

# COMBINING INTERACTIVE THERMODYNAMICS SIMULATIONS WITH SCREENCASTS AND CONCEPTTESTS

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The interactive simulations method of instruction has been shown to improve learning<sup>[1-4]</sup> by actively engaging students so they create knowledge for themselves. Students can manipulate parameters and receive instant feedback so that abstract concepts become more tangible. Students can experiment and use simulations at their own speed; they can slow down or speed up processes and observe behavior that would be hard to observe in real time or would be too expensive.<sup>[1]</sup> Simulations promote self-directed inquiry and exploration.<sup>[5]</sup>

Interactive simulations have been used extensively in physics education,<sup>[1,6]</sup> and more than 130 PhET simulations (<[www.phet.colorado.edu](http://www.phet.colorado.edu)>) have been developed for science and math. The PhET simulations employ graphics that show molecular motion and realistic representations of physical situations. They also typically have a significant number of options, and each simulation costs about \$60,000 to prepare. The thermodynamics simulations for chemical engineering described here are less sophisticated than the PhET simulations, but take less time and are less expensive to prepare. They retain many of the PhET attributes, however: they encourage inquiry, show visual models, present multiple representations, and provide interactivity. They were prepared using *Mathematica*, which has powerful commands that create interactivity, but the simulations can be used without a *Mathematica* license or a knowledge of *Mathematica*.

We first reported on preparing *Mathematica* simulations in 2014,<sup>[7]</sup> and most of those simulations, which were for kinetics/reactor design, involved solving ordinary differential equations and presenting the results as x-y plots. We have extended these interactive simulations to chemical engineering thermodynamics and created simulations that involve animations and more interactive graphical representations. Simulations can be particularly useful for thermodynamics because many of its concepts confuse students and because graphical representations are used extensively.

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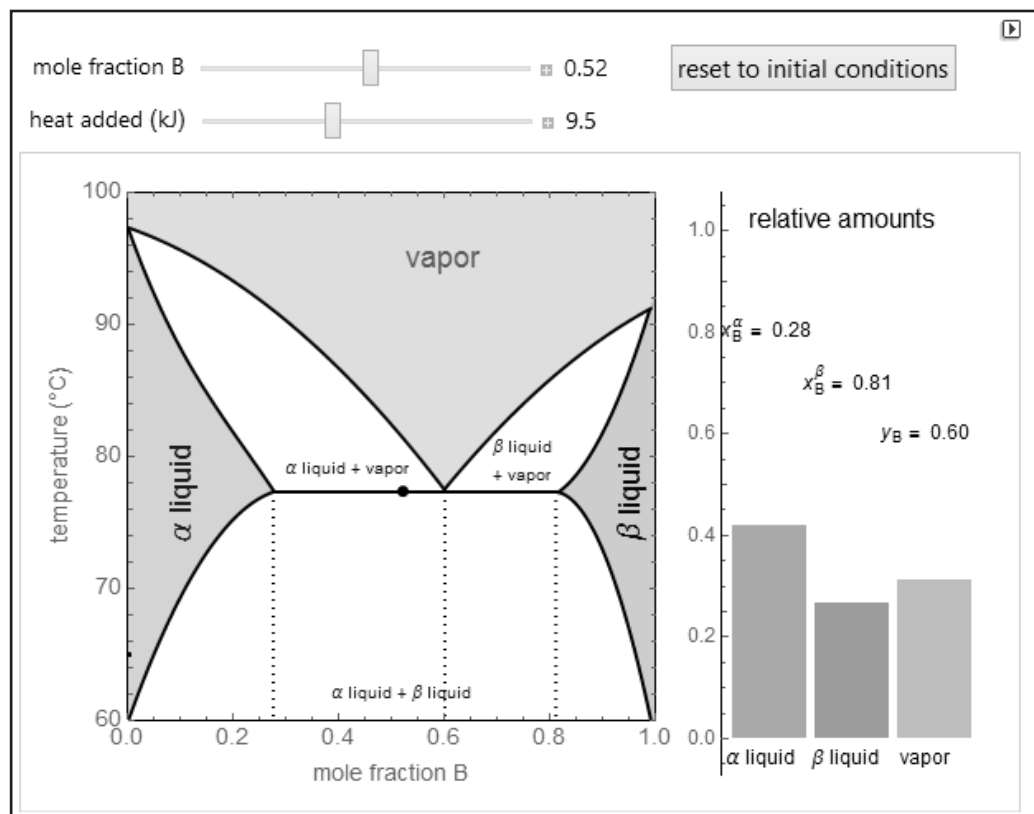


