:

 $QPH = Fadj * C_n (Tout - Tin)$

= (1.631 kmol/h)(76.28 kJ/kmol-K)(62.6-20)(h/3600 sec) = 1.473 kW(4)

Thus the total heat removed from the overhead vapor is 7.41 kW according to these cold-side calculations.

They can be checked by energy calculations on the hot process side. The heat removed in the three heat exchangers condenses and subcools the process vapor, which is the sum of the reflux and the distillate (0.464 + 0.345 = 0.809 kmol/h) with a composition of 0.954 mole fraction methanol. The enthalpy of the vapor leaving Tray 14 at 66.3 °C is 39,450 kJ/kmol, and the enthalpy of the subcooled liquid (reflux + distillate) is 37,900 kJ/kmol). Thus the total heat removed from the process vapor is:

$$Qtotal = (D+R)(H14-hR)$$

= (0.809 kmol/h)(39,450-3790 kJ/kmol)(h/3600 sec) = 8.104 kW (5)

This independent check of the heat transferred in the overhead system is quite close to the 7.41 kW calculated from the cold sides of the preheater and condenser and is well within experimental error. There are some heat losses to the atmosphere from the hot vapor, so we would expect the hot-side heat removal to be higher than the cold-side heat pickup, which these calculation show to be the case.

The overall energy balance for the whole system shows a very significant heat loss. Most of the column shell is not insulated and at temperatures significantly higher than ambient. The reboiler duty is calculated from the

The overall energy balance for the whole system shows a very significant heat loss. condensate flowrate and the difference between saturated steam at 35 psig and saturated condensate at 5 psig.

QR = FS(H35 - h5)	
= (0.433 kg/min)(2731 - 4546 kJ/kg)(min/ 600 sec) = 16.4 kW (6)	
The overall energy balance is $\Delta H = Q - W$ $Dh_{\rm p} + Bh_{\rm B} - Fh_{\rm F} = QR - QCW - Qloss$ (0.2451 h = 11) (2500 h H = 1) = (1.200 h = 11) (2500 h H = 1)	Under total reflux condi-
(0.345 kmol/h)(3790 kJ/kmol) + (1.286 kmol/h)(7131 kJ/kmol) -(1.631 kmol/h)(1526 kJ/kmol) = 16.42 kW - 5.94 kW - Qloss (7) 2.22 kW = 10.48 kW - Qloss Qloss = 8.26 kW	tions, there
Half of the reboiler duty is lost to the atmosphere.	are no feed and
TOTAL REFLUX	no products.

Under total reflux conditions, there are no feed and no products. The liquid and vapor flowrates are the same in all sections of the column, which means the slope of the operating line is unity. Hence the operating line is the 45° line on the McCabe-Thiele diagram as shown in Figure 4.

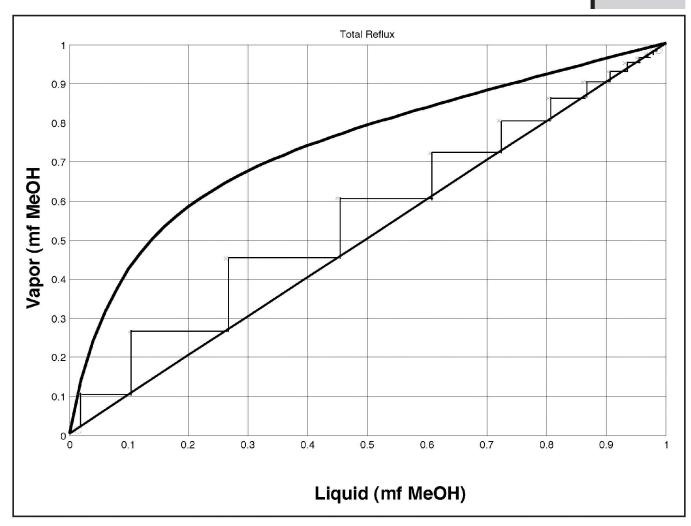


Figure 4. McCabe-Thiele.

Data from a total reflux run are given in Table 3. The specific gravity data are used to calculate the compositions of the reflux ($x_R = 0.987$) and of the base ($x_B = 0.0143$). Both of these purities are higher than in the feed run, as expected since the reflux ratio is infinite and more fractionation should occur.

The heat duty in the condenser from the cooling water data is 7.038 kW. From the overhead vapor, which is now only reflux, the duty is 8.368 kW. Heat losses could account for this difference.

The reboiler duty is calculated from the steam flowrate (13.54 kW). Since no streams are fed or leave the process, the Δ H term in the overall

energy balance is zero. Therefore the heat added in the reboiler should equal the heat lost in the condenser plus heat lost to the surroundings. The loss is 13.54 - 7.038 = 6.50kW, which is similar to the heat loss in the feed run.

Figure 5 gives the experimental temperature profile (the circles) under total reflux conditions. The other curves come from the simulation and are discussed in the next section. Notice that the experimental temperature profile is fairly flat at both ends of the column, indicating quite high product purities.

COMPUTER SIMULATION

TABLE 3 Data from total reflux run					
	sp. gr.	Flowrate	Composition (mole fraction methanol)		
Base	0.997	0	0.005		
Reflux	0.793	559 cm ³ /min	0.995		
Steam		0.357 kg/min			
CW		14.7 kg/min			
	Temperatures (°C)				
CW Into Condenser	6.0				
CW Out Condenser	12.9				
Reflux Drum	38.6				
Tray 1	99.4				
Tray 14	64.7				

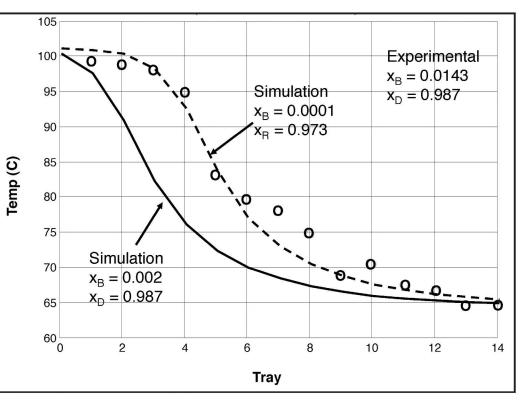


Figure 5. Temperature profiles; total reflux; simulation and experimental.

An Aspen Plus simulation is developed to model

the process. An Aspen "Radfrac stripper" model (reboiler but no condenser) is used for the column. Aspen "HeatX" models are used for the feed preheater and condensers. The NRTL physical property package is used. The process flow diagram is given in Figure 6.

Feed run

The experimental values that were specified for input data to the simulation are listed below.

1. Adjusted feed flowrate = 1.631 kmol/h

- 2. Adjusted feed composition = 0.2191 mole fraction methanol
- *3. Feed tank temperature = 20 \degree C*
- 4. Bottoms flowrate = 1.286 kmol/h
- 5. Reflux flowrate = 0.464 kmol/h
- Table 4 Comparison of experimental and simulation results; feed run Simulation Experiment mf methanol 0.965 0.956 $\mathbf{X}_{\mathbf{D}}$ mf methanol 0.022 0.021 X_B kW 1.473 1.547 Q_{PH} kW 5.938 6.797 Q_{CW} kW 16.40 9.404 Q_R °C Tovhd 66.3 65.8 $^{\circ}C$ Treflux 50.6 46.9
- 6. Cooling water flowrate = 0.433 kg/min
- 7. Cooling water inlet temperature = $5.8 \degree C$
- 8. Partial reboiler stage efficiency = 100%
- 9. Stage efficiency = 65%

All of the other variables are calculated by the model. Table 4

compares experimental and simulation results. The agreement is quite good. Figure 3 compares the temperature profiles.

Total reflux run

How to set up a total reflux simulation is not completely obvious. The Aspen Plus "Radfrac" model requires feed and product streams, but these are all zero under total reflux operation. The reflux flowrate is set at the experimental value (0.8343 kmol/h). Efficiency is set at 65%.

A small feed flowrate (0.01 kmol/h) is specified with composition 0.211 mole fraction

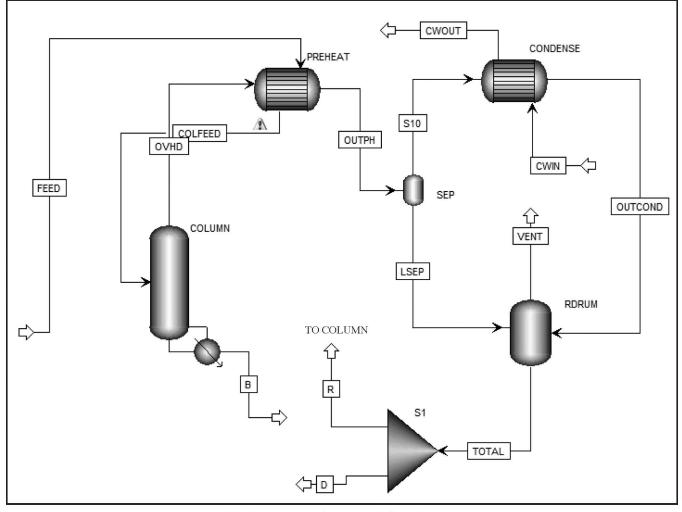


Figure 6. Aspen Plus process flow diagram.

methanol. Then the bottoms flowrate is varied and the calculated values of the reflux x_R and the base x_B are observed. A bottoms flowrate of 0.0078 kmol/h gives a reflux composition ($x_R = 0.987$) that matches the experimental value. But the base composition is 0.002, which is much smaller than the experimental $x_B = 0.0143$. The predicted temperature profile under these conditions is the solid line shown in Figure 5.

The predicted temperature profile is not as flat in the lower part of the column as the experimental profile. This indicates that the real bottoms composition is lower than that calculated from density. Considerable inaccuracy is to be expected when purities are high.

A very small decrease in the specified bottoms flowrate to 0.00775 kmol/h changes the calculated compositions to $x_R = 0.973$ and $x_B = 0.0001$. The resulting temperature profile is the dashed line in Figure 5.

There are multiple experimental temperature measurements and only one bottoms composition measurement, so it is logical to assume that the composition measurement is inaccurate.

ASSESSMENT OF STUDENT LEARNING

Several student comments about the utility of the experiment are given below. The major contribution is permitting students to relate theory with real equipment.

- "The pilot-scale distillation experiment is very useful in understanding how a distillation column operates in real life. We were able to familiarize ourselves with proper start-up and shutdown procedures of the plant, and also how to make measurements of physical parameters such as the flow rate and the purities of the components. In addition, the energy requirements of the plant are also computed, which makes it very relevant to industrial operation."
- 2. "I was honestly most excited to run this experiment because we had learned so much in theory and my design project was based upon distillation. It made it more real and helped with understanding how flow rates are actually measured and how the temperature rises up the column during start-up before reaching steady state. Those sorts of things aren't taught in the classroom."
- 3. "The distillation experiment gave a lot of insight to how a distillation actually operates. We spent a lot of time in class studying how separations take place in distillation columns, and this lab allowed us to apply and actually

see the theories in action. The most interesting part about this experiment for me was seeing the difference between theory and actuality. Comparing the physical data to what is expected from theory and seeing how heat loss and efficiencies affect the results was a good learning experience."

4. "In my opinion it was the most valuable experiment in the lab. The distillation experiment solidified the core foundations of mass transfer, as well as provided insight into proper unit operation beyond the textbook aspects. The experiment truly required teamwork. The construction of the unit allowed thorough understanding of the possible degrees of separation for a two-component system. The full-size column gave a unique experience in the senior operations lab."

CONCLUSION

The experimental procedure and analysis of a realistically complex distillation experiment is described in detail. Educational objectives include reviewing mass transfer theory, developing a safe startup procedure, adjusting imperfect raw data, calculating tray efficiencies, and performing energy balances. Three generations of Lehigh chemical engineering students have found this experiment the most industrially relevant part of our two-semester senior-year process analysis laboratory. They gain very useful experience in operating a fairly complex process with multiple inputs and outputs that challenge their technical skill and develop their common sense.

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ChE classroom

IMPROVED PERFORMANCE VIA THE INVERTED CLASSROOM

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ecturing in the classroom has been the historical method of delivering information to students at the university level. However, this method of delivery has been shown to not be the most effective with millennial students (born between 1982 and 2005)^[1, 2] that are our current traditional college-aged population. These students have had technology consistently in their lives and particularly computer use is an integral part of their personal and education experiences.^[3]

Active learning, where students do something courserelated in the classroom other than just watching and listening to the instructor and taking notes, has been used for a while in higher education and has been shown to improve student learning.^[4-7] The flipped or inverted classroom is the extreme of active learning where all lecture material is delivered outside of class (by online videos or other modules) and the time spent in class is dedicated to working on problems or projects, asking questions, and taking assessments. The inverted concept is not novel,^[8] but improved technology and software along with the ease of implementation has made the inverted classroom recently accessible to a large number of faculty without significant assistance.^[9]

Using the inverted classroom, student performance has been shown to be improved compared to a traditional lecture version of the course. Various metrics were used to show improved learning including pre- and post-material testing compared to a previous year,^[10] content coverage whereby students' time to comprehend material is shorter compared to previous year as measured by examinations,^[11] and through self-evaluations via surveys.^[9] Some studies have shown no significant student learning enhancements.^[12] However, there are subtleties in the way the inverted classrooms are implemented that could account for the differences in measured student learning enhancements. For example in an inverted classroom study by Lape and coworkers^[12] students were not given daily assessments to force their watching and understanding of material in advance of class. The first 10-15 minutes of class were spent reviewing the material from the videos; therefore, students could gain knowledge of material presented in the videos from the instructor without ever having to watch them. At the end of the class period the instructor reviewed and often presented the solutions to problems done

in class and therefore students could get the answers without having to do the problems. Interestingly, the investigators themselves identified that in future implementations students would be required to do some work based on the videos prior to coming to class and hence force the students to be responsible for the material. Another inverted classroom study^[13] found that on average only about 50% of the students watched the lecture material before coming to class. There were no daily assessments given in this study. Pre-class work based on the lectures that had an influence on the student's grade helps ensure students' full use of the inverted class material.^[14] The literature does not present clear evidence supporting

The literature does not present clear evidence supporting or refuting the use of the inverted classroom for improving student learning.^[15] The inverted classroom can be implemented for many reasons including improving student learning, increasing student-teacher interactions, providing opportunities for real-time feedback, allowing for self-paced learning, improving the homework problems and practice provided to students, and enhancing student engagement with the material.^[15]

METHOD

An inverted class was implemented in a first-semester junior-level chemical engineering thermodynamics course at Villanova University—a medium-sized private university with undergraduate enrollments of 6,800 students—in Fall 2013 and 2014 for the purpose of determining if students learned better under this mode. There were four sections totaling 108 students for an average section size of 27 students. The inverted class was compared to the previous four years (Fall 2009-2012) of traditional lecture classes consisting of

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seven sections and 188 students for an average section size of 27 students. Each class met for 50 minutes three times a week for 14 weeks. This course had been taught 15 times prior to the inverted class by the same instructor as a traditional lecture course. An identical set of course notes prepared by the instructor was given to all sections (inverted and lecture). Each section was also given identical sample problems (158) and their solutions. Three in-class exams and a comprehensive final were given to each section. All sections were given approximately weekly homework problem sets done in teams. The inverted class had video lectures assigned (one to four) for each class consisting of the same material that would have been given in a lecture class from the previous years. Daily inclass quizzes were given to the inverted class that were closed book, but a one-page hand-written set of notes was allowed along with a calculator. In 2011, unannounced quizzes were given at the end of several lecture periods. Table 1 provides a quick reference for how each course offering was handled.

Performances on the three exams and final exam were compared between the lecture and inverted classes. Identical exams were not given since these tend to be available to students and in fact were handed out by the instructor as practice exams. Instead exam questions were developed based upon historical performance of the students on the material. The exams will be the primary method of determining the performance of the students.

An exam consisted of four questions. One question was targeted to have a 60% average and the remainder were targeted to have an 80% average producing an overall average target of 75% on the exam. The exam questions from Fall 1998-2008 and their student results were used to find types of questions that produce the desired average scores. Besides passing the t-Test (described in Statistical Analysis section) to verify equal means, exam questions had to address similar concepts and have the same number of steps and types of calculations to be considered the same, but obviously they were not identical questions. Calculations were broken down into unit conversions, algebra, and calculus steps.

Approximately weekly homework sets were assigned to all sections and were completed in teams of two to three students. Homework groups have been shown to be beneficial to student learning if implemented well.^[16] All homework problems were created by the instructor. Homework length and difficulty were designed to be the same from year to year. Each of the years of 2009-2012 when compared to its previous year produced statistically similar mean scores on the cumulative homework average using the two sample t-Tests for equal means verifying that the homework degree of difficulty was consistent from year-to-year. Students also reported similar hours for time spent outside of class on assignments. For the years 2009-2012, the traditional lecture model was used and all homework was completed outside of class. For the inverted class in 2013, homework assignments were identical to that of the class of 2006 (a traditional lecture class not included in this study); however, a significant amount of class time was spent allowing students to work on their homework and ask questions of the instructor. For the inverted class in 2014, new homework assignments were developed. The average homework grade for the inverted classes was not statistically the same as the any of the previous five years of classes, having a higher average (92 \pm 1.8 % versus 85 \pm 2.3%).

For the inverted class, lecture videos were prepared using voice and screen capture software on a tablet. The course notes provided to all classes had blanks in them and these were filled in with writing during the lecture as would have been done during a traditional lecture class. A typical 50-minute lecture was broken down into one to four videos of varying lengths. Each video was targeted at covering one topic, concept, or problem. If students were allowed to work on a problem or a question as part of the lecture as would have been done in the traditional lecture class an opportunity for them to do so was provided in the video. The time the students spent on these active-learning activities was not included in the video length. Students were required to log in to watch the videos and the system tracked student access to the videos. At the start of each class, students were given an online 10-minute quiz consisting of four to five questions on the material in the videos assigned for that class. The quizzes were closed book but each student was allowed to prepare their own page of notes for the quiz. Calculators were allowed. Each question was targeted to a particular video and aimed at the basic concepts of the lower levels of Bloom's taxonomy of learning objectives in the

	TABLE 1 Format of the course each year							
	Lecture Notes Provided	Practice Problems Provided	Daily Quizzes	Random Pop Quizzes	Weekly Homework	3 Exams and Final	Inverted Video Lectures	Traditional in-Class Lectures
2009	Х	Х			Х	Х		Х
2010	Х	Х			Х	Х		Х
2011	Х	Х		Х	Х	Х		Х
2012	Х	Х			Х	Х		Х
2013	Х	Х	Х		Х	Х	Х	
2014	Х	Х	Х		Х	Х	Х	

cognitive domain: knowledge, comprehension, and application. Only exam questions addressed the higher levels of analyzing, synthesizing, and evaluating.

For the lecture classes of 2009, 2010, and 2012 daily quizzes were not given. However in 2011 quizzes were given 20 times during the last 10 minutes of the lecture. These were

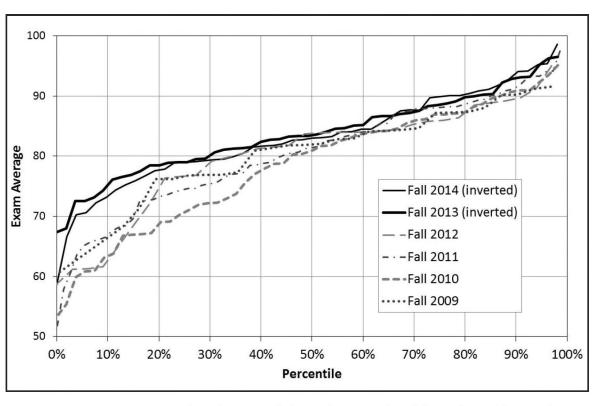


Figure 1. Average exam scores from the inverted classes (2013-2014) and the traditional lecture classes (2009-2012) based upon class rank percentile.

not announced at the start of the class so students would not know if they would receive a quiz based upon the day's lecture while listening to the lecture. This was instituted to see if the students would gain more knowledge during the lecture if they were immediately held responsible for the lecture material once it was delivered. These quizzes were not given online and were open notes as compared to the 33 quizzes given during the inverted course (which were online with students only allowed a one-page sheet of notes). Both sets of quizzes addressed lower-level learning objectives and 48% of the questions were identical in both sets. A comparison of the exam results from the class in 2011 to those in 2009. 2010, and 2012 can explore the effect of frequent quizzing of the lecture material on student learning. The lecture course in 2011 with quizzes can be used as a control to compare student learning to the inverted courses in 2013 and 2014, which also utilized frequent quizzing, and potentially eliminate the quizzes as having an effect on student learning objectives.

STATISTICAL ANALYSIS

To compare two data sets to verify if they were from different populations a two-sample t-Test for equal means^[17] if normally distributed or Welch's adaptation of the t-Test^[18] if not normally distributed was implemented. The normal distribution was tested using the Shapiro-Wilk normality test which has been shown to be a very accurate method for testing normality. $^{[19]}\,\mathrm{A}\,95\%$ confidence interval was selected for this analysis.

Averages throughout the manuscript are reported at 95% confidence intervals. The Mann-Whitney non-parametric test^[20] was used to show that there was a significant difference between the average scores from one set of data when compared to another set.

RESULTS AND DISCUSSION

Exam Performance: The three exams and final exam were averaged (equal weight given to each) and the Mann-Whitney non-parametric test^[20] verified that there was a difference between the averages from the lecture classes when compared to the inverted class. With all four lecture classes combined the significance value of the test was 0.031 and is below 0.05 for 95% confidence limits. If each year was examined separately versus the inverted years, there was still statistical difference between the data sets. Even the lecture course from 2011 that instituted frequent quizzes to hold students accountable for the lecture material showed statistical difference when compared to the results from the inverted class, which also had frequent quizzing. Therefore frequent quizzing alone could not account for the improved student performance observed in the inverted class. The averages for all four exams combined (equally weighted) are shown in Figure 1. The exam averages (95% confidence interval)

Average er	TABLE 2 Average exam scores (95% confidence limit) for inverted versus traditional classes. Class was partitioned based upon average exam score.						
	2009-2012 2013-2014 Normal (Traditional) (Inverted) Distribution t value p value						
Overall	79.8 ± 1.4	83.2 ± 1.3		3.29	0.001		
Top 1/3	89.2 ± 0.7	91.1 ± 1.0		3.04	0.003		
Middle 1/3	81.4 ± 0.6	83.3 ± 0.6	Х	3.98	0.00007		
Bottom 1/3	68.6 ± 1.6	75.3 ± 1.5	Х	5.62	< 0.00001		

	TABLE 3 Average scores (95% confidence interval) for the bottom third (partitioned using exam average) of the class based upon question type for traditional lecture versus inverted classes.						
	2009-2012 (Traditional)	2013-2014 (Inverted)	t value	p value			
Overall	68.6 ± 1.6	75.3 ± 1.5	5.62	<0.00001			
Questions 1-3	70.9 ± 0.4	76.0 ± 0.4	4.89	<0.00001			
Question 4	60.1 ± 0.6	73.7 ± 0.6	5.56	<0.00001			

are also presented in Table 2 along with t and p values from the two-sample t-Test for equal means^[17] for normal distributions or for Welch's adaptation when the distributions were not normal.^[18] The bottom and middle third averages were normally distributed while the overall and top third averages were not.

Interestingly, the lower third of the class (based upon exam average) performed significantly better in the inverted class compared to their lecture-class counterparts. Their exam average went from a D+ to a C on the traditional grading scale, improving almost seven points. The top third of the class only increased exam averages by two points. It is important to note that the qualifications (cumulative GPA and math and verbal SAT scores) between these classes were not statistically different. For example the inverted cohort had their SAT scores only 1 point higher than the traditional cohort and the populations were deemed identical.

