

# INTERACTIVE MATHEMATICA SIMULATIONS in Chemical Engineering Courses

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An effective approach to demonstrate the behavior of a chemical engineering system is to use interactive simulations that allow the user to manipulate variables and observe the effects on the system behavior. They can be designed to focus on a specific—or model a complex—unit process. Interactive simulations have been used extensively in physics education,<sup>[1-2]</sup> and more than 125 PhET simulations are available online (<http://phet.colorado.edu/>). PhET simulations cover topics in physics, chemistry, biology, earth science, and math. They contain physical representations of the system under study (e.g., individual molecules moving around in a container) and many use graphical representations to describe particular relationships. Student interaction with computer simulations is known to have positive effects on learning<sup>[3-5]</sup> and promote student inquiry and exploration.<sup>[6-7]</sup> Podolefsky, *et. al.* showed that simulations are effective at engaging students in “acting like a scientist” and promoting self-directed inquiry.<sup>[7]</sup> Virtual labs created for chemical engineering also promote this type of learning without the large expense of physical laboratories.<sup>[8-11]</sup>

Many chemical engineering textbooks include simulation codes that solve example problems, and some have these codes available online. Mathematica<sup>®</sup>-based interactive simulations have some advantages over these textbook simulations: 1) the values of variables can be changed quickly over a wide range using user-friendly controls (sliders, checkboxes, buttons, tabs, zoom, location drag) instead of command line prompts; 2) a repository of free simulations is available online with explanations so that a specific textbook is not required; and 3) these simulations can be run without a software license—they can be run online using a browser plugin or the executable version can be downloaded to use offline.

Mathematica is a registered trademark of Wolfram Research, which holds the copyright to the Wolfram Mathematica software system. Mathematica simulations can be submitted to the Wolfram Demonstrations Project (<http://demonstrations.wolfram.com/>) for publication. The site currently has more than 400 chemical engineering simulations. Mathematica interactive simulations are not as sophisticated

as PhET simulations, written in Java and Flash, or process simulations prepared with Aspen, SuperPro, or ChemCad. However, they can be prepared with much less effort because of the built-in functions in Mathematica and the relative ease of programming in Mathematica.<sup>[12,13]</sup>

In this paper, we present examples of simulations available for chemical engineering courses and discuss how they can be used. Initial feedback from students in courses where simulations were used is reported. Information on preparing Mathematica-based simulations is also presented, but faculty and students do not need to know how to prepare simulations in order to use the simulations already available.

## WHAT ARE INTERACTIVE SIMULATIONS?

Many of the Mathematica simulations for chemical engineering are solutions to differential equations (ordinary and partial) or algebraic equations. The output is plotted graphically and/or presented through visual animation, and many simulations allow switching between outputs. One

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key advantage of these simulations, over those generated in MathCAD® or MatLAB® for instance, is that the calculations are done in real time while input parameters are manipulated using user-friendly controls, and the graphical output appears almost instantaneously. In the example simulation in Figure 1, the sliders shown at the top of the figure can be moved on the screen to change the indicated variables. In addition to sliders, simulations can use the following methods for interaction:

*Buttons* – choose options or variables to plot.

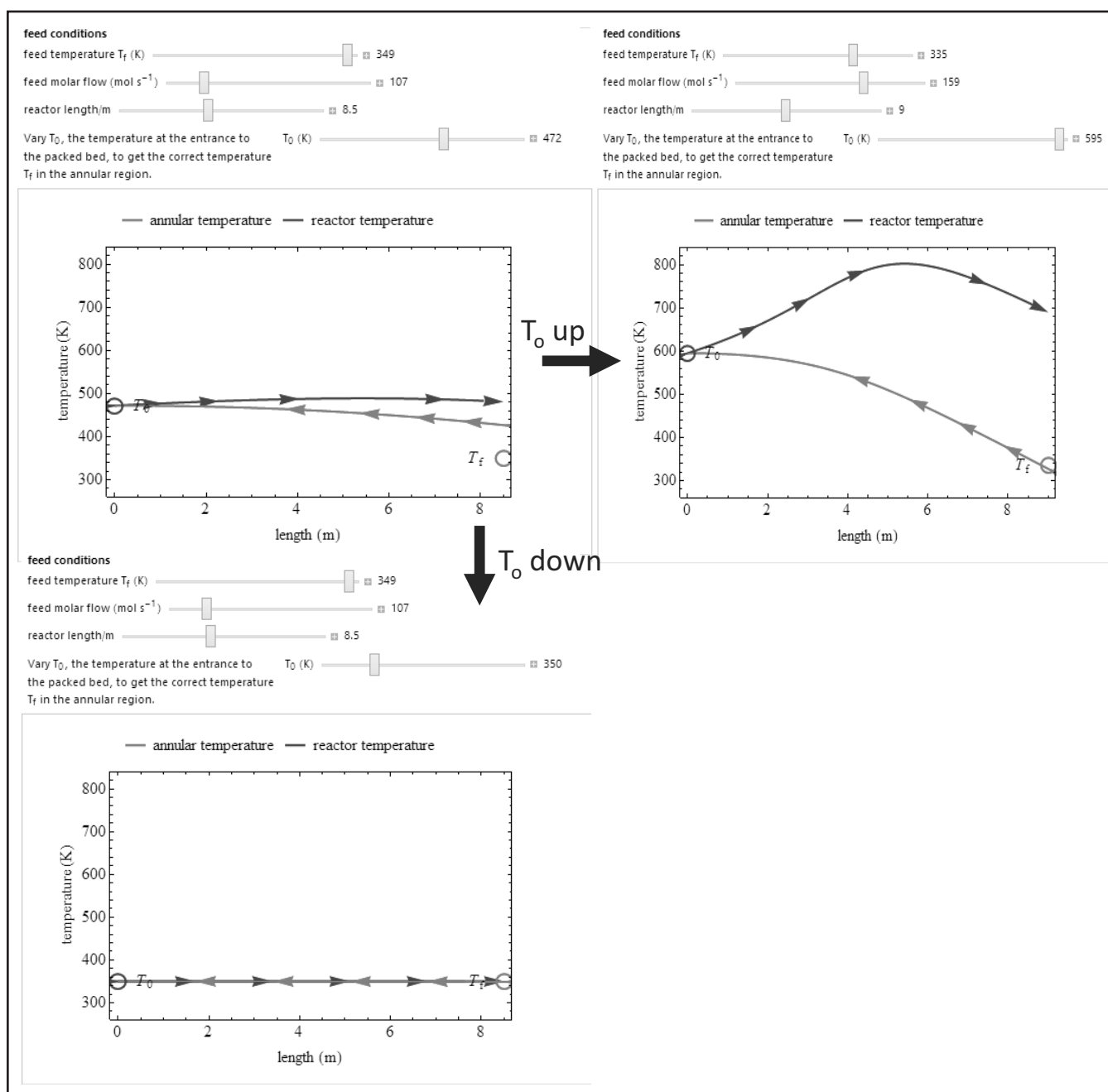
*Location drag* – point to location within plot or figure.