<b>TABLE 1</b> <b>Interactive thermodynamic simulations (&lt;<a href="http://www.learncheme.com/simulations/thermodynamics">http://www.learncheme.com/simulations/thermodynamics</a>&gt;)</b>	
Energy Balances and Entropy:	Temperature Changes in an Ideal Gas
	Reversible and Irreversible Expansion or Compression Work
	Throttling High-Pressure Water
	Evaporative Cooling of Water
	Energy Balance on Pressurizing a Tank
	Entropy Changes in Mixing Ideal Gases
	Heat Water/Air Mixture in a Closed Container
Cycles:	Carnot Cycles with Irreversible Heat Transfer
	Rankine Cycle
	Ordinary Vapor Compression (OVC) Cycle for Refrigerant R-134a
Phase Equilibrium in Pure Fluid/Phase Diagrams/Water-Air Mixtures:	Reading a Psychrometric Chart
	Phase Behavior on a Pressure-Volume Diagram
	Single-Component P-V and T-V Diagrams
	Inject Liquid Into Evacuated Tank
	Circumnavigating the Critical Point
	Heat a Water/Air Mixture
Fugacity and Departure Functions:	Fugacity From Equation of State for Water
	Fugacities in a Can of Soda
	Fugacity as a Driving Force for Mass Transfer
	Fugacities in an Ideal Binary Mixture
	Enthalpy and Entropy Departure Functions
Multi-Component VLE for Ideal Solutions:	P-x-y and T-x-y Diagrams for Vapor-Liquid Equilibrium (VLE)
	Adding a Second Component to a Single-Component Vapor-Liquid Equilibrium (VLE) Mixture
	Adding One Component to a Binary Vapor-Liquid Equilibrium (VLE) Mixture
	Adiabatic Flash Drum with Binary Liquid Feed
	Basic Ternary Phase Diagram
Multi-Component VLE for Non-Ideal Solutions:	Partial Molar Enthalpy
	Three Intermolecular Potential Models
	Mass Balances for Binary Vapor-Liquid Equilibrium (VLE)
	Vapor-Liquid Equilibrium Diagram for Non-ideal Mixture
	Non-Ideal Vapor-Liquid Equilibrium (VLE) Modeled by the Margules Equation
	Add a Component to a Mixture With an Azeotrope
Partially Miscible and Immiscible Solutions:	Vapor-Liquid-Liquid Equilibrium (VLLE)
	Partially Miscible Liquids
	Immiscible Liquids on Pressure-Composition Diagram
	Temperature-Composition Diagram for Immiscible Liquids
	Solid-Solid-Liquid Equilibrium
	Ternary Phase Diagram With Phase Envelope
	Ternary Phase Diagram With Alternate Phase Envelope
	Right and Equilateral Triangle Ternary Phase Diagrams
Reaction Equilibrium:	Chemical Equilibrium in the Haber Process
	Gas-phase Chemical Equilibrium at Constant Pressure or Volume
	Heterogeneous Chemical Equilibrium With Calcium Carbonate
	Reversible Reaction in an Adiabatic Plug-Flow Reactor

The thermodynamics simulations use x-y plots (P-V, P-T, T-V, P-H, T-S, T-x-y, P-x-y), bar graphs (to show amounts of components in different phases or amounts of reactants and products), and simple animations (moving pistons, opening valves, changing liquid levels). Numerical values of parameters are changed with sliders that are manipulated with a mouse, and in some cases parameters are changed by selecting buttons. Different displays (different plots or physical representations) are also selected with buttons, and most animations start when a play button is selected. On some phase diagrams, a point can be moved around the diagram (and values calculated at that point) by clicking and dragging.