As noted before, each exam consisted of four questions. Three of the questions were targeting an 80% average while the fourth was targeting a 60% average. The first three questions addressed the fundamental lower-level Bloom's Taxonomy in the cognitive domain of knowledge, comprehension, and application learning objectives while the more difficult problem also required analysis, synthesis, and/or evaluation. Since the bottom third of the class performed significantly better on their exams it was desired to see if their skills increased across Bloom's Taxonomy. Exam averages were created using just the fourth problem and then another average created using just the fourth problem across all exams. In all cases the scores were normally distributed. The results are shown in Table 3. Similar trends were not observed in the better performing students.

In all groupings the exam averages were higher for the inverted cohort compared to the traditional lecture cohort and the data sets are different. For the traditional lecture cohort the averages from questions 1-3 were statistically different than the averages from question 4 using the Mann-Whitney non-parametric test.^[20] For the inverted cohort there was no statistical difference between

the averages of questions 1-3 compared to question 4 at the 95% confidence limit. The weaker students in the lecture course tended to perform poorly on problems requiring higher-level learning objectives compared to problems requiring lower-level skills. However, the students in the inverted course showed equal performance across exam questions addressing different levels of learning outcomes. The inverted method showed a 5.1 exam point increase in lower-level skills

and a 13.6 point increase on higher-level skills when compared to the lecture method. The inverted classroom method appears to help the weaker students more than the stronger students in the course. A larger increase in higher-level skills occurs with the inverted method.

Student Perception: It has been shown that the students in the inverted class perform better than the students in the traditional lecture class. A common belief for this enhancement is that the students in the inverted class do more work or put in more time outside of class to achieve their performance enhancement. In the third to last week of the semester of the inverted classes the students were asked to rank their perception of the inverted class on a five-point scale where 1 represented strongly disagree and 5 represented strongly agree. There was one student out of the 107 who had previous experience in an inverted course before this one. The results of this survey are present in Table 4.

TABLE 4 Survey of student perceptions of the inverted classes, 1 = strongly disagree and 5 = strongly agree.				
I feel the format of this course improved my overall learning compared to a traditional lecture course.	4.5 ± 0.3			
I feel the format of this course required a substan- tial amount more time compared to a traditional lecture course.	4.4 ± 0.3			
Solving problems in class prepared me better for solving problems on my own.	4.1 ± 0.4			
I feel that because of the format of this course, I received more personal attention compared to a traditional lecture course.	4.3 ± 0.4			

From the survey results it appears that the students believe they are putting in more work when compared to a lecture course; however, this may not actually be the case. On the last day of class anonymous course surveys are administered to the students in all courses. One of the questions asks the students in the thermodynamics course to identify on average how many hours a week outside of class they spent on this class. For the inverted sections students identified 6.2 ± 0.5 hours per week spent on the class. For the four previous years of the lecture version of the

	TABLE 5 Daily quiz averages (95% confidence interval) for inverted class in 2013 (full credit for attempt) compared to identical quizzes given to the 2014 class where quiz grades counted.					
	2013 Quiz Average credit for attempt Week 6	2014 Quiz Average graded quizzes Week 6	2013 Quiz Average graded quizzes Weeks 1-5, 7-14			
Overall	50 ± 3.1	80 ± 1.6	82 ± 1.8			
Top 1/3	68 ± 3.7	94 ± 1.4	92 ± 1.4			
Middle 1/3	59 ± 3.7	81 ± 1.4	84 ± 1.9			
Bottom 1/3	23 ± 6.9	66 ±3.7	69 ± 4.3			

course the students reported that they spent 5.8 ± 0.6 hours per week outside of class, an average time that was shown to be statistically the same as for the inverted course using the t-Test even though there can be errors in students self-reporting data. When taking an inverted course and other lecture courses at the same time the students believe the inverted course takes much more time than their lecture courses. However, in reality they may not be spending any different amount of time outside of class on their material for the inverted class. Their time is spent differently and one might say more effectively to achieve higher exam scores based upon the course material. More of the student time is spent on the video lectures and comprehending the material and less time on the homework and studying for exams.

Holding Students Accountable: After reviewing the literature on the inverted classroom it appears that students must be held accountable for the material presented outside of class. The viewing and comprehension of the material must somehow affect their course grade. This was accomplished in this study by having the students take a 10-minute quiz based upon the assigned videos every day. The quizzes were closed book but a hand-prepared one-page sheet of notes was allowed. The students had 33 quizzes throughout the 14-week course and were allowed to drop their 10 lowest scores assuming they missed fewer than two classes (unless excused for illness or other reason). As an experiment in week 6 (about halfway thought the course) in the 2013 inverted sections the students were given full credit for the 3 quizzes as long as they attempted the quiz no matter what they actually scored on the quiz; they were made aware of this change prior to the assignment of the videos. Results are shown in Table 5.

In the 2013 version of the inverted class, when students were given full credit for attempting the quiz they performed significantly worse when compared to the rest of the quizzes they took when the quiz scores counted. This was even observed for the high-performing students. The identical quizzes for week 6 were given to the two sections of the inverted course in 2014 (52 students); however, the quiz scores counted in their grade and when this occurred the students performed significantly higher when compared to their 2013 counterparts. In 2013 there were on average 1,025 videos accessed during a typical non-exam week (excluding week 6).

This corresponded to 172 student accesses per video or each student accessing each video three times on average. During week 6 there were only 435 videos accessed and there were 22 students (39% of the class) that did not access any videos that week. During all the other weeks there was never a student observed to not access videos. These results clearly show that the students must be held accountable for the inverted material before they come to class.

Effect of Frequent Quizzing: A common criticism of the inverted classroom in the way it was implemented in this study focuses on the daily quizzing, and it is postulated that it is this change in the course that improves the student learning and not the inverted method. In 2011, during the traditional lecture version of this course there were 73 students in two sections and the students were told at the beginning of the course that at the end of a lecture it was possible they would be given a 10-minute quiz based upon the day's material. They would be allowed to use their notes taken that day as well as a calculator during the quiz. Twenty quizzes were actually given during 2011. The quiz average for 2011 based upon 20 quizzes was 86% while for inverted sections based upon 33 quizzes it was 80%. The students did perform slightly better on the guizzes in 2011 than in the inverted course and if an examination of just the quiz scores was the only method for evaluating the inverted classroom one could conclude that there was no difference in student performance or even that the students in the traditional lecture class retained information better and performed better on the material. However, when examining the exam scores shown in Figure 1 and Table 2 it is clear that the inverted class performed better than the lecture class even if the lecture class was given frequent assessments to facilitate the students learning the material. Therefore it is the inverted part of the course and its implementation and not the frequent assessment that increases student performance. It is possible that the mere action of students having to summarize the notes for the quiz could

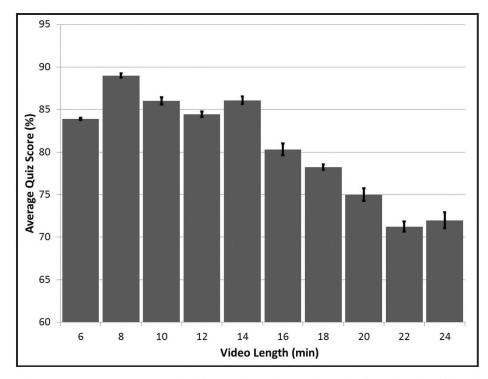


Figure 2. Average quiz score (95% confidence interval) tracked to video length containing the material for the question. There were 64 videos for the course and some videos had multiple questions associated with them.

also lead to improved performances and this is part of the method of implementing an effective inverted classroom that goes beyond just the recording of lectures. The ability for the students to watch the lectures when they want and as many times as they want, along with their frequent interaction with the instructor in the class while working on problems, helped increase their knowledge, understanding, and application of the course material. The daily quizzing in the inverted course helped to facilitate a level of comprehension of the material before the class so that it could be applied to problems and situations quickly during class time. The students could even go back and access the videos during the class while working on problems and often were observed doing so.

Video Length: Lectures were prepared for each class and were broken into 1-4 videos per day keeping major topics and problems in one video. Videos were then grouped into length categories by 2-minute intervals. The set of videos for each day was matched to the set of lectures that would have been given that day in the traditional lecture course. If a lecture included a break for students to work on a problem/question that break was provided in the video by asking students to pause the video and work on the problem. There was no monitoring of how long students actually spent on the problem. The time a student would spend working on a problem was not included in the measured video length. The problem/question was generally reviewed in the video by the instructor, as

would have been done in the lecture course, and this time was included in the video length. Typically the traditional 50-minute class did not contain 50 minutes of lecturing as there were always some active-learning activities built into the lectures and these were maintained to keep the content delivery identical between the inverted and lecture courses. Each video also had quiz question(s) associated with it and the performance of the class on each question was tracked. Results of the student quiz scores based upon video length is presented in Figure 2.

All of the quiz questions addressed learning objectives associated with knowledge, comprehension, and application. The videos covered these learning objectives as well as those related to analyzing, synthesizing, and evaluating. Many of the higher-level learning objectives were also covered in the example problems provided to the class. There was no partial credit given on quiz responses. Students tended to test better on materials as-

sociated with shorter videos. There was a drop off in student understanding and applying thermodynamic concepts if they were presented in videos longer than 15 minutes.

After reviewing these results it was questioned whether the longer videos contained topics that were a different degree of difficulty or addressed higher levels of learning objectives on Bloom's scale even though the quiz questions only addressed the lower levels. Therefore the set of learning objectives written for the course was examined. There were 168 learning objectives previously written. These were initially developed in 2001 and edited for three years. Since 2004 they have remained the same for the course and have been provided verbatim to the students in all classes at the start of the course. The verb in each learning objective was analyzed and matched to a learning outcome in Bloom's cognitive domain using the work of Huitt^[21] as a guide to help classify the objectives. Each objective was grouped into either the lower three levels or higher three levels. Of the 168 learning objectives, 81% of them were in the lower levels while the remainder was classified in the higher levels.

There were 64 videos for the course presented over 33 days of lectures. Each video addressed multiple learning objectives. The 32 higher-level learning objectives were traced to 12 videos, each being longer than 15 minutes. There were only three other videos longer than 15 minutes that did not address higher-level learning objectives. The

quizzes only asked questions related to lower-level learning objectives even though the video lectures covered material across all levels. Two conclusions could be drawn from the learning objective analysis. First, for better student comprehension, topics addressing lower-level learning objectives should be separated from the higher-level ones when preparing the lecture videos. It appears students would get wrapped up in the higherlevel skill acquisition and not grasp the lower-level skills as well when both were presented together. The other conclusion would be to shorten the video lengths to below 15 minutes without having to separate the different levels of learning objectives. These conclusions would need to be verified as the data cannot definitively support either one, but suggest them as possibilities.

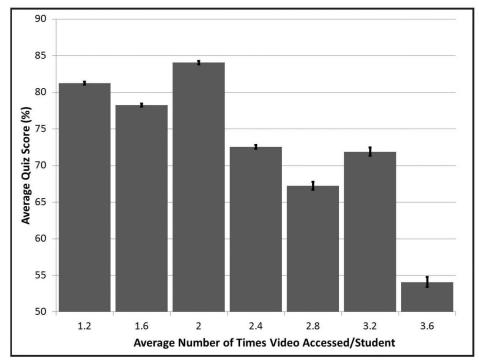


Figure 3. Average quiz score (95% confidence interval) tracked to number of times a video was accessed. Data are a composite for all 64 videos.

Video Access: The online system was able to track when students accessed videos. There was no correla-

tion between the time or day when the students accessed the videos and their quiz scores. There was a correlation between how many times a video was accessed and the average quiz score on the material related to that video (Figure 3). The data were collected up until the quiz time. Students did access videos after the quiz when doing problems, reviewing materials, and studying for exams but those accesses were not included in this data.

The results in Figure 3 provide information to the instructor about what material is difficult for the students to comprehend without having to test the students. One could examine material in videos that were accessed more than twice for this course and assume students need additional instruction on this material. In fact, the instructor could, in future offerings of the course, monitor the video access up until the time of class and enter class with some prior knowledge about where the students are struggling and provide instantaneous instruction on that material via a mini lecture, an example problem, or other means.

CONCLUSION

Students in an inverted class tended to perform better on exams than their counterparts in a traditional lecture course. Students with lower exam scores saw the biggest improvement in their performance with the bottom third of the class increasing their average exam score by seven points. The method of implementation of the inverted course is important and several factors were found to be required for improved student performance. Students must be held responsible for material presented outside of class by video. This was accomplished by daily quizzing. Videos needed to be kept short as videos longer than 15 minutes were found to be not as effective in transferring knowledge as shorter ones. Tracking student access of the online material can also provide data to the instructor on student learning prior to formal assessment.

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ChE JUNIOR LABORATORY AND THE NEW KINETICS EXPERIMENT AT THE UNIVERSITY OF DELAWARE

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comprehensive laboratory course is an important component for adequately preparing engineering students for future careers in industry.^[1] The University of Delaware (UD) Department of Chemical and Biomolecular Engineering (CBE) has recognized the importance of such a course and has committed significant resources and effort towards continuous improvement. Chemical Engineering Laboratory I, more commonly known as Junior lab or J-lab, is offered to students in the Spring semester of their junior year, and seeks to reinforce ChE fundamentals, technical writing, oral presentation, teamwork, leadership skills, and safety practices. Five experiments focused on chemical kinetics, fluid mechanics, thermodynamics, heat and mass transfer, and engineering instrumentation provide the connection with the theory taught in the core ChE courses. This article provides an overview of the Junior lab taught at UD and a detailed analysis of the recently introduced chemical kinetics experiment.

CHEMICAL ENGINEERING LABORATORY I

The Junior lab provides the first opportunity for undergraduate students to apply the knowledge and skills acquired from coursework to actual chemical engineering experiments. The undergraduate lab provides a comprehensive and well-developed program that can lead to significant academic growth for the students. The UD CBE department dedicates significant resources for the Junior lab. A team of four professors, four graduate teaching assistants (TAs), and two laboratory technicians operate, maintain, and work to

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continuously improve the laboratory. The laboratory consists

of five different experiments: fundamentals of measurement

(FOM), heat exchange (HEX), vapor-liquid equilibrium

(VLE), fluid mechanics (FLO), and chemical kinetics (KIN).

The FOM laboratory introduces students to the operation of

basic temperature, pressure, and flow measurement devices.

The lab also provides students with background on analog

and digital data acquisition and control hardware and an

introduction to LabView[®] computer programming. The FLO

experiment features a series of pipes and instrumentation to

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study flow in the laminar, transition, and turbulent regimes. The VLE experiment consists of four ebulliometers for measuring infinite dilution activity coefficients to calculate binary phase behavior.^[2] The HEX experiment features tube and tube, shell and tube, and plate and frame heat exchangers for evaluating and comparing heat transfer correlations. The KIN experiment measures the reaction order and activation energy for the iodination or bromination of acetone reaction. A detailed description of the KIN experiment is provided in the next section.

All students start by running the FOM experiment, which is focused on understanding the principles and operation for a variety of temperature, pressure, and flow measuring devices. The instruments are mounted on portable racks that can be moved between the laboratory and classroom. The FOM experiment provides students with a thorough understanding of engineering instrumentation before they need to use it in the four additional experiments (FLO, VLE, HEX, KIN). Students select two out of the four remaining experiments to complete during the rest of the semester. The experiments are based on the core chemical engineering classes that serve as prerequisites for the lab: CHEG341 (Fluid Mechanics), CHEG231 and CHEG325 (Thermodynamics), CHEG342 (Heat and Mass Transfer), and CHEG332 (Chemical Kinetics).

To complete three experiments with approximately 80 to 100 students within a 13-week semester requires a rigorous schedule be followed. The lab is split into three cycles with each cycle lasting approximately four weeks (and the oral/ video presentations lasting one week). At the beginning of a cycle, the laboratory groups, typically consisting of four students, each elect a group leader. The group leader is responsible for division of labor, organization of the group, assignment submission, and student-teacher correspondence. A new group leader is elected for each cycle so that all students have the opportunity to lead an experiment or an oral presentation.

Given such a demanding schedule, professors, TAs, and students utilize Sakai^[3] for exchanging course information. Sakai provides professors and TAs the ability to post resources, schedule meetings, send out messages, announce assignment deadlines, and provide grades, all of which are archived and easily accessible by the students. In addition, students are able to electronically submit draft and final reports via Sakai to eliminate the need for hard copy submissions. The electronically submitted reports provide users with a confirmation email, which includes the attached files and time of submission. TAs grade draft reports and the professors grade the final reports. Due to the short time frame between experiments, the professors and TAs aim for a two- to threeday turnaround on their comments and grades. This provides students with important feedback before beginning the next experiment. Significant improvement in report writing and lab performance is often seen from the first to third cycle.

During the first week of the semester, faculty and TAs provide

150

lectures on topics such as instrumentation, statistics, error analysis, and how to write an effective engineering report. The first week of each cycle features a prelab lecture given by the assigned professor for the experiment and a prelab tour given by the TA so that students can become familiar with the laboratory equipment. Instructional videos of experiments are also available online for students to watch and see the equipment in operation.^[4] A prelab meeting is held with the assigned faculty member and TA for each experiment. The prelab meetings are one to two hours and include a 20-minute presentation by the students to the professor and TA as a demonstration of their preparedness for the upcoming lab. The prelab meetings provide the faculty member time to thoroughly cover the theory for the experiment and any safety concerns for the lab to ensure all students understand the hazards. The prelab meeting also provides the opportunity for the students to ask in-depth questions. The professors assigned to each experiment meet individually with all groups, which is a significant time commitment, but ensures that the students are well prepared for the lab.

During the second week, the students work in the lab as organized groups and each experiment can be completed within the allotted 4-hour time period. The third week provides time for analysis and report writing. The report is due two weeks after the groups' completion of the in-lab experiments. The average report consists of approximately 20 pages with a supplemental appendix. Students are allowed to submit a rough draft of their report to the TA up to 72 hours before the report deadline so that the TA can provide comments on data analysis and report writing.

The first cycle is identical for all groups, with every group completing the FOM lab. Cycles two and three vary between groups, with each group completing two of the four possible remaining labs. The fourth cycle is a presentation on one of the completed experiments. Each group is given the option of either creating an instructional laboratory video or giving a professional oral presentation. The videos are presented during a video night at the end of the semester, with the best videos receiving awards. The best videos are also used to help instruct the next year's students on the operation of the equipment and how to successfully complete each experiment.^[4] The oral presentation is given in a television studio at UD, in front of the Junior lab professors and TAs. The other student groups are also invited to attend. The presenters have access to an "Oral Communication Fellow," usually a senior communications major, to assist them in the design and delivery of the presentation. Following a period of questions after the presentation, the students are provided a DVD copy of their presentation, and asked to write a critique of both their speaking skills and overall presentation quality.

In 2014, 92 students were enrolled in the Junior lab, and these students worked in groups to complete three of the five labs over the course of the semester. The students were given

TABLE 1 Junior laboratory schedule in 2014					
Timeline	Group 1	Group 2	Group 3	Group 4	
		Cycle 1			
WEEK 1	Prelabs	Prelabs	Prelabs	Prelabs	
WEEK 2	FOM in-lab	FOM in-lab	FOM in-lab	FOM in-lab	
WEEK 3	Data Analysis	Data Analysis	Data Analysis	Data Analysis	
WEEK 4	Final Report	Final Report	Final Report	Final Report	
		Cycle 2			
WEEK 5	Prelabs	Prelabs	Prelabs	Prelabs	
WEEK 6	FLO in-lab	KIN in-lab	VLE in-lab	HEX in-lab	
WEEK 7	Data Analysis	Data Analysis	Data Analysis	Data Analysis	
WEEK 8	Spring Break	Spring Break	Spring Break	Spring Break	
WEEK 9	Final Report	Final Report	Final Report	Final Report	
		Cycle 3			
WEEK 10	Prelabs	Prelabs	Prelabs	Prelabs	
WEEK 11	KIN in-lab	FLO in-lab	HEX in-lab	VLE in-lab	
WEEK 12	Data Analysis	Data Analysis	Data Analysis	Data Analysis	
WEEK 13	Final Report	Final Report	Final Report	Final Report	
WEEK 14	Oral & Video Presentations				

CHEMICAL KINETICS EXPERIMENT

The growing number of students in the UD CBE department required another experiment be added to the Junior lab course. In 2013, we added a KIN experiment in combination with the FLO, VLE, and HEX experiments. In the KIN lab, the undergraduate students run either the iodination or bromination of acetone reaction. During Spring 2014 the students studied the iodination of acetone. The reaction is shown in Eq. (1) and uses HCl as a catalyst. The following sections will describe in

the option of creating their own laboratory groups, and these groups needed to be determined before the semester began. During the previous semester students take a fluid mechanics course that also utilizes four-person groups for its projects, and students are encouraged to use this as a test run for their Junior laboratory group. The result was 23 groups completing a total of 69 experiments. The scheduling used during the Spring 2014 semester can be seen in Table 1.

detail the critical elements for the KIN lab.

$$\begin{array}{c} H^{+} \\ Ac+I_{2} \rightarrow Acl+HI \\ H_{2}O \end{array}$$
 (1)

Apparatus and safety

The kinetics laboratory is equipped with two identical reac-

tors. An example of one of the reactor setups can be seen in Figure 1. The 1-liter glass reactor (fabricated

Figure 1. Image of reactor setup in laboratory with the following equipment labeled: Spectrophotometer (1), Sipper Pump (2), Reactor (3), Impeller (4), Circulating Water for Temperature Regulation (5), Sampling and Return Needles (6), Thermocouple (7), Impeller Motor (8), Syringe Port (9), Waste Beaker (10), Impeller Speed Control (11), Impeller Speed Readout (12), Thermocouple Readout (13), Water Bath (14), Computer Monitor (15), Keyboard (16), Computer Mouse (17), Spectrophotometer Dust Cover (18). Secondary Container (19).



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by Ace Glass) is mounted on the wall for easy access and improved visibility. Each reactor includes a drain spout to empty the reactor, an outer jacket for temperature control, and three ports located on the top of the vessel. A glass beaker inside a secondary container is placed under the drain spout to prevent chemical spills and to collect waste after each run. The impeller extends into the reactor through the central top port and is powered by a motor through a flexible coupling system. A tachometer displays the impeller speed through an LCD display on the control panel. A sipper pump (Jenway, 632002 SIPPER) uses peroxide-cured silicone tubing (Cole Parmer, Masterflex) to transport the chemical samples through one of the outer top ports to a flow cell. Absorbance readings are collected using the Jenway 6300 spectrophotometer at a continuous, specified rate during the experiment. The spectrophotometer software provided by Jenway (63-Zero version 1.10.2207.27293, Jenway) allows for real-time monitoring and data collection. The two reactor setups allow for the completion of the laboratory in a 4-hour period, and ensure that if one reactor malfunctions, students have a backup reactor to complete the experiment. In total, each reactor setup cost about \$10,000 when the experiment was constructed in 2012.

The chemicals (HCl, acetone, and iodine-water solution) are weighed on analytical balances inside a chemical fume hood. Several graduated cylinders (30, 50, 100, 1000 mL) are available for students to weigh acetone and water, and 10 mL plastic syringes (BD Luer-LokTM) with detachable needles (18 gauge, BD PrecisionGlide) are used for volumetric measurement of HCl and iodine water solution. The graduated cylinders and syringes are all weighed on mass balances (OHAUS Scout Pro SPE2001) to obtain the most accurate weights.