*Check boxes* – select specific parameters or analysis methods.

*Tabs* – select output for analysis; switch between picture and plots.

*Figure zoom/pan* – rotate, zoom, pan across figures (2D and 3D).

*Animate* – automatically move the sliders to visualize effects.



**Figure 1.** Mathematica simulation demonstrating the use of sliders and instant visual feedback. Source: Rachael L. Baumann and John L. Falconer. "Autothermal Reactor" Wolfram Demonstrations Project. Published: July 10, 2013. (<<http://demonstrations.wolfram.com/AutothermalReactor/>>)

## HOW CAN THEY BE USED IN COURSES?

One way to use these simulations in class is to ask students to predict the behavior of a system. For example, this can be done as part of a ConcepTest that students answer with clickers. For the simulation in Figure 1, a packed bed catalytic reactor is used for an exothermic reactor; heat transfer from the reactor preheats the feed gas that enters in an annular region. The solutions of these initial-value ODEs are obtained by adjusting the temperature at the entrance to the packed bed in order to obtain the correct feed temperature. Using a slider to adjust the temperature makes this trial and error solution easy. The bottom slider in Figure 1 can be adjusted until the calculated feed temperature is the same as the temperature represented by the circle. Students are shown Figure 1a and asked to predict whether the gas temperature entering the packed bed should be increased or decreased (or both) to obtain the correct feed temperature to the annular region; this feed temperature is represented

by the circle on the right side of the plot. Students answer using clickers and then discuss the question with their peers. Figures 1b and 1c show that both increasing and decreasing the temperature at the entrance to the packed bed yield solutions. The presence of multiple steady states can be easier to visualize and explain with this interactive simulation than by using stagnant images and equations. This visual feedback can help teach concepts.

Another ConcepTest example is shown in Figure 2. In this question, a plug flow reactor with heat transfer through the walls is used for an exothermic gas-phase reaction. The original temperature versus distance down the reactor is plotted in the top right of Figure 2. The ConcepTest asks which plot represents the new temperature versus distance when the total molar flow rate into the reactor doubles, but other parameters do not change. The four answers were generated with a Mathematica simulation. After the students select their answers and then discuss the question with their classmates,

the interactive simulation can be used in class to demonstrate the behavior. Doubling the inlet flow rate results in the same temperature behavior, but over twice the distance (answer B). That is, if the two curves were plotted versus residence time they would be identical. The simulation presents the system behavior visually and can be used to show behavior when other variables are changed.

Typically, in-class examples are designed to solve for a particular set of conditions, whereas the interactive simulations can demonstrate parametric sensitivity. A simulation can be prepared with multiple parameters treated as variables that can be adjusted using interactive sliders. A problem with specific conditions can be solved using the simulation, and then students could vary the sliders to see how sensitive that solution is to the parameters used. The simulation in Figure 3 (next page) shows a series reaction in a PFR. Students can use the simulation to determine how sensitive the output is to the