Efforts were made to make these simulations readily useable by someone just learning the material. This means minimizing options, labeling curves (instead of using a legend), using words instead of symbols, using bar graphs instead of presenting numerical values, and providing options to display only parts of complicated plots. In addition, short screencasts (3 – 5 minutes) that describe how to use the simulations were prepared in response to student feedback; 10 – 15% of students in the thermodynamics course felt that some simulations were difficult to understand. A separate web page was created on <www.LearnChemE.com> for each simulation, which can be used while simultaneously watching the screencast. Studies have shown that developing an appropriate hypothesis, evaluating results, and using simulations systematically can be difficult.<sup>[8]</sup> Indeed, Rieber et al. showed that students who were given interactive simulations with short explanation videos scored better than students who were just given interactive simulations.<sup>[9]</sup> The simulations are also available on the Wolfram Demonstration Project (<<http://demonstrations.wolfram.com/>>), and the *Mathematica* code for these simulations can be downloaded from that site and modified.

These simulations can be used by students outside of class for self-study and as part of assignments, but they are also



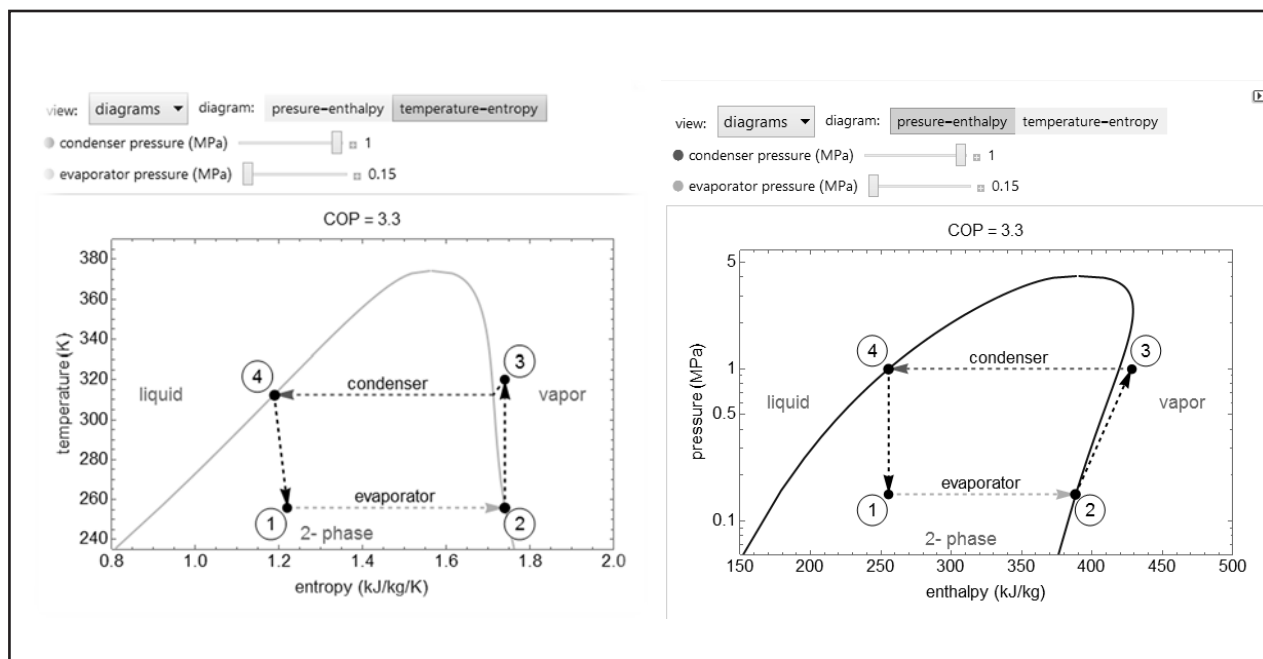
**Figure 1.** Snapshot of the interactive Mathematica simulation Vapor-Liquid-Liquid Equilibrium (VLE). The temperature-composition diagram is on the left, and the bar graph on the right shows the relative amounts of each phase for conditions corresponding to the black dot.

particularly useful in class to demonstrate concepts and diagrams. Thus, for each simulation, at least one in-class ConcepTest was prepared. Bodemer et al. showed that first studying static representations before exploring dynamic visual simulations improved student performance and understanding.<sup>[8]</sup> To use these simulations in class, clickers are used to obtain student responses to ConcepTests, and then students discuss the question with their neighbors (peer instruction). They can then change their answers before the simulation is shown in class and discussed. Peer instruction and clickers have been shown to significantly improve student understanding of concepts.<sup>[10-14]</sup> Students are also given a link to the simulation so they can use it outside of class.