During the prelab meeting, the faculty members assigned to the experiment ask the students a series of safety questions to make sure they are aware of all the experimental hazards. In addition, all students are required to take a mandatory 1-hour safety training course before entering the lab. Students must also thoroughly cover all aspects of safety during their prelab presentation. Specifically for the kinetics experiment, the concentrations of the iodine (or bromine) and HCl used are 0.1 N and 1 N, respectively. The dilute nature of these chemicals is a designed safety feature for this laboratory. In addition to the mandatory safety training, all students must wear personal protective equipment (splash goggles, lab coat, nitrile and Chloroflex[™] gloves, closed-toe shoes, and long pants) and dispense hazardous chemicals in a ventilated chemical fume hood. Students are required to read and become thoroughly familiar with the chemical Safety Data Sheets (SDS) and calculate amounts that if spilled could exceed allowable exposure limits (AEL) and flammability limits such as lower and upper explosivity limits (LEL and UEL). The laboratory is also equipped with a safety shower, eyewash station, and spill kit. OSHA-certified waste disposal containers are provided for the

reactor products, wash solutions, and solid waste such as paper towels. The waste jugs are located in secondary containers for spill protection. A sharps bin is available for disposal of used syringe needles. Plastic transfer trays are used to minimize safety risks when moving syringes around the laboratory and syringes have protective covers. Needles are removed using a special tool to prevent finger pricks. Glass funnels are used when pouring large volumes of reagents such as water and acetone into the reactor to reduce the possibility of spills. Finally, in lab long hair is tied back and loose clothing, such as ties and jewelry, are removed to prevent contact with the rotating agitator shaft. Process safety management is a constant theme throughout Chemical Engineering Lab I, with the other experiments having equally strong safety features in place. Finally, adjunct professors from industry often participate or teach experiments in Junior lab and reinforce the importance of maintaining a strong safety culture.

Methodology and data analysis

The reaction mechanism for the iodination of acetone can be written in three elementary steps. The first step [Eq. (2)] is an equilibrium reaction between acetone (Ac) and the acid (HCl) to form the protonated acetone intermediate (AcH+). The second step [Eq. (3)] is the slow step to form the enol intermediate (Ac*). The fast step [Eq. (4)] between the Ac* and the iodine (or bromine) produces the iodoacetone (or bromoacetone). The rate-determining step is the slow step and the rate equations for each step can be written in order to determine the overall rate expression for the reaction, which is shown in Eq. (5). The reaction is first order in acetone and HCl and zero order in iodine (or bromine).

$$Ac+H_3O^+ \xleftarrow{k_1} AcH^+ + H_2O(equilibrium step)$$
 (2)

$$AcH^{+} + H_{2}O \xrightarrow{k_{2}} Ac^{*} + H_{3}O^{+} (slow step)$$
(3)

$$Ac^* + I_2 \xrightarrow{k_3} AcI + HI(fast step)$$
 (4)

$$\mathbf{r} = \mathbf{k}(\mathbf{T}) \cdot \mathbf{A} \mathbf{c}^{\alpha=1} \cdot \mathbf{I}_{2}^{\beta=0} \cdot \mathbf{H} \mathbf{C} \mathbf{I}^{\gamma=1}$$
(5)

Students are taught how to use the method of initial rates [Eq. (6)] to solve for the rate constant and orders of reaction^[5,6]:

$$\frac{\mathbf{r}_{1}}{\mathbf{r}_{2}} = \frac{\mathbf{k}_{1}(\mathbf{T}) \cdot [\mathbf{Ac}]_{1}^{\alpha} \cdot [\mathbf{I}_{2}]_{1}^{\beta} \cdot [\mathbf{HCI}]_{1}^{\gamma}}{\mathbf{k}_{2}(\mathbf{T}) \cdot [\mathbf{Ac}]_{2}^{\alpha} \cdot [\mathbf{I}_{2}]_{2}^{\beta} \cdot [\mathbf{HCI}]_{2}^{\gamma}}$$
(6)

where r is the reaction rate, k is the rate constant, [Ac], $[I_2]$, and [HC1] are reactant concentrations, and α , β , and γ are the orders of reaction, and the subscripts 1 and 2 denote two individual reactions.

The iodination (and bromination) of acetone reaction is a color change reaction. The water, acetone, and HCl solution are added in order and the mixture is colorless. Once the iodine (or bromine) is added the reaction mixture changes to a yellowish-brown color and the reaction begins. The final product iodoacetone (or bromoacetone) is colorless so a spectrometer can be used to measure the change in color from yellow-brown to clear. The spectrometer measures the change in intensity of the iodine at a wavelength of 510 nm (450 nm for bromine). Concentration is obtained from absorbance data using the Beer-Lambert Law:

$$A = \varepsilon bc$$
 (7)

where A is absorbance, ε is the molar absorption coefficient, b is the sample path length, and c is the molar concentration.^[7] Calibration standards are prepared by the TA and a calibration curve can be constructed to determine ε b, which over the range of iodine concentrations measured remains essentially constant.

During the prelab meeting, students will provide a detailed analysis of their methodology and experimental plan for obtaining the kinetic parameters. Typically, students perform one baseline experiment and then vary the concentration of one component at a time while holding the others constant including temperature which results in seven to 10 experiments. These experiments are typically run by two of the four students in one of the reactor setups.

The activation energy for the reaction can be determined using the Arrhenius equation:

$$\mathbf{k}(\mathbf{T}) = \mathbf{A}\mathbf{e}^{\frac{-\mathbf{L}_{3}}{\mathbf{R}\mathbf{T}}} \tag{8}$$

where k is the reaction constant, A is the Arrhenius parameter, E_a is the activation energy, R is the ideal gas constant, and T is the temperature.^[8] Typically, the other two students in the group will also run the baseline experiment in the second reactor and focus on changing the temperature of the reaction while keeping the concentrations constant in order to determine the activation energy. Students usually run three to five experiments at temperatures from about 298 K to 308 K. Changing temperature can take longer than changing concentrations so having a second reactor allows all four students to run experiments and finish within the 4-hour time period. The key to high-quality measurements is maintaining a constant concentration or temperature depending on which variables students plan to keep fixed and understanding the impact of any deviations in the detailed error analysis for the order and activation energy.

Conceptually, the ideas are simple; however, the biggest problem students encounter with the initial rates method involves the difficulties in keeping reactant concentrations constant when preparing their solutions, and keeping temperature constant when performing each of the reactions. Each group of students must determine a value and an uncertainty for the orders of reaction for iodine, acetone, and hydrochloric acid, as well the Arrhenius parameter and activation energy. Students who are well prepared with good lab skills and who analyze their data in lab typically obtain excellent results.

Iodine concentration data as a function of time is shown in Figure 2. The spectrometer is turned on before any iodine is

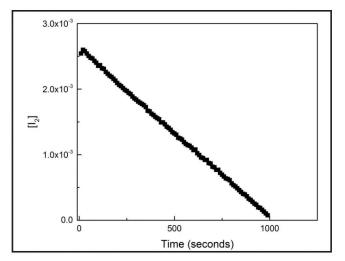


Figure 2. Concentration of iodine as a function of time.

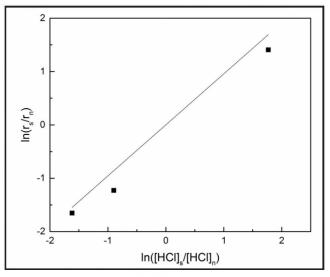


Figure 3. Application of initial rates method used to determine the order of reaction for HCl when used as a catalyst. The trend line was fit through the intercept (0,0) with a slope of 0.956.

added so the initial baseline concentration (or absorbance) is zero. When the iodine is added, the concentration immediately increases as shown and the reaction begins. As the reaction progresses the iodine concentration steadily decreases to produce iodoacetone. The change in iodine concentration as a function of time can be fit using linear regression to determine the rate of reaction. As shown in Figure 2, a typical reaction takes about 15 to 20 minutes (900 – 1200 seconds) so 12 to 16 experiments can be completed in a 4-hour lab period.

To determine the reaction order for HCl, the concentration of iodine and acetone along with the temperature must be kept constant with respect to the initial baseline experiment. This simplifies Eq. (6) so that the rate constant (k) and the acetone and iodine concentrations cancel out. Next, Eq. (6) can be linearized by taking the natural log of both sides. Figure 3 is a

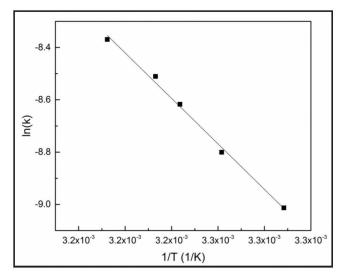


Figure 4. Application of the Arrhenius Equation to determine kinetic parameters.

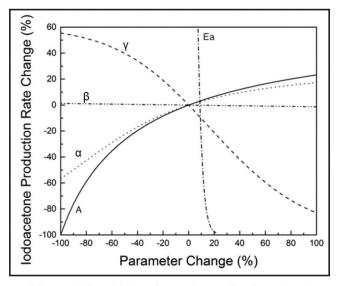


Figure 5. Sensitivity of experimentally determined kinetic parameters to percent changes in their value in a CSTR reactor. The values of E_a , A, α , β , and γ used were 86.22 kJ/mol, 8.68·10¹⁰ L/(mol s), 0.99, -0.04 and 0.99, respectively.

plot of the ratio of the rates versus the ratio of the HCl concentrations where the slope is the reaction order of interest for HCl. The same procedure is repeated for determining the orders for acetone and iodine (or bromine). Again, the method appears simple, but in practice how close the students maintain the concentrations and temperature they plan to cancel out determines how well they can obtain the theoretical orders for the reaction while minimizing their uncertainty.

To determine the activation energy and the Arrhenius parameter for this reaction, the rate constant k must be determined as a function of temperature assuming either the theoretical or the experimentally determined orders. Eq. (8) can be linearized and ln(k) can be plotted versus the inverse of the absolute temperature as shown in Figure 4. The activation energy can be calculated by multiplying the slope of the trend line by the gas constant, R. The Arrhenius parameter can then be determined by taking the exponential value of the vertical intercept.

Non-linear regression can also be applied to solve the reaction orders simultaneously using all the rate data. The data has to be good quality and an initial guess for the orders provided based on the theoretical orders for acetone, HCl, and iodine (or bromine) of 1.0, 1.0, and 0. In some cases if the temperature-dependent data is also high quality the activation energy and Arrhenius parameter can also be determined along with the orders. In 2013, the use of non-linear regression was not mandatory; however, many students were able to develop a model and make comparisons with the initial rates method. In 2014, students were provided background on non-linear modeling and required to include this analysis in their final report. All groups were able to successfully model their data using non-linear regression and make comparisons with the initial rates method. Students typically employed Microsoft Excel for the linear regressions, and either MATLAB or Mini-Tab for the non-linear regressions.^[9,10] In most cases when the data were of high quality the results using both methods were similar to within the experimental uncertainty.

ASPEN modeling

Students were taught the basics of ASPEN Plus, so that they could model the iodoacetone reaction and perform a sensitivity analysis.^[11] Video tutorials were prepared using Camtasia® software so students could watch and learn online how to create a reactor ASPEN model.^[4] The videos can be run simultaneously while students create their own model in a separate ASPEN window on the computer. This method of teaching engineering software has been popular with students at UD because they can watch the videos on their own as many times as necessary to learn the fundamentals while performing the exercises. Most groups chose the CSTR model (RCSTR) to evaluate the effect of changing kinetic parameters such as the reaction orders for acetone (α), I₂ (β) and HCl (γ), activation energy (E) and Arrhenius parameter (A) on the production of iodoacetone as shown in Figure 5.

As expected the reaction order for iodine has no effect on the production of iodoacetone (*i.e.*, zero order), increasing the reaction order for acetone increases the production of iodoacetone (*i.e.*, [acetone] > 1.0), and increasing the HCl reaction order decreases the production of iodoacetone (*i.e.*, [HCl] < 1.0). The activation energy (E_a) and/or temperature have the largest effect on the production of iodoacetone, which is expected since both are within the exponential as shown in Eq. (8). A few groups also modeled the reactor using the batch ASPEN model (RBATCH), which provided the change in iodine concentration as a function of time. A good fit between the experimental and model data was obtained as shown in Figure 6. This provides students with a model comparison of their time-dependent concentration data.

Students use their ASPEN models to estimate the reactor size and operating conditions necessary for commercial-scale production of iodoacetone (or bromoacetone). This is the first opportunity students get to use ASPEN to model an experiment and although they only have time to go to lab once to run this experiment, they can use their models to expand upon the effect of changing operating conditions such as reactor temperature and volume or operating a continuous flow reactor versus a batch reactor. In other words, the students can run additional experiments using their ASPEN models without having to return to the laboratory.

Assessment and experiences

The average kinetic parameters obtained for the KIN experiment in 2013 and 2014 are provided in Table 2. The bromination of acetone in 2013 was run by 13 groups (52 students) and the iodination of acetone in 2014 was run by 12 groups (48 students). In both years, students came close to obtaining the theoretical orders for the halogen (I_2 or Br₂) of 0, the acetone of 1.0, and the catalyst (HCl) of 1.0. The activation energy (E_a) for the bromination of acetone was about 84.1 ± 2.0 kJ/mol, which is in good agreement with reported literature values (86.7 ± 0.5 kJ/mol).^[12] The activation energy and Arrhenius factor were expected to be similar for both reactions as shown because the rate limiting step is not a function of the halogen [see Eq. (3)].

Students are encouraged to be creative in Junior lab. During their prelab meetings with the faculty member and TAs other experiments and modeling are discussed that the group might try if time allows. A few examples in 2014 include one group performing a mixing experiment to evaluate the speed of mixing on the rate of reaction and another group performing a basic heat transfer analysis on the temperature difference between inside the reactor versus inside the spectrometer cuvette cell. In some cases these additional experiments have improved the design of the experiment. For example, a group brought to our attention the fact that the cooling/heating jacket around the reactor did not completely envelop the 1 liter fill volume recommended for each experiment. The group determined if the reactor were filled to approximately 0.6 liters the temperature was easier to maintain and control; however, the reduced volume did lead to larger experimental errors when preparing reactant concentrations because smaller masses for each reactant must be weighed.

CONCLUSIONS

The undergraduate Junior laboratory at the University of

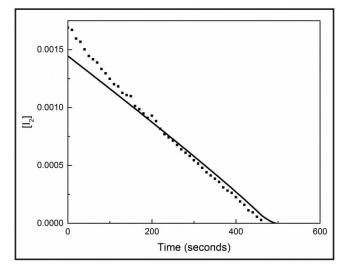


Figure 6. Comparison of experimental batch reactor data, and data generated by ASPEN. The black dots represent the experimental data and the solid line represents the ASPEN model.

TABLE 2 Average values of experimentally determined kinetic parameters from all groups in 2013 and 2014					
	2013 Bromination	2014 Iodination			
Halogen Order	0.097±0.020	0.002±0.065			
Acetone Order	0.943±0.031	1.010±0.049			
HCl Order	0.960±0.026	1.020±0.039			
A [L/(mol s)]	$8.26 \cdot 10^{11} \pm 6.17 \cdot 10^{11}$	$8.60 \cdot 10^{11} \pm 2.72 \cdot 10^{11}$			
E _a [kJ/mol]	84.1±2.0	88.5±1.3			

Delaware has evolved over several decades and each year continues to implement improvements based on student feedback. Students have responded very positively to the Junior laboratory when surveyed at the end of the course. As part of the survey, students were asked to rate whether or not the following three ABET objectives were achieved:

- Plan an optimum set of experiments that meet welldefined objectives;
- (2) Recognize and properly use laboratory safety procedures. Identify major hazards in an experiment. Collect data, analyze and interpret experimental measurements, and compare to existing theories, and;
- (3) Learn to communicate results and conclusions effectively through both written reports and oral presentations.

During the Spring 2014 semester, 70 out of 92 students

responded to our survey. On a scale of 1 to 5, with 1 being very dissatisfied and 5 being very satisfied, these questions received average scores of 4.53, 4.75, and 4.59, respectively.

Many students also take a special interest in Junior lab after completing the course and want to know what they can do to improve the lab for the future. Students have assisted instructors during the summer and winter sessions with many upgrades including the design, construction, and documentation for the KIN experiment and modifications and calibrations to the VLE, FLO, HEX, and FOM experiments. Currently a group of students is studying the iodination of 2-butanone and another student is evaluating other strong acids that can catalyze the iodination reaction as future kinetic experiments.

Chemical Engineering Laboratory I features an informative instrumentation experiment and four unique labs each directly relating to a core course in the ChE curriculum. The KIN experiment has been successfully demonstrated for both the iodination and bromination of acetone. ASPEN modeling provides the opportunity for students to run additional experiments on the computer outside of laboratory time with results that are comparable to their laboratory data.

Many students describe the Junior lab as one of the most memorable courses they take during their undergraduate education at UD. The course prepares students to not only connect the theory from core courses with actual experiments, but also to work together efficiently in teams, to have the opportunity to lead a project, to learn how to effectively write and present engineering reports, and to operate equipment safely. The Junior lab provides a comprehensive learning environment to help prepare students for future careers as chemical engineers.

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STUDENT CHEMICAL ENGINEERING **REFLECTIVE ePORTFOLIOS** ChE Student Perceptions of Learning From Reflective ePortfolio Creation

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ngineering educators and employers value and prioritize communication skills as evidenced by desired student learning outcomes and job descriptions defining new positions; however, developing and assessing such skills in an engineering program is challenging. ABET's criteria for accrediting engineering programs comprises General Criterion 3, student outcomes, including the ability to effectively communicate.^[1] Effective oral and written communication outcomes frequently appear in higher education course syllabi and industry job requirements. Employer feedback, however, indicates new graduates lack communication skills.^[2]

In an Association of American Colleges and Universities (AACU)-sponsored study, employers prioritized communication skills: "More than three in four employers say they want colleges to place more emphasis on helping students develop five key learning outcomes, including: critical thinking, complex problem solving, written and oral communication, and applied knowledge in real-world settings."[2] Furthermore, they believed company success depends on innovation and recognize that employees face increasingly complex problems requiring broader skill sets; therefore, employers prioritized "critical thinking, communication, and complex problemsolving skills . . . when making hiring decisions."

Although educators and employers value and prioritize communication skills, developing and assessing such skills in a higher education engineering course is difficult. In addition, engineering courses include rigorous science, math, and engineering curricula, but rarely require students to reflect, write, and articulate how new learning connects to prior experiences and transfers across or to new contexts.^[3] Therefore, students do not connect learning from assignment to assignment,

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course to course, and course to experience, such as an internship. Even when students demonstrate communication skills through formal assessments, they may be unaware of their thought processes and unable to articulate what they know and how they solve problems, a critical engineering skill.^[4,5] Incorporating technical writing into engineering courses and, more specifically, incorporating multiple reflection opportunities, enhances the student's ability to communicate within the discipline. Requiring students to go further and draw together experiences through a reflective portfolio gives them an opportunity to describe how and why they know what they know.

Reflective ePortfolios can develop students' communication skills by requiring multiple writing assignments integrated into engineering curricula.^[6] Lorenzo and Ittelson defined an ePortfolio as "a digitalized collection of artifacts, resources, and accomplishments" that showcases a student's work and provides opportunities for metacognitive, reflective, critical, creative, and logical thinking.^[7] In addition, ePortfolios address the six areas employers identified for higher education emphasis in student learning: critical thinking and analytical reasoning; complex problem solving and analysis; written and oral communication; knowledge and skill application in real-world settings; locating, organizing, and evaluating information from multiple sources; and innovation and creativity.^[2] Furthermore, 80% of employers indicated an ePortfolio would be helpful in the hiring process to demonstrate student knowledge, skills, and experience.

THE COURSE AND REFLECTIVE ePORTFOLIO ASSIGNMENT

To develop effective communication skills, Texas A&M University's chemical engineering department requires CHEN 301, Engineering Workplace Writing, a technical communication course (see <https://sites.google.com/site/tamuchen301/ home>).^[9] The instructor provided students, typically juniors and seniors, the following welcome, which connects communication learning outcomes to discipline-specific ABET outcomes and broader university undergraduate learning outcomes:

Engineering Workplace Writing integrates best-use practices of technical communication instruction including high-impact learning activities while also meeting university student learning outcomes. The course stresses the principles of rhetoric, i.e., understanding the audience and purpose of communication in different workplace contexts, in order to effectively prepare and deliver the message. You, the student, will practice the essentials of technical communication while addressing a variety of communication challenges, thus reinforcing communication, critical thinking, lifelong learning, and collaboration outcomes as stated in the TAMU Undergraduate Learning Outcomes and ABET Program Educational Outcomes.^[9]

As the culminating course assignment, chemical engineering students created a ChemE-folio, hereafter referred to as a reflective ePortfolio (see <https://sites.google.com/site/ chemefolioassignment/home>)^[10] to house a collection of their work representing academic accomplishments as well as academic and career goals. Using an ePortfolio template (see

The purpose of this three-year qualitative case study was to investigate the use of reflective ePortfolios in an undergraduate chemical engineering course. Three research questions guided the study: a) How do reflective ePortfolios affect chemical engineering students' perceived learning?, b) Why are chemical engineering students motivated to create reflective ePortfolios?, and c) What are chemical engineering students' preferences (likes and dislikes) in creating reflective ePortfolios?[8]

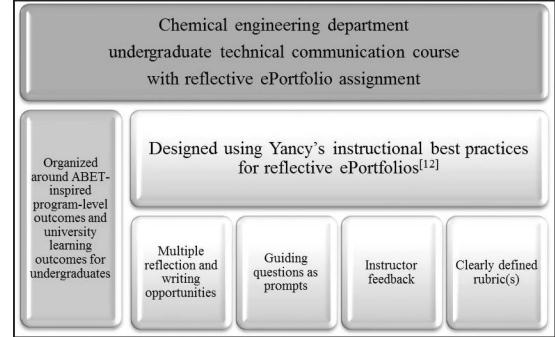


Figure 1. CHEN 301, Engineering Workplace Writing, a technical communication course.

<https://sites.google.com/site/chemefoliotemplatespring 2013/>),^[11] students selected relevant chemical engineering outcomes and customized the reflective ePortfolio based on their unique skills and accomplishments. In addition to ABET-inspired program-level outcomes and the university's learning outcomes, Yancey's best practices for reflective ePortfolios guided the design (see Figure 1). According to Yancey, instructional best practices for reflective ePortfolios include a) multiple reflection and writing opportunities, b) guiding questions that prompt student identification of what they are learning and why it matters, c) instructor feedback on interim reflections, and d) a clearly defined rubric with specific expectations.^[12]

First, this course provided multiple reflection and writing opportunities to reinforce communication competencies assessed in the final reflective ePortfolio. For example, course assignments required students to understand how rhetorical context influences the message, prepare multiple assignments addressing different workplace contexts, and reflect on how the assignment context influenced the development, organization, etc., of their created messages. Furthermore, students prepared and revised reflections demonstrating workplace writing processes (*e.g.*, invention or defining the problem, planning, drafting, editing, revising) and writing competencies (*e.g.*, developing logical arguments supported by adequate evidence, effective paragraph development, professional writing style, conventions, and document design). Second, the course used guiding questions that prompted students to reflect on their broader learning across the engineering curriculum (see Table 1).^[12] For example, the reflective ePortfolio assignment, organized by university and ABET learning outcomes, used guiding questions to prompt student responses demonstrating chemical engineering skills. For students to make sense of projects and experiences beyond the communication course, guiding questions scaffolded learning from lower- to higher-order thinking. Related to engineering projects, for example, lower-level thinking skill questions asked students about what they did (including when, where, and how) followed by higher-level thinking questions asking why it matters and to whom.