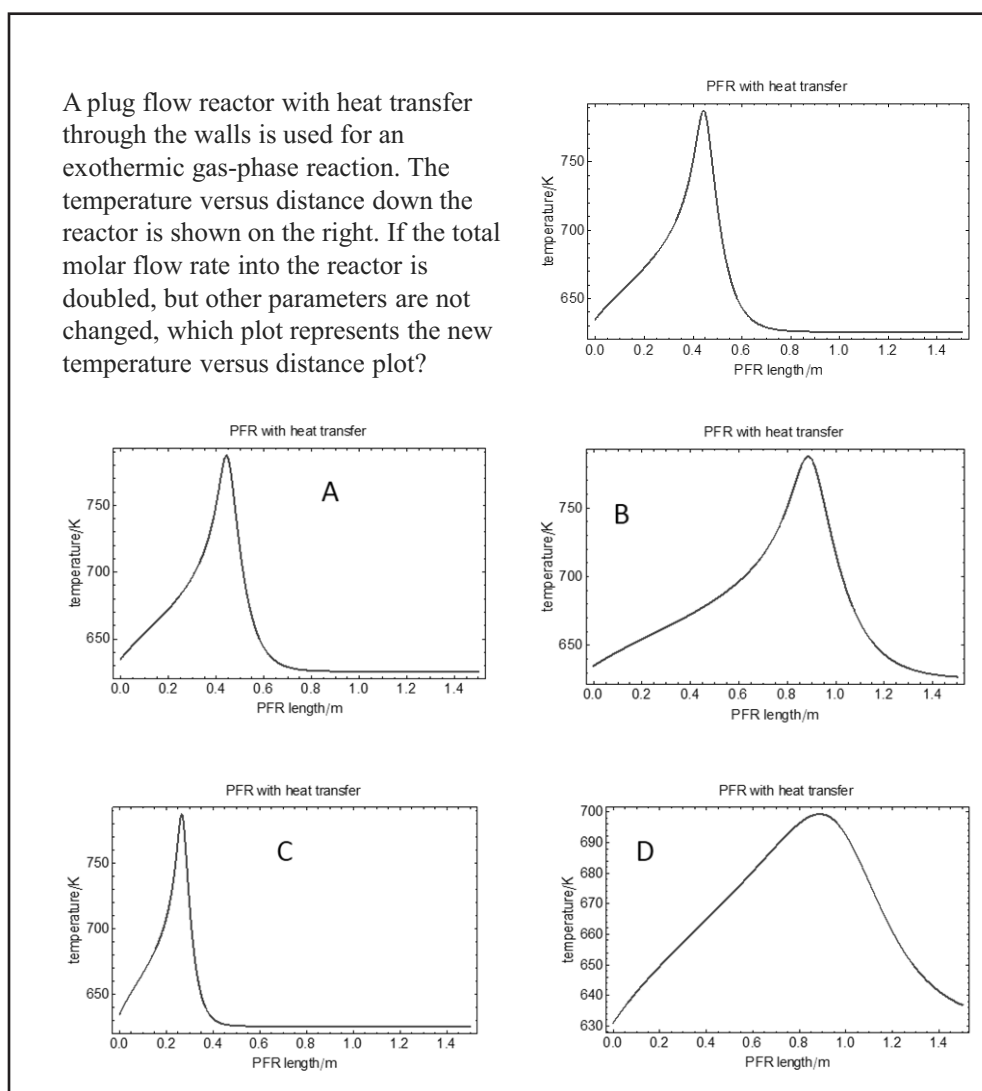


Figure 2. ConcepTest used in class based on a Mathematica simulation.

value of the activation energy used, for example. A simulation can also be used like an experiment in which students try to elucidate relationships between variables to understand governing equations. Interactive simulations can also be used as part of pre-class or post-class assignments. Students can be given questions to answer in a pre-class quiz as preparation to problem solving in class. This initial exposure to the simulation allows students to formulate their own ideas about the material and test them.

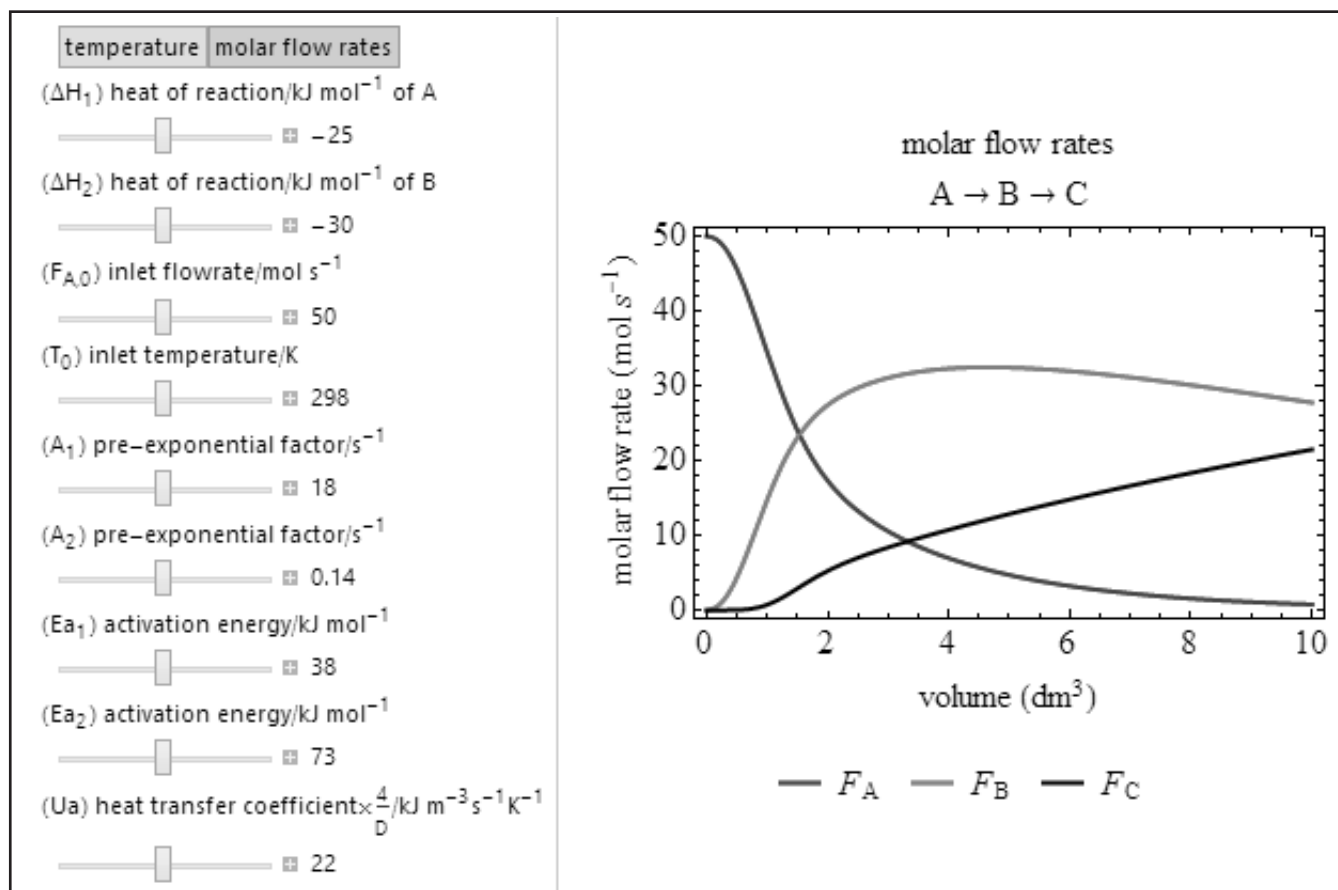
Simulations can also be assigned as homework. Students can be asked to use the simulations and then describe physically why the system exhibits the observed behavior. In courses where students know Mathematica, assignments can ask students to prepare interactive simulations. For instructors, a generic simulation with multiple sliders can be used to design multiple homework or exam problems by changing slider settings and obtaining a new solution. For example, a generic PFR simulation with multiple sliders can be used to change the reactor from isothermal to adiabatic, add or remove pressure drop, change the reaction stoichiometry, change the number of reactions, and change other

variables. The example in Figure 3 has nine sliders but more could be readily added.