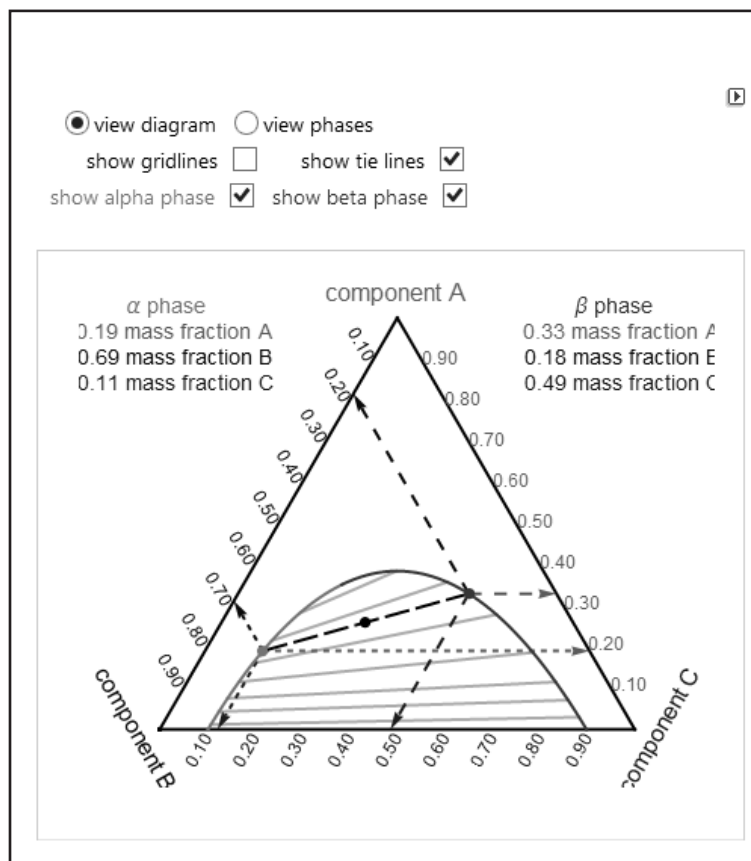
## INTERACTIVE SIMULATIONS EXAMPLES

Table 1 lists the thermodynamic simulations currently available by topic; additional simulations are being prepared. Many of these simulations can also be used in separations or material and energy balances courses. Snapshots of a few simulations are presented here to demonstrate the type of simulations available and the capabilities of *Mathematica*.

The simulation in Figure 1 represents vapor-liquid-liquid equilibrium for a partially miscible, binary system. The black



**Figure 2.** Snapshot of an interactive Mathematica simulation Ordinary Vapor Compression (OVC) Cycle for Refrigerant R-134a.

