



## **Interactive Mathematica Simulations for Chemical Engineering**

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# Interactive *Mathematica* Simulations for Chemical Engineering

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## Abstract

More than 75 interactive *Mathematica* simulations have been prepared for four chemical engineering courses: kinetics/reactor design, thermodynamics, fluid mechanics, and heat transfer. These simulations, which do not require *Mathematica* to use, are located on the Wolfram Demonstration Project website. They allow the user to change parameters and see how the system responds. Short screencasts that demonstrate how to use the simulations were also prepared for many of the kinetics and thermodynamics simulations. These simulations have been used in class as part of ConcepTests with clickers, and they have also been used as part of homework assignments.

## Introduction

An effective method to demonstrate complex system behavior is to use interactive simulations, which allow the user to manipulate variables and receive instant feedback on how these changes affect the system. Because users manipulate the simulation at their own speed, fewer demands are placed on working memory and students can focus on understanding.<sup>1</sup> Interactive simulations have been used extensively in physics education<sup>2,3</sup> and 130 PhET simulations are available online ([phet.colorado.edu](http://phet.colorado.edu)). Student using simulations has been found to have positive effects on learning.<sup>4-6</sup> Podolefsky et al. showed that they promote self-directed inquiry and exploration.<sup>7</sup> Although not as sophisticated as the PhET simulations, *Mathematica*-based interactive simulations are advantageous because they are easier to program.

Simulation-based learning has the potential for a high impact on education.<sup>8</sup> Students get immediate feedback and they can experiment. However, interactive simulations on their own may not be the best learning tool. Users have difficulties developing an appropriate hypothesis, evaluating simulation results, and using the simulation systematically.<sup>9</sup> Rieber et al. showed that students who were given interactive simulations with short explanation videos scored better than students who were given just interactive simulations.<sup>8</sup> Creating screencasts that show how an interactive simulation works allow the advantages of interactive simulations to be utilized while keeping students focused on learning objectives and outcomes.

## Preparing interactive simulations

Interactive simulations were created using the *Mathematica*, and they are available on the Wolfram Demonstration Project website (<http://demonstrations.wolfram.com/>). They can be used without a *Mathematica* license, and only require a free plug-in that can be downloaded from the site. The simulations use the powerful Manipulate command in *Mathematica* to create on-screen controls that allow users to change system parameters. One key feature of these simulations is that the calculations are done in real-time as input parameters are manipulated using user-friendly controls, and the graphical output appears almost instantaneously.

## Examples of chemical engineering simulations

A few examples are presented here to demonstrate the types of simulations that are possible in Mathematica and the types of options available for manipulation by students. In Figure 1, a vapor-liquid-liquid equilibrium diagram is shown for a partially-miscible binary system. The black dot in the middle of the phase diagram can be moved by moving the sliders located above the T-x-y diagram. On the right side, the fractions of each phase present are shown in a bar graph, and the composition of each phase is above the bar for that phase. In order to represent the behavior on the T-x-y diagram when three phases are present, a slider for heat added is manipulated instead of temperature. In this way, when more heat is added at the temperature where three phases exist, the relative amounts of each phase change, but the temperature remains constant until one of the phases disappears.

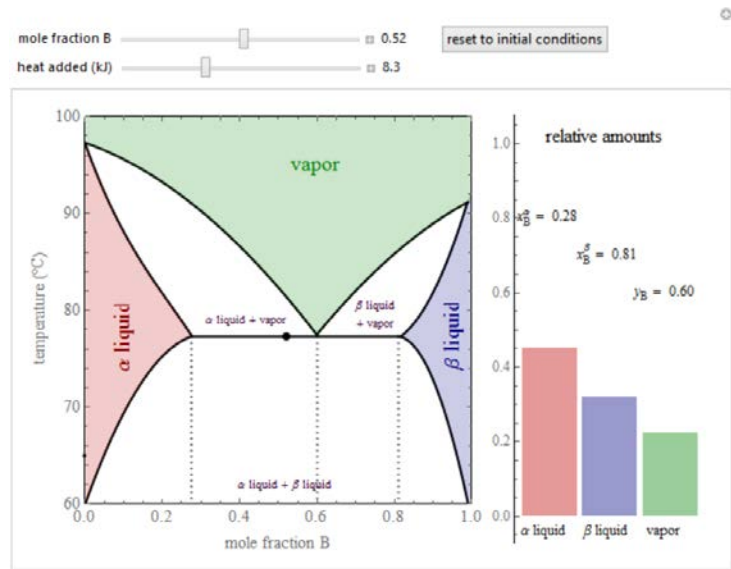


Figure 1 Interactive simulation for vapor-liquid-liquid phase equilibrium. This simulation is located at: <http://demonstrations.wolfram.com/VaporLiquidLiquidEquilibriumVLE/>.