### WHAT IS AVAILABLE?

More than 440 interactive simulations, prepared by authors at a number of institutions, are currently available for chemical engineering topics (<http://demonstrations.wolfram.com/search.html?query=chemical%20engineering>). Many of these simulations are specific examples that may be best suited for advanced topics. A significant number focus on core concepts, and the open source nature of the simulations allows for easy manipulations to the code to modify them. We have published 42 simulations, and our first 16 simulations were viewed more than 10,000 times in the first seven months that they were available. We also prepared YouTube screencasts that describe how to prepare interactive simulations and how to use some simulations that we prepared. They are linked on [www.LearnCheme.com](http://www.LearnCheme.com) under the simulations tab.

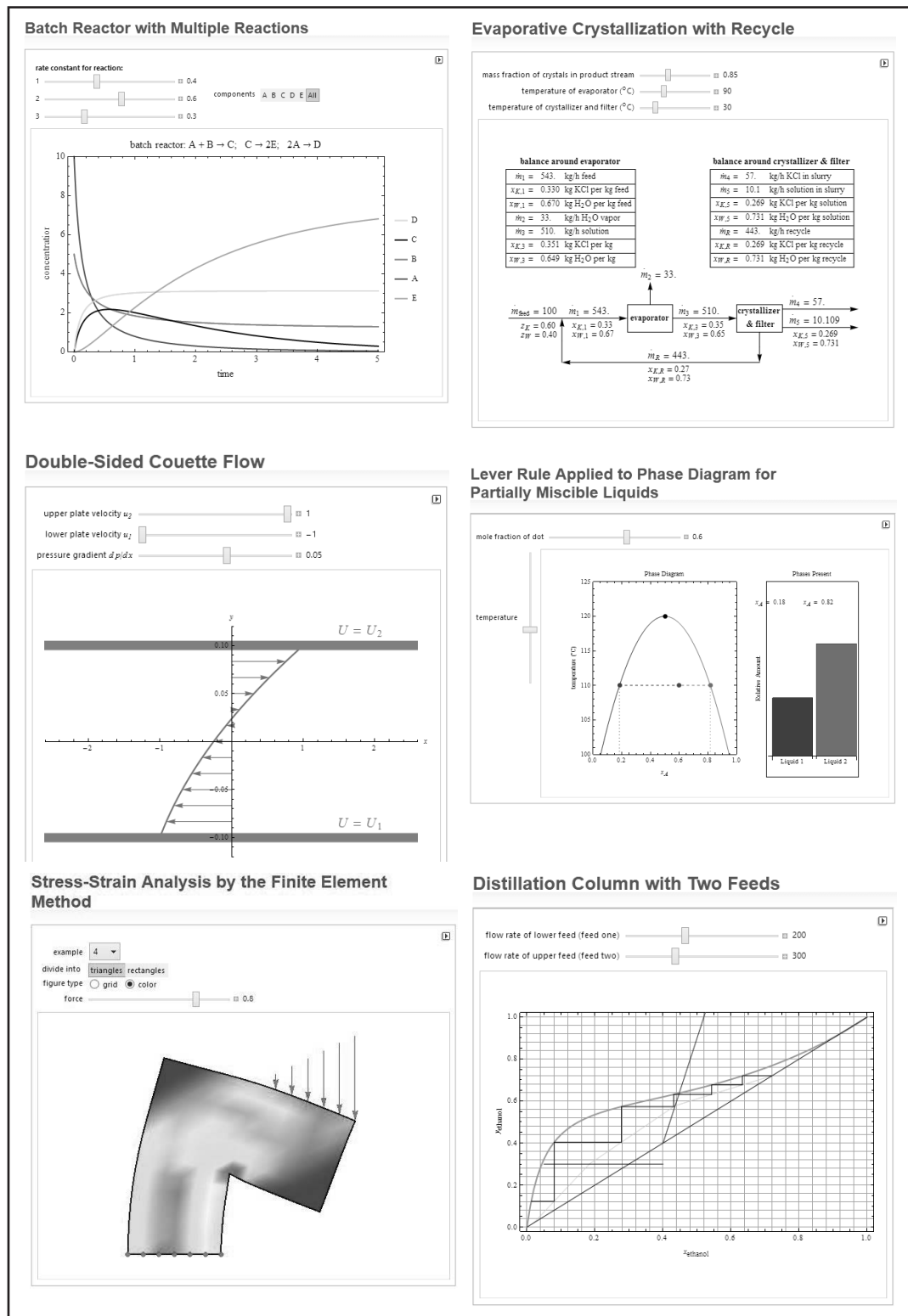
The Wolfram site currently has more than 9,400 interactive simulations that cover a range of fields including engineering,



**Figure 3.** Simulation demonstrating relationships between variables and system behavior. All relevant model parameters can be adjusted using sliders to observe system sensitivity. Source: Rachael L. Baumann and John L. Falconer. "Parametric Sensitivity of Plug Flow Reactor with Heat Exchange." Wolfram Demonstrations Project Published: June 17, 2013. (<http://demonstrations.wolfram.com/SensitivityOfAPlugFlowReactorToModelParameters/>)

science, mathematics, and computation. They are searchable and subdivided by general topics such as mechanical, civil, and chemical engineering. Unfortunately, the chemical engineering simulations are not further subdivided, but are listed by the date they were added to the site. We have created

links to the simulations on <[www.LearnChemE.com](http://www.LearnChemE.com)> where we have subdivided the chemical engineering simulations by courses to make them easier to use. Examples of different types of chemical engineering simulations are shown in Figure 4.