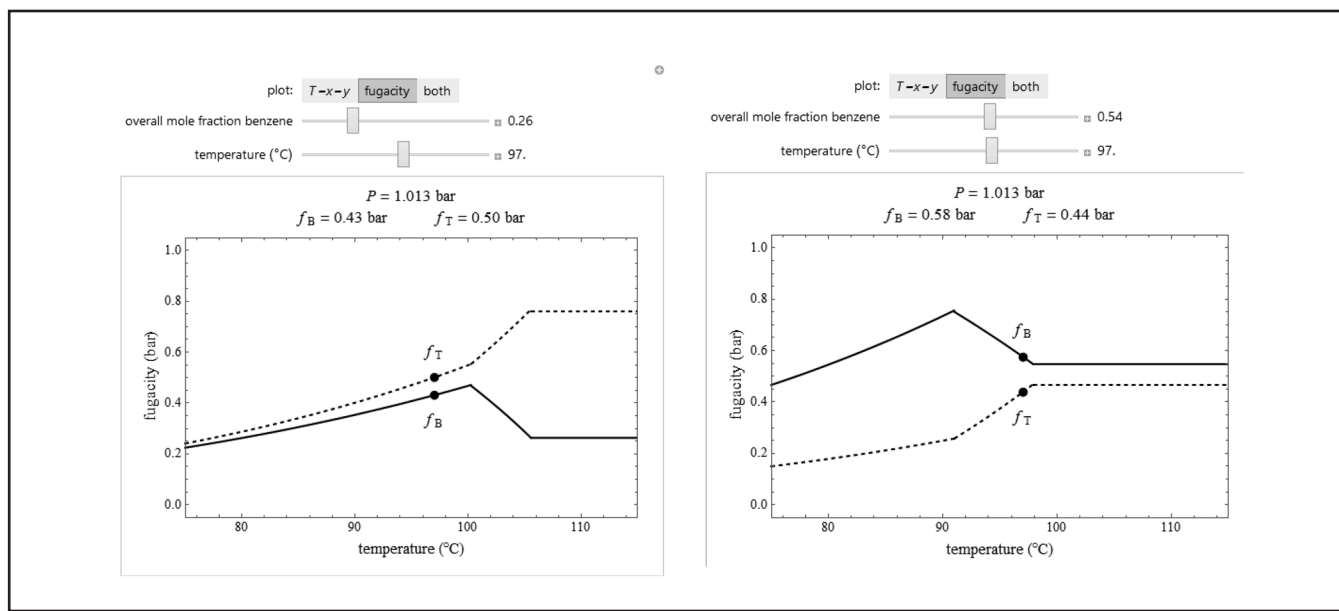


**Figure 3.** Snapshot of an interactive Mathematica simulation Ternary Phase Diagram with Phase Envelope.

dot on the temperature-composition diagram moves as the sliders at the top of the figure for mole fraction and heat-added are changed. The bar graph on the right indicates the relative amounts of each phase ( $\alpha$  liquid,  $\beta$  liquid, vapor) present. Heat added is used as a variable instead of temperature so that the three-phase behavior can be better represented. When heat is added at about  $77^\circ\text{C}$ , both liquids evaporate and vapor forms, but the temperature does not change until one of the liquids completely evaporates.

A snapshot of a simulation for a refrigeration cycle is shown in Figure 2. Either the temperature-entropy or the pressure-enthalpy diagram can be displayed by clicking on one of the rectangles in the top right of the simulation. The diagrams are redrawn when the condenser or evaporator pressure is changed with the sliders, and a new coefficient of performance is calculated. The pull-down menu in the upper left displays the T-S, the P-H diagram, or a schematic of the cycle.

In the ternary phase diagram with phase separation in Figure 3, the black dot can be moved on the phase diagram by clicking and dragging, and the corresponding mixture composition(s) is displayed. In the two-phase region, the compositions of the two phases in equilibrium are displayed when the boxes “show  $\alpha$  phase” and “show  $\beta$  phase” are checked, and the dashed lines show how the compositions are read from the diagram. Similarly, tie lines and



**Figure 4.** Two snapshots of an interactive Mathematica simulation, *Fugacities of an Ideal Binary Mixture*. Fugacity versus temperature is shown for two benzene mole fractions in a benzene/toluene mixture.

gridlines can be hidden or displayed by checking the appropriate box so that the phase diagram is easier to understand.

The simulation in Figure 4 calculates fugacities of each component in an ideal mixture as a function of temperature. A T-x-y diagram can also be viewed, and the black point moves on both diagrams as the mole fraction and the temperature change when the sliders are moved. This simulation demonstrates how fugacities increase for each component as temperature increases when only liquid is present because the saturation pressure increases. When only vapor is present, the fugacities do not change with temperature for either component because the partial pressures do not change at constant total pressure. In the two-phase region, the fugacity of the more-volatile component decreases with temperature, but the fugacity increases for the less-volatile component, and the accompanying T-x-y diagram demonstrates the reason for this behavior. Fugacity tends to be one of the more difficult concepts in chemical engineering thermodynamics, and thus several simulations related to fugacity were prepared.