Third, the instructor provided feedback to students on their reflections, including written and voice comments on writing strengths and weaknesses. For example, student feedback included how effectively their reflective ePortfolios provided well-developed short essays supported by clear, substantial, relevant evidence, communicated through coherent paragraphs and a professional writing style. In addition, students received feedback in class through large group discussions on their low-stakes reflections, introducing or reinforcing key writing skills. Fourth, the instructor created clearly defined rubrics with specific expectations: to provide constructive

TABLE 1 Examples of reflective ePortfolio reflective writing prompts for chemical engineering students				
	Where, in what context, was this project completed? Was it part of a course? Internship? Co-op?			
	What were the purposes of the project, as a whole?			
What was the context?	What was the problem or topic your project addressed? Was a project description (or problem) stated, or were you required to identify the problem and describe it yourself?			
	What were you required to do to complete the project? How did you prepare for the project? What tasks or steps did you complete? Did you create a management plan?			
	What did the project requirements assume that you already knew? Were there pre-requisites regarding terminology, use of equipment, safety standards, etc.?			
	Did the project require you to design something to address the problem?			
	Did your recommendation, plan, or design require you to compare options?			
	Did your project require you to determine the resources needed to produce a given product or service?			
	Did your research require you to read, understand, and incorporate information from technical sources such as peer- reviewed journals? Which ones?			
What did you do?	Did your research require documentation? Did you comply with established guidelines?			
	Did your research require you to use databases in your discipline? Which ones?			
	Did your research require you to network with professionals whose expertise would help you solve a problem, comp options, recommend a best solution?			
	Did you present any of the information in a graphical form? What was the purpose(s) of these graphics?			
	Did this project require you to maintain a level of confidentiality?			
	What did you learn (equipment, skills, safety, time management, collaboration, patience) by completing this project?			
W7h-4 J: J 19	What challenges did you face to complete the project? Did anything unexpected happen?			
What did you learn?	How did you overcome the challenges? Provide details.			
	Did you receive feedback from your instructor or supervisor? If so, what did he or she say?			

feedback on essential writing competencies and to direct the development of the ePortfolio. Writing competencies addressed in the rubric included content development according to the audience, purpose, and context; organization; design; graphics; style; and convention. ePortfolio development addressed in the rubric included the required portfolio sections (*e.g.*, overview or cover letter, resume, academic interests, experiences and skills, university and ABET-related learning outcomes).

LITERATURE REVIEW

According to Davis, Davis, Leiffer, McCormack, Beyerlein, Khan, and Brackin, engineers must reflect on what they know, how they learned it, and why it matters in order to problem solve and to transfer learning to new contexts.^[13] Therefore, this literature review focuses on reflection's central role in engineering students' professional skill development, professional identity development, and integrated learning. In addition, this section reviews the role of ePortfolios within integrated learning curricula and engineering education.

First, reflection is central to professional skill development. Research in engineering undergraduate curricula emphasizes the importance of reflection in developing professional skills, particularly in capstone courses where students complete design projects requiring skill sets they will use as practicing engineers.^[13] However, students tend to focus on project completion, not on how and why they problem solve the way they do. Therefore, the National Science Foundation (NSF) funded a project to create Integrated Design Engineering Assessment and Learning System (IDEALS) modules to scaffold formative and summative reflection in a capstone course curriculum. While working on capstone projects, students moved through professional skill sets, reflecting on what works, how it works, and why it works. As a result, they made and expressed sound judgments regarding engineering standards and constraints as well as sound judgments regarding the broader impact of engineering solutions. Assessment examples from programs using the IDEALS modules "illustrate student reflection on past experiences, relating causes and effects, making decisions on actions to achieve goals, taking necessary actions, showing new understandings emerging from experiences, and taking control of thoughts in order to be more constructive."[13]

Second, *reflection is central to professional identity development*. Light, Chen, and Ittelson emphasized the importance of reflection to students' individual professional development, team contributions, and overall professional responsibility.^[5] Eliot and Turns analyzed post-surveys from professional portfolio workshops to investigate engineering undergraduate identity-related impacts and processes and identified internal and external frames of reference for professional identity construction.^[14] The internal frame of reference focused on students' "emerging realization of their own values and

interests as professional engineers," and the external frame of reference focused on students' understanding of future employers' expectations. Last, Magolda and King as well as Light, Chen, and Ittelson advocated that self-authorship, in which students organize, connect, and evaluate information, facilitates identity development.^[15,5]

Beyond making connections between information, learners also need to think through how that information helps them to know and understand the world—in other words, to understand how their existing knowledge provides a framework for their understanding, how their values shape those frameworks, and how the relationships they engage in provide alternate perspectives.^[5]

Third, reflection is central to integrated learning. Reflection encourages students to build "across the curriculum and co-curriculum, from making simple connections among ideas and experiences to synthesizing and transferring learning to new, complex situations within and beyond the campus."^[16] Based on cognitive research by Ambrose, Bridges, DiPietro, Lovett, and Norman, Brent and Felder identified five instructional strategies.^[17,18] In their fourth strategy, helping students learn to function like experts, they encouraged engineering educators to require students to "reflect on what they learned and what they will do differently in the future. When you first ask them to strategize and reflect, explain why you are doing it and give several good and bad examples of both processes."[18] To develop mastery, students must acquire component skills, practice integrating them, and know when to apply what they have learned.

In addition, *creating reflective ePortfolios supports integrated learning*. Continuing with Brent and Felder instructional strategies, engineering educators can design reflective ePortfolios with explicit learning goals, objectives, outcomes, and expectations (strategy two) and scaffold complex tasks (strategy three).^[18] In addition, ePortfolios can use structured reflective pedagogy, asking students to outline their problem-solving steps, explain their thinking (metacognition), describe encountered problems, and identify most helpful learning aspects.^[19]

Last, *reflective ePortfolios support engineering education*. Recent research on the use of ePortfolios in engineering education includes studies of knowledge construction, identity development, creative behaviors, prior educative experience, and lifelong learning skills awareness and development.^[14,20-23] Additional research examined learning portfolios as a collaborative learning application and an assessment tool.^[24-26] For example, Dunsmore, Turns, and Yellin analyzed mechanical engineering undergraduate portfolios to investigate how students construct their understanding of engineering.^[20] They concluded students perceive engineering practice as real-world knowledge, but knowledge acquired through school as not integral to such practice. Rojas analyzed construction engineering and management graduate portfolios to examine collaborative learning in engineering.^[24] The instructor positively viewed the teaching and learning experience and concluded students "look at the virtual portfolio as a symbol of their achievements, and therefore, they develop a sense of pride that inspires them throughout the semester." In addition, the portfolios provided benefits to prospective students in evaluating the skill set they would learn, to incoming students in benchmarking expected work quality and scope, and to alumni in demonstrating abilities to prospective employers.

This literature review focused on reflection and ePortfolios and situated the study. The next section describes the research design.

METHODOLOGY

Based on the purpose and research questions, this study used a qualitative case study methodology. Qualitative case studies research real-life cases bounded by space and time.^[27] Therefore, this study investigated the use of reflective ePortfolios in an undergraduate chemical engineering course during six semesters spanning three academic years. To achieve this purpose, we defined the case (see The Course and Reflective ePortfolio Assignment section), identified participants, and collected and analyzed data. This study's participants included 313 mostly junior and senior students in the chemical engineering department at Texas A&M University. The students took a technical communication course, CHEN 301: Engineering Workplace Writing, and created reflective ePortfolios as the course's culminating assignment.

Data collection included anonymous post-course surveys initially comprised of seven closed- and open-ended questions (six semesters, 2011-2104, n=313), later expanded to eight questions (two semesters, 2013-2014, n=228). This study used data from four questions: a) Do you believe that reflecting (*i.e.*, writing about your knowledge, skills, and experiences) in the ChemE-folio has enhanced your learning within your degree program? If so, how?, b) What did you like most about creating your ChemE-folio?, c) What did you like least about creating your ChemE-folio?, and the question added for the final two semesters, d) What motivated you to complete your portfolio to the best of your ability (spend time on it)? Data analysis included reviewing the study's purpose and research questions and using Creswell's qualitative case study procedures (see Table 2).^[27]

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This study investigated the use of reflective ePortfolios in an undergraduate chemical engineering course. Guided by the research questions and based on the data, this study identified themes related to chemical engineering students creating reflective ePortfolios: perceptions of learning, motivations, and preferences (see Table 3, following page). This section discusses the findings using student quotes as illustrations.

Student perceptions of learning

The first analyzed survey question asked, "Do you believe that reflecting (*i.e.*, writing about your knowledge, skills, and experiences) in the ChemE-folio has enhanced your learning within your degree program? If so, how?"

Survey responses indicated 67% of students believed reflecting very likely or likely enhanced their learning with regard to the chemical engineering program (see Table 4, following page). In addition, this analysis includes data from 13%

Qualitative	Case Study	This Study Organized the anonymous student feedbac survey responses about the reflective ePortfolio assignment by question, specific cally student reflection, motivations, and combined likes/dislikes	
Organize data	Create and organize data files		
		Read survey responses in their entirety for an overall sense of the data	
Read and memo	Read text, make margin notes, form initial codes	Focusing on specific questions, read all responses	
		Made notes about initial codes	
Describe data using codes and themes/categories	Describe the case and context	Drafted an overview of the course and reflective ePortfolio assignment to provide context	
		Sorted related survey question responses	
		Assigned codes	
Classify data into codes and	Establish themes using categorical categoriza-	Grouped related or overlapping codes	
themes/categories	tion	Established themes	
		Verified each other's sorting, coding, and themes	
T	Interpret data and de-	Identified major themes, based on greates numbers of survey responses	
Interpret data	velop generalizations of what was learned	Used the literature to interpret data and generalize findings	
	Present case using nar-	Presented the case	
Represent data	rative, tables, and/or figures	Represented the findings using participant quotes, tables, and figure	

TABLE 2

of students who responded unsure, but narratively provided evidence of enhanced learning through reflective ePortfolios. Findings included that students a) connected reflection and learning, b) connected learning to real-world application, c) connected learning to future employability, d) learned about themselves, and e) enhanced communication skills. First, students described how they connected reflection and learning. For example, one student professed new understanding of ABET outcomes:

"Yes! I honestly never look at ABET outcomes, but looking and reflecting on them helped me understand why professors do some of the things they do for our classes; also helped reiterate why employers ask certain questions."

Another student wrote,

"Yes, it helped me to understand the purpose and importance of my classes."

Second, students connected the knowledge and skills they were learning to how they would apply such knowledge and

skills in the real world. One student shared,

"Writing my ChemE-folio required me to slow down and take time to reflect on my academic (and other) undergraduate experiences. This reflection has helped me to better understand where I will apply what I have learned as well as its value."

Third, students connected learning to future employability in two ways. First, reflection supported critical thinking about how classroom and work experiences connect and why resulting skills would be useful following graduation. One student summarized,

"By reflecting on my qualities, I gained a better understanding of what values engineers should possess to succeed."

In addition, for many students, analyzing gained knowledge and skills increased confidence and reaffirmed career choice:

"It has showed me that I have tools to succeed. It has made me more confident in my ability to excel in chemical engineering."

TABLE 3 Major themes emerged from undergraduate chemical engineering reflective ePortfolio surveys				
Survey Question	Major Themes			
	Connected reflection and learning			
Do you believe that reflecting (i.e., writing	Connected learning to real-world application			
about your knowledge, skills, and experiences) in the ChemE-folio has enhanced your learning	Connected learning to future employability			
within your degree program? If so, how?	Learned about themselves			
	Enhanced communication skills			
What motivated you to complete your portfolio to the best of your ability (spend time on it)?	Extrinsic • Future • Employability • Course grade	Intrinsic • Self-reflection • Pride • Fun		
	Reflection			
What did you like most about creating your ChemE-folio?	Future employability			
	Creativity or creating the deliverable			
What did you like least about creating your	Time			
ChemE-folio?	Technology or tool			

Second, reflection helped students prepare for interviews with potential employers. Some students used their ePortfolio reflections in job interviews, for example,

"It made it much easier to talk about myself in my recent interview. I just mentioned each reflection point briefly."

Specifically, students thought through how specific skills relate to future work in chemical engineering and how reflecting in their ChemE-folios better prepared them for job interview questions.

Fourth, students learned more about themselves, including values, attributes, and how experiences shaped them. For example, one

	TABLE 4 Students' percentage responses to survey question: Do you believe that reflecting (<i>i.e.</i> , writing about your knowledge, skills, and experiences) in the ChemE-folio has enhanced your learning within your degree program?						
Semester	Very likely	Likely	Not sure	Unlikely	Highly unlikely	Course responses	
2011 Fall	10	16	9	2	1	38	
2012 Spring	15	16	12	1	3	47	
2012 Fall	10	16	8	1	0	35	
2013 Spring	14	12	6	3	0	35	
2013 Fall	20	21	9	7	5	62	
2014 Spring	15	44	31	5	1	96	
Total responses	84	125	75	19	10	313	
	27%	40%	24%	6%	3%	100%	

Chemical Engineering Education

student described how reflection enhanced learning:

"I believe it has helped me learn about myself, and how to improve aspects about me.... This ultimately will help enhance learning within my degree program."

Another student responded,

"By reflecting on my qualities, I gained a better understanding of what values engineers should possess to succeed."

Last, students reported reflective ePortfolios enhanced communication skills, including effectively expressing themselves in writing. One student stated,

"My writing skills did get better, that's for sure,"

and another commented,

"I feel that I have improved my communication ability from this assignment, and I have a better grasp of new technology."

In contrast, 9% of students believed reflecting unlikely or very unlikely enhanced their learning with regard to the chemical engineering program (see Table 4). In addition, this analysis includes data from 11% of students who responded *unsure*, but narratively provided evidence of no enhanced learning through reflective ePortfolios. For example, some responses indicated students did not feel they were far enough along in their chemical engineering program and, therefore, could not see how reflection yet influenced their learning.

Student motivations

The second analyzed survey question asked, "What motivated you to complete your ChemE-folio to the best of your ability (spend time on it)?"

Students indicated extrinsic and intrinsic motivations. Extrinsically, students first identified future employability as motivation. Specifically, creating reflective ePortfolios prepared students for interviews and provided evidence of knowledge, skills, and accomplishments. For example, one student responded,

"I was motivated by the fact I could use the portfolio to help present my credentials and set myself apart from other job candidates. It was nice to have a finished product I could use after the class ended."

Second, students identified the course grade, of which the reflective ePortfolio comprised 25%, as the primary motivation. In addition to the grade, some students identified motivations prior to or during the creation of their reflective ePortfolios. One student shared,

"At first I was motivated to get a good grade, but as I went through it I began to envision seeing the folio come together."

Other students acknowledged future use,

"I wanted to be able to use the ChemE-folio in the future. I would not have spent the time if it was just for the grade," "At first I was motivated to get a good grade, but as I went through it I began to envision seeing the folio come together." — Student feedback

and

"Either I was going to do a bad job and not use the ChemEfolio again, or do a really good job so I could use it. I chose the latter."

In contrast to extrinsic, student intrinsic motivations were more self-reflective. For example, one student described,

"The fact that the ChemE-folio is a direct reflection of who I am. I want it to be clear, accurate, honest, professional, and aesthetically pleasing."

Other students expressed pride in their work, especially when they saw the reflective ePortfolio coming together. For example,

"I want to be proud of my work."

and

"It looks good and felt good to see the fruits of my labor."

Last, fun motivated a few students; as one student shared,

"It was fun to do it and I was motivated to do it well since I plan on keeping it for a while."

Student preferences

The third analyzed survey question asked, "What did you like most about creating your ChemE-folio?"

Students generally liked creating reflective ePortfolios and specifically liked the reflection, preparation for future employability, and creativity or creating the deliverable. First, students most liked the reflection, and findings included closely related and overlapping aspects of reflection, such as thinking about self, reminiscing about the past, reflecting and writing about experience, thinking about learning, and learning about self. For example, students wrote,

"The ChemE-folio made me think about my experiences and how to present them," and "It made me sit down and reflect on my past experiences, especially on how they could apply to a job application."

Second, students most liked how reflective ePortfolios prepared them for future employability, including job interviews and providing a job search tool. Generally, one student acknowledged,

"The ChemE-folio got me thinking," and asked, "What do I really have to offer employers? What can I talk about in an interview? [I] liked being able to reflect on my academic career, and what I had done at Texas A&M."

Specific to job interview preparation, one student shared,

"I liked putting what I have [accomplished] on paper and writing it out. It made me think of what I would say instead of stuttering through an interview with only points."

Other students most liked the reflective ePortfolio as a job search tool,

"It was like creating an online super resume and it is easy to update and track every changing experience and qualification."

Similarly,

"I liked that it can be used for career purposes and gives me an advantage against other applicants."

Third, students most liked creating a reflective ePortfolio or using their creativity. Several students described creating reflective ePortfolios as "fun" and enjoyed the "creativity" in and "freedom" to design a visual representation of their experiences.

In contrast, the last analyzed survey question asked, "What did you like least about creating your ChemE-folio?"

Students identified time and the technology or tool as dislikes. First, many students least liked the time required to create their reflective ePortfolios, for example,

"The heavy time commitment; To create a high quality, robust portfolio takes time," and "Very lengthy and takes a lot of time to think and write."

Second, a few students least liked the technology or tool.

Overall, chemical engineering students who created reflective ePortfolios believed such reflection enhanced their learning with regard to the chemical engineering program. They connected reflection and learning, further connected learning to real-world application and future employability, learned about themselves, and enhanced communication skills. Connection to future employability motivated students to create their reflective ePortfolios, in addition to the course grade, pride in work, and fun. Student preferences in creating their reflective ePortfolios divided into likes (reflection and future employability), and dislikes (time required to create such a large project) and, to a lesser extent, the technology or tool used for creation.

DISCUSSION OF THE FINDINGS

The purpose of this three-year qualitative case study was to investigate the use of reflective ePortfolios in an undergraduate chemical engineering course. Student motivations to create reflective ePortfolios included future employability, the course grade, pride in work, and enjoyment. Student preferences divided into likes (reflection and future employability), and dislikes (time required to create such a large project), and, to a lesser extent, the technology or tool. Influenced by such motivations and preferences, chemical engineering students created reflective ePortfolios, perceived enhanced learning, and connected their learning to job knowledge and skills, future employability, and professional identity (see Figure 2).

First, chemical engineering students connected their learning to job knowledge and skills. Creating reflective ePortfolios scaffolded student reflection on their learning, which they connected to job knowledge and skills. This finding reinforces Davis, Davis, Leiffer, McCormack, Beyerlein, Khan, and Brackin's conclusion that engineers must reflect on what they know, how they know it, and why it matters to problem solve and transfer learning to new contexts.^[13] For

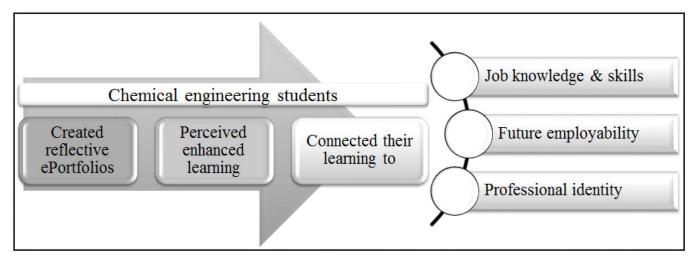


Figure 2. Study findings.

example, students connected ABET-inspired program course learning outcomes to course content and then connected these outcomes to internship experiences. Furthermore, students connected the knowledge and skills they were learning to real-world applications. As Brent and Felder concluded, to develop mastery, students must acquire component skills, practice integrating them, and know when to apply them.^[18] In addition, some students enhanced communication skills through their reflections by striving to be clear and concise, yet descriptive, while demonstrating knowledge and experiences in meaningful ways.

Second, chemical engineering students connected their learning to their employability. Creating the chemical engineering reflective ePortfolios scaffolded student reflection on their learning through writing, which they connected to future employability. Students felt better prepared for job interviews because they reflected on their knowledge gained from coursework and experiences, such as capstone projects, studies abroad, or internships. Furthermore, they described how understanding course content and resulting knowledge and skills applied to future chemical engineering jobs. This finding is important because ABET student outcomes reference the ability to effectively communicate in program accreditation standards, and job descriptions often reference such standards, and employers prioritize critical thinking, problem solving, and communication skills when making hiring decisions.^[1,2] In addition, students reported reflective ePortfolios provided an effective job application and interviewing tool. ePortfolios address the six areas employers identified for higher education emphasis in student learning: critical thinking and analytical reasoning; complex problem solving and analysis; written and oral communication; knowledge and skill application in real-world settings; locating, organizing, and evaluating information from multiple sources; and innovation and creativity.^[3] Furthermore, 80% of employers indicated an ePortfolio would be helpful in the hiring process to demonstrate students' knowledge, skills, and experience.

Last, students connected learning to their professional identity. Creating the chemical engineering reflective ePortfolios scaffolded student reflection on their learning, which they connected to their professional identity as chemical engineers. Students learned about themselves and desired portfolios that professionally and personally reflected them. Guided reflection helped students develop self-authorship and identity by prompting them to ask what they know and how they know it.^[5] Eliot and Turns found students constructed professional identities by realizing their engineering-related values and interests.^[14] Last, students develop professional identity through self-authorship, by organizing, connecting, and evaluating information.^[5,15]

In summary, students believed creating reflective ePortfolios enhanced their learning with regard to their chemical engineering program. Specifically, influenced by motivations and preferences, chemical engineering students created reflective ePortfolios, connecting their learning to job knowledge and skills, future employability, and professional identity.

IMPLICATIONS AND FUTURE RESEARCH

This study investigated the use of reflective ePortfolios in an undergraduate chemical engineering course and offers implications for theory, policy, and practice as well as suggestions for future research. First, the study contributes to the reflection, integrative learning, and reflective ePortfolio literature generally and within engineering and chemical engineering contexts. In addition, the findings contribute to literature on student learning, employment preparation, and professional identity both generally and in a chemical engineering context.

Second, this study contributes to higher education policy and engineering education policy. For example, ABET requirements could expand the accreditation criteria to explicitly include reflective writing and integrative learning exemplified through reflective ePortfolios. ABET reviewers could more clearly see the connection and achievement of program learning outcomes in student reflective ePortfolios. In addition, higher education institutions and engineering colleges and programs can institute cross-curricula reflective ePortfolios to enhance student job knowledge and skill acquisition, future employability, and professional identity development. Furthermore, incorporating reflection throughout engineering curricula will scaffold the development of communication skills from students' first year through their entire college careers.

Last, this study contributes to instructional practice generally in higher education and more specifically in engineering and chemical engineering. For example, instructors can integrate reflective ePortfolios in course-level instructional design to scaffold student reflection and learning and to reinforce writing skills. In addition, they can assist students in strategically selecting what artifacts to include in reflective ePortfolios and prompt reflection and learning. Furthermore, instructors can provide reflective ePortfolio feedback to motivate and support student development in writing and assist with making connections to learning in the discipline. Finally, instructors can model reflection in their teaching to exemplify and reinforce the value of reflection to students.

Based on the findings, chemical engineering students created reflective ePortfolios, perceived enhanced learning, and connected their learning to job knowledge and skills, future employability, and professional identity. For future research, we recommend adding more discipline-specific reflection questions to course components and the reflective ePortfolio assignment to enhance students' understanding and the assessment of engineering conceptual knowledge.

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SIMPLIFY UNCERTAINTY ANALYSIS WITH EXCEL MACROS

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stimating and reporting reliability in experiments and calculations is an important part of engineering design and analysis. Reporting results from calculations and experiments without some estimation of reliability may invalidate our results. To illustrate, if we report a volume from designing a chemical reactor without taking into account the uncertainty in the design parameters, we risk under sizing a cooling system, which can have catastrophic consequences for exothermic runaway reactions. One measure of reliability comes from uncertainty analysis. Chemical engineering students may learn simple concepts of experimental error and uncertainty analysis in physics and chemistry labs. Their first impressions and experiences with uncertainty are not typically positive. In some cases, this is their first exposure to statistics. Students find the process tedious, labor intensive, and sometimes irrelevant in the context of their limited science and engineering experience. When we bring up the topic of uncertainty analysis in our engineering instructional labs, students groan in anticipation of the laborious, monotonous calculations.