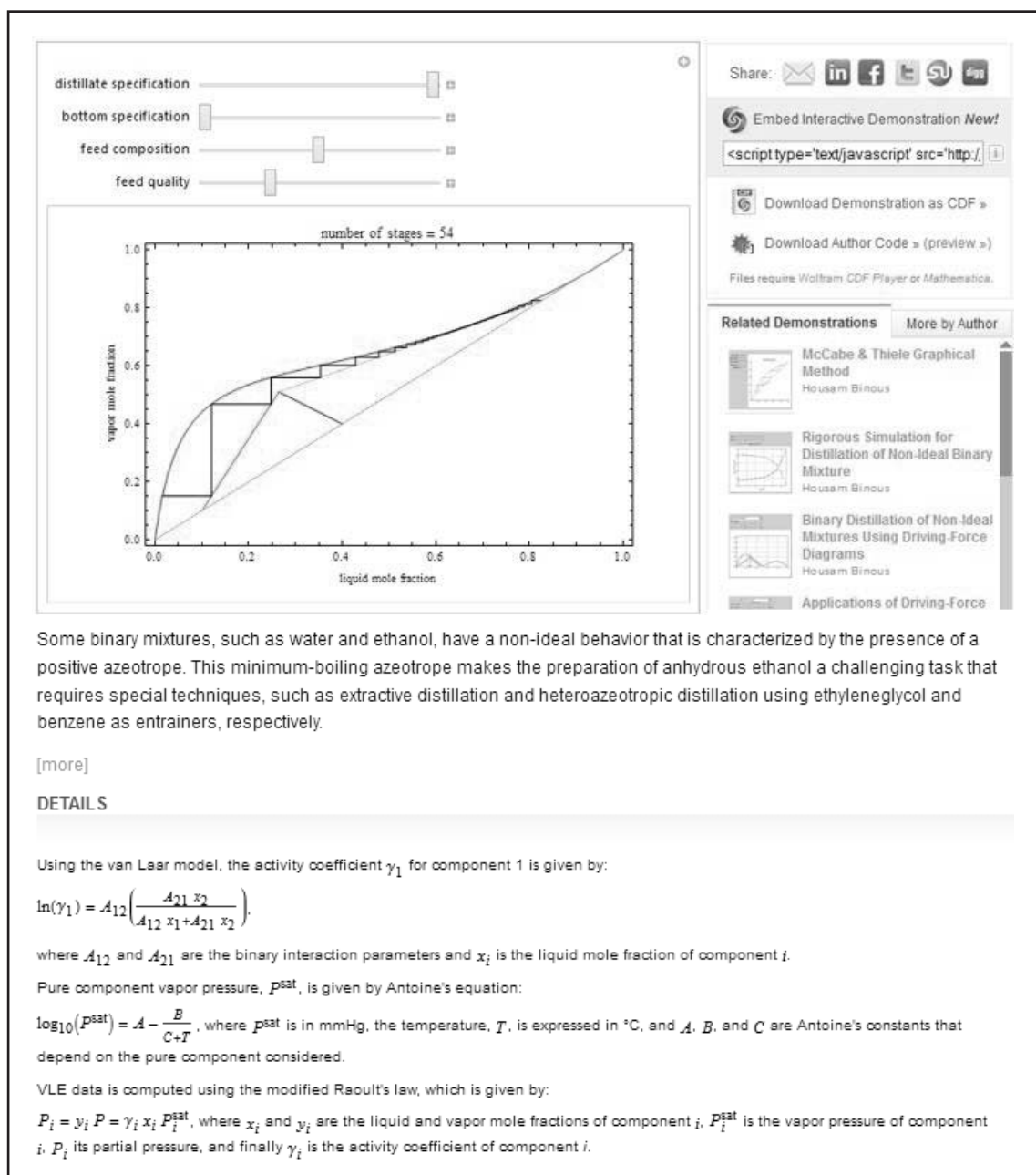
**Figure 4.** Examples of useful screen-casts related to core chemical engineering topics. Source: Wolfram Demonstrations Project, Accessed: October 24, 2013. Simulations listed from top left to bottom right: “Batch Reactor with Multiple Reactions,” John L. Falconer and Rachael L. Baumann. “Evaporative Crystallization with Recycle,” Rachael L. Baumann, Janet deGrazia, and John L. Falconer. “Double-Sided Couette Flow,” David Gerhardinger and William C. Guttner. “Lever Rule Applied to Phase Diagram for Partially Miscible Liquids,” Lisa M. Goss. “Stress-Strain Analysis by the Finite Element Method,” Yuncong Ma. “Distillation Column with Two Feeds,” Housam Binous.



According to the Wolfram site, each demonstration is reviewed by experts for “content, clarity, presentation, quality, and reliability” before it is published on the site. The simulation is then posted in a format that can be used without owning a copy of Mathematica. Instead, a CDF (Computable Document Format) player can be downloaded free from the Wolfram site (<http://www.wolfram.com/cdf-player/>). One important attribute of these simulations is that the code is provided so that others can use it to create their own simulations. Use of the simulations and code follows the Creative Commons Attribution-NonCommercial-ShareAlike 3.0 Unported License and MIT License (<http://www.wolfram.com/legal/terms/wolfram-demonstrations-project.html>).

Each demonstration provides a description of the physical system and most also present the equations used in the simulation. The Mathematica code is presented as a downloadable file. An example of how an interactive simulation for separations appears on the Wolfram site is shown in Figure 5. This simulation shows a McCabe-Thiele diagram for distillation of a binary non-ideal mixture. Typically this topic might be taught using an example with a specific set of conditions to determine the number of stages for the separation. This type problem is ideal for a simulation because variables such as distillate composition, bottoms composition, feed composition, and feed quality can be easily changed and their direct influence on the separation observed. The simulation also