### COMBINED SCREENCASTS AND SIMULATIONS

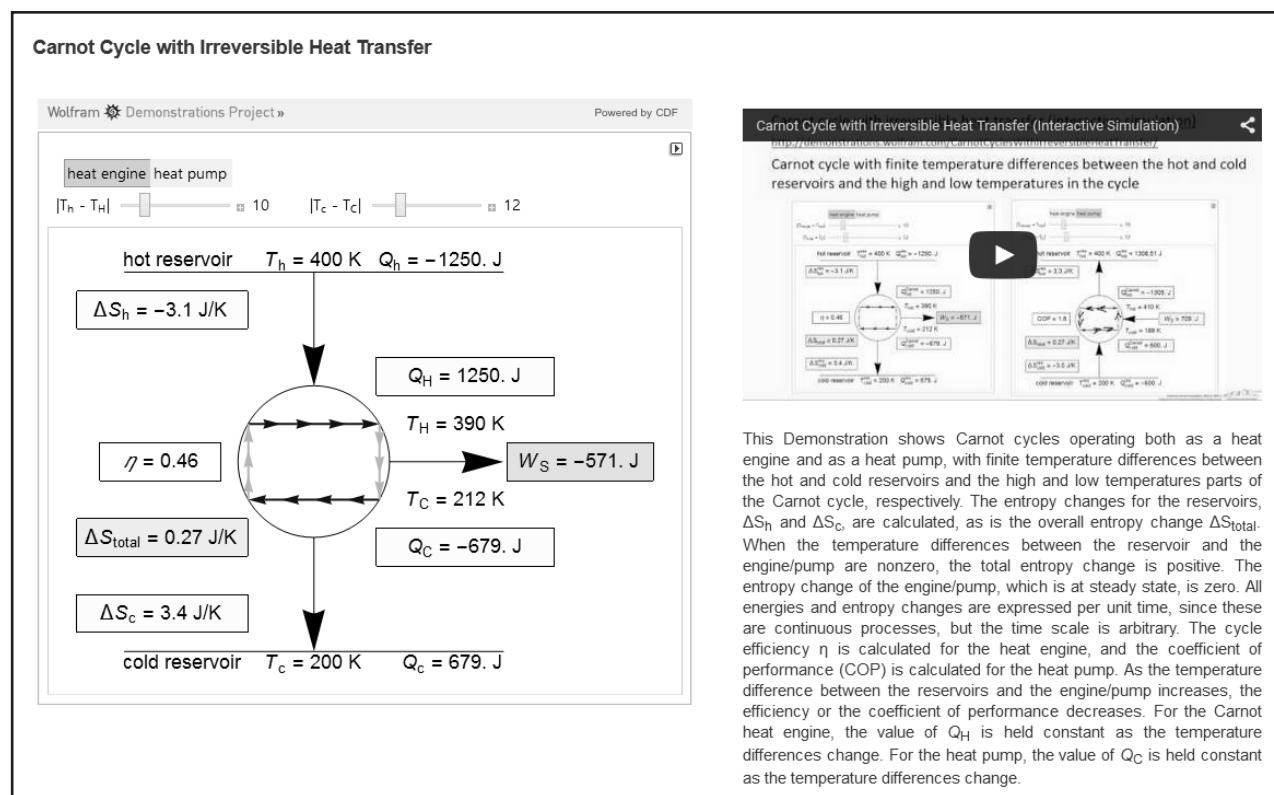
We prepared a 3 – 5 minute screencast for each simulation and put both on a web page so that the simulation can be used while simultaneously playing the screencast that describes how to use it. Figure 5 (following page) shows a screenshot of the page for Carnot Cycles with Irreversible Heat Transfer; the temperature differences between the low and high temperatures of the cycle and the reservoir temperatures can be changed with sliders, and the simulation calculates entropy changes of the reservoirs and the efficiency of the cycle.

