



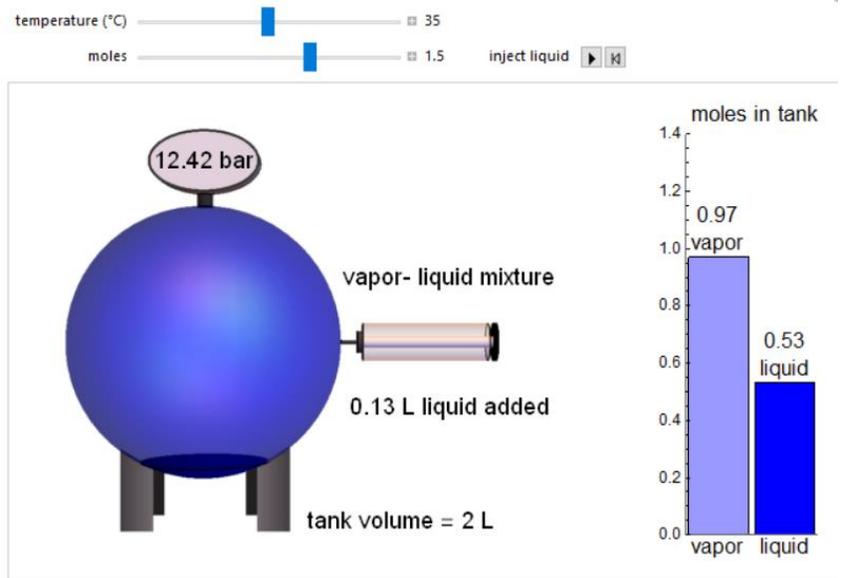
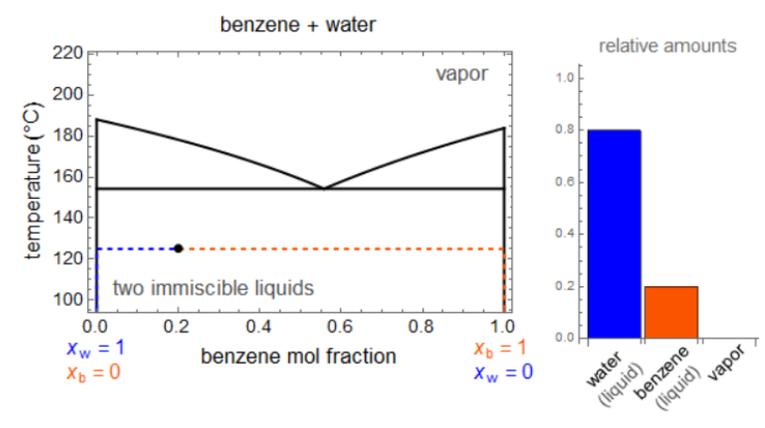
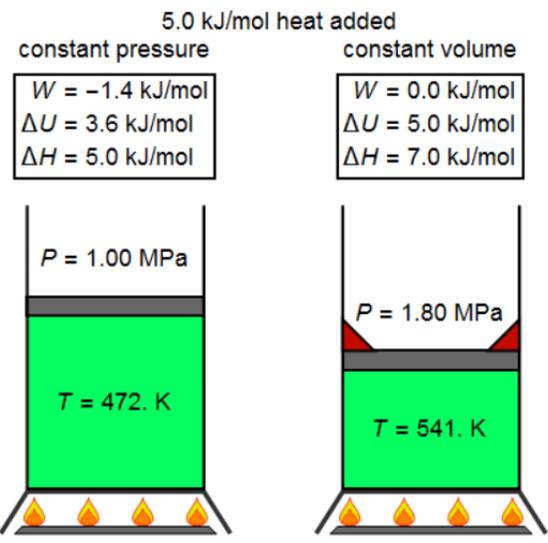
Combining Interactive Thermodynamics Simulations with Screencasts and ConcepTests