To reinforce the principles of uncertainty analysis and provide students with tools for uncertainty calculations that help to alleviate their anxiety, we have incorporated uncertainty analysis earlier in our program in a one-semester required course on computational methods for engineering problem solving. Our students typically take this course in the second year of our program, about midway through their chemistry, physics, and engineering lab sequences. Prior to our computational methods course, students receive a basic introduction to descriptive statistics and uncertainty in their chemistry and physics courses. Most students in the course have also completed another course on statistical design of engineering experiments.

In our computational methods course, we introduce students to concepts of random and systematic uncertainty in measurements, degrees of freedom, propagation of uncertainty, and expanded uncertainty (confidence intervals). We outline steps for uncertainty analysis and develop spreadsheet tools to simplify the implementation. We use a simple, hands-on classroom demonstration to generate experimental data and help students experience the differences between uncertainties in analog and digital measuring instruments. The exercise involves calculating the density of an object from replicated measurements of dimensions and weight. The students first perform the steps of uncertainty analysis in an Excel worksheet to experience the calculations "by hand." In a follow-up class exercise, students create an Excel macro that calculates the expanded propagation of uncertainty according to the conventional Guidelines for Analysis of Uncertainty in Measurements (GUM).^[1] The macro incorporates basic programming methods of loops, logical statements, input and output, user functions, and subroutines. Students finish the course with a deeper understanding and appreciation of their responsibility for reporting reliability of results in terms of uncertainty. They also move on to other courses equipped with tools for simplifying the implementation of uncertainty analysis for most situations they will encounter in their undergraduate experience.

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UNCERTAINTY ANALYSIS

In an interactive lecture, we present the well-known principles of uncertainty analysis.^[1-4] We also discuss case studies to promote the value of uncertainty analysis, including a qualitative example of a nuclear reactor.^[5] For brevity in this paper, we skip theories of uncertainty analysis that are readily available in the literature and outline the steps for students to follow when calculating the propagation of uncertainty through their engineering calculations. The reader is encouraged to review the literature for background information on uncertainty analysis.^[3] The analysis presented here is limited by the assumptions of normally distributed random errors in replicated measurements with no bias or correlation between independent variables. We also assume that systematic errors are uniformly distributed between the limits of precision in the measurement. Students learn to reduce bias and correlation between independent variables by careful calibration of instruments and randomization of experiments.

Eq. (1) represents the functional relationship between inputs, x (e.g., experimental measurements), and the output, y:

$$y = f(x_1, x_2, ...)$$
 (1)

The function, f, represents any combination of calculation steps that incorporate the input values from experimental measurements x needed for obtaining y. The question we answer with uncertainty analysis is how the uncertainties in the input variables propagate through the function to give an uncertainty in the output. Ultimately, we want to know y with some degree of confidence:

$$y = f(x_1, x_2, ...) \pm U_y$$
 (2)

where U_y represents the expanded uncertainty, or confidence interval for the calculated value of y.

Uncertainty in the values of the input variables comes from a variety of sources that may include measurement mistakes, systematic errors due to our inability to take precise measurements, and random errors that are the results of our inability to control the environment of the experiment.^[1,4] We use descriptive statistics of mean and standard deviation as the basic building blocks for predicting the value of replicated measurements and their corresponding uncertainty from random errors. We recommend a conservative calculation for the uncertainty from systematic errors according to the precision of the instruments of measurement. Unfortunately, there is no good way to quantify unknown mistakes in uncertainty analysis. We should take steps in our experimental design and data collection to minimize the possibility for mistakes. For our analysis, we follow the Guidelines for the Analysis of Uncertainty in Measurements.^[1] The following steps of uncertainty analysis are illustrated with a simple hands-on classroom exercise:

1. Begin with a model of the uncertainty in the experimental inputs from the combined effects of random and systematic errors:

$$\mathbf{x} = \overline{\mathbf{x}} \pm \mathbf{u}_{\mathbf{x}} \tag{3}$$

where $\overline{\mathbf{x}}$ is the expected value for *x* calculated from the mean value of *n* replicated measurements:

$$\overline{\mathbf{x}} = \frac{1}{n} \sum \mathbf{x} \tag{4}$$

and u_x is the combined uncertainty due to random (u_R) and systematic (u_7) errors in the measured values:

$$\mathbf{u}_{\mathrm{x}} = \sqrt{\mathbf{u}_{\mathrm{R}}^2 + \mathbf{u}_{Z}^2} \tag{5}$$

2. Assume random errors are normally distributed and use the standard error in Eq. (6) for the random uncertainty in terms of the standard deviation s, and the sample size, n:

$$u_{R} = \frac{s}{\sqrt{n}} \tag{6}$$

Students discover that they may reduce the random uncertainty in Eq. (6) by taking more measurements. However, this revelation is tempered by Eq. (5) when they realize that systematic uncertainties are always present for any measurement due to the limitations of precision in our instrumentation.

3. Assume that systematic (fixed) errors are uniformly distributed between the limits of readability of the instrument of measurement, $\pm \delta$, for a probability density function $p = 1/(2\delta)$ when $\overline{\mathbf{x}} - \delta \leq \mathbf{x} \leq \overline{\mathbf{x}} + \delta$, and p = 0 otherwise. Calculate the variance for the fixed uncertainty in the measurement:

$$\mathbf{u}_{Z}^{2} = \int_{\overline{\mathbf{x}}-\delta}^{\overline{\mathbf{x}}+\delta} \frac{(\mathbf{x}-\overline{\mathbf{x}})^{2}}{2\delta} = \frac{\delta^{2}}{3}$$
(7)

or

$$u_z = \frac{\delta}{\sqrt{3}} \tag{8}$$

Eq. (7) represents a conservative estimate for the fixed error by assuming an equal probability for error over the range of readability of the instrument.

4. Use the law of propagation of uncertainty (ignoring parameter correlation) for calculating the standard uncertainty in the output in terms of the combined uncertainties of the inputs calculated from Eq. (5):

$$\mathbf{u}_{y} = \sqrt{\sum (\mathbf{c}\mathbf{u}_{x})^{2}} \tag{9}$$

where u_y is the standard uncertainty in the output y from Eq. (1). The parameter c is the sensitivity coefficient, defined as the partial derivative of the function with respect to x evaluated at the mean value of measurement x:

$$c = \frac{\partial f}{\partial x}\Big|_{\overline{x}}$$
(10)

Chemical Engineering Education

5. Finally, calculate the expanded uncertainty in y, symbolized here with a capital U_y, to give a level of confidence for the interval of uncertainty by multiplying the standard uncertainty in Eq. (9) by the 95% coverage factor, or Student t-statistic:

$$\mathbf{U}_{\mathbf{y}} = \pm \mathbf{t}_{\mathbf{95\%}, \mathbf{v}_{\mathbf{y}}} \mathbf{u}_{\mathbf{y}} \tag{11}$$

We use the conventional 95% coverage, but are certainly free to use any level. The evaluation of the coverage factor from the t-distribution requires the degrees of freedom, v_y . We obtain an estimate for the degrees of freedom for the pooled variances in Eq. (9) from the Welch-Satterthwaite formula.^[1]

$$v_{y} = \frac{u_{y}^{4}}{\sum \left[\frac{(c \cdot u_{x})^{4}}{v_{x}}\right]}$$
(12)

The degrees of freedom, v_x , for each variable in Eq. (12) are calculated individually from the Welch-Satterthwaite formula applied to Eq. (5) assuming infinite degrees of freedom for systematic errors, and n-1 degrees of freedom for the random value:

$$\mathbf{v}_{\mathbf{x}} \cong \frac{\mathbf{u}_{\mathbf{x}}^{4}}{\frac{\mathbf{u}_{\mathbf{R}}^{4}}{\mathbf{n}-1} + \frac{\mathbf{u}_{\mathbf{z}}^{4}}{\infty}} \cong \frac{(\mathbf{n}-1)\mathbf{u}_{\mathbf{x}}^{4}}{\mathbf{u}_{\mathbf{R}}^{4}}$$
(13)

The ubiquitous spreadsheet software Excel is primed to carry out these analysis steps with relative ease using built-in statistical functions and custom macros.^[6] We illustrate the implementation of the analysis with a simple exercise that students complete in a single class period using inexpensive materials and basic measuring instruments. A second follow-up class period is used to guide students in programming Excel macros designed to simplify and automate the analysis in an Excel worksheet.

HANDS-ON LEARNING EXERCISE

A simple classroom experiment was devised to allow students to generate data with random and systematic errors for calculating the density of wood from the dimensions of rectangular wooden blocks with a cylindrical hole drilled through their centers, as shown in the schematic of Figure 1. The small wood blocks were rough cut from the same piece of wood, with slight deviations from the mean values of each dimension to introduce noise into the experimental data. This example extends the simpler uncertainty exercise proposed by Yates, who distributed sheets of paper with hand-drawn rectangles to chemistry students for measuring dimensions to calculate the circumference and area.^[7] In our wood block exercise, however, students use combinations of analog and digital instruments for measurement. By extending the exercise to a density calculation, we allow for two different types of instruments that

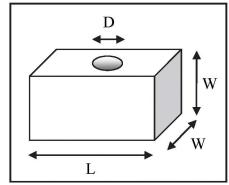


Figure 1. Schematic of wooden block with length L, width W, and hole diameter D.

must be treated differently in uncertainty analysis.

Students first derive an expression for the density of the block from the ratio of the mass to volume in terms of mass (m), length (L), width (W), and diameter (D).

ρ

$$=\frac{\mathrm{m}}{\mathrm{V}}$$
 (14)

$$V = W \left(LW - \frac{\pi D^2}{4} \right)$$
(15)

Students form teams with a minimum size of three members. Each team member is provided with a similar block of wood, an inexpensive plastic ruler for measuring length dimensions in two-unit systems of inches and centimeters, and a portable digital scale for measuring the mass in grams, as shown in Figure 2. The ruler serves as a simple example of an analog instrument. Students must visually interpolate between the graduation marks on the scale for a measurement reading. We have a brief discussion of the issues of reading values from scales using different examples of analog instruments in our labs including liquid thermometers, titration pipettes,

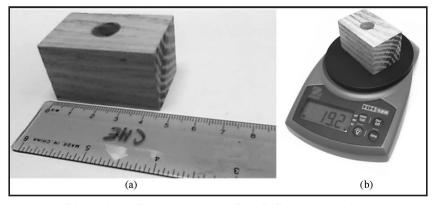


Figure 2. (a) Analog ruler for measuring length dimensions. The precision in the graduation marks is 0.1 cm or 1/16 in. The readability is ± 0.05 cm or $\pm 1/32$ in (0.03125 in). (b) Digital scale for measuring mass in grams. The precision is 0.1 gm, with a readability of ± 0.05 gm.

	А	В	С	D	Е
1	Team	L/in	W/cm	D/cm	m/gm
2	1	1.8125	2.65	1.12	18.4
3	2	1.8125	2.75	1.15	19.4
4	3	1.78125	2.6	1	18.7
5	4	1.8125	2.85	1.1	18.8
6	5	1.78125	2.7	0.9	18.6
7	6	1.78125	2.7	0.9	19.2
8	7	1.75	2.71	0.96	18.4
9	8	1.8125	2.6	1.1	19.8
10	9	1.8125	2.7	0.95	18.6
11	10	1.8125	2.75	1	18.9
12	11	1.84375	2.7	1.1	18.9
13	12	1.8125	2.75	0.95	18.7

Figure 3. Student-derived experimental data for wooden block dimensions.

Excel fo	TABLE 1 Excel formulas for calculating measurement uncertainty in length. Use similar formulas for the other measurements.										
Variable Symbol Cell Worksheet Formula R											
Average Length	L	B14	= AVERAGE(B2:B13)	1.8021 in							
Number of measurements	n	B15	= COUNT(B2:B13)	12							
DoF (n-1) of Average	DoF	B16	= B15-1	11							
Standard Deviation	s	B17	= STDEV(B2:B13)	0.0243 in							
Random Uncertainty	u _R	B18	= B17/SQRT(B15)	0.0070 in							
Readability	δ	B19	= 1/32	0.03125 in							
Systematic Uncertainty	u _z	B20	= B19/SQRT(3)	0.0180 in							
Combined Uncertainty	u _x	B21	= SQRT(B18 + B20)	0.0194 in							
Combined DoF	v	B22	= (B15-1)*(B21/ B18)^4	635							

Bourdon-tube pressure meters, rotameters for fluid flow rates, manometers, and barometers. The readability of an analog instrument is subject to our comfort level in determining the precision of our interpolation between the graduation marks. The precision of the graduation marks on the ruler is 0.1 cm on one side and 1/16 in on the other, but students report the readability of the ruler as ranging from ± 0.05 cm down to ± 0.025 cm or 1/32 in (depending on a student's confidence in his or her ability to interpolate the scale).

The electronic balance is an example of a digital meter

that interpolates the signals for the user. We build on our discussion of how to incorporate uncertainty from examples of digital meters in our labs, including conductivity meters, refractometers, thermocouple digital thermometers, pressure gauges, flow meters, and humidity meters, to name a few. The readability of a digital instrument for use in Eq. (8) is determined from the least significant digit. The precision and readability of the digital balance scale is 0.1 gm, for a uniform systematic uncertainty of $\pm 0.05/\sqrt{3}$ gm.

All student teams pool their measurement results and record the values in an Excel worksheet, like Figure 3. Although this is a team-based exercise, each individual student creates a copy of the Excel worksheet for personal reference and use later in the program and future lab courses. Students calculate the combined uncertainty in each variable using worksheet functions. To illustrate, we refer to the data for the measurement of length (L) of the block listed in column B on the Excel worksheet, shown in Figure 3. Table 1 contains a summary of the measurement uncertainty calculations including the Excel formulas and worksheet functions for L. By mixing dimension of inches with centimeters we also illustrate how numerical derivative approximations in terms of the input values handle the challenge of unit conversions in uncertainty analysis.

The volume and density of the wood are calculated from the average values for the dimensions and mass in Eqs. (14) and (15). The length units of inches are converted to centimeters

in the volume calculation. Figure 4 shows the results in the Excel worksheet. The uncertainty analysis uses these values for evaluating the derivatives in the sensitivity coefficients.

The analytical formulas for the sensitivity coefficients are listed below:

$$\mathbf{c}_{\mathrm{L}} = \frac{\partial \rho}{\partial \mathrm{L}} = -\mathbf{m} \left(\frac{\mathrm{W}}{\mathrm{V}} \right)^2 \tag{16}$$

$$\mathbf{c}_{\mathrm{w}} = \frac{\partial \rho}{\partial \mathrm{W}} = -\mathbf{m} \left[\frac{1}{\mathrm{WV}} + \frac{\mathrm{LW}}{\mathrm{V}^{2}} \right]$$
(17)

$$c_{\rm D} = \frac{\partial \rho}{\partial D} = \frac{\pi D W m}{2 V^2}$$
(18)

$$c_{m} = \frac{\partial \rho}{\partial m} = \frac{1}{V}$$
(19)

The results for c using the average values of the variables are shown in row 23 of the Excel worksheet in Figure 5.

Unlike the simple linear derivative results of the perimeter and area of a rectangle in the uncertainty exercise of Yates,^[7] the derivative formulas for density in terms of mass and block dimensions are nonlinear, and prone to formulation errors in a worksheet

calculation. At this juncture, it is important to remind the students that uncertainty analysis is by its own nature "uncertain." High-precision calculations for the sensitivity coefficients are unnecessary. We can take our first step toward simplification of the general process of uncertainty analysis by introducing first-order, finite difference approximations for the sensitivity coefficients:

$$\mathbf{c}_{i} = \frac{\partial \rho}{\partial x_{i}} \cong \frac{\rho(x_{i} + \varepsilon) - \rho(x_{i})}{\varepsilon}$$
(20)

where ε is a small value used to perturb the average value of a variable in the formula for density. The perturbation value must be small relative to the magnitude of the variable. In our exercise, students find that a value of $\varepsilon = 10^{-4}$ is sufficiently small to yield good values for the sensitivity coefficients of each variable. We use the VBA user-defined function in Figure 6 for evaluating the density from the dimensions to simplify the calculations in a worksheet. We use the following worksheet formula to illustrate the calculation of the sensitivity coefficient relative to the wood block length measurement using finite difference derivative approximation:

The epsilon term refers to a named cell on the worksheet that contains a small perturbation value of 0.0001 used in Eq. (20).

By using absolute worksheet cell references for the average values of the variables, we can fill the formula in Eq. (21) across the row of cells in the worksheet for each variable. Then, we simply change the addition of the perturbation value for each variable in turn to get the complete set of sensitiv-

	G	Н
1	V/cm ³	=C14*(CONVERT(B14,"in","cm")*C14-PI()*(D14^2)/4)
2	ρ/(gm/cm3)	=E14/H1

Figure 4. Wood block volume and density formulas evaluated at the average values for the experimental measurements of L, W, D, and m.

ity coefficients. The values in rows 23 and 24 compare the results from the analytical formulas to the finite-difference approximations where we observe good agreement. Finite-difference derivative approximations become important for obtaining good sensitivity coefficients for complicated calculations that involve multiple mathematical operations between the inputs to the output. For working with more complicated problems, we help the students write a VBA

	А	В	С	D	E
1	Team	L/in	W/cm	D/cm	m/gm
14	X _{ave}	1.8021	2.71	1.02	18.9
15	n	12	12	12	12
16	DoF	11	11	11	11
17	s	0.0243	0.0690	0.0900	0.4163
18	u _R	0.0070	0.0199	0.0260	0.1202
19	δ	0.03125	0.025	0.025	0.050
20	uz	0.0180	0.0144	0.0144	0.0289
21	u _x	0.0194	0.0246	0.0297	0.1236
22	v	635.36	25.61	18.84	12.31
23	c analytical	-0.3582	-0.4616	0.0835	0.0320
24	c finite difference	-0.3582	-0.4616	0.0835	0.0320
25	c macro	-0.3582	-0.4616	0.0835	0.0320

Figure 5. Measurement uncertainty and sensitivity coefficients for the wood density exercise, evaluated in an Excel worksheet.

B24 - (DENS(B\$14 + epsilon, C\$14, D\$14, E\$14) - DENS(B\$14, C\$14, D\$14, E\$14)) / epsilon (21)

```
Public Function DENS(L, W, D, m)
With WorksheetFunction
    DENS = m / (.Convert(L, "in", "cm") * W ^ 2 - W * .Pi() * (D / 2) ^ 2)
End With
End Function
```

Figure 6. VBA user defined function for calculating the density of a wood block.

macro like the listing in Figure 7 to automate the evaluation of the sensitivity coefficients.

Students create their macros in the same workbook that contains their worksheet for uncertainty analysis of the wood density calculations. The macro employs input boxes for selecting the ranges of data and writing the results on the worksheet. The algorithm cycles through the variables perturbing the average values one at a time to calculate the derivative approximation. The average value of the variable is reset to its original cell contents before perturbing the next variable for partial derivative evaluations. By default, Excel worksheets automatically recalculate the value of the density function for each small change in the variables. Be sure to turn on automatic calculations if it is not previously set in the Excel worksheet.

With the sensitivity coefficients, we now have all of the information needed to calculate the propagation of the uncertainty in the measurements for the variables (L, W, D, and m) through the calculation of density. First, we calculate the standard uncertainty from the law of propagation of uncertainty. Figure 8 shows the values for the product of the sensi-

dent in identifying which variable(s) contribute most to the uncertainty in y. We find that the contribution from the width measurement in column C is larger than the other variables by at least an order of magnitude. We can take steps to reduce the uncertainty in the width by taking more measurements, or using a higher precision ruler. We report the density with standard uncertainty as

 $\rho = 0.603 \pm 0.014 \text{ gm/cm}^3 \text{ (standard uncertainty)} (22)$

Note that the uncertainty is rounded up. Some practitioners recommend the retention of just one significant figure in the uncertainty, rounded up to ρ =0.61±0.02 gm cm³.

Finally, students calculate the expanded uncertainty for a 95% confidence interval. We need the degrees of freedom from the Welch-Satterthwaite formulas in Eqs. (12) and (13). Table 2 summarizes the worksheet formulas and functions for calculating the propagation of uncertainty and coverage factor. Note how we rounded the result for the combined degrees of freedom down to the nearest integer value for a conservative value of the coverage factor. It is important to help students learn to match the precision in their reported

tivity coefficient and combined uncertainty re- quired by Eq.		TABLE 2 Excel worksheet formulas for calculating the propagation of uncertainty in the wood density exercise.						
quired by Eq. (9).	Variable	Symbol	Cell	Worksheet Formula	Result			
The results for	Standard Uncertainty	u _y	B28	=SQRT(SUMSQ(B26:E26))	0.014 gm/cm ³			
the square of the	Degrees of Freedom	V _y	B30	=ROUNDDOWN((B28^4)/(SUM(B29:E29)),0)	58			
product $(c \cdot u)^2$	Coverage Factor	t	B31	=TINV(0.05,B30)	2.002			
guide the stu-	Expanded Uncertainty	Uy	B32	= ROUNDUP(B28*B31,3)	0.029 gm/cm ³			

```
Public Sub dfdx()
 Get sensitivity coefficients from finite difference derivative approximations
' Get input from the worksheet
With Application
    Set x = .InputBox(Type:=8, prompt:="Select range of average variables:")
    Set f = .InputBox(Type:=8, prompt:="Select cell with function result:")
    Set c = .InputBox(Type:=8, prompt:="Select range for sensitivity coefficients:")
End With
 Specify number of variables, perturbation factor & save function value
n = x.Count: eps = 0.0001: finit = f
 Loop through variables to calculate sensitivity coefficients
For j = 1 To n
    temp = x(j).Formula
                             ' save worksheet formula for average variable j
                             ' perturb value of variable j in the worksheet
    x(j) = x(j) + eps
    c(j) = (f - finit) / eps ' calculate the sensitivity coefficient for variable j
    x(j) = temp
                             ' replace value/formula of variable j in the worksheet
Next j
End Sub
```

Figure 7. VBA macro for calculating sensitivity coefficients in an Excel worksheet.

result to the precision in the uncertainty. We now have the expanded uncertainty for wood density:

$$\rho = 0.61 \pm 0.03 \text{ gm/cm}^3 (95\% \text{ confidence})$$
 (23)

or

$$\rho = 0.61 \text{ gm/cm}^3 \pm 5\% (95\% \text{ confidence})$$
 (24)

Figure 9 shows the Excel worksheet results for expanded uncertainty in density.

JITTER MACRO

A macro named JITTER that automates the complete analysis for uncertainty propagation is provided to the students.^[4] The macro incorporates the VBA code from the student-generated macros from the class exercises. To use the macro, students must set up a worksheet with a cell containing the final value of the function ultimately calculated from the average values of experimental inputs. In addition, the worksheet must include ranges of values for the average variables. random uncertainties, readability, and degrees of freedom. In most cases, the degrees of freedom for averaged values are the number of replicated experiments, less one (n-1). An example of a different

number of degrees of freedom is the use of leastsquares regression parameters, such as the slope or intercept of a line, where the degrees of freedom are the number of regression data points less two. The macro uses input boxes to prompt the user for the required information. The input boxes displayed in Figure 10 show the cell and range addresses used for the wood density exercise with the density calculated in Cell B34 on the worksheet.

The JITTER macro output for our class exercise

in Figure 11 shows the absolute and relative expanded, standard, and maximum standard uncertainties. In addition, the output includes the sensitivity coefficients and contributions from each variable to the propagation of uncertainty. We see that variable 2, corresponding to width, contributes approximately 65% of the uncertainty and should be a target for refining the experiments to reduce uncertainty in our density

	А	В	С	D	E
1	Team	L/in	W/cm	D/cm	m/gm
26	c∙u _x	-0.007	-0.011	0.002	0.004
27	(c·u _x) ²	4.81E-05	1.29E-04	6.16E-06	1.56E-05
28	u _γ	0.014			

Figure 8. Excel worksheet calculation of standard uncertainty.