### CONCEPTTESTS AND SIMULATIONS

The ConcepTest in Figure 6 (following page) uses a simulation that applies the first law to a piston/cylinder system. When a play button is selected in the simulation, the stops below the piston are removed and the pistons move down to their final volumes. For irreversible compression or expansion, the weights are fixed at the final value, whereas for the reversible cases, additional weights are added to or removed from the pistons as they move in order to approximate a reversible process. Since this simulation allows reversible and irreversible, adiabatic and isothermal, and compression and expansion, multiple ConcepTests were made that utilize it. The ConcepTests are available on <[www.LearnChemE.com](http://www.LearnChemE.com)>; faculty must register to obtain access.

### STUDENT FEEDBACK

Approximately 10 – 12 of the simulations were used in the Fall 2014 thermodynamics course, and many of those were related to vapor-liquid equilibrium; the other simulations were not completed in time to use. Students were asked to submit anonymous feedback at the end of the semester where they were asked to comment on the interactive simulations. Of the students who did so, 77% thought the interactive simulations were useful. Many of the remaining 23% also thought the interactive simulations were useful, but indicated that they sometimes had trouble understanding how to use them. This feedback provided motivation to create the screencasts that describe how to use the simulations. Comments from 10 students (out of 45 students who had positive responses about the simulations) are listed below verbatim to demonstrate



**Figure 5.** Screenshot of an embedded Mathematica simulation for Carnot Cycles With Irreversible Heat Transfer (on the left), with the corresponding screencast describing how to use the simulation (on the right), and text explaining the simulation (on the right).

how strongly many students felt about the simulations, and also to show that students used them outside of class. Many similar comments were obtained from the other students.

*“The simulations were very helpful to me. I’m a visual learner, so lectures don’t always stick but diagrams always have been very helpful. Once the interactive aspect was added to these diagrams, I was completely sold on concept and the topics illustrated stuck more. I think they are very well executed and are very powerful learning tool.”*

*“They were incredibly useful.”*

*“I enjoyed using the interactive simulations. Thought they provided an excellent visual learning tool that added tremendous value to the class.”*

*“The interactive simulations were very useful because I could test every scenario on my own rather than just seeing a few general ones.”*

Two identical piston/cylinders each contain 1 mol of a gas at 0.1 MPa and 300 K. They are each compressed with a constant external pressure of 1.5 MPa until their pressures are each 1.5 MPa. One is compressed isothermally and one adiabatically. The final volume is \_\_\_\_\_ system(s).

A. larger for the isothermal  
 B. larger for the adiabatic  
 C. the same for both  
 D. insufficient information

isothermal | adiabatic

**Figure 6.** A ConcepTest that utilizes the interactive Mathematica simulation Reversible and Irreversible Expansion or Compression Work. The stops indicate that the piston is constrained from moving until the play button is selected in the simulation. The correct answer is B.

“These interactive simulations were amazing!”

“The interactive simulations were the best thing that could even imagine.”

“Interactive simulations are also very useful. The ability to visualize the more complicated systems was key to understanding the phase equilibrium problems involving vapor-liquid-liquid equilibrium especially. They are also pretty fun to mess around with in general.”

“The interactive simulations were helpful because sometimes it’s really difficult to visualize what we are talking about in class. It was helpful to go home after class and try simulations on my own to make sure that you understand the concept.”

“The interactive simulation were very helpful. Helps to visualize what exactly is going on and especially in vapor-liquid equilibrium”

“The interactive simulations are incredibly useful in understanding the material, especially vapor-liquid equilibrium and vapor liquid-liquid equilibrium.”

## SUMMARY

More than 40 interactive simulations were developed for chemical engineering thermodynamics and made available on <www.LearnChemE.com> and on the Wolfram Demonstration Project (<<http://demonstrations.wolfram.com/>>). Screencasts were prepared that explain how to use the simulations and are located on the same page in LearnChemE as the corresponding simulation. ConceptTests were prepared for the simulations and also posted on LearnChemE. Approximately 45 other chemical engineering simulations were prepared for kinetics, heat transfer, fluids, and material and energy balances. Students indicated the simulations were very useful for helping them understand thermodynamics.

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