Interactive Mathematica Simulations for Chemical Engineering

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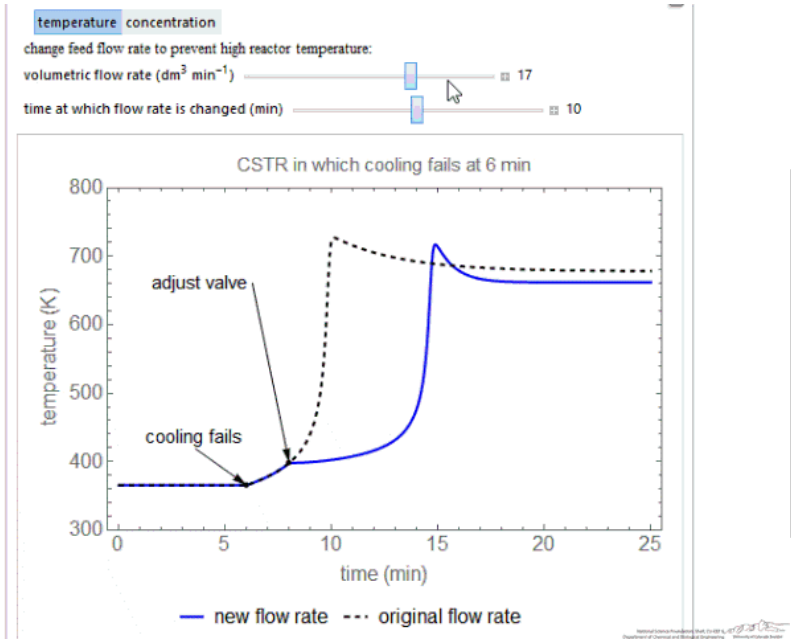
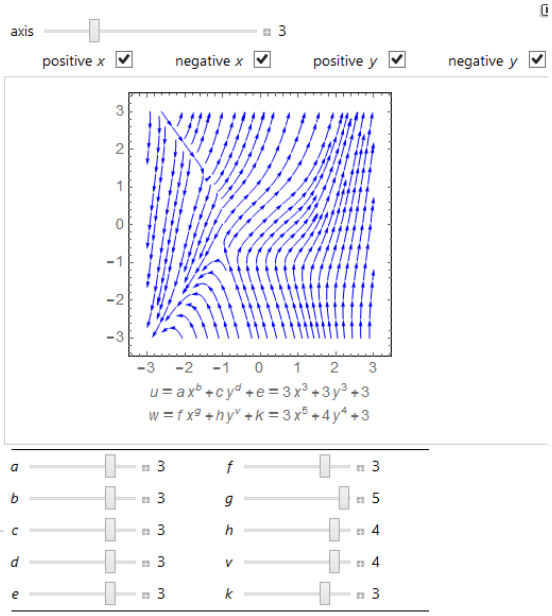
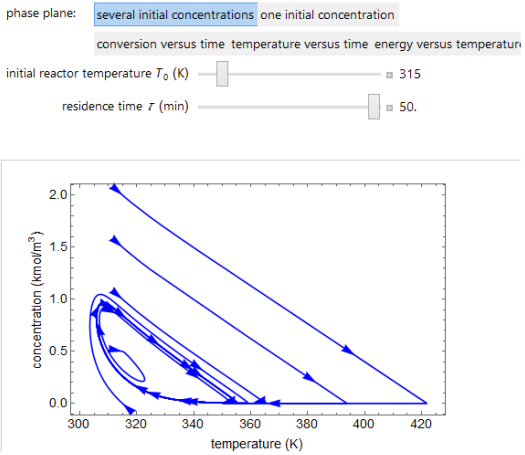
Funding: NSF







