Interactive Virtual Laboratories

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Issue

For many students, thermodynamics is a challenging, and even scary, class.

It deals with abstract concepts such as internal energy, enthalpy, exergy, and entropy. These properties are "emergent". They are the result of the ensemble behavior of the system's constituent particles. We believe that students lack a grounded understanding of how these macroscopic properties arise from this lower-level behavior, and that the current educational process insufficiently teaches these abstract ideas.

Our hope is that the simulations will provide fundamental understanding which will be applicable to real world engineering problems such as the air conditioning system show in Figure 1.