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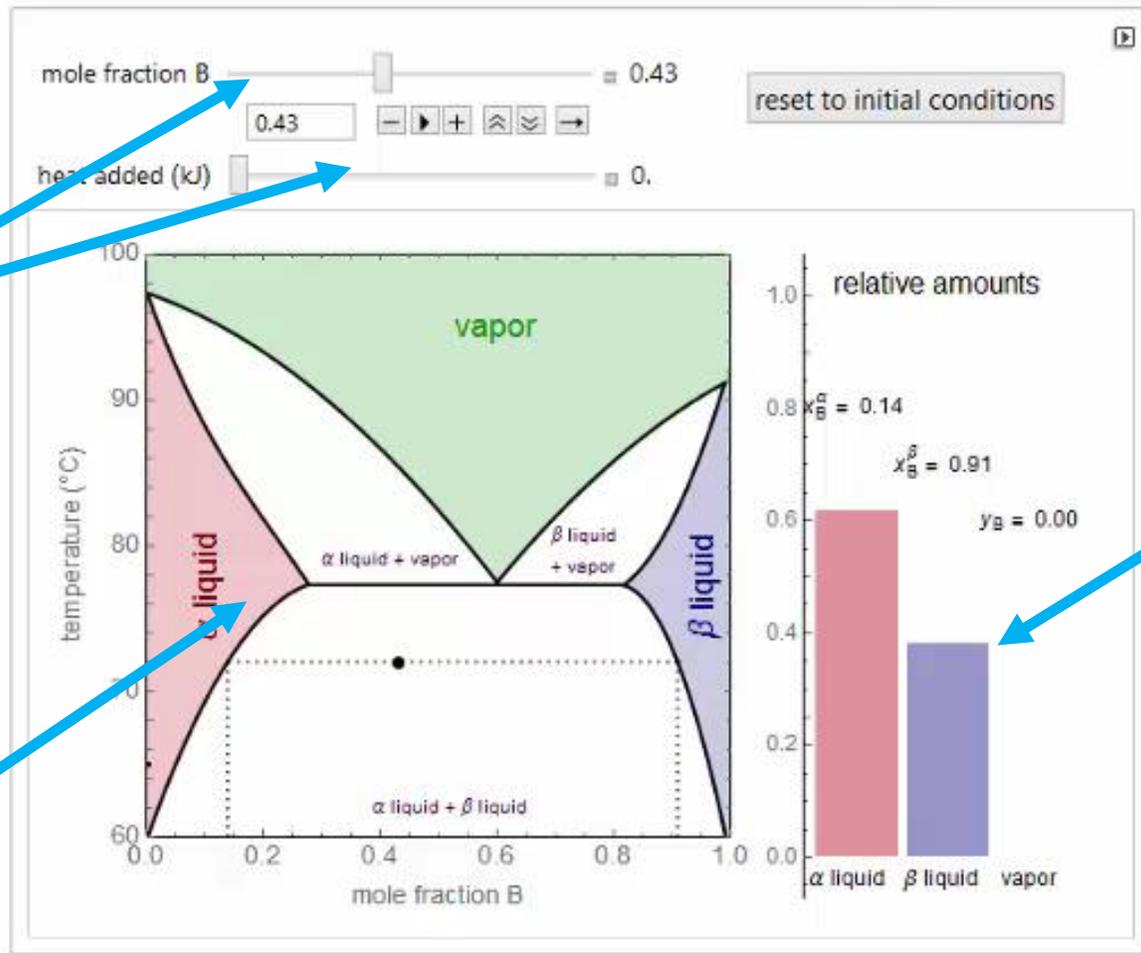
Boulder, Colorado

Funding: NSF



Simulation options

Vapor-Liquid-Liquid Equilibrium (VLLE)



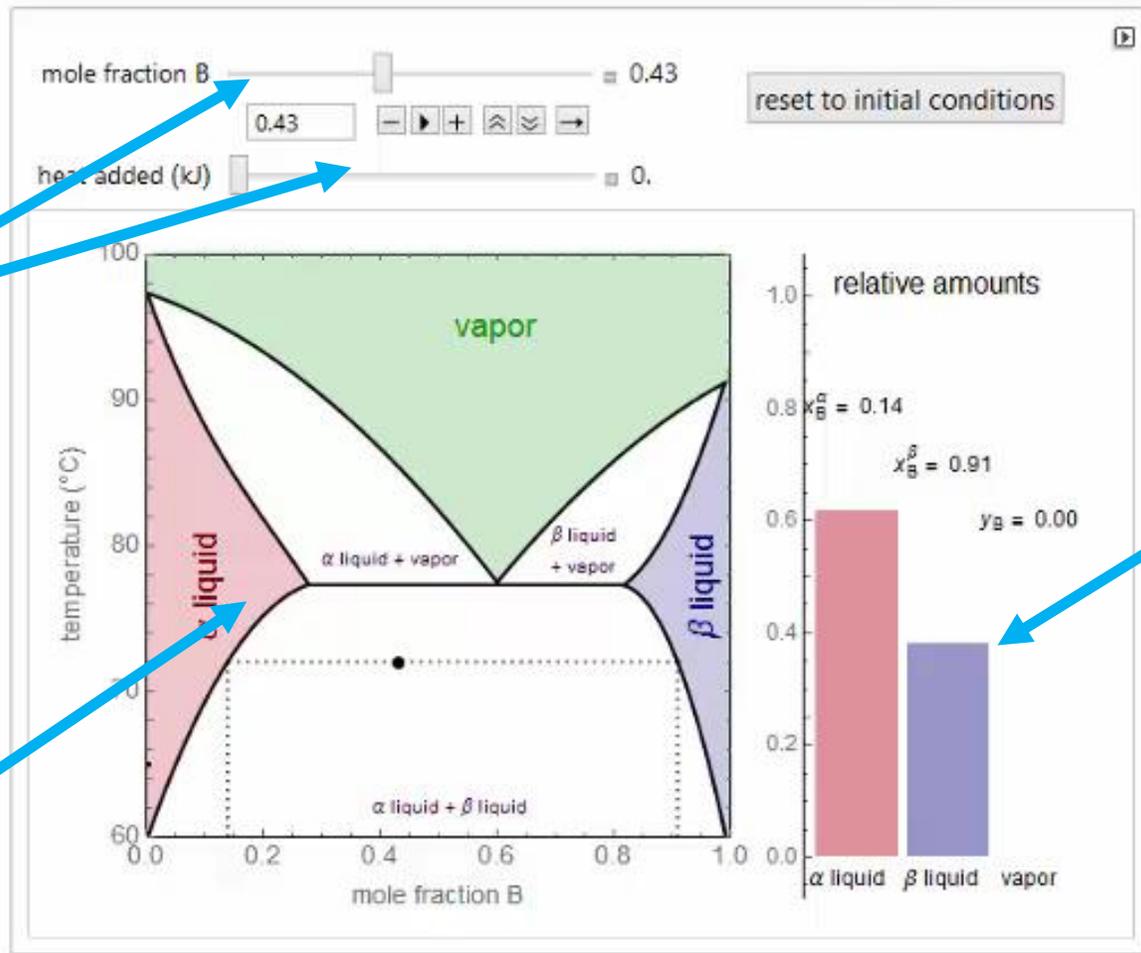
sliders

diagrams

bar graphs

Simulation options

Vapor-Liquid-Liquid Equilibrium (VLLE)