	А	В	С	D	E
1	Team	L/in	W/cm	D/cm	m/gm
29	(c∙u _x) ⁴ /v	3.64E-12	6.48E-10	2.01E-12	1.98E-11
30	v _y	58			
31	t	2.002			
32	U _y	0.029			

Figure 9. Excel worksheet with results for expanded uncertainty in density.

Figure 11 . Results	U _{95%} = ±	2.8E-02	= ±	4.7%
from	$u_{max} = \pm$	2.5E-02	= ±	4.1%
macro JIT-	u = ±	1.4E-02	= ±	2.3%
TER for the propaga-	t _{95%} =	2.00	DoF =	58
tion of	c ₁ =	-3.58E-01	$(c \cdot u_1)^2 =$	24.2%
uncer- tainty in	c ₂ =	-4.62E-01	$(c \cdot u_2)^2 =$	64.8%
the wood density	c ₃ =	8.35E-02	$(c \cdot u_3)^2 =$	3.1%
exercise.	c ₄ =	3.20E-02	$(c \cdot u_4)^2 =$	7.9%

JITTER: Propagation of Uncertainty	JITTER: Propagation of Uncertainty
Click on FUNCTION cell, f(x): \$B\$34	Select range of AVERAGE (MEAN) VARIABLES, x: \$B\$14:\$E\$14
,	
Select range of STANDARD (RANDOM) UNCERTAINTIES, ±u_r: \$B\$18:\$E\$18	Select range of mean DEGREES of FREEDOM: \$B\$16:\$E\$16
Select range of READABILITIES, ±d:	Click on the first OUTPUT cell:
\$B\$19:\$E\$19	\$C\$34

Figure 10. JITTER macro input boxes with worksheet ranges for wood density exercise.

calculation. An Excel workbook with the data and calculations for the example exercise, as well as the general-purpose JITTER macro, is available for download from the author's website (<www.d.umn.edu/~rdavis/cee>).

RESULTS

Students develop tools in these exercises that are applicable to a wide variety of problems involving uncertainty analysis in their remaining coursework, but particularly in our program's unit operations lab courses. Armed with an understanding of the basic assumptions and data requirements, students may use other software tools for uncertainty analysis available freely on the Internet or commercially.

We evaluate our students' ability to transfer their skill with the formulas and Excel tools for uncertainty analysis by an exam question where they are allowed to use their Excel worksheets and macros from the class exercises. We find that over 90% of the students are consistently able to transfer their uncertainty analysis skills from the class exercise to correctly analyze the uncertainty in the exam problem.

We also see improvements in uncertainty analysis conducted by students in our lab courses. Evidence includes an increased discussion and application of analysis of uncertainty in lab reports with more appreciation for reporting reliability of experimental results. Students are also careful to include estimates of uncertainty in all final reported values. Although we warn the students that they will need these tools in courses later in the program, a few students have a habit of compartmentalizing their learning. Once they are finished with the computational methods course, they do not automatically make the connection of applying the analysis later in the program. However, when we provide them with a copy of the wood density exercise, they are able to quickly relearn and apply these skills.

In one particularly complicated lab analysis, students use the macro to estimate the uncertainty in the calculation of chemical equilibrium constants. Experimental measurements of volume and mass to calculate reagent concentration and extent of reaction are fed into a worksheet set up to perform a complex series of stoichiometric mass conservation calculations to arrive at a value of the equilibrium constant. These calculations may be spread across multiple worksheets. Propagating the uncertainty through these involved series of calculations by hand is tedious and prone to mistakes. The JITTER macro efficiently performs the analysis requiring little effort setting up the worksheets for the macro inputs. The students also appreciate the additional VBA programming skills developed as part of this exercise and report using this additional skill in academic and industrial settings.

CONCLUSIONS

A simple hands-on active-learning exercise provides students with experience collecting and analyzing experimental data with random and fixed uncertainties. The exercise uses data collected from analog and digital instruments that give the students experience interpreting fixed uncertainties from readability. Students create an Excel worksheet that serves as a template of the steps for calculating the propagation of measurement uncertainty in engineering analysis. This worksheet template, coupled with VBA macros, gives the students powerful tools for including measures of reliability in their calculated results. By making the process simple, relatively easy, and painless, students who formerly avoided uncertainty analysis are now more willing and able to conduct proper uncertainty analysis. Similar tools may be developed in other computational platforms, such as Matlab or Python, as needed by a department to meet the needs of its constituents. We elected to focus on Excel based on the feedback we receive from our own graduates who report using Excel with macros as their primary computational software.

NOMENCLATURE

- c = sensitivity coefficient
- D = diameter, cm
- f = relationship between input variables and output variable
- L =length, cm
- m = mass, gm
- n = number of replicated measurements
- s = sample standard deviation
- t = coverage factor, or Student's t-statistic
- U_{y} = expanded uncertainty in the output value y
- $I_{\rm p}$ = random uncertainty or standard error
- u_{x} = combined uncertainty in measurements
- u_{y} = standard uncertainty in the output value y
- u_{τ} = systematic uncertainty degrees of freedom
- \tilde{V} = volume, cm³
- $v_{x} = degrees of freedom$
- $v_y^{"}$ = degrees of freedom for pooled variances in expanded uncertainty
- W = width. cm
- x = input variable from experimental measurements
- y = output value calculated from input values
- δ = readability
- ϵ = perturbation in x
- $\rho = \text{density, gm/cm}^3$

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SPREADSHEET PROCEDURE FOR SIMULATING SETPOINT TRACKING IN SISO BY DYNAMIC MATRIX CONTROL

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The objective of this work is to present a spreadsheet tool that illustrates an ideal case of dynamic matrix control (DMC) calculations. The ideal case presented in this work is a hypothetical single-input-single-output DMC control system for setpoint tracking, in the absence of disturbance and mismatch between the measured and predicted process variable, at various move suppression coefficients. Students in an undergraduate process control class who followed the procedure to build the spreadsheet would gain a good basic understanding of DMC.

A BRIEF OUTLINE OF DYNAMIC MATRIX CONTROL METHOD

Dynamic matrix: prediction of future process response based on present and future control moves

Industry has widely accepted control strategies based on model predictive control (MPC), primarily in multiple-inputmultiple-output processes. The first known industrial application of linear MPC was known as dynamic matrix control (DMC). Initially, DMC was introduced for the single-inputsingle-output (SISO) cases.^[1] The development of DMC and its recent status has been reported in the literature.^[2]

Moving horizon control is a key feature of dynamic matrix

control. This type of controller employs a model internal to the controller architecture to predict the process variable for n_p steps into the future based on control moves for n_p steps in the past. The future process response predicted from the past control moves is called "free response."^[3] Then, the algorithm calculates the predicted error (setpoint–free response, with model mismatch and disturbance taken into consideration) for future n_p steps, followed by an optimization scheme to calculate the present and future control moves needed to minimize or suppress the net error (predicted error–future

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process response due to the present and future control moves). Once the computation is done, only the first calculated control move is implemented and the algorithm moves one time step ahead. The free response is predicted and new control moves are calculated again for this new time step. The procedure of predicting the future free response, calculating the present and future control moves to suppress error, and implementing the first calculated control move is carried out as time moves on.

The first crucial step in implementing DMC in a SISO case is to obtain information about how the process responds to a step change in the controller output. This procedure is very much like the traditional approach of finding the dynamic model of a process by making a step change in the controller output (in the manual mode) and observing the response of the process variable, followed by fitting the response curve to the model chosen (such as the first-order-plus-dead-time (FOPDT) model). With the model parameters (such as process gain, first-order time constant, and dead time), an engineer may use well-established tuning rules, such as Ziegler-Nichols method, Cohen-Coon method, and Internal Model Control (IMC) method, to find appropriate tuning parameters for a proportional-integral-derivative (PID) feedback controller. However, instead of fitting response data to a particular model, the DMC method calculates the coefficients of the system's step response model (SRM).^[1]

Assuming that the system is initially at steady state and the initial value of the process variable is 0, the coefficient can be defined as follows:

Coefficient of SRM =
$$a_i = \frac{y(t_i)}{\Delta u(t_0)}$$
 (1)

where $\Delta u(t_0)$ is the magnitude of step change made (and held constant) in the controller output at $t = t_0$ and $y(t_i)$ is the response of the process variable at $t = t_{i}$. We may consider the t's as discrete times of choice and/or sampling times. In DMC applications, at least 10 discrete time steps are needed between t_0 and t_{ee} (time to reach the next steady state). The number of time steps taken to reach steady state is called model horizon (denoted as m in this work). If the controller output changes from the previous value by the magnitudes of $\Delta u(t_0)$, $\Delta u(t_1)$,..., $\Delta u(t_{nc-1})$, at present and future times (t = $t_0, t_1, ..., t_{n_0-1}$) and held constant thereafter, we may predict the response of the process at any future time t_i (i = 1, 2,..., n) by the principle of superposition. The effect of a control move made at t_o would take t time steps to reach t. Likewise, the effect of a control move made at t, would take t, steps to reach t, and so forth. Since the effect is additive, we have Eq. (2).

$$\mathbf{y}(\mathbf{t}_{i}) = \mathbf{a}_{i} \Delta \mathbf{u}(\mathbf{t}_{0}) + \mathbf{a}_{i-1} \Delta \mathbf{u}(\mathbf{t}_{1}) + \dots (\text{for } \mathbf{n}_{c} \text{ terms}), \qquad (2)$$

Assuming that one is making 12 steps of prediction ahead (*i.e.*, the *prediction horizon* $n_p = 12$) based on the subsequent control moves for 5 steps (at t_0 , t_1 , t_2 , t_3 , and t_4) and held con-

stant thereafter (*i.e.*, the control horizon $n_c = 5$), Eq. (2) may be rewritten in the matrix form [Eqs. (3) and (4)]:

$$\begin{bmatrix} y(t_1) \\ y(t_2) \\ y(t_3) \\ \vdots \\ y(t_{12}) \end{bmatrix} = \begin{bmatrix} a_1 & 0 & 0 & 0 & 0 \\ a_2 & a_1 & 0 & 0 & 0 \\ a_3 & a_2 & a_1 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{11} & a_{10} & a_9 & a_8 & a_7 \\ a_{12} & a_{11} & a_{10} & a_9 & a_8 \end{bmatrix} \begin{bmatrix} \Delta u(t_0) \\ \Delta u(t_1) \\ \Delta u(t_2) \\ \Delta u(t_3) \\ \Delta u(t_4) \end{bmatrix}$$
(3)

$[y]_{12 \times 1} = [A]_{12 \times 5} [\Delta u (present and future)]_{5 \times 1}$ (4)

The first term on the right-hand side of Eqs. (3) and (4) $([A]_{12\times 5})$ is called the dynamic matrix. Note that the present and future control moves $\Delta u(t_0)$, ..., $\Delta u(t_4)$ are not known *a priori*. We need to use the procedure below to calculate them.

FREE RESPONSE: PREDICTION FOR FUTURE PROCESS RESPONSE BASED ON PAST CONTROL MOVES

Free response is defined as the predicted process response for $t > t_0$ (at $t_1, t_2,..., t_{np}$) based on the past control moves $(\Delta u(t_{np}), \Delta u(t_{np+1}),...., \Delta u(t_1))$ if no further controller outputs are changed at $t_0, t_1, t_2,...$ The effect of the control move made at t_1 would take 2 steps to reach t_1 , 3 steps to reach t_2 , ..., and so forth. Likewise, the effect of the control move made at t_2 would take 3 steps to reach t_1 , 4 steps to reach t_2 ,..., and so forth. Therefore, for a system in which $n_p = 12$, we would obtain the prediction vector $[y_p]_{12\times 1}$ for the free response (due to past control moves only) as

$$\begin{bmatrix} y_{p}(t_{1}) \\ y_{p}(t_{2}) \\ \vdots \\ \vdots \\ y_{p}(t_{12}) \end{bmatrix} = \begin{bmatrix} y(t_{-12}) \\ y(t_{-12}) \\ \vdots \\ y(t_{-12}) \end{bmatrix} + \begin{bmatrix} a_{13} & \vdots & a_{3} & a_{2} \\ a_{14} & \vdots & a_{4} & a_{3} \\ \vdots & \vdots & \ddots & \vdots \\ a_{24} & \vdots & a_{14} & a_{13} \end{bmatrix} \begin{bmatrix} \Delta u(t_{-12}) \\ \Delta u(t_{-11}) \\ \vdots \\ \Delta u(t_{-1}) \end{bmatrix}$$
(5)

or

$$\left[\mathbf{y}_{p}\left(\mathbf{future}\right)\right]_{12\times1} = \left[\mathbf{y}\left(\mathbf{t}_{-\mathbf{n}_{p}}\right)\right]_{12\times1} + \left[\mathbf{A}_{p}\right]_{12\times12} \left[\Delta \mathbf{u}\left(\mathbf{past}\right)\right]_{12\times1}$$
(6)

where

$$[\mathbf{A}_{\mathbf{p}}]_{12 \times 12} = \begin{bmatrix} a_{13} & \cdots & a_{3} & a_{2} \\ a_{14} & \cdots & a_{4} & a_{3} \\ \vdots & \vdots & \ddots & \vdots \\ a_{24} & \cdots & a_{14} & a_{13} \end{bmatrix}$$

where $y(t_{.np})$ is the value of the process variable at the beginning of prediction n_p steps in the past. For a system at initial steady state, the process variables at the beginning of prediction during moving horizon control $\{y(t_{.np}), y(t_{.np+1}), ..., y(t_{.1})\}$ are all zero for $t < t_0$.

If the setpoint profile y_{sp} for $t > t_0$ is known, we may define the free-response error vector as

$$\begin{bmatrix} E(t_1) \\ E(t_2) \\ . \\ . \\ E(t_{12}) \end{bmatrix} = \begin{bmatrix} y_{sp}(t_1) \\ y_{sp}(t_2) \\ . \\ . \\ y_{sp}(t_{12}) \end{bmatrix} - \begin{bmatrix} y_p(t_1) \\ y_p(t_2) \\ . \\ . \\ . \\ y_p(t_{12}) \end{bmatrix}$$
(7)

or

$$[\mathbf{E}]_{12\times 1} = \left[\mathbf{y}_{sp}\right]_{12\times 1} - \left[\mathbf{y}_{p}\right]_{12\times 1}$$
(8)

To reduce or suppress the free-response error, DMC must instruct the final control element to make control moves for n_c steps at the present and future time steps ($t_0, t_1, t_2, ..., t_{nc-1}$).

Calculation of present and future control moves

If the controller makes control moves of $\Delta u(t_0)$, $\Delta u(t_1)$, $\Delta u(t_2)$, $\Delta u(t_3)$, and $\Delta u(t_4)$ for n_o steps (= 5 in this work), we may anticipate that such present and future control moves would cause the process to respond by the magnitudes given by Eqs. (3) and (4). Therefore, the free response error may be reduced due to the present and future control moves, resulting in an effective or net error expressed as a net error vector $[NE]_{12\times 1}$:

Net Error = (Free response error due to past control moves $\Delta u(t < t_0)) -$ (Process response due to present and future control moves $\Delta u(t \ge t_0)$

$$\begin{bmatrix} NE(t_1)\\ NE(t_2)\\ \vdots\\ NE(t_{12}) \end{bmatrix} = \begin{bmatrix} E(t_1)\\ E(t_2)\\ \vdots\\ E(t_{12}) \end{bmatrix} - \begin{bmatrix} a_1 & 0 & \vdots & 0 & 0\\ a_2 & a_1 & 0 & \vdots & 0\\ a_3 & a_2 & a_1 & 0 & 0\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ a_{11} & a_{10} & a_9 & a_8 & a_7\\ a_{12} & a_{11} & a_{10} & a_9 & a_8 \end{bmatrix} \begin{bmatrix} \Delta u(t_0)\\ \Delta u(t_1)\\ \Delta u(t_2)\\ \Delta u(t_3)\\ \Delta u(t_4) \end{bmatrix}$$
(9)

$$\left[\text{NE}\right]_{12\times 1} = \left[\text{E}\right]_{12\times 1} - \left[\text{A}\right]_{12\times 5} \left[\Delta u \text{ (present and future)}\right]_{5\times 1} \quad (10)$$

It can be said that the present and future control moves would serve to reduce or suppress the free response error. In Eqs. (9) and (10), it is assumed that disturbance does not exist and that there is no mismatch between the measured and predicted process variable. It is also assumed that the controller does not reach saturation and there is no constraint on the control moves. To compute the present and future control moves, an objective function Φ is defined as

$$\Phi = \sum_{i=1}^{n_p} \left\{ \left[NE(t_i) \right]^2 + \lambda \left[\Delta u(t_i) \right]^2 \right\}$$
(11)

where λ is defined as the move suppression coefficient.

Moving horizon control is a key feature of dynamic matrix control. This type of controller employs a model internal to the controller architecture to predict the process variable for n_p steps into the future based on control moves for n_p steps in the past.

Optimization of DMC gives the required present and future control moves that will serve to minimize Φ for a given $\lambda^{[1,3]}$

 Δu (present and future)]_{5×1} =

$$\begin{aligned} & \Delta u(t_0) \\ \Delta u(t_1) \\ \Delta u(t_2) \\ \Delta u(t_3) \\ \Delta u(t_4) \end{aligned} = \left(\begin{bmatrix} \boldsymbol{A}^T \end{bmatrix}_{5 \times 12} \begin{bmatrix} \boldsymbol{A} \end{bmatrix}_{12 \times 5} + \lambda \begin{bmatrix} \boldsymbol{I} \end{bmatrix}_{5 \times 5} \right)^{-1} \begin{bmatrix} \boldsymbol{A}^T \end{bmatrix}_{5 \times 12} \begin{bmatrix} \boldsymbol{E} \end{bmatrix}_{12 \times 1}$$
(12)

where $[A^T]$ is the transpose of the dynamic matrix [A] and [I] is a 5×5 identity matrix for $n_c = 5$. Apparently, the greater the move suppression coefficient λ , the smaller the $\Delta u(t_i)$ values or a more conservative control action; and vice versa the control action becomes more aggressive.

Once the calculation is done, only the first control move $\Delta u(t_0)$ is implemented and the horizon moves one time step further. By treating t_1 as the present time, t_0 is then one time step in the past, and so forth. In the next step of calculation at t_1 , the previously calculated $\Delta u(t_0)$ would be considered as the control move one step in the past. So, its value (and only this Δu) should be entered at the bottom of the [$\Delta u(past)$] vector for the past control moves [second term on the righthand side of Eqs. (5) and (6)]. Then [y_p], [E], [NE], and the new [Δu (present and future)] are recalculated at t_1 . The whole procedure may be repeated for n_p steps.

If there is no mismatch between the measured and predicted process response, then the actual process response for future steps at $t_1, t_2, ...$ should be the sum of the free response and

the process response due to present and future moves [Eq. (13)]

$$\mathbf{y} \Big[(\text{actual response}) \Big]_{12\times 1} = \Big[\mathbf{y}_{p} \Big]_{12\times 1} + [\mathbf{A}]_{12\times 5} \big[\Delta \mathbf{u} (\text{present and future}) \big]_{5\times 1}$$
(13)

However, since only the first control move $\Delta u(t_0)$ is implemented at t_0 , we may predict the actual process response of $y(t_1)$ only [Eq. (14)]

$$y(t_1) = y_p(t_1)$$
 (predicted at t_0 based on $y(t_{12})$ and $[\Delta u(past)] + a_1 \Delta u(t_0)$ (14)

As the control horizon moves forward, the whole calculation repeats. In a system where $a_1 = 0$ (due to dead time), the actual process response $y(t_1)$ is the same as the free response $y_p(t_1)$ predicted at t_0 due to past control moves.



Based on the MPC theory and DMC strategy outlined above, the authors developed a spreadsheet procedure using data for a hypothetical first-order-plus-dead-time model with process gain $K_p = 1.5$, time constant $\tau_p = 1$, and deadtime $\theta_p = 1$. The SRM coefficients for this process model are shown in Table 1 and Figure 1. The size of time step $\Delta t = 1$ is chosen in this work. This process stabilizes in 10 time steps or model horizon m = 10. The established DMC guidelines recommend that the pre-

	TABLE 1 Coefficient of step response model (SRM) used in this work												
a ₁	\mathbf{a}_1 \mathbf{a}_2 \mathbf{a}_3 \mathbf{a}_4 \mathbf{a}_5 \mathbf{a}_6 \mathbf{a}_7 \mathbf{a}_8 \mathbf{a}_9 \mathbf{a}_{10}												
0.00	0.948	1.297	1.425	1.473	1.490	1.496	1.499	1.499	1.500				
a ₁₁	a ₁₂	a ₁₃	a ₁₄	a ₁₅	a ₁₆	a ₁₇	a ₁₈	a ₁₉	a ₂₀				
1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500				
a ₂₁	a ₂₂	a ₂₃	a ₂₄	a ₂₅	a ₂₆	a ₂₇	a ₂₈	a ₂₉	a ₃₀				
1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500				

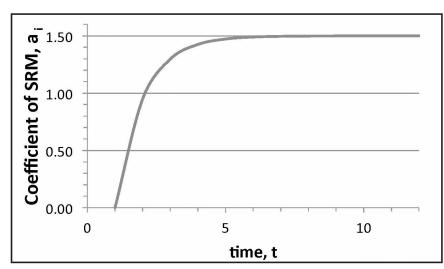


Figure 1. Plot of SRM Coefficient a, versus time.

TABLE 2Dynamic matrix $[A]_{12x5}$ for prediction horizon $n_p = 12$ and control horizon $n_c = 5$ using the coefficients a_i (i = 1, 2,, 12) from the SRM.											
0.000	0.000	0.000	0.000	0.000							
0.948	0.000	0.000	0.000	0.000							
1.297	0.948	0.000	0.000	0.000							
1.425	1.297	0.948	0.000	0.000							
1.473	1.425	1.297	0.948	0.000							
1.490	1.473	1.425	1.297	0.948							
1.496	1.490	1.473	1.425	1.297							
1.499	1.496	1.490	1.473	1.425							
1.499	1.499	1.496	1.490	1.473							
1.500	1.499	1.499	1.496	1.490							
1.500	1.500	1.499	1.499	1.496							
1.500	1.500	1.500	1.499	1.499							

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As the control horizon moves forward, the whole calculation repeats.

	TABLE 3 Matrix ([A ^T] [A]+ λ [I]) ⁻¹ [A ^T] for move suppression coefficient λ = 3.0										
0.000	0.160	0.127	0.071	0.033	0.012	0.004	0.002	0.001	0.000	0.000	0.000
0.000	-0.091	0.087	0.085	0.050	0.020	0.009	0.005	0.003	0.003	0.003	0.003
0.000	-0.044	-0.127	0.065	0.070	0.031	0.017	0.012	0.010	0.010	0.009	0.009
0.000	-0.018	-0.059	-0.140	0.046	0.033	0.028	0.026	0.026	0.026	0.025	0.025
0.000	-0.007	-0.026	-0.073	-0.172	-0.026	0.028	0.048	0.055	0.058	0.059	0.059

diction horizon $n_{\rm p}$ exceeds the model horizon by 20% or 50% ($n_{\rm p} \sim 12\text{-}15$) and that the control horizon $n_{\rm c} = 0.5$ m $\sim 5.^{(1)}$ Since the purpose of this module is to illustrate the concept of DMC without using Visual Basic (or other sophisticated software), the authors choose $n_{\rm p} = 12$ and $n_{\rm c} = 5$ for illustrating the procedure.