A second example from thermodynamics is shown in Figure 2 for a refrigeration cycle. The cycle is shown on a pressure-enthalpy diagram on the left, and as the upper and lower pressures are changed with sliders, the cycle diagram is redrawn, and a new coefficient of

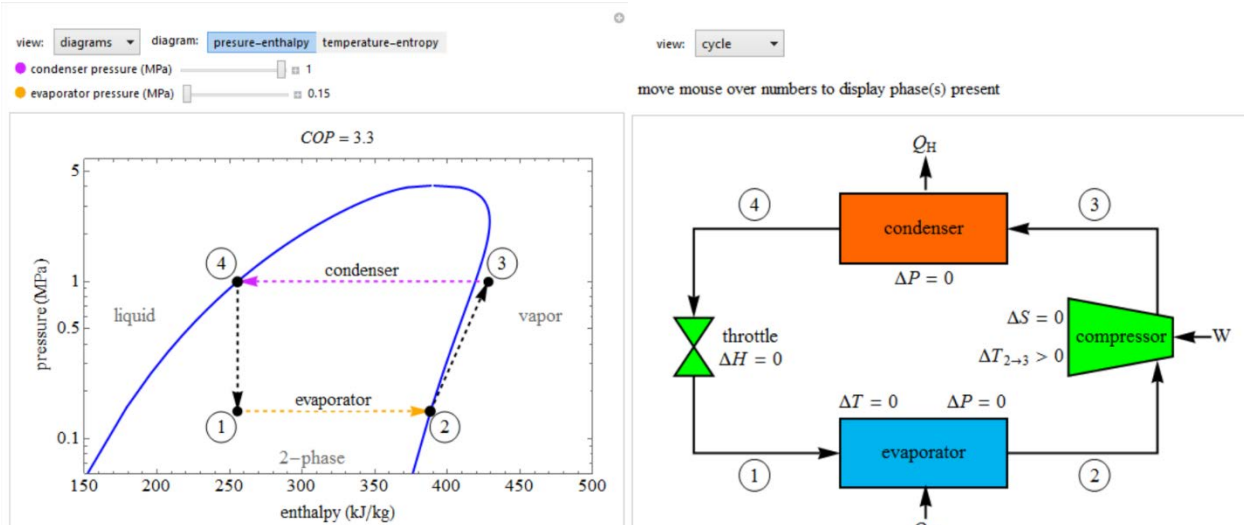


Figure 2 Interactive simulation for vapor compression cycle. This simulation is located at: <http://demonstrations.wolfram.com/OrdinaryVaporCompressionOVCCycleForRefrigerantR134a/>

performance is calculated. By clicking on the button on the top right, a temperature-entropy diagram for the same cycle is displayed instead. The pull-down menu on the left allows a diagram of the cycle to be seen, as shown on the right side of Figure 2.

An example from kinetics is shown in Figure 3 for an autothermal reactor. In this simulation, differential equations are solved for a catalytic reactor in which the reacting gases are fed to an annular region around the catalyst bed. These equations are solved by guessing the entrance temperature to the catalyst bed. The feed temperature to the annular region is known, but the temperature of the fluid entering the catalyst bed is unknown. The amount of reaction in the catalyst bed determines how much the feed is preheated, and the amount of reaction depends on the temperature of the fluid entering the bed. The bottom slider allows the user to adjust the feed temperature to the bed to obtain the correct feed temperature (red circle on the bottom right).