sliders

diagrams

bar graphs

compression expansion

choose two conditions:

reversible isothermal irreversible isothermal

final pressure (MPa) 1.5

reversible isothermal
 $W = 0.0 \text{ kJ/mol}$
 $T = 300. \text{ K}$
 $P_{\text{ext}} = 0.1 \text{ MPa}$
 $P = 0.1 \text{ MPa}$

irreversible isothermal
 $W = 0.0 \text{ kJ/mol}$
 $T = 300. \text{ K}$
 $P_{\text{ext}} = 1.5 \text{ MPa}$
 $P = 0.1 \text{ MPa}$

select buttons

drop-down menus

slider

play button

animations

The image shows a software interface for a thermodynamics simulation. At the top, there are two tabs: 'compression' (selected) and 'expansion'. Below them, a label 'choose two conditions:' is followed by two dropdown menus: 'reversible isothermal' and 'irreversible isothermal'. A slider for 'final pressure (MPa)' is set to 1.5. To the right of the slider is a play button. Below these controls are two diagrams of gas cylinders. The left cylinder is labeled 'reversible isothermal' and shows a piston with a weight that is being removed in small steps, with $P_{\text{ext}} = 0.1 \text{ MPa}$ and $P = 0.1 \text{ MPa}$ inside. The right cylinder is labeled 'irreversible isothermal' and shows a piston with a large weight that is suddenly removed, with $P_{\text{ext}} = 1.5 \text{ MPa}$ and $P = 0.1 \text{ MPa}$ inside. Red areas at the top of the gas in the right cylinder indicate compression work. Blue arrows point from text labels to various UI elements: 'select buttons' points to the 'compression' tab; 'drop-down menus' points to the 'reversible isothermal' dropdown; 'slider' points to the 'final pressure' slider; 'play button' points to the play button; and 'animations' points to the red areas in the right cylinder.

compression expansion

choose two conditions:

reversible isothermal irreversible isothermal

final pressure (MPa) 1.5

reversible isothermal
 $W = 0.0 \text{ kJ/mol}$
 $T = 300. \text{ K}$
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select buttons

drop-down menus

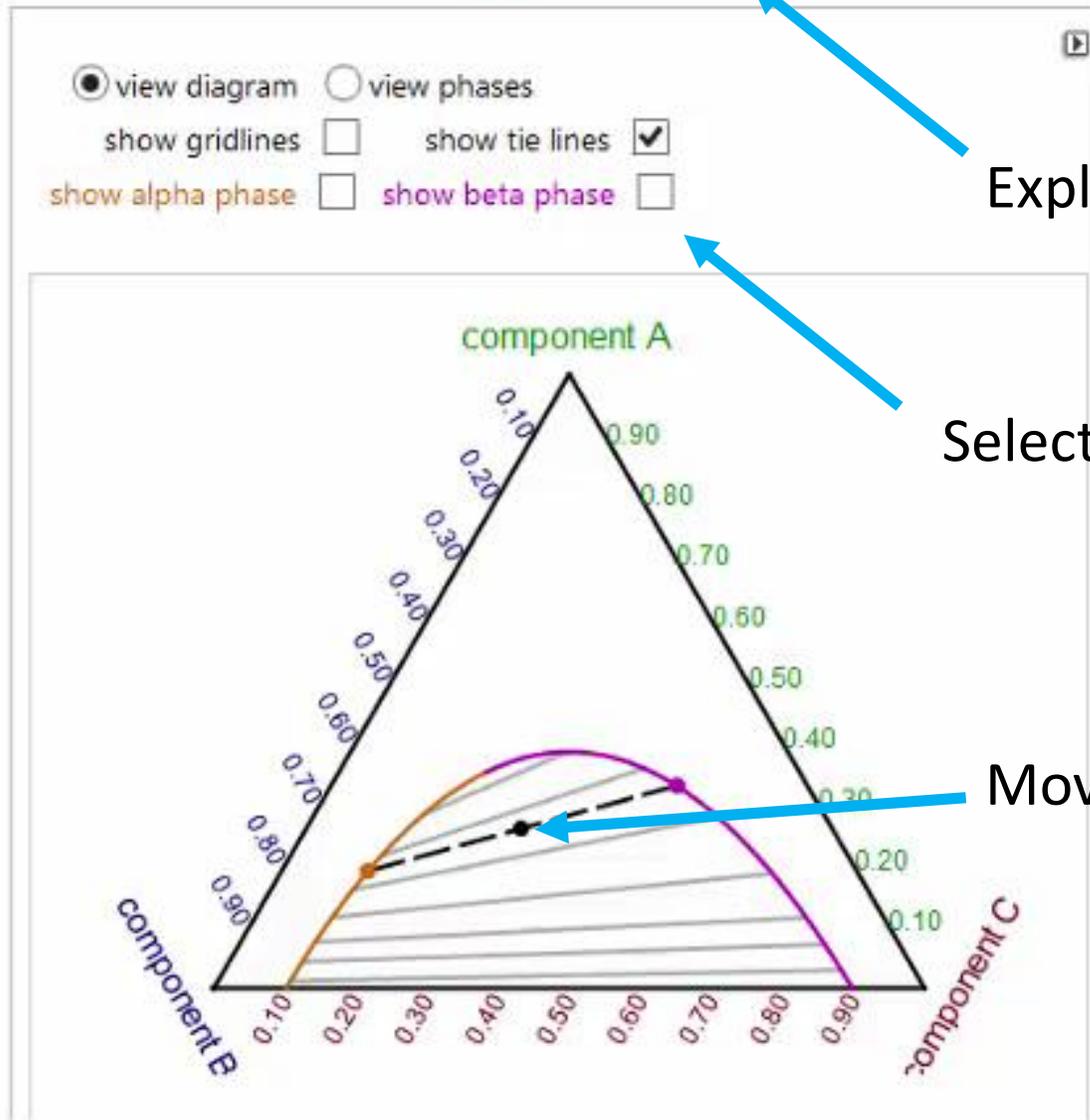
slider

play button

animations

The image shows a software interface for simulating thermodynamic processes. At the top, there are two tabs: 'compression' (selected) and 'expansion'. Below them, a label 'choose two conditions:' is followed by two dropdown menus: 'reversible isothermal' and 'irreversible isothermal'. A slider for 'final pressure (MPa)' is set to 1.5, with a play button to its right. The main area contains two diagrams of gas cylinders. The left cylinder is labeled 'reversible isothermal' with $W = 0.0 \text{ kJ/mol}$, $T = 300. \text{ K}$, $P_{\text{ext}} = 0.1 \text{ MPa}$, and $P = 0.1 \text{ MPa}$. The right cylinder is labeled 'irreversible isothermal' with $W = 0.0 \text{ kJ/mol}$, $T = 300. \text{ K}$, $P_{\text{ext}} = 1.5 \text{ MPa}$, and $P = 0.1 \text{ MPa}$. The right cylinder shows a piston with a stack of blue weights and a red wedge at the bottom, indicating a sudden increase in external pressure. Blue arrows point from text labels to various UI elements: 'select buttons' points to the 'compression' tab; 'drop-down menus' points to the 'reversible isothermal' dropdown; 'slider' points to the 'final pressure' slider; 'play button' points to the play button; and 'animations' points to the piston and weights in the irreversible cylinder diagram.

Ternary Phase Diagram with Phase Envelope

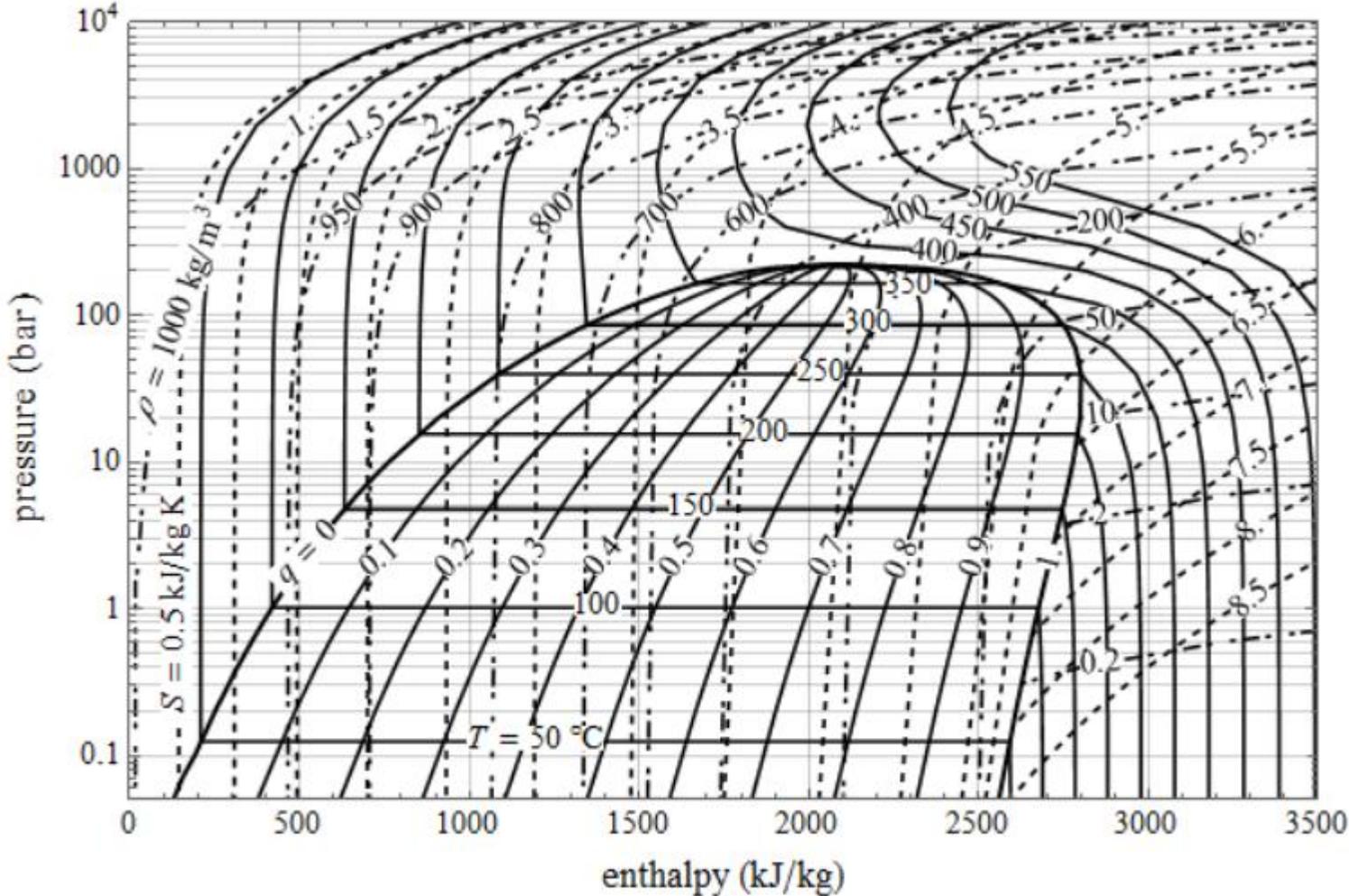


Explain diagram

Select info displayed

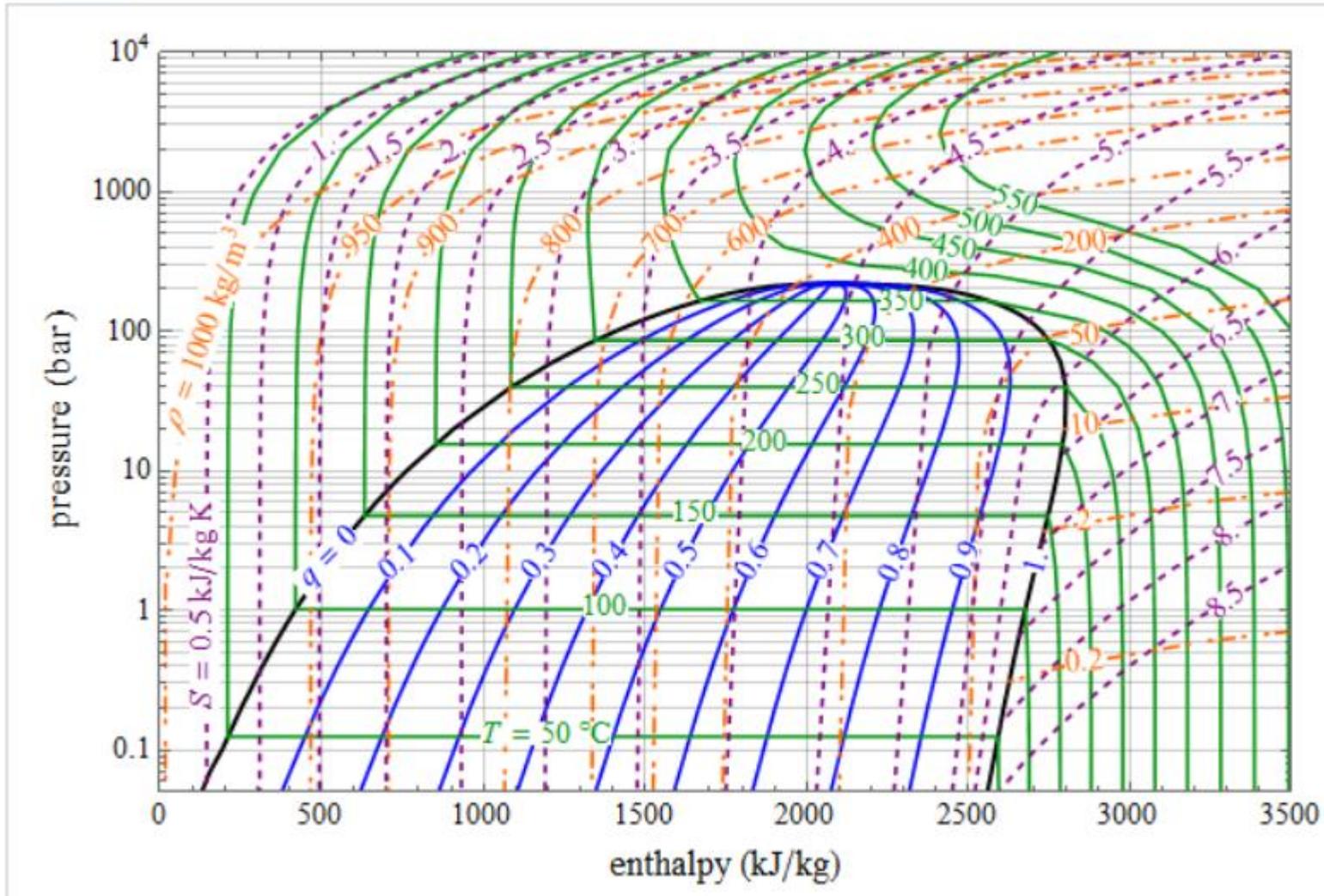
Move point with mouse

Pressure-enthalpy diagram



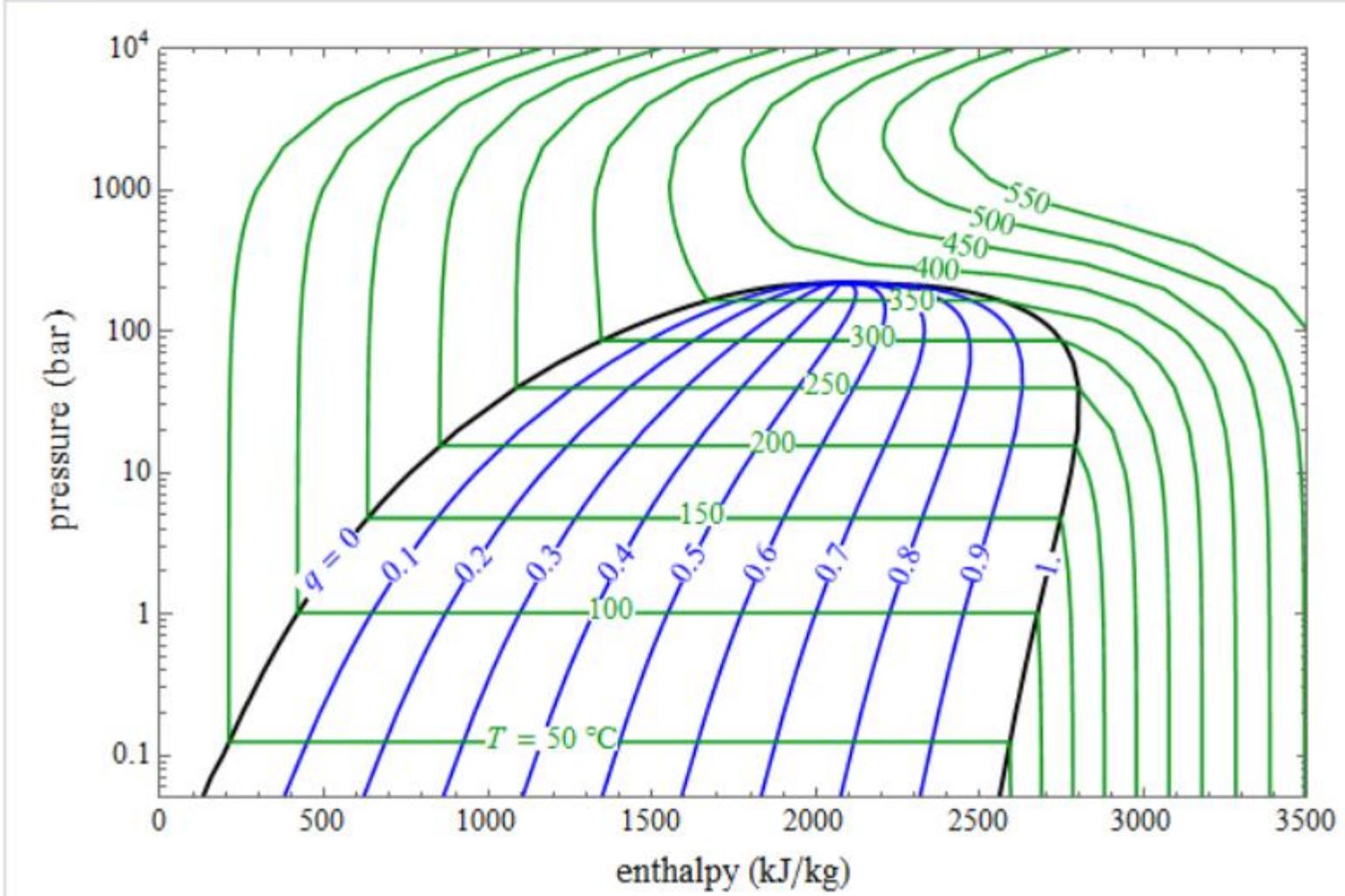
Pressure-enthalpy diagram

view lines of constant: vapor quality isotherms density entropy
color black & white grid lines



Pressure-enthalpy diagram

view lines of constant: vapor quality isotherms density entropy
color black & white grid lines



Objectives of interactive simulations

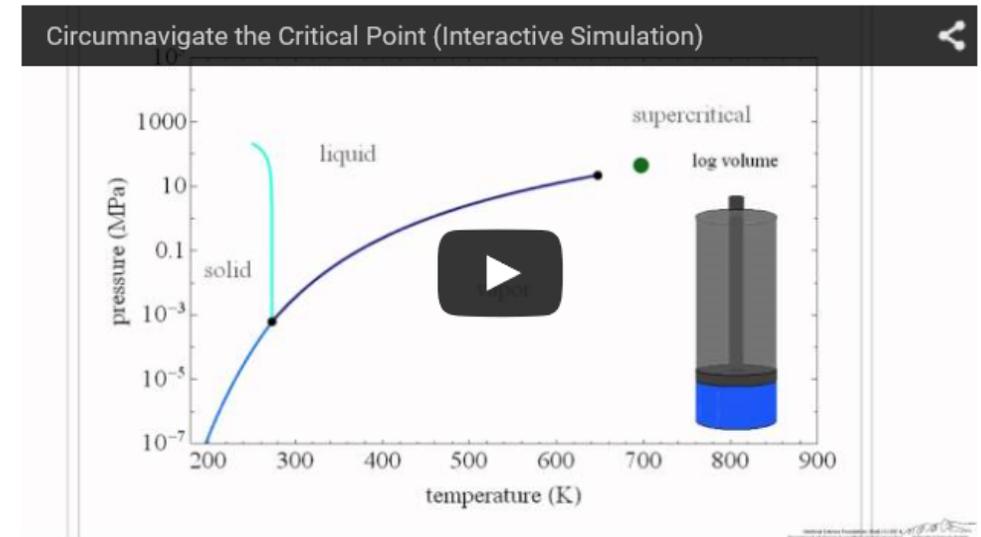
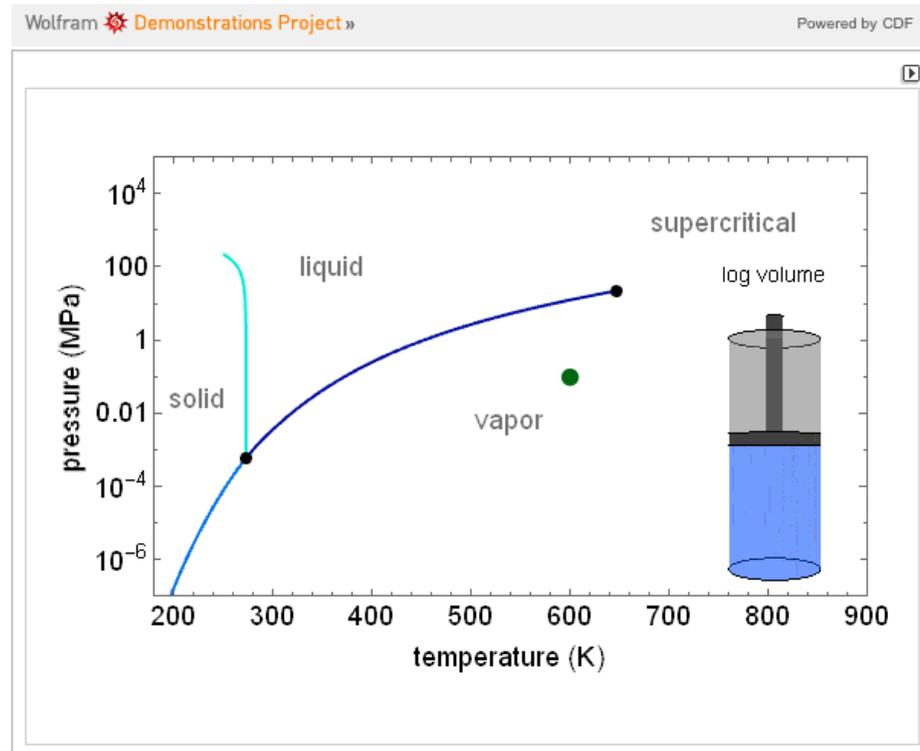
- Demonstrate concept, explain diagram
- Minimize options, parameters to change
- Easy to use - corresponding screencast

Mathematica simulations

- Simple commands to make interactive
- CDF format- *Mathematica* not required
- <http://demonstrations.wolfram.com/> (download code)
- www.LearnChemE.com/simulations

Simulation and short screencast

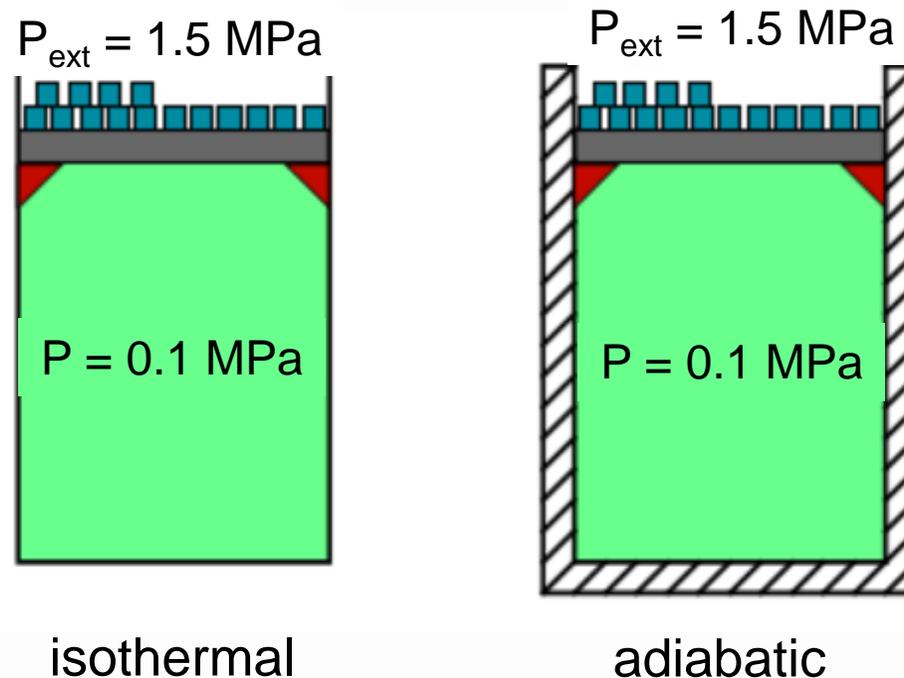
Circumnavigating the Critical Point



The pressure-temperature phase diagram for water is used to illustrate the concept of state functions and the possibility of going from the liquid phase to the vapor phase (or the other way) without a phase change (a single phase throughout the process) by circumnavigating the critical point, which is the highest temperature and pressure where two distinct phases exist (647 K, 22.1 MPa for water).

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



- 45 interactive Mathematica simulations for thermodynamics
 - Energy balances and entropy changes
 - Cycles
 - Single-component phase equilibrium
 - Fugacity and departure functions
 - Multi-component VLE, ideal solutions
 - Multi-component VLE, non-ideal solutions
 - Partially-miscible and immiscible solutions
 - Chemical reaction equilibrium
- 100 ConcepTests using simulations
- 36 screencasts

Questions ?

Why interactive simulations?

Studies show simulations improve student learning^{1,2}

Actively engage students

Observe behavior that hard to observe in real time

Student like them

Why screencasts?

Improve student learning³

Students like and use them

Why ConcepTests?

Numerous studies demonstrate effectiveness

Students like them

1. Wieman, C. E., Adams, W. K., Perkins, K. K. PhET, *Science*. **322**, 682 (2008)
2. Wieman, C. E., Perkins, K. K., *Nat. Phys.* **2**, 290 (2006)
3. Rieber, L. P., Tzeng, S. C., Tribble, K., *Learn. Instr.* 14, 307 (2004).

Positive feedback from students

“These interactive simulations were **amazing!**”

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

“The interactive simulations are **extremely useful.**”

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

“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.

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

“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.”

Positive feedback from students

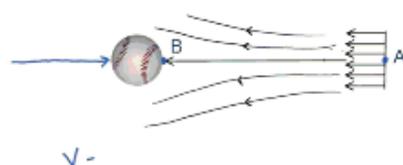
“Interactive simulations on assignments and used in class were very valuable. With thermodynamics your intuition may not be good to determine how the system will actually change when you change a parameter. **The simulations are the best** because you could vary parameters and visually see what actually happened to the system.”

“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 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.”



Acceleration
- Eulerian Approach $f(x, y, z, t)$



www.khanacademy.com

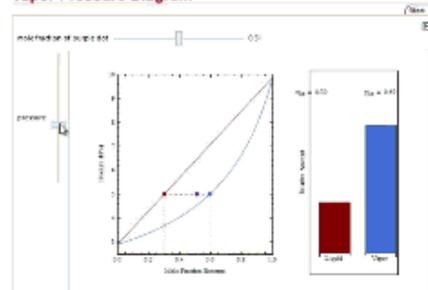
Screencasts

[see all screencasts](#)

Screencasts are short screen captures, usually of a tablet PC, with instructor narration. They are solutions to example problems, explanations of concepts, software tutorials, introduction to topics, descriptions of diagrams, and reviews of material. Screencasts supplement textbooks, classes, and office hours and allow students to learn at their own pace. Many of the screencasts are organized by textbook table of contents found on each topic page.

[Interactive screencasts](#) present a multiple choice question where the viewer chooses an answer within the video. The video response guides the user to the correct answer and explanation. For more information, see our [interactive screencasts](#).

Lever Rule Applied to the Benzene-Toluene
Vapor Pressure Diagram



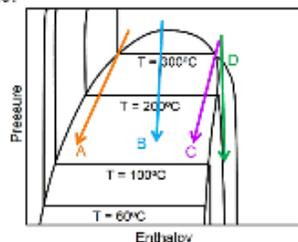
Interactive Simulations

[see all interactive simulations](#)

Wolfram *Mathematica*-based simulations (Wolfram Demonstrations) are available for a number of chemical engineering topics. These simulations allow the user to determine how system behavior changes when variables are changed using sliders. The simulations can be accessed using free Wolfram based browser plug-ins or using the free [Wolfram CDF](#) player that enables the simulation to be loaded offline; a *Mathematica* software license is not required. For more information about the simulations and their use, go to [Wolfram Demonstrations](#).

All simulations are copyrighted © 2013 Wolfram Demonstrations Project & Contributors. Visit Wolfram Demonstrations Project [Terms of Use](#) for more details.

Which line is most likely to represent a reversible turbine?



Department of Chemical & Biological Engineering, University of Colorado Boulder

Instructor Resources

[see all instructor resources](#)

ConceptTests challenge students with qualitative questions that are not answered by memorization. Used in tandem with peer instruction, ConceptTests can dramatically improve functional understanding while allowing instructors to gauge students understanding immediately and tailor their instruction accordingly.

Course packages provide digital OneNote based resources containing class notes, ConceptTests, reading assignments, screencast recommendations, homework problems and exam questions.

Instructors: [Check out the resources](#) to request access our 1300+ ConceptTest inventory or course packages.

Summary

- 45 thermodynamics simulations
- 97 total simulations (kinetics, fluids, heat transfer)
- Accompanying screencasts
- ConcepTests
- www.LearnChem.com

www.LearnChemE.com

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

Mathematica programming: *Rachael Baumann, Megan McGuire, Garrison Vigil,
Derek Machalek, Nathan Nelson*

Screencasts and web pages: *Katherine McDanel, Michelle Medlin, Nathan Nelson,
Isaac Dillon*

ConcepTests: *Katherine McDaniel*