With $n_p = 12$ and $n_c = 5$, the dynamic matrix $[A]_{12\times5}$ based on the SRM coefficients (Table 1) is given in Table 2. By following the standard matrix operations in Excel for transpose, multiplication, and addition, the matrix $([A^T][A] + \lambda[I])^{-1}[A^T]$ for $\lambda = 3.0$ is calculated and summarized in Table 3. The matrix $[A_p]_{12\times12}$ (for predicting the free response of the process) is given in Table 4. Note that the elements of $[A_p]_{12\times12}$ should be entered according to Eq. (6), where the values of the elements are from Table 1.

To initialize the calculation, it is assumed that the system is at steady state at t_0 and that the process variable and the past control moves are both zero for $t < t_0$ for at least n_p steps in the past. The spreadsheet shown in Table 5 (following page) illustrates the calculation for the time step at t_0 . The following procedure was used to create Table 5:

- Column G is created to count the past and present time steps -12, -11,..., -1, 0. Column H is created to count the present and future time steps 0, 1, 2,..., 12;
- Assign 0.00 values to Q65-Q77 for present and past values of process variable;
- (3) Highlight cell I65 and perform "=\$Q65 " (the beginning process variable (t_{.12}) for prediction of free response). Highlight cell I66, perform "= 165," and copy downward. In this manner, elements in Column I have the y(t_{.12}) value;
- (4) Assign 0.0 to J65-J76 (for past control moves [$\Delta u(past)$];
- (5) Highlight cell K-65-K76 and perform matrix multiplication [A_p] [Δu (past)] (=MMULT(\$E\$37:\$P\$48,J65:J76), followed by the combined key stroke, control+shift+enter, in Excel, where [A_p] is located in the cells E37-P48 and [Δu(past)] is located in the cells J65-J76. The \$ sign is needed to fix the column number and the row number for [A_p] when copying the content of Table 5 down below. However, the cell positions for [Δu(past)] do not need the \$ sign in front of the column number or the row number; Excel will automatically reference to the appropriate cell positions when the content of Table 5 is copied downward;
- (6) Add Column I and K and put the results in L65-L76, that gives (future) free response of process variable due to past control moves;
- (7) Assign setpoint of 1.00 to M65-M76, assuming that there is a unit step change of 1.000 occurring at t₀⁺ and calculate the free response error [E] (Column N) by subtracting Column L from Column M;

	t < t ₀)	0.948	1.297	1.425	1.473	1.490	1.496	1.499	1.499	1.500	1.500	1.500	1.500
	er outputs (1.297	1.425	1.473	1.490	1.496	1.499	1.499	1.500	1.500	1.500	1.500	1.500
	ast controll	1.425	1.473	1.490	1.496	1.499	1.499	1.500	1.500	1.500	1.500	1.500	1.500
	hanges in pa	1.473	1.490	1.496	1.499	1.499	1.500	1.500	1.500	1.500	1.500	1.500	1.500
	t_0) due to c	1.490	1.496	1.499	1.499	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500
,E 4	ble $[y_p]$ (t >	1.496	1.499	1.499	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500
TABLE 4	rocess varia	1.499	1.499	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500
	esponse of p	1.499	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500
	uture free re	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500
	$A_p]_{12x12}$ for f	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500
	Prediction matrix $[A_p]_{12x12}$ for future free response of process variable $[y_p]$ (t > t ₀) due to changes in past controller outputs (t < t ₀)	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500
	Predict	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500

,	(t_{12})	and p	ast $\Delta \iota$	1(t)	" t _{.11} ,	d future)] _{5x} .t _{.1}). Note tl	at onl	y the fir	st of th	e prese	nt and f	uture 2	$\Delta u (0.$	410) is ac	tually ca	rried of	t_{0}
	A	В	C	D	E	FG	н	1	J	K	L	M	N	0	P	Q	R
2								y@t()									
53				t	0	count, now & past	count, now & future	-12	∆u(past)	[A _p] [Δu(past)]	y _p (free response)	Укр	[E]	Δu(now & future)	y(next)	y(now & past)	
54					'=165 & c	opied downwards	0	`=\$Q65			'=165+K65		'=M65-	0.410	"=L65+O64" \$E\$7		
5	-					-12	1	0.000	0.000	0.000	0.000 /	1.000	1.000	0.176	0.000	0.000	
6						-11	2	0.000	0.000	0.000	0.000	1.000	1.000	0.064		0.000	
37						-10	3	0.000	0.000	0.000	0.000	1.000	1.000	0.018		0.000	
38						-9	4	0.000	0.000	0.000	0.000	1.000	1.000	0.001		0.000	
39	-					-8	5	0.000	0.000	0.000	0.000	1.000	1.000			0.000	
70						-7	6	0.000	0.000	0.000	0.000	1.000	1.000	'=MMULT(\$ E\$28:\$P\$32, N65:N76)		0.000	
71						-6	7	0.000	0.000	0.000	0.000	1.000	1.000	Sec. Sec.		0.000	
72						-5	8	0.000	0.000	0.000	0.000	1.000	1.000			0.000	
73						-4	9	0.000	0.000	0.000	0.000	1.000	1.000			0.000	
14						-3	10	0.000	0.000	0.000	0.000	1.000	1.000			0.000	
15						-2	11	0.000	0.000	0.000	0.000	1.000	1.000			0.000	
15 16						-1	12	0.000	0.000	0.000	0.000	1.000	1.000			0.000	
77						0			0.410							0.000	

TABLE 6

Calculation of Δu to be carried out at $t_1, t_2, ..., t_5$ based on predicted process variable $y_p(t_2, t_3, ...,, t_{13})$ and past $\Delta u(t_{11}, t_{33}, ..., t_0)$. Only the first of the present and future Δu (0.176) is actually carried out at t_1 . Important cell operations are explained in the text.

21	A	8	C	D	E	F	G	н	1	1	K	L	M	N	0	P	Q	R
79								'=163+1	y@t()									
80				t	1		count, now & past	count, now & future	-11	Δu(past)	[A _p] [Δu(past)]	γ _p (free response)	Yu	[E]	∆u(now & future)	y(next)	y(now & past)	
81					'=063+1	_		1	`=\$Q82						0.176			
82							11	2	0.000	0.000	0.389	0.389	1.000	0.611	0.064	0.389	0.000	
82 83					'=G65+1-	_	-10	3_	0.000	0.000	0.532	0.532	1.000	0.468	0.018		0.000	
84							-9	4	0.000	0.000	0.585	0.585	1.000	0.415	0.002		0.000	
85						-	-8	5	0.000	0.000	0.604	0.604	1.000	0.396	-0.002		0.000	
86					`=182		-7	6	0.000	0.000	0.611	0.611	1.000	0.389			0.000	
87							-6	7	0.000	0.000	0.614	0.614	1.000	0.386			0.000	
88							-5	8	0.000	0.000	0.615	0.615	1.000	0.385			0.000	
89							-4	9	0.000	0.000	0.615	0.615	1.000	0.385			0.000	
90							-3	10	0.000	0.000	0.615	0.615	1.000	0.385			0.000	
91							-2	11	0.000	0.000	0.615	0.615	1.000	0.385			0.000	
90 91 92							-1	12	0.000	0.000	0.615	0.615	1.000	0.385		=Q77	0.000	
93 94 95							0	13	0.000	0.410	0.615	0.615	1.000	0.385		and copied	0.000	
94					1		1			0.176	1					upwards	- 0.000	
95				1			1			`=O81 /	'=J77 (and (copied upwa	rds)			'=P65		

- (8) Highlight cell 064-068 and perform matrix multiplication according to Eq. (12), where the([A^T][A]+ λ [I])⁻¹ [A^T](for λ=3.0) is given in Table 3. Again, in the matrix multiplication "=MMULT(\$E\$28:\$P\$32,N65:N76)," E28-P32 is the matrix [A^T] [A]+ λ [I])⁻¹ [A^T] and its column number and row number must be fixed by placing the \$ sign in front of them. However, the cell positions in the [E] vector do not need the \$ sign. The cells 064-068 are the predicted control moves to be made at t₀, t₁, ...,t₄. But only the first one (064, with calculated value of 0.410) will be actually implemented;
- (9) Highlight cell J77 and assign " = O64." In this way, the present $\Delta u(t_o)$ is entered to the bottom of Column J;
- (10) Highlight cell P65 to calculate the actual process variable y(next) or $y(t_1)$ according to Eq. (14) to show the effect of the present control move $\Delta u(t_2)$. In the au-

thors' spreadsheet, the coefficient of SRM a_1 is located at cell E7.

To perform the calculation for the moving horizon control, the cells in Table 5 are copied and pasted somewhere else on the spreadsheet for calculations at the next time step at t_1 . The pasted cell needs revision before the final outcome (Table 6) is obtained:

- Highlight the cell G82 and perform "= G65 +1" and copy downward. The count for now and past will be advanced by 1 from corresponding cells of Table 5. Do the same for H81-H93 and cell 180;
- (2) Highlight Q94 and perform "= P65." Doing so will put the y(next) calculated at t₀ as the value of the process valuable y(now) at t₁;
- (3) Highlight Q93, perform "= Q77," and copy the formula upward. In this manner, the process vari-

		_		0 -2 1		1			0					ewhere bel	
A	D	E	F	G	н	1	J	K	L	M	N	0	Р	Q	R 🔺
96						γ@t									
97	t	2.000		count, now & past	count, now & future	-10.000	∆u(past)	[A _p] [∆u(past)]	y _p (free response)	Y _{sp}	[E]	∆u(now & future)	y(next)	(now & past)	
98					2							0.064			
99				-10	3	0.000	0.000	0.699	0.699	1.000	0.301	0.018	0.699	0.000	
00				-9	4	0.000	0.000	0.813	0.813	1.000	0.187	0.003		0.000	
01				-8	5	0.000	0.000	0.855	0.855	1.000	0.145	-0.002		0.000	-
02				-7	6	0.000	0.000	0.870	0.870	1.000	0.130	-0.002		0.000	
03				-6	7	0.000	0.000	0.876	0.876	1.000	0.124			0.000	
04				-5	8	0.000	0.000	0.878	0.878	1.000	0.122			0.000	
05				-4	9	0.000	0.000	0.879	0.879	1.000	0.121			0.000	
06				-3	10	0.000	0.000	0.879	0.879	1.000	0.121			0.000	
07				-2	11	0.000	0.000	0.879	0.879	1.000	0.121			0.000	
08				-1	12	0.000	0.000	0.879	0.879	1.000	0.121			0.000	
09				0	13	0.000	0.410	0.879	0.879	1.000	0.121			0.000	
10				1	14	0.000	0.176	0.879	0.879	1.000	0.121			0.000	
11				2			0.064							0.389	
12															
13						y@t									
				count.	count.							∆u(now			100

1	D	F	F	G	н	1	1	K	1	M	N	0	р	Q	R	\$	
263	*			10	23	0.000	0.000	1.000	1.000	1.000	0.000			1.001			1
264				11			0.000							1.000			
265																	
266						y@t											1
267	t	12.000		count, now & past	count, now & future	0.000	∆u(past)	[A _p] [∆u(past)]	y _e (free response)	$\gamma_{\rm sp}$	(E)	∆u(now & future)	y(next)	now & pa	st)	u	
268					12							0.000			*=\$268+J269		
269				0	13	0.000	0.410	1.000	1.000	1.000	0.000	0.000	1.000	0.000	and copied	0.410	
270				1	14	0.000	0.176	1.000	1.000	1.000	0.000	0.000		0.000	downwards	0.586	
271				2	15	0.000	0.064	1.000	1.000	1.000	0.000	0.000		0.389		0.650	
272				3	16	0.000	0.018	1.000	1.000	1.000	0.000	0.000		0.699		0.668	
273				4	17	0.000	0.003	1.000	1.000	1.000	0.000			0.874		0.671	
274				5	18	0.000	-0.001	1.000	1.000	1.000	0.000			0.955		0.670	
275				6	19	0.000	-0.001	1.000	1.000	1.000	0.000			0.988		0.668	
276				7	20	0.000	-0.001	1.000	1.000	1.000	0.000			0.999		0.667	
277				8	21	0.000	0.000	1.000	1.000	1.000	0.000			1.001		0.667	
278				9	22	0.000	0.000	1.000	1.000	1.000	0.000			1.001		0.667	
279				10	23	0.000	0.000	1.000	1.000	1.000	0.000			1.001		0.667	
280				11	24	0.000	0.000	1.000	1.000	1.000	0.000			1.000		0.667	
281				12			0.000							1.000		0.667	
282																	
283			C. C. IA		A					and the second							

able calculated in the time step before will move up one position;

- (4) Highlight J93, perform "= J77" (the bottom of J column in Table 5), and copy the formula upward. In this manner, the ∆u(past) from the previous table will move up by one position;
- (5) The users will then see the revised result of cells 081-085. Finally, Highlight J94 and perform "= 081" to enter the present control move just calculated.

Once Table 5 and Table 6 are established, the content of Table 6 can be copied and pasted somewhere down below without any further revisions because the relationships between two successive tables are already established. The result of calculations at t_2 is given in Table 7. If the contents of Table 6 are pasted for subsequent time steps, the final results of calculations for t_{12} are shown in Table 8. In Table 8, the cell S269 is highlighted and "= S268+J269" is performed and copied downward. In this way, the cumulative controller output may be calculated from the control moves since t_0 (Column J).

Figure 2 shows the process response (y), control moves at every time step (Δu), cumulative controller output (u) and setpoint ($y_{setpoint}$) for time steps up to $n_p = 12$ (Table 8). Once the calculations are done for $\lambda = 3$, the contents of this worksheet may be copied and pasted on several other worksheets. By simply changing the cell that stores the λ value, the results for $\lambda = 1$, 5, 8, and 20 would appear immediately. Figures 3 and 4 summarize the effects of moving suppression coefficient λ on the process variable y as well as cumulative controller output u. It is clear that the greater the λ value, the more conservative the control action and the more sluggish in process response.

DISCUSSION

This work focuses on setpoint tracking in the absence of disturbance for perfectly linear process models. In reality, many real-world processes exhibit non-linear behaviors, with SRM coefficients (a,'s) varying with steady-state conditions. Also, it is assumed that there is no process or model mismatch between the predicted and measured values of process variable at t_0 . If such a mismatch exists, the magnitude $\varepsilon = y_{sp}(t_0) - y_p(t_0)$ must be subtracted from every element of the vector [E] in Eqs. (7) and (8) to make the prediction more accurate.

With the model having the first-order-plus-dead-time behavior, there are many well-established tuning rules available to tune the feedback controller for this process. However, DMC offers several benefits. DMC is able to predict the future errors and the present and future control moves in order to minimize predicted net errors for future steps. This ability of changing controller outputs based on the predicted future process condition is absent in traditional feedback control. Or, we may say that a DMC system having a very short prediction horizon (n_{n}) behaves more like a traditional feedback controller. In this work, the authors choose n, m, and n according to recommended guidelines. Because the control action cannot change after the control horizon ends, a short control horizon n results in a large initial controller output, but a few careful changes in control action. The large control action in a short control horizon might overshoot the setpoint. However, as the controller continues to execute, the process variable will eventually settle around setpoint. On the other hand, a long control horizon produces a small initial controller output but more *aggressive changes* in control action. These aggressive changes in control action in a long control horizon can result in oscillation. In general, a control horizon of about one-half model horizon is recommended. Although a long prediction horizon increases the predictive ability of the DMC, the performance of the controller may suffer due to the extra calculations required.

The spreadsheet procedure developed here allows students to track step-by-step changes of a moving horizon control system with great ease. Interested users may revise this spreadsheet by

(1) using SRM coefficients obtained from real-world 82

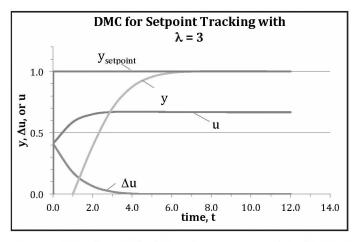


Figure 2. Results of calculation for setpoint tracking by DMC with move suppression coefficient $\lambda =3$. Since $a_i = 0$ in this case, $y = y_p$.

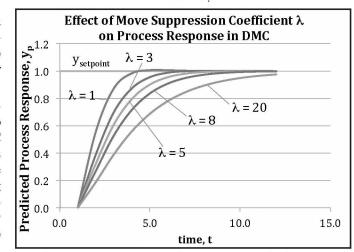


Figure 3. Effect of move suppression coefficient λ on the actual process response y or free response y_p , same for this case with $a_i = 0$.

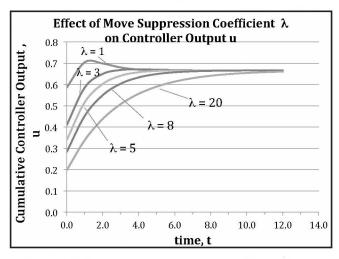


Figure 4. Effect of move suppression coefficient λ on the controller output u.

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processes or real plant data;

- (2) removing or changing the amount of dead time to explore the effects of dead time on y and u. In the absence of dead time, the free response $y_p(next)$ and actual response y(next) will differ by a magnitude of $a_1^* \Delta u(present)$, where $a_1 \neq 0$;
- (3) consulting with publications that use more sophisticated software^[4] once they are confident in the basic concept; or
- (4) exploring the effects of using different values for various horizons (model horizon, prediction horizon, and control horizon).

The topic of DMC was covered in our department's process control class for the first time in the Fall 2014 semester, as suggested by our department's industrial associates. The topics covered in this class are listed below:

- Introduction to the course, control practice, elements of typical control systems, design of data acquisition using modern software such as LabVIEW
- Case study of process dynamic model: heated stirred tank—from energy balance to closed-loop control system, and case studies including laboratory control experiments
- Derivation of dynamic models for industrially important process units
- *Review of essential mathematical tools (differential equations and Laplace Transform)*
- Dynamic behavior of first-order systems (first experience of Loop Pro software); Dynamic Matrix
- Dynamic behavior of second-order systems
- Higher order systems and approximate models for poorly understood systems
- Overall transfer function of closed-loop feedback control systems
- Stability analysis
- Process identification of typical chemical engineering processes
- Industrial procedure of controller tuning (process reaction curve method, continuous cyclic response method, frequency response method)
- Industrial procedure of controller tuning (Internal Model Control (IMC))
- Advanced Control Methods—Cascade, Feedforward/Feedback, Smith Predictor, Gain Scheduling
- Introduction to Dynamic Matrix Control

Besides two hours of lecture each week, this course has a Laboratory/Problem (L/P) component that meets three hours each week. During the L/P hours, students have opportunities running real-world experiments, performing simulation using Loop-Pro software (Workshop 1 through 3 below), and designing spreadsheet procedures (Workshop 4):

- Workshop #1: Level control in gravity drained tanks
- Workshop #2: Temperature control in shell-n-Tube heat exchangers
- Workshop #3: Level control in pumped tanks
- Workshop #4: Spreadsheet procedure for Dynamic Matrix Control calculations

Although the topic of DMC and the associated spreadsheet workshop were covered toward the end of the semester for one lecture and one L/P activity, students had a chance to learn the basics of this advanced concept.

CONCLUSIONS

1. An easy-to-follow spreadsheet procedure is developed for an undergraduate process control class to learn basic aspects of moving horizon control in a dynamic matrix controller (DMC);

2. Based on coefficients of step response model (SRM) obtained from plant data, a dynamic matrix can be constructed for a DMC;

3. The DMC calculates the present and future control moves required to decrease the predicted future errors (and steer the process variable toward setpoint) according to the rules of DMC and a selected value of move suppression coefficient λ ; and

4. The greater (smaller) the λ value, the more conservative (aggressive) the control action.

ACKNOWLEDGMENT

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Chemical Engineering at ... Lafayette College

JAMES K. FERRI

afayette College is a small, private college located in Easton, Pennsylvania. It enrolls approximately 2,400 undergraduate students, about half of whom are en-

gineering and science majors. Founded in 1826, Lafayette enjoys a unique connection between liberal arts and engineering; a strategic combination that meets the increased demand for science and technology as well as providing the creativity and insight imparted by the arts and humanities.

In addition to its strong tradition of liberal arts and engineering, Lafayette College is also known for its longstanding football rivalry; we hosted the 150th meeting of Lafayette and Lehigh at Yankee Stadium in November 2014. Begun in 1884, Lafayette-Lehigh is the nation's most-played college football rivalry, and it has been played every year since 1897 without interruption—the longest streak of consecutive years for any rivalry in college football.

The 150th also marked the kick-off of the capital campaign, *Live Connected*, *Lead Change*, celebrating the accomplishments of the college and its alumni. The college is enabled by an endowment-per-student in the top eight percent of all colleges and universities in the country, Lafayette has a

strong record of achievement in the chemical industries with distinguished alumni including John Townsend Baker (founder, J.T. Baker Chemical), Alvin and Andy Deitz (founders, Spectra Gases), and Stephen D. Pryor (CEO, ExxonMobil Chemical). This alumni base coupled with the strong relationships with industry leaders ExxonMobil, Air Products, DuPont, BASF, GlaxoSmithKline, and Merck and Company enable Lafayette chemical engineers to routinely secure post-graduation job placement in these companies, as well in programs for advanced study. In the last five years, graduates have enrolled in programs at Princeton, Johns Hopkins, Cornell, the University of California–Santa Barbara, and the University of Delaware,



among others. Since 2010, five Lafayette chemical engineers have been awarded National Science Foundation Graduate Research Fellowships, and eight since 2003. In a study recently

reported by PayScale.com, Lafayette boasts a seven percent annual return on investment over 20 years; it is ranked 8th among liberal arts colleges in the nation.

In 2016, engineering at Lafayette will celebrate 150 years; chemical engineering at Lafayette is celebrating its centennial in 2015.

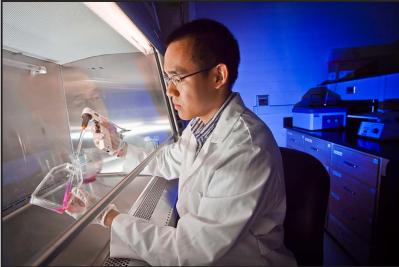
THE HISTORY OF ChE AT LAFAYETTE

The origin of chemical engineering at Lafayette can be traced to Dr. Edward Hart. Hart received his Ph.D. in chemistry from the Johns Hopkins University in 1878, studying with Dr. Ira Remsen. Joining the faculty of the chemistry department at Lafayette shortly thereafter, Hart immediately began inspiring students to pursue opportunities in chemical manufacturing. Together with John Townsend Baker (B.S., Chemistry, 1882; M.S., Chemistry, 1885), Hart founded the partnership of

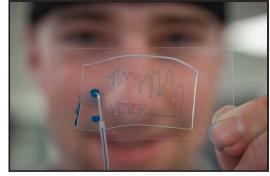
Top, above: Edward Hart, co-founder of Baker and Hart Chemical and the founder and editor of Analytical Chemistry. Hart was the chair of the Industrial and Engineering Chemistry Division of the American Chemical Society and department head of chemistry before becoming the first professor of chemical engineering at Lafayette College.

Bottom, above: Eugene C. Bingham, co-founder of the field of rheology and author of Fluidity and Plasticity (McGraw-Hill; New York, NY). Bingham was the organizer of the first Plasticity Symposia of the American Chemical Society. He was head of chemistry at Lafayette College.