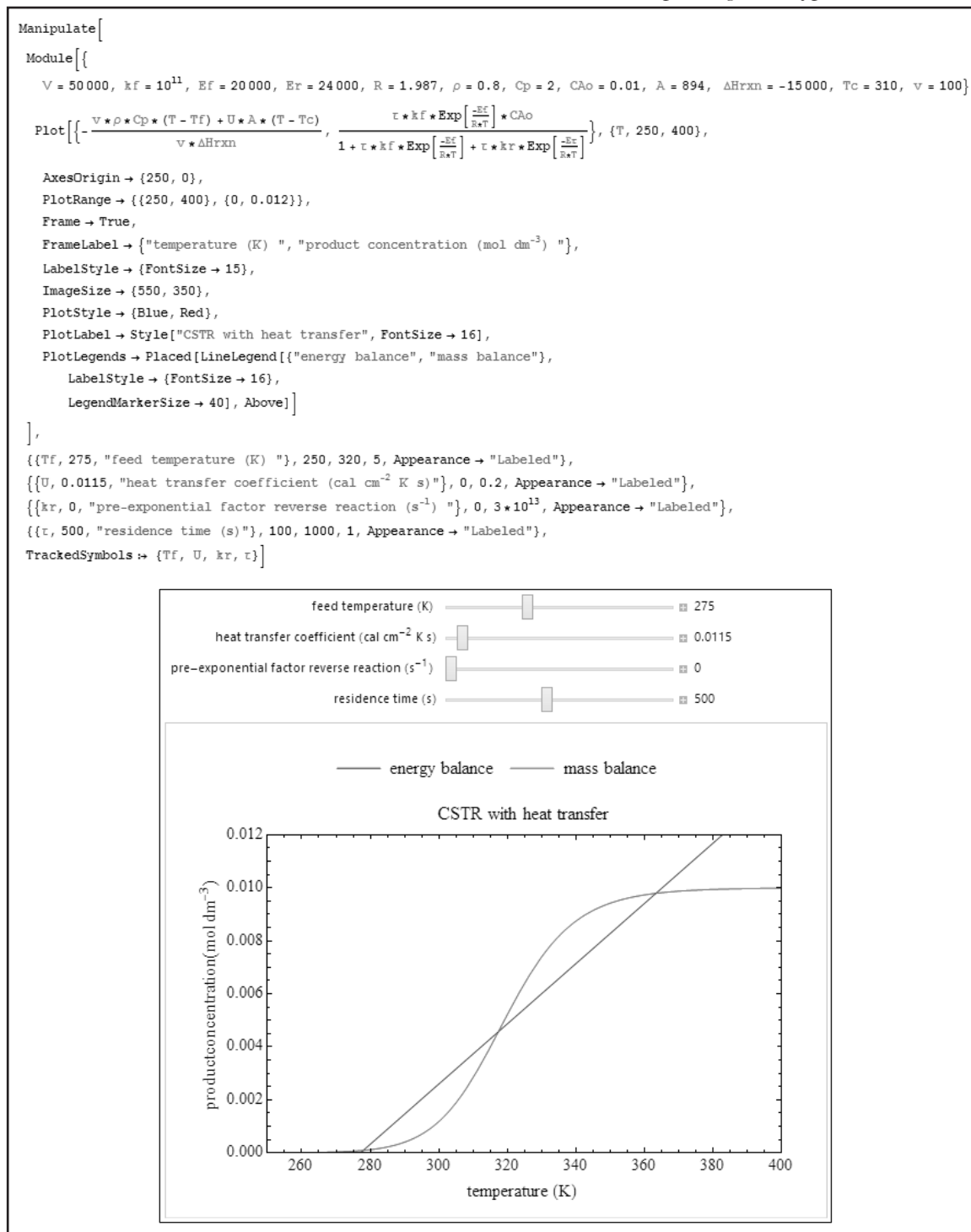
**Figure 5.** Simulation that uses distillation to separate a binary non-ideal mixture. Source: Housam Binous. “McCabe-Thiele Graphical Method for a Non-Ideal Binary Mixture,” from the Wolfram Demonstrations Project. Accessed: Oct. 24, 2013. (<http://demonstrations.wolfram.com/McCabeThieleGraphicalMethodForANonIdealBinaryMixture/>)



shows how the number of stages changes both graphically and numerically as the sliders are moved to change system parameters. A description and details of the mathematical analysis are presented below the simulation. To the right of the simulation are links to download and use the simulation offline (CDF format), to download the author's code, and to embed the simulation on another website. Related simulations are also listed.

## PREPARING MATHEMATICA SIMULATIONS

Mathematica simulations can be made interactive by adding the Manipulate function command. For example, the Mathematica code to generate plots of mass and energy balances (product concentration versus temperature) for a steady-state CSTR with heat transfer is shown with the program output in Figure 6. Most of the code consists of formatting options for the plot (e.g., font type and size, axis labels, figure labels,



**Figure 6.** Simulation code and output for a simulation involving material and energy balances for a CSTR with heat transfer. Source: John L. Falconer and Rachael L. Baumann. "Multiple Steady States in a Continuously Stirred Tank Reactor," *Wolfram Demonstrations Project* Published: June 7, 2013. (<<http://demonstrations.wolfram.com/MultipleSteadyStatesInAContinuouslyStirredTankReactor/>>)

annotations, and legends), and only a few lines of code are needed to create the sliders and their range of variables. Although some effort is involved in learning a computer language, sophomore students with little Mathematica background were able to prepare good interactive simulations in a fluids course. Simulations that are numerical solutions to sets of differential equations are also relatively easy to prepare, as shown by the Mathematica program (Figure 7a) for an isothermal batch reactor with multiple reactions and the corresponding interactive simulation in Figure 7b. Note that the ODEs were solved with the NDSolve function and most of the rest of the code is formatting for the plot and the constants needs in the ODEs.

## STUDENT FEEDBACK

Simulations were used in a 5-week intensive summer session of fluid mechanics. They were used in pre-class quizzes to introduce concepts to students with questions like, “What happens when...” and “Where is the point in which...”. Simulations were also used in class to demonstrate a system and support an example problem performed in class, as well as used in conjunction with a ConcepTest to ask students to predict system behavior when conditions were changed. During a lesson on pipe flow and viscous losses, the simulation Fractional Pressure Drop in a Pipe (Figure 8, page

174) was used to show students how flow variables affect the friction factor. Students were asked to predict the system behavior before being shown the simulation. An advantage of using this in class is to help students see relationships before doing calculations. Students also earned extra credit by designing fluid mechanics simulations. On an end-of-course survey, 40% of students indicated that they used the simula-