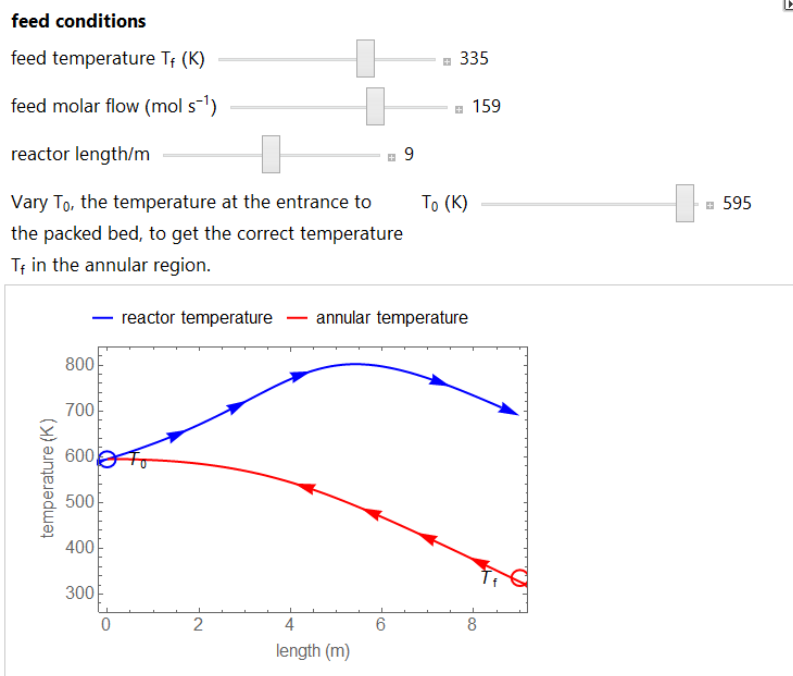


Figure 3 Interactive simulation for autothermal reactor. This simulation is located at:

<http://demonstrations.wolfram.com/AutothermalReactor/>

Using the simulations

These simulations have been used in class after asking students to predict system behavior as part of a ConcepTest with student-held clickers. For example, students answered the ConcepTest in Figure 4 using clickers and peer instruction. Then, the interactive simulation was shown, and various changes from different starting points were presented. These simulations have also been used outside of class as part of assignments and in office hours to help students understand important concepts. Students also use them on their own to help understand confusing aspects of a topic. For example, they are excellent for demonstrating the idea of parametric sensitivity. These interactive simulations have also been used as part of screencasts prepared for information delivery outside of class (flipped classroom); these screencasts are posted on [www.LearnChemE.com](http://www.LearnChemE.com).

We used some of these simulations in thermodynamics in fall 2014, and anonymous written feedback was collected from students at the end of the semester as part of an assignment. Of the 75 students who responded to the question “How useful were the interactive

simulations?”, 77% said they were useful and were very positive with statements like:

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

“the interactive simulations are incredibly useful”

“Really liked the simulations. You should use more of these”.

Some of the remaining 23% of the students found them useful in some cases, but said they would be more useful if better explained. As a result, we prepared short screencasts that demonstrate how to use many of the simulations. As pointed out earlier, Rieber et al. found that interactive simulations with short explanation videos improved learning.<sup>8</sup>

### Acknowledgments

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### References

1. Beaulieu, J. R. A dynamic, interactive approach to learning engineering and mathematics. (2012).
2. Wieman, C. E., Adams, W. K. & Perkins, K. K. PhET: simulations that enhance learning. *Science*. **322**, 682–683 (2008).
3. Wieman, C. E. & Perkins, K. K. A powerful tool for teaching science. *Nat. Phys.* **2**, 290–292 (2006).
4. Bodemer, D., Ploetzner, R., Feuerlein, I. & Spada, H. The active integration of information during learning with dynamic and interactive visualisations. *Learn. Instr.* **14**, 325–341 (2004).
5. Van der Meij, J. & de Jong, T. Supporting students’ learning with multiple representations in a dynamic simulation-based learning environment. *Learn. Instr.* **16**, 199–212 (2006).
6. Kadiyala, M. & Crynes, B. L. A review of literature on effectiveness of information technology in education. *J. Eng. Educ.* **89**, 33–37 (2000).
7. Podolefsky, N. S., Perkins, K. K. & Adams, W. K. Factors promoting engaged exploration with computer simulations. *Phys. Rev. Spec. Top. Phys. Educ. Res.* **6**, 020117 (2010).
8. Rieber, L. P., Tzeng, S. C. & Tribble, K. Discovery learning, representation, and explanation within a computer-based simulation: finding the right mix. *Learn. Instr.* **14**, 307–323 (2004).
9. Bodemer, D., Ploetzner, R., Bruchmuller, K. & Hacker, S. Supporting learning with interactive multimedia through active integration of representations. *Instr. Sci.* **33**, 73–95 (2005).

What happens when this system is heated until the amount of vapor doubles?

- A.  $\alpha$  liquid completely evaporates
- B.  $\beta$  liquid completely evaporates
- C. some of each liquid evaporates
- D. none of the above

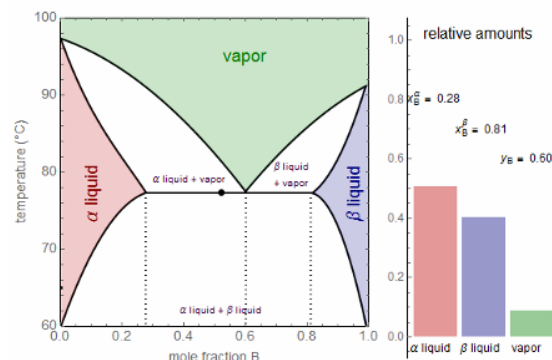


Figure 4 ConceptTest that uses an interactive simulation