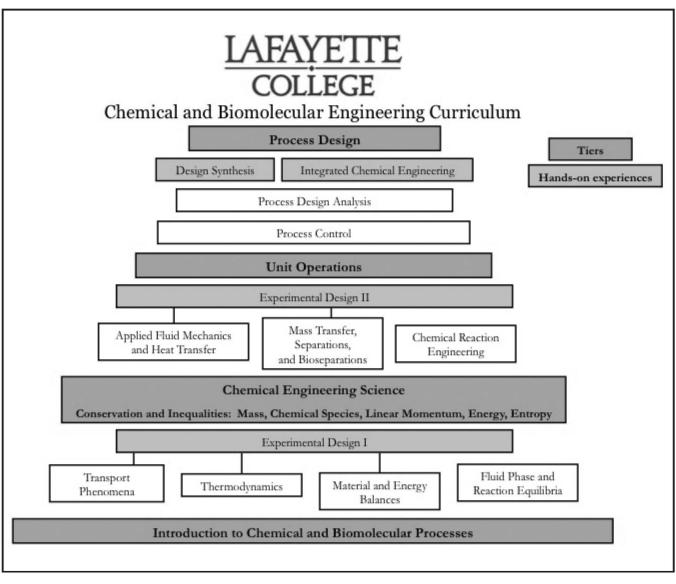
Baker and Hart in 1882, and began the production of refined chemicals in a small plant that they constructed together on College Hill, several blocks from campus. In 1884, another of Hart's students, George Purseglove Adamson (B.S., chemistry, 1884; M.S., chemistry, 1887) joined their partnership,



Top: The Inaugural Chemical Engineering Spring Symposium included commissioning and ribbon-cutting ceremony of the twincolumn distillation plant in the Lafayette Unit Operation Laboratory by Stephen D. Pryor, CEO, ExxonMobil Chemical.

Left above: Kevin Ling explores experiential molecular bioengineering in the LafChBE Tissue Cultural Facility (2012).

Right above: Student Victor D'Ascenzo, class of 2017, made a name for himself—literally— in Lafayette's Introduction to Engineering/ChBE module, which teaches the art of engineering small/microfluidic device fabrication.



The Chemical and Biomolecular Engineering (ChBE) curriculum at Lafayette College: hierarchical organization.

which then became known as the Baker and Adamson Chemical Company. It was reckoned that Hart's name was omitted from the enterprise because Lafayette College preferred that the business activities of its staff remained unpublicized. Nonetheless, Hart served as president of Baker and Adamson Chemical from its incorporation in 1890 until 1913. Revenues in 1890 were \$10,000 per month! (*The Octagon*, May 1960, Vol. 43, No. 5)

Another of Hart's students was Richard Kidder Meade (B.S., chemistry, 1899; M.S., chemistry, 1908). Meade founded and edited *The Chemical Engineer*, a journal of practical, applied, and analytical chemistry. Perhaps most noteworthy, in a forceful editorial first published in October 1905 and re-printed in October 1907, titled "Why not 'The American Society of Chemical Engineers'?" Meade argued that "...mining, civil, electrical, and mechanical engineers are organized and each has a strong

society ... the chemical engineers must also organize and the time is now opportune for the formation of an American Society of Chemical Engineers." (The Chemical Engineer, Volume 3, 1905) A committee of six, including Arthur D. Little, William H. Walker, and Richard Meade, was formed to explore the need for such a society, and the American Institute of Chemical Engineers was established in January 1908. Among the 40 charter members. George Adamson was a member of the Council of the Institute from 1908 until 1911. Also a charter member of the AIChE, Hart served on the council from 1911 through 1913. The first Finance Committee was comprised of Hart, Adamson, and Meade, while Hart was also a member of the publications committee. (Volume 1, Transactions of the American Institute of Chemical Engineers, 1908) It is significant that these Lafayette chemists were at the forefront of the movement to organize the AIChE and took such an active part in its early life.

At Lafayette, the college catalog for academic year 1915– 1916 first listed a "Course of Study in Chemical Engineering" in the summer of 1915. In the following year, Hart stepped down as head of the Department of Chemistry to become the first professor of the chemical engineering at Lafayette; he was succeeded by Dr. Eugene C. Bingham, also an industrial chemist.

The first students of the chemical engineering course of study at Lafayette graduated in 1919. The B.S. in chemical engineering was first conferred at Lafayette in 1920. In 1921 Hart published the first textbook in the United States to bear the title *Chemical Engineering* (Chemical Publishing Company; Easton, Pa.).

As the Program in Chemical Engineering grew, the tradition of industrial chemistry was strong at Lafayette under Bingham in the 1920s. His milestone text, *Fluidity and Plasticity* (McGraw-Hill; New York, NY) in 1922, first described his observations that certain fluids did not flow until the imposed shearing stress reached a critical value, the yield stress, τ_0 . The first and third Plasticity Symposia of the American Chemical Society were hosted at Lafayette in 1924 and 1928, the latter of which spawned the Society of Rheology, organized in April 1929 in Columbus, Ohio. Leveraging the connection between the humanities and science and technology, the term "rheology" was coined at Lafayette by a classics professor at the request of Bingham and Marcus Reiner, then frequent visiting scientist, to make the subject more approachable.

An independent Department of Chemical Engineering was established in 1938. From 1938 through 1961, chemical engineering was led by Dr. E. L. McMillan. During this time, a student section of the AIChE was established (1940) and the program was first accredited (1956). Other major milestones in the department include its merger with the Department of Metallurgical Engineering in 1976; the closure of Metallurgical Engineering as a program in 1990; and the expansion of the department to include biomolecular engineering in 2008. Presently, the department maintains nine faculty positions and has more than 150 undergraduates across all class years — the fourth-largest degree program at Lafayette.

CURRICULUM

Chemical engineers bridge from the molecular sciences to the consumer through the creation and optimization of valueadded processes and products. The curriculum in the Department of Chemical and Biomolecular Engineering (ChBE) at Lafayette seeks to train undergraduates to not only traverse this bridge, but ultimately provide its foundation. As such, the plenary curriculum is organized into four hierarchical levels: Introduction to Chemical and Biomolecular Processes, Chemical Engineering Science, Unit Operations, and Process Design. Additionally, the curriculum provides flexibility for all ChBE students to fully participate in the Common Course of Study (CCS) at Lafayette College.

Experiential learning

Experiential learning is, and always has been, one of the hallmarks of chemical engineering education at Lafayette College. Students at Lafayette have been attracted to the notion of applying concept to practice since the days of Edward Hart. In the 1970s, Dr. George M. Hoerner, then associate professor of chemical engineering, convened 33-hour (voluntary!) laboratory sessions focusing on continuous manufacturing of solvent-based products in the Unit Operations Laboratory. Shifts began on Friday at 1 p.m. and continued through 10 p.m. on Saturday with operators (the inexperienced students) and crew chiefs (seniors with previous operating experience), while the shift supervisor, Dr. Hoerner, was on-hand the entire time with his sleeping bag in a room across the hall.

Currently, we seek to elaborate the complementary nature of theory and practice in our Experimental Design I (CHE312), Experimental Design II (CHE322), and Integrated Chemical Engineering (CHE412) hierarchy. This three-course sequence is composed of hybrid courses that emphasize experiential learning, increasing complexity from the bench to the unit operation to the pilot plant scale.

Experimental Design I (ED1) focuses on thermophysical properties characterization, such as viscometry, rheometry, diffusion, and calorimetry. In addition to illustrative lab experiences that utilize a range of bench scale equipment, students are exposed to lectures in the systematic empirical approach of statistical design of experiments (DOE). In ED1, emphasis is placed on full-factorial DOE together with both descriptive and inferential statistical tools enabling students to parameterize and characterize highly coupled complex chemical systems. There is also a focus on integrating laboratory and writing skill through reports and both oral and poster style presentations.

Experimental Design II (ED2) focuses on the unit operations of chemical engineering, such as fluid and heat transfer and multiphase flow, fluid phase equilibrium, and an introduction to feedback controlled processes. In ED2, lectures on statistical design of experiments are continued with an emphasis on fraction factorial and central composite design of experiments. The communications emphasis shifts to memo-style results reporting and continues to build on oral presentation skills.

Integrated Chemical Engineering (ICE) focuses on integrated pilot and industrial scale processes, such as continuous gas absorption, stripping, liquid-liquid extraction, distillation, and reverse osmosis, as well as experiments demonstrating dynamic interacting systems reactors in series, bioreactor mass transfer and kinetics, and advanced manufacturing processes. In ICE, student learn approaches to safety and hazards analysis; working in teams, all students complete and document Hazards and Operability Studies (HazOp) for a process. Students are assessed on full laboratory and HazOp reports, and oral presentations on advanced topics in the chemical process industry such as statistical process control; environmental, health, and safety regulations; risk; and compliance.

Pedagogical innovation takes the form of flipped laboratories to empower students to personally control hands-on learning with the overarching goal to enhance student understanding and operability of chemical engineering processes and equipment. A flipped laboratory is a pedagogical model that essentially inverts the instructor-to-student passage of information regarding operation of key pieces of equipment. Students have access to a library of short videos that explain standard operating procedures, common protocols, and troubleshooting tips. Students watch the videos for pre-lab assignments and can have access to the video protocols with them in the laboratory using tablet-style devices.

The LafayetteChBE YouTube channel (<https://www.youtube.com/user/LafayetteChBE>) hosts short tutorial videos for each major piece of equipment focusing on SOPs, quick start and instrument familiarity, and troubleshooting guides. Students and faculty can access these videos and learn how to operate the equipment. With over 40,000 views on these videos, based on an average in-class laboratory class size, we are demonstrating impact well beyond our institution.

Capstone design

Capstone design is a highlight of the student experience in ChBE through the diversity of projects offered. In 2015 projects feature industry/academy partnerships in conductive plastic process development and characterization in cooperation with Zzyzx Polymers and full-density digital part materialization through additive manufacturing with the ExOne Company. In these projects, students are involved and receive first-hand perspectives to the challenges and rewards associated with innovation and entrepreneurship in start-up enterprises.

Specializations and electives

The breadth in ChBE technical electives within the department enables wide exposure to chemical engineering subdisciplines. We have created speciality hybrid courses across several sub-disciplines including materials and interfaces, micro and nanofabrication, molecular bioengineering, and energy and the environment.

One example, CHE 344 Interfacial Phenomena, is an elective course that includes topics such as the thermodynamics of surfaces and interfaces, adhesion, intermolecular forces, DLVO theory, electrostatic and electrokinetic effects in colloidal systems, and characterization techniques such as scanning force microscopy, light scattering, and microscopy. The course is approximately evenly divided between lectures, lab experiences, and seminars in current literature. We use seminar and laboratory experiences as didactic opportunities to train students in lifelong learning methods. For each weekly twohour seminar or lab experience, self-selected student groups identify a topic or method from a list of 15 or so subjects designed to complement the lectures. Each group of three or four is mentored to develop a hosting strategy to engage the rest of the class in a meaningful experience. For seminars, this means selecting (and learning how to select) current literature and developing study/discussion questions for the class by serial jury-like selection of articles. For laboratory experiences, this means setting up rotating stations that enable all students in the course to learn sophisticated research techniques such as dynamic light scattering and zeta potential measurement, axisymmetric drop shape analysis, confocal microscopy, and scanning force microscopy while simultaneously mitigating the risks associated with new users and expensive equipment by pre-training the hosting group.

The feedback we have received from both students and faculty at Lafayette and in national venues, such as the American Society for Engineering Education (ASEE), has been highly positive suggesting that our approach would be well received in a variety of other venues.

Individualized learning

Lafayette ChBE faculty are active in diverse contemporary research areas such as energy and the environment, materials and interfaces, micro and nanofabrication, molecular bioengineering, and pedagogical innovation.

The eight faculty in the department during the last four years have published more than 30 peer-reviewed journal publications—many including student co-authors—and garnered more than \$2M in federally funded research grants while hosting more than 100 individual student experiences.

At Lafayette, individualized learning opportunities take on many different forms. Students can participate in the Lafayette EXCEL Scholars Program, which enables high-performing students to assist faculty members with their scholarship. The purpose of the EXCEL Program is to encourage collaboration in learning between faculty and students. The work of the student must, therefore, be research-oriented and not clerical in its primary emphasis. Faculty members supervising EXCEL Scholars receive assistance in accelerating the progress of their research efforts. Students can also undertake research for credit. The department permits one semester of student research toward the chemical engineering elective requirements. The highest achieving students often choose to undertake a two-semester senior honors thesis in order to earn departmental honors. These students are supervised or co-supervised by department faculty.

FACILITIES AND EQUIPMENT

In 1938, the department was granted an initial fund of \$10,000 provided by the Trustees of the College to equip the Chemical Engineering Laboratory. Much of the equipment was designed and installed by senior chemical engineering students and Dr. McMillen, including heat transfer, filtration, fluid flow, drying, air conditioning, and gas absorption. The utilization of students in the construction of simpler laboratory units enabled most of the funds to be used to purchase commercial pilot scale equipment units for distillation, evaporation, and continuous vacuum filtration.

Since 2010, the department has acquired new capital assets (~\$1.7M) associated with experiential learning through new state-of-the-art instrumentation and equipment to help us maintain our standing as one of the premier locations for undergraduate education including an additive manufacturing suite featuring a ProMetal 3D printer that enhances the capstone design sequence; a new Custom Separations Technologies independently operated



Assistant Professor Lindsay Soh and students participate in Introduction to Engineering/LafChBE: renewable biofuel and the global energy challenge.

twin-column distillation plant featuring digital controls that enhances experimental design and integrated chemical engineering courses; a micro/nanofabrication laboratory featuring photo and soft lithography as well as a scanning electron microscope that has been integrated into our first-year engineering design experiences; and a Center for Molecular Bioengineering enabled by a Nikon Eclipse Ti-E inverted microscope with C1 Plus confocal imaging system, a biaxial micromaterials mechanical test frame, and many tools from molecular biology helping to meet the growing demand for student experiences in molecular bioengineering.

CO-CURRICULAR PROGRAMS

In collaboration with the department, the Lafayette Chapter of the American Institute of Chemical Engineers (AIChE) has helped in the development of upcoming professional chemical engineers through out-of-class academic enrichment, studentfaculty interaction, and career path support. This co-curricular program of student engagement includes many outward facing programs such as informal lunchtime talks to inform students on opportunities within Lafayette's chemical engineering department including course scheduling, study-abroad, and research opportunities. Seminars also include presentations by professionals to help students explore career opportunities in chemical engineering and advanced industrial concepts that have not been extensively covered in curriculum. The department and AIChE Student Chapter also host regular networking and social events to facilitate student, faculty, and alumni interactions. This programming is complemented by specific events including off-campus trips, participation in college-wide events, and outreach opportunities. There are about 30 programmed events per year.

In March 2014, the department and the Lafayette AIChE Student Chapter hosted the inaugural Chemical Engineering Spring Symposium, "Engineering re-Connections: Framing Future Networks" featuring a celebration of the commissioning of the new twin-column distillation plant—bring-ing together more than 150 students, faculty, and alumni with representatives from 11 different companies including ExxonMobil, Pinnacle Foods, Air Products and Chemicals, AstraZeneca, BASF, Dow, and O'Brien & Gere.

STUDENTS AND ALUMNI

In 1919, there were six graduates of the Chemical Engineering Program. After the separate department was established in 1938, enrollments grew—and in 1959, it was reported that the freshman enrollment numbered 43 students, with "many of the abler men entering the College among this group." (Annual Report of the Department of Chemical Engineering, 1959-1960).

Lafayette chemical engineers have always been engaged in campus life and extra-curricular activities. In academic year 1967-1968, Lafayette was the host for the AIChE Student Conclave. Two papers were read by Lafayette seniors, and William Flis received honorable mention for his presentation. The annual report of the department recorded: "In what is becoming almost typical for Lafayette's scholar-athletes, [Flis] accomplished this by entering the MAC Track Meet preliminary time trials at the University of Delaware on Friday afternoon, presenting his paper to the conclave in Easton on Saturday morning, and returning to Delaware for the balance of the track meet later this Saturday."

The trend of scholar-athletes has continued across the years. David Klaus, a chemical engineer, was the captain of the Lafayette basketball team that won the Patriot League tournament in 1999 and went on to play in the NCAA Tournament. The Lafayette record for receiving yardage in football, set by John Weyrauch in 2003, stood for nearly a decade. Athletics, however, is only one of many extra-curricular activities undertaken by ChBEs.

Due to the strong mentorship from ChBE faculty, many Lafayette students have placed in the AIChE Mid-Atlantic Student Research Paper competition, including Daniel Connolly and Tyler Fruneaux who went on to the national competition in 2002 and 2014, respectively.

The bond between faculty and students has also been a constant. During the civil unrest in the late 1960s, Department Head Zbigniew D. Jastrzebski recorded, "although the academic year has witnessed considerable unrest and some demonstrations on the Lafayette campus, our chemical engineering students ... are in close personal contact with their professors so that the spirit of comradeship between faculty and students is welldeveloped." The same is true today; chemical engineering faculty plan, prepare, and host a midnight breakfast for students in the department once each semester.

Between 1919 and 1938, there were 120 graduates of the chemical engineering program. The total number of undergraduate students has ranged from as few as six in 1919 to 144 in 2014. On average 66 percent of ChBE students study abroad, while staying on track for graduation in four years. Lafayette engineering faculty lead semester-long programs tailored to engineering majors in Bremen, Germany, and Madrid, Spain.

Lafayette chemical engineers meet with success beyond our campus. There is a 90 percent placement rate for all graduates within 12 months of graduation including a high rate of placement among premier employers such as ExxonMobile, Air Products and Chemicals, DuPont, BASF, and many others. Students continuing for advanced study enroll in top graduate programs, often supported by prestigious fellowships and awards. National Science Foundation Graduate Research Fellowship winners from Lafayette ChBE include Lauren Sefcik (2004), Gabriella Engelhart (2005), Scott Crown (2010), Ashley Cramer (2010), Melissa Gordon (2011), and Ashley Kaminski (2013).

FACULTY AND STAFF

Having grown from only one professor of chemical engineering in 1916, to five tenure track faculty in 1980, Chemical and Biomolecular Engineering (ChBE) at Lafayette now has nine tenure-track lines in the department. These include:

- James K. Ferri, (department head and James T. Marcus 1950 Professor), Ph.D. chemical engineering, The Johns Hopkins University; interfacial phenomena, stability of disperse systems, additive manufacturing
- Lauren S. Anderson, associate professor, Ph.D. biomedical engineering, University of Virginia; tissue engineering, biomaterials, cell-substrate interaction
- Christopher R. Anderson, assistant professor, Ph.D. biomedical engineering, University of Virginia; molecular imaging, protein expression, and controlled drug delivery
- Polly R. Piergiovanni, professor, Ph.D. chemical engineering, University of Houston; biochemical engineering, pedagogical innovation
- James P. Schaffer, professor, Ph.D. mechanical engineering, Duke University; composite materials, non-destructive evaluation, engineering pedagogy
- Michael J. Senra, assistant professor, Ph.D. chemical engineering, University of Michigan; cold flow properties of petroleum, biofuel crystallization
- Lindsay Soh, assistant professor, Ph.D. chemical and environment engineering, Yale University; sustainable energy, biofuel production.

In addition, the department is presently searching to fill two tenure-track faculty positions with a focus in advanced materials and manufacturing, energy and the environment, or micro nanofabrication.

CONCLUDING REMARKS

As we draw near to the completion of nearly a century of chemical engineering at Lafayette, the department continues to build on its strong tradition and reputation of excellence. We welcome you to contact us to find out more about the exciting developments at Lafayette College in ChBE.

ACKNOWLEDGMENTS

I wish to thank Dr. J.R. Martin for directing me to the unpublished manuscript of Dr. E. L. McMillen regarding the history of chemical engineering at Lafayette, Dr. James P. Schaffer, director of Institutional Research for providing statistical information, and College Archivist Diane Shaw, who helped verify the dates and facts associated with the milestones and people who shaped the department. \Box

Random Thoughts . . .

TO FLIP OR NOT TO FLIP

RICHARD M. FELDER AND REBECCA BRENT

In traditional teaching, students first encounter new course material in class and then apply it to problem solving in out-of-class assignments. In a *flipped classroom*, the opposite approach is taken—new material outside class, followed by application in class.

Flipping has some attractive features and moderate research support, but as with every other teaching method, there are good and bad ways to do it. Here are two common bad ones:

How NOT to flip a classroom

- Before students come to class, assign them to read some of the course text or watch slides or a video of a complete lecture.
- (2) Assign new material before class, and then present more new material in a lecture.

What's wrong with those approaches? If you ever assigned students a technical reading and expected them to apply the content next morning, you've known disappointment. Having students sit through a straight online lecture is no better—they have little chance of understanding the content without being able to ask questions about it or get feedback on their initial attempts to apply it. And assigning readings or online lectures before class and then giving more lectures in class is not flipping anything—it's just doubling the rate of fire-hosing the students with information.

So if those methods of flipping don't work, what does? Effective classroom flipping has two components: *interactive* online presentation of information before class, and active learning in class.^[1,2] The online materials might include short videos, lecture clips, and screencasts; hands-on experiences with virtual labs, control rooms, and plants; and quizzes on presented material. Each presentation segment should be roughly six minutes: when it goes much above that, students' attention starts drifting.^[3]

Here are several suggestions to consider before flipping your class.

• Don't try flipping until you're comfortable with active learning and know how to deal with student resistance to it.

Flipping gives students the responsibility for their own learning that active learning always imposes, and it also forces them to learn on their own before they come to class. Many students are not thrilled about either feature of this teaching method, and some aren't shy about letting their instructors know about it. If you're not prepared for pushback, your first flipped classroom experience could be grim for both you and the students. If you can, teach for several semesters using active learning in an otherwise traditional course, and if student resistance starts becoming uncomfortable, take steps to defuse it.^[2,4] When you are confident that you can handle



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the resistance, if you still want to flip (not every teacher has to), go for it.

• Have good online lessons with integrated assessments in place for every class session you plan to flip.

If slide shows and complete taped lectures are the only online resources you have, hold off on flipping until you can assemble interactive materials of the kinds we mentioned above. Screencasts and simulations suitable for most core courses in chemical engineering can be found at *<www*. *learncheme.com>* and by entering *"Tutorial (topic)"* or *"Simulation (topic)"* into a search engine, and Koretsky^[5] and Velegol *et al.*^[6] offer excellent examples of online materials and assignments.

A powerful component of online instruction is quizzes during and following online lessons, with immediate affirmative or corrective feedback on the students' responses.^[7,8] The quizzes should not just be simple tests of factual information but should include assessments of deep understanding of the online material, such as the conceptual questions found in the AIChE Concept Warehouse (*<http://jimi.cbee.oregonstate. edu/concept_warehouse/>*).

Make class sessions mainly activities that build on previous online lessons.

Structure the sessions using active learning techniques, especially *thinking-aloud pair problem solving* for working through complex problems.^[2,9] Be flexible during the sessions, paying careful attention to what the students are doing, and be prepared to intervene with a mini-lecture when common stumbling blocks and misunderstandings arise.

When you decide to flip, get help if you can, and start gradually.

If you have colleagues who have successfully flipped their classrooms or a campus center for teaching and learning that provides consulting assistance, call on them for guidance. Instead of trying to flip an entire course, identify a small portion of the course that you feel enthusiastic about teaching and for which good online materials are available, and try flipping only that portion. Learn from that experience and continue expanding your use of the method in subsequent course offerings.

• Consider flipped flipping.

In a flipped class, the basic material is presented in online modules and some or all of the application is done in a subsequent class. Another approach is to introduce new material via active/interactive exploration in class, *then* send the students out to view the screencasts and work through the tutorials online. Researchers at Stanford University refer to this approach as the "flipped flipped classroom," and have found it superior to flipping in many respects.^[10]

Jensen *et al.*^[11] carried out a well-designed study in which students' performance and attitudes in a flipped classroom and a flipped flipped classroom were compared. No significant between-section differences were found in the students' learning gains or in their attitudes about their instruction. The authors concluded that the key to the effectiveness of both approaches is the extensive use of active student engagement (which has been repeatedly shown to be superior to straight lecturing^[12]) in both the online and in-class instruction.

In short, flip your class if you want to, observing the precautions we suggested—and if you don't want to flip, don't flip. As long as you keep students actively engaged in both flipped classrooms (new material out of class, problem solving in class) and nonflipped classrooms (vice versa), you should see the learning you're looking for.

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