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Manipulate[
Module[{t, z, sol, p1, p2, p3, p4, Ea1, Ea2, R, A1, A2, Cao, k1, k2},
Ea1 = 145; Ea2 = 155; R = 8.314*10-3; A1 = 3.6*1016; A2 = 1.8*1017; Cao = 2.0;
z = If[T ≤ 465, 15, 5]; k1 = A1*Exp[-Ea1/(R*T)]; k2 = A2*Exp[-Ea2/(R*T)];
sol = NDSolve[{Ca'[t] == -k1*Ca[t], Cb'[t] == k1*Ca[t] - k2*Cb[t], Cc'[t] == k2*Cb[t],
Ca[0] == Cao, Cb[0] == 0, Cc[0] == 0}, {Ca, Cb, Cc}, {t, 0, z}];
p1 = Plot[{Ca[t] /. sol}, {t, 0, z}, PlotRange → {0, 2},
PlotLabel → Style["A → B → C Ea2 > Ea1", FontSize → 15],
PlotStyle → Thick, Frame → True, FrameLabel → {"time/h ", "concentration/mol dm-3 "},
LabelStyle → {FontSize → 14, FontFamily → Arial},
PlotLegends → Placed[LineLegend[{"CA"},
LabelStyle → {FontSize → 14, FontFamily → Arial}, LegendMarkerSize → 20], Above],
ImageSize → {450, 380}, ImagePadding → {{50, 5}, {40, 10}}];
p2 = Plot[{Cb[t] /. sol}, {t, 0, z}, PlotRange → {0, 2},
PlotLabel → Style["A → B → C Ea2 > Ea1", FontSize → 15],
PlotStyle → {Thick, Red}, Frame → True,
FrameLabel → {"time/h ", "concentration/mol dm-3 "},
LabelStyle → {FontSize → 14, FontFamily → Arial},
PlotLegends → Placed[LineLegend[{"CB"},
LabelStyle → {FontSize → 14, FontFamily → Arial}, LegendMarkerSize → 20], Above],
ImageSize → {450, 380}, ImagePadding → {{50, 5}, {40, 10}}];
p3 = Plot[{Cc[t] /. sol}, {t, 0, z}, PlotRange → {0, 2},
PlotLabel → Style["A → B → C Ea2 > Ea1", FontSize → 15],
PlotStyle → {Thick, Green}, Frame → True,
FrameLabel → {"time/h ", "concentration/mol dm-3 "},
LabelStyle → {FontSize → 14, FontFamily → Arial},
PlotLegends → Placed[LineLegend[{"CC"},
LabelStyle → {FontSize → 14, FontFamily → Arial}, LegendMarkerSize → 20], Above],
ImageSize → {450, 380}, ImagePadding → {{50, 5}, {40, 10}}];
p4 = Plot[{Cb[t]/Cc[t] /. sol}, {t, 0.5, z}, AxesOrigin → {0.5, 0},
PlotLabel → Style["A → B → C Ea2 > Ea1", FontSize → 15],
PlotRange → All, PlotStyle → {Thick, Black}, Frame → True,
FrameLabel → {"time/h ", "selectivity "},
LabelStyle → {FontSize → 14, FontFamily → Arial},
ImageSize → {450, 380}, ImagePadding → {{50, 5}, {40, 10}}];
Switch[plt, 1, Show[p1], 2, Show[p2], 3, Show[p3], 4, Show[p4], 5, Show[p2, p1, p3]],
{{plt, 5, ""}, {1 → "CA", 2 → "CB", 3 → "CC", 4 → "SB/C", 5 → "all"}, ControlType → SetterBar},
{{T, 460, "temperature/K ", 450, 480, 1, Appearance → "Labeled"}]

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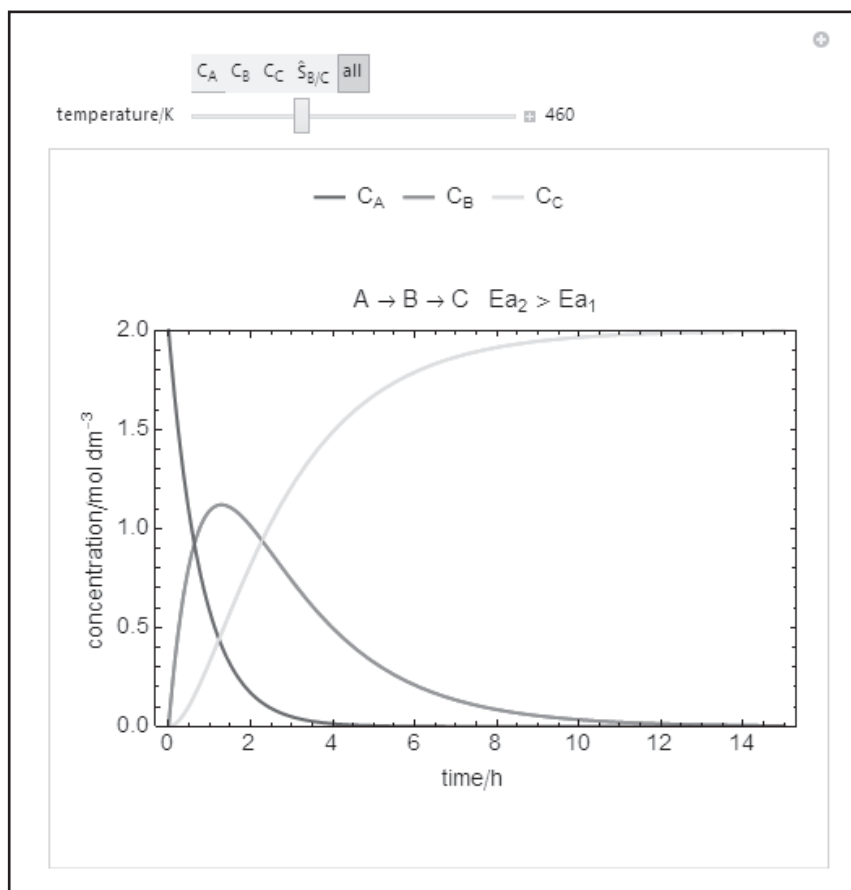
**Figure 7a (above) and 7b (facing page).** Simulation designed to solve an isothermal batch reactor with multiple reactions. The demonstration code (7a) and visual output (7b) are shown. Source: Rachael L. Baumann and John L. Falconer. “Series Reactions in a Batch Reactor,” *Wolfram Demonstrations Project* Published: June 17, 2013. (<<http://demonstrations.wolfram.com/SeriesReactionsInABatchReactor/>>)



tions on their own beyond the demands of the course, and 90% said they would use them again for other courses. When asked about how the simulations affected their confidence in the material, answers ranged from “extremely confident” to “confused me even more” with the average indicator suggesting they improved the students’ confidence in the material (Value 6.2/10 where 5 = no difference). Students also indicated that the simulations enhanced their understanding beyond the use of the textbook (Value 6.8/10, where 5 = no difference).