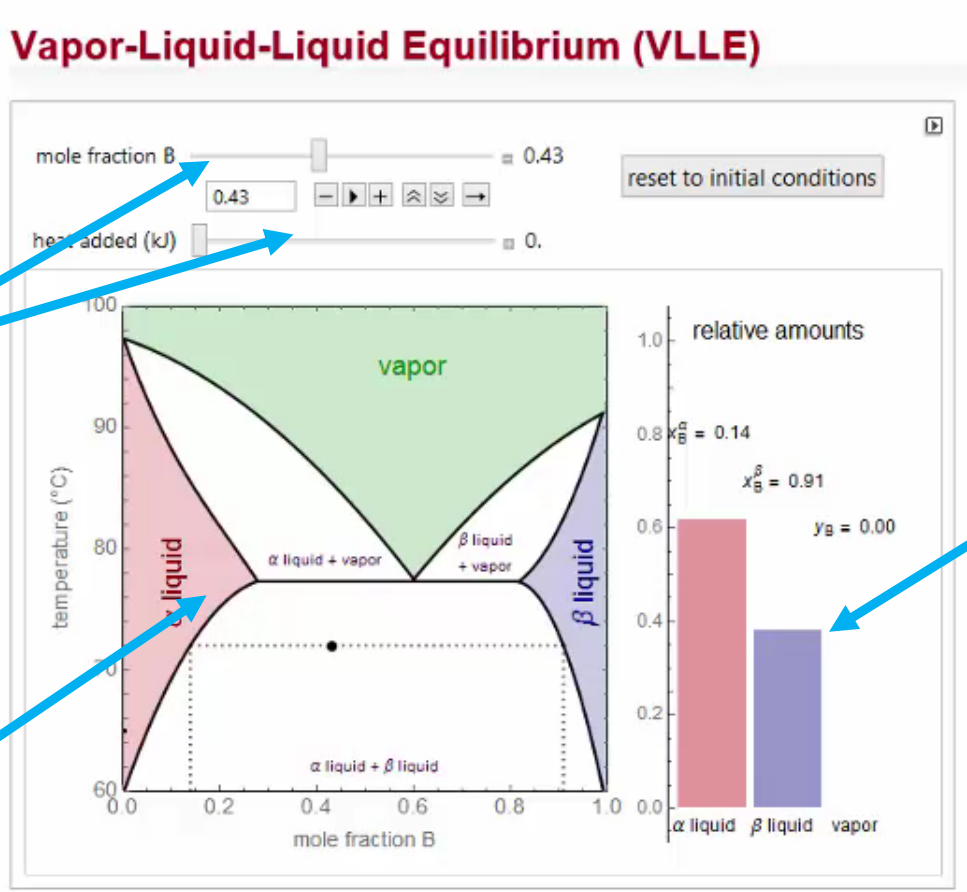
Objectives of interactive simulations

- 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

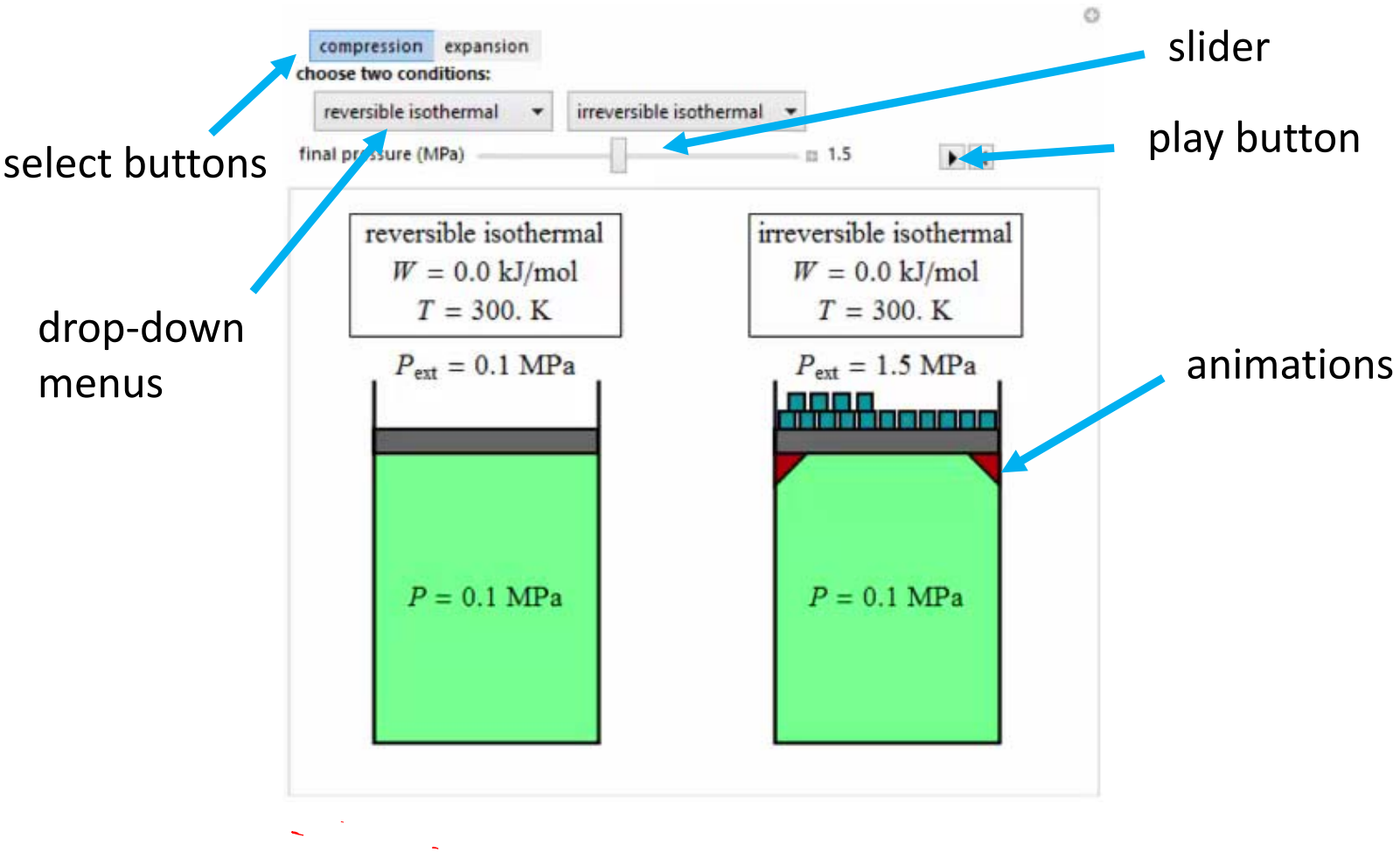
Simulation options

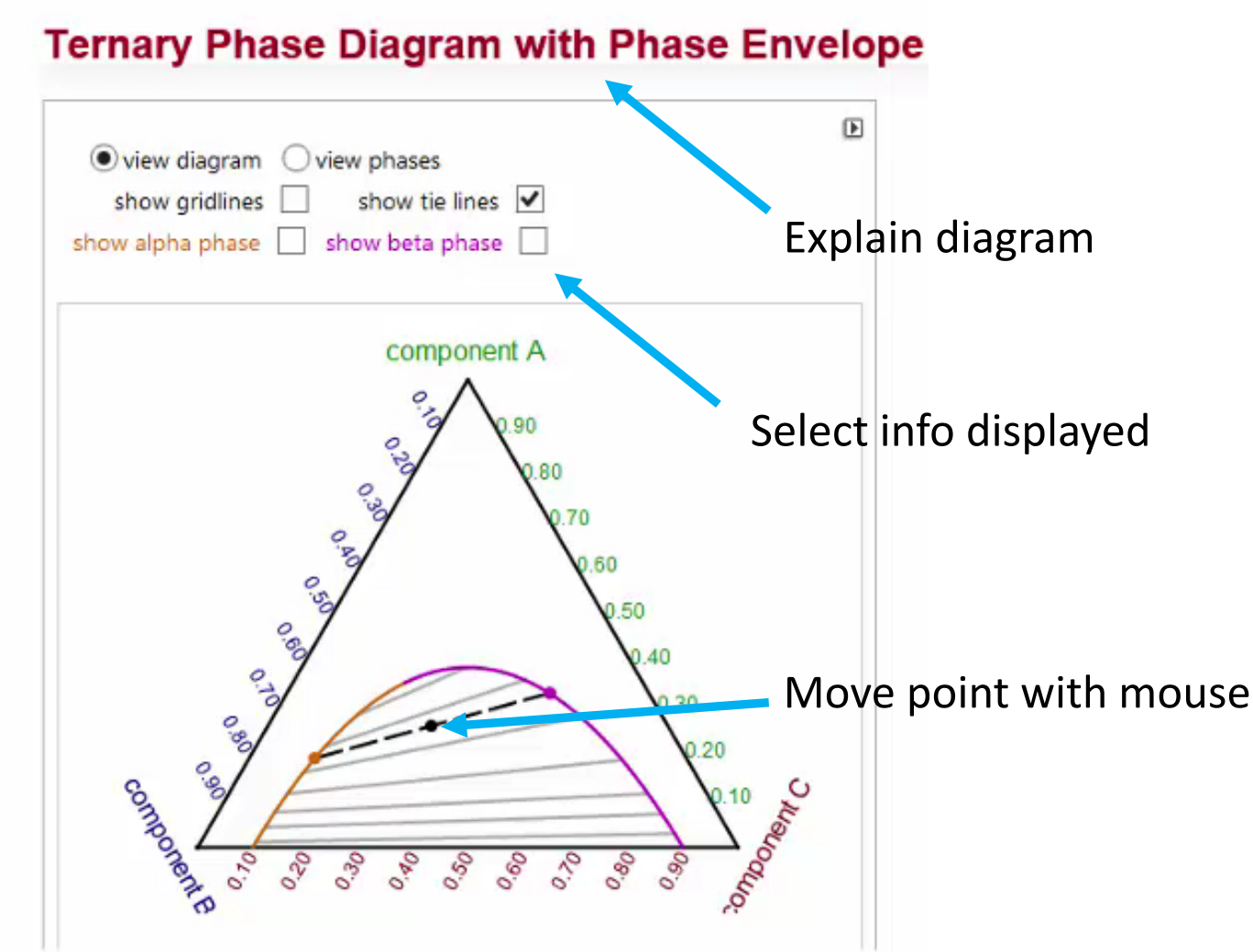


sliders

diagrams

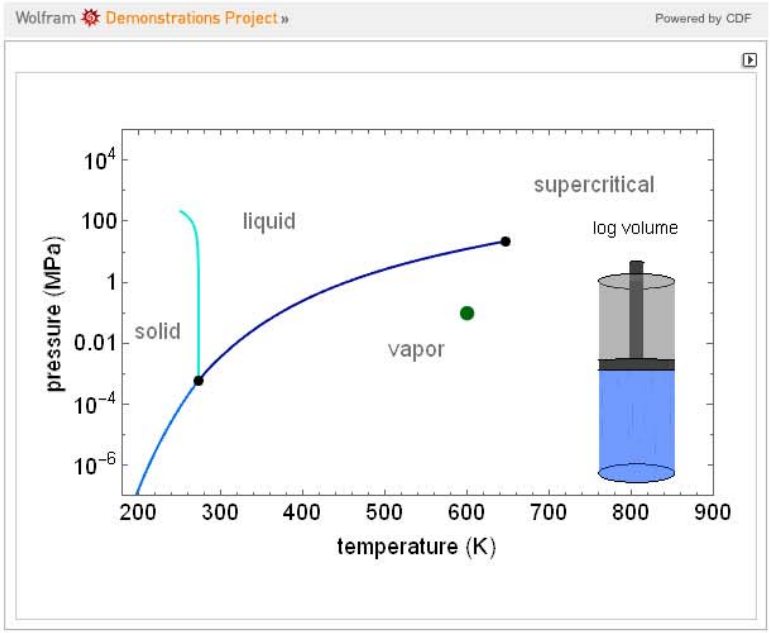
bar graphs

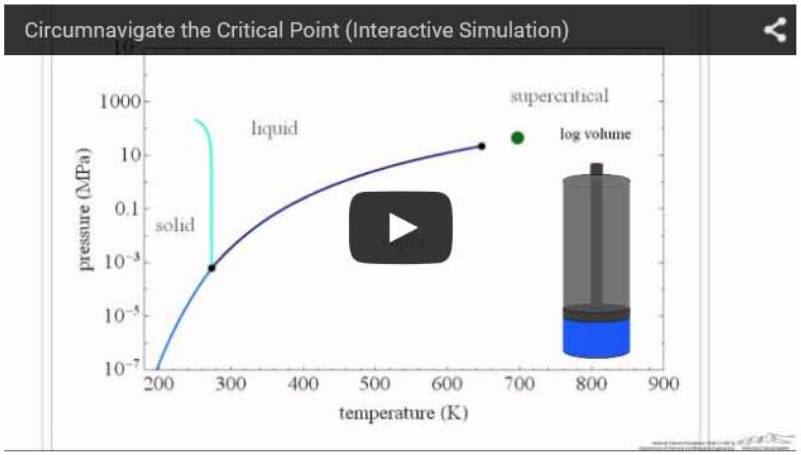

compression
expansion
choose two conditions:
reversible isothermal
irreversible isothermal
final pressure (MPa)
1.5
reversible isothermal
W = 0.0 kJ/mol
T = 300. K
irreversible isothermal
W = 0.0 kJ/mol
T = 300. K
P_ext = 0.1 MPa
P_ext = 1.5 MPa
P = 0.1 MPa
P = 0.1 MPa
select buttons
drop-down menus
slider
play button
animations


Ternary Phase Diagram with Phase Envelope
view diagram
view phases
show gridlines
show tie lines
show alpha phase
show beta phase
component A
component B
component C
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
Explain diagram
Select info displayed
Move point with mouse

Simulation and 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).

Why interactive simulations?

- Studies show simulations improve student learning[1,2]
- Student like them

Why screencasts?

- Improve student learning [3]
- Students use 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).

How to use simulations

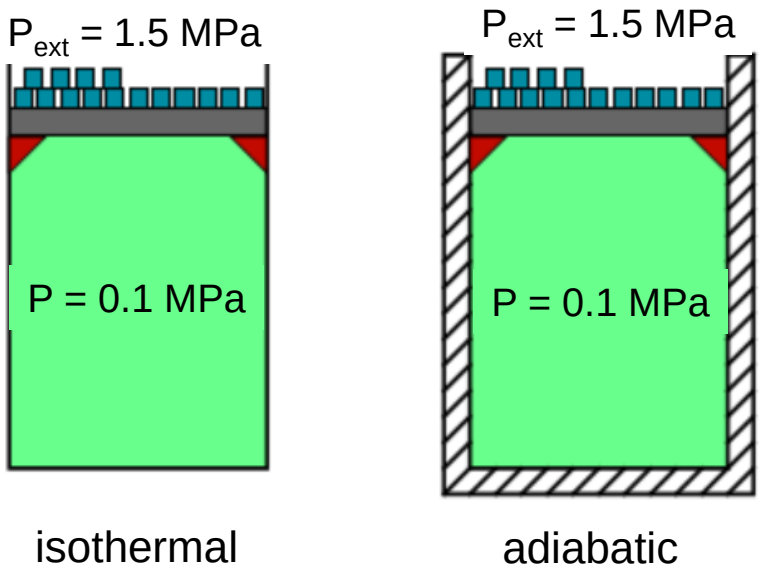
- Supplement textbook
- Office hours
- Assignments
- ConcepTests in class

  Static representations before dynamic simulations improves performance [1]

1. Bodemer, D., Ploetzner, R., Bruchmuller, K., Hacker, S., *Instr. Sci*. 33, 73 (2005).

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



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 imagin**e."

"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.”

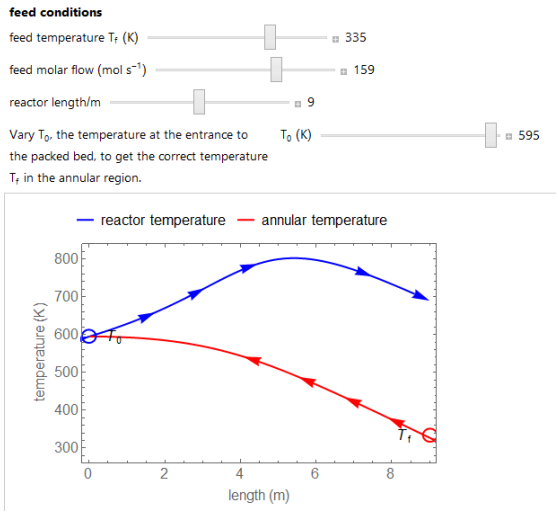
“Interactive simulations are also very useful. The ability to visualize the more complicated systems was key to understanding the phase equilibrium problems involving vapor-liquid-liquid equilibrium especially. They are also **pretty fun to mess around with in general**.”

“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.”

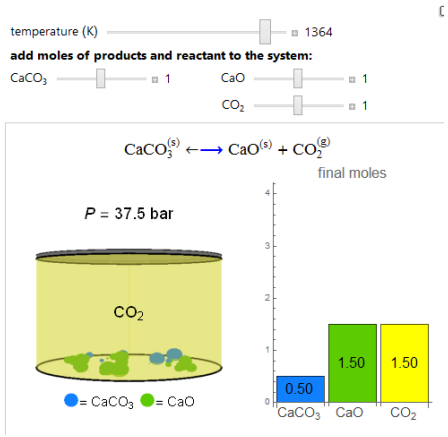
> 110,000 plays on Wolfram site

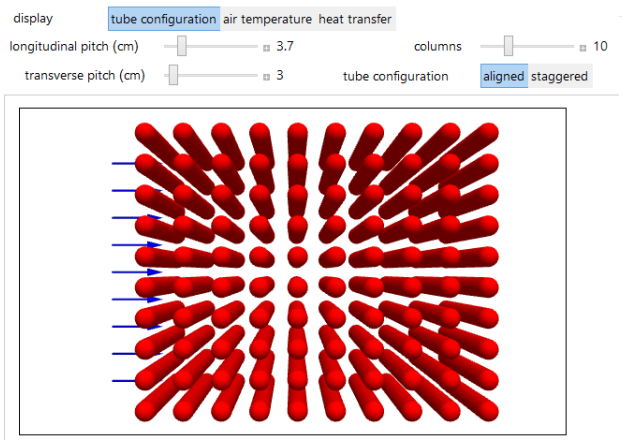
> 43,000 plays in 2015

Kinetics (25)

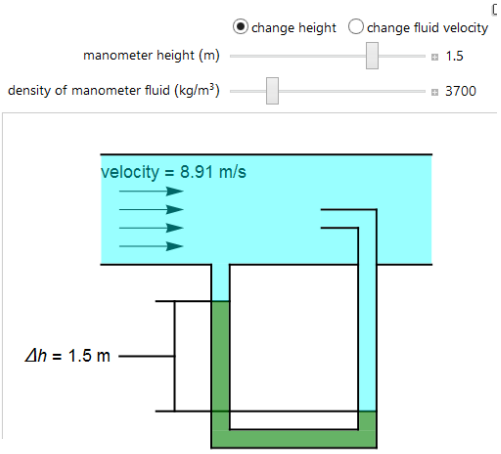


Thermodynamics (41)





Fluids (11)

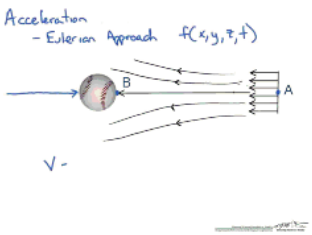


Heat transfer (6)

LearnChemE

Educational Resources for Chemical Engineering
University of Colorado **Boulder**

Department of Chemical & Biological Engineering

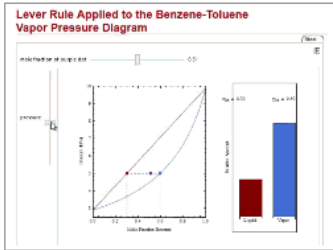


Screencasts

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.

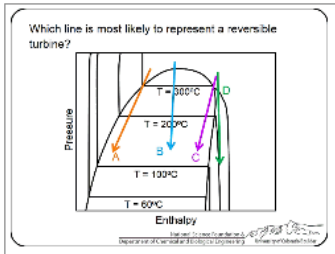
Interactive screencasts present a multiple choice question where the viewer chooses an answer within the video. The video response guides the user to the correct answer and explanation. For more information, see our interactive screencasts.



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.



Instructor Resources

see all instructor resources

ConcepTests challenge students with qualitative questions that are not answered by memorization. Used in tandem with peer instruction, ConcepTests 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, ConcepTests, reading assignments, screencast recommendations, homework problems and exam questions.

Instructors: Check out the resources to request access our 1300+ ConcepTest inventory or course packages.

Summary

- 85+ interactive simulations, 40+ for thermo
- Accompanying screencasts
- ConcepTests
- www.LearnChem.com

www.LearnChemE.com

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

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

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

ConcepTests: *Katherine McDaniel*