Some student comments that represent typical feedback about the simulations include:

- “The demos were a great way to visualize a concept and analyze the relationship between an equation or theory and the variables involved.”
- “The Wolfram demos were helpful because I could see how things changed instead of just having one question and one answer like in a quiz, clicker, or screencast.”
- “Would have been nice to incorporate more demos. Found them very useful.”
- “The demo could use better explanations of what is being observed and controlled. It was confusing at first to determine this on our own.”
- “The demos were useless. Most of the time we had no idea what we were looking at.”



Simulations were also used in a 100-student, junior-level separations and mass transfer course. They were used during class to help explain a concept [*e.g.*, McCabe Thiele diagram (Figure 6), Ponchon-Savarit method, Murphree efficiency, membrane separations] and also so that students could predict system behavior. Sometimes the question was posed as a ConcepTest and other times it was used to start discussions. Out of the 45 students who responded to an end-of-the-semester survey, 67% said they would use the simulations again on their own, but the average response found them less than helpful in improving their understanding of a concept. This was primarily due to the lack of details or directions provided with the simulations. Most of the students found the simulations, “confusing” and “not clearly described,” while a few comments regarding their use in class matched one student’s feedback that “there wasn’t enough of them to be consistently useful.” Some students suggested the simulations would be more useful by giving explanations of what students were visualizing along with the simulation.

Thus, a concern expressed by a number of students is that many of the simulations are not explained sufficiently to make them easy to use: the system is not described sufficiently, and often the plots and sliders contain variables that are depicted as symbols and not described clearly. Indeed many simulations on the Wolfram site have brief descriptions, and this was part of our motivation to prepare our own simulations. We have provided more-detailed descriptions of our simulations, and in some cases prepared screencasts that explain the system and how to use the simulation.

We also used simulations in a graduate kinetics course (24 students) in Fall 2013. Eighty-five percent of the students provided positive feedback about the simulations at the end of the semester. Some of their comments were:

- “They (simulations) were really useful because they allowed us to run them again after class and think about the physical process that is occurring and how the different parameters affect the behavior of the system.”
- “Mathematica simulations are cool and informative, and I think they could be better served if you have us look at them outside of class to do the manipulation.”
- “They (simulations) were more useful and clearer than the typical whiteboard sketches of lectures I have encountered.”
- “Mathematica simulations are useful in demonstrating the behavior of reaction systems. It helps my understanding of the clicker questions when I actually play with the simulations.”

In general the feedback from these students was more positive, which we attributed to the use of simulations with better descriptions and explanations.

## CONCLUSIONS

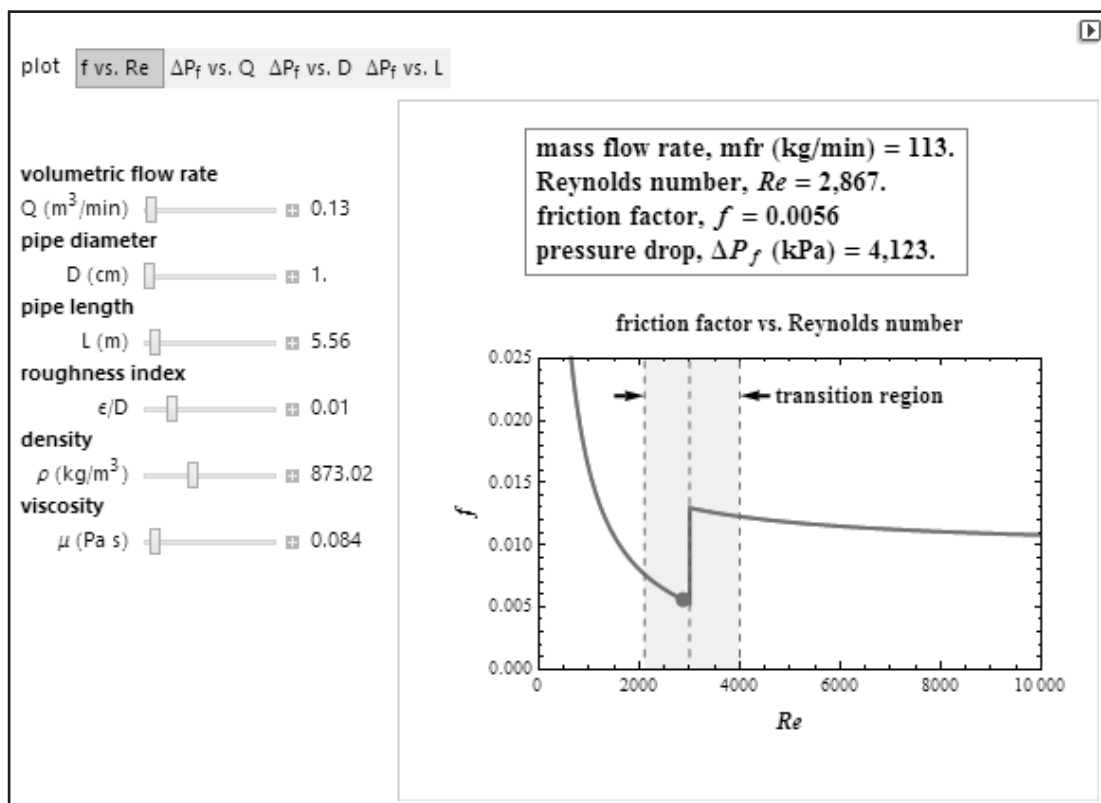
Mathematica simulations on the Wolfram demonstration site can be used in chemical engineering courses to enhance student interaction with course material. They can be used in class or as part of assignments. Modification of Mathematica simulations to make them interactive is relatively simple. The biggest concern raised by students is that many simulations on the Wolfram site do not provide sufficient instructions or explanation for someone just learning the material. We have prepared simulations with more descriptions of the systems to make them easier to use. Simulations that we found relevant to course topics are listed on our website (<http://www.learncheme.com/page/simulations>).

## ACKNOWLEDGMENTS

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**Figure 8.** Simulation used to introduce viscous losses and friction in pipe flow. Source: Mark D. Normand and Micha Peleg. "Frictional Pressure Drop in a Pipe," *Wolfram Demonstrations Project*, Accessed: Oct. 27th, 2013. (<http://demonstrations.wolfram.com/FrictionalPressureDropInAPipe/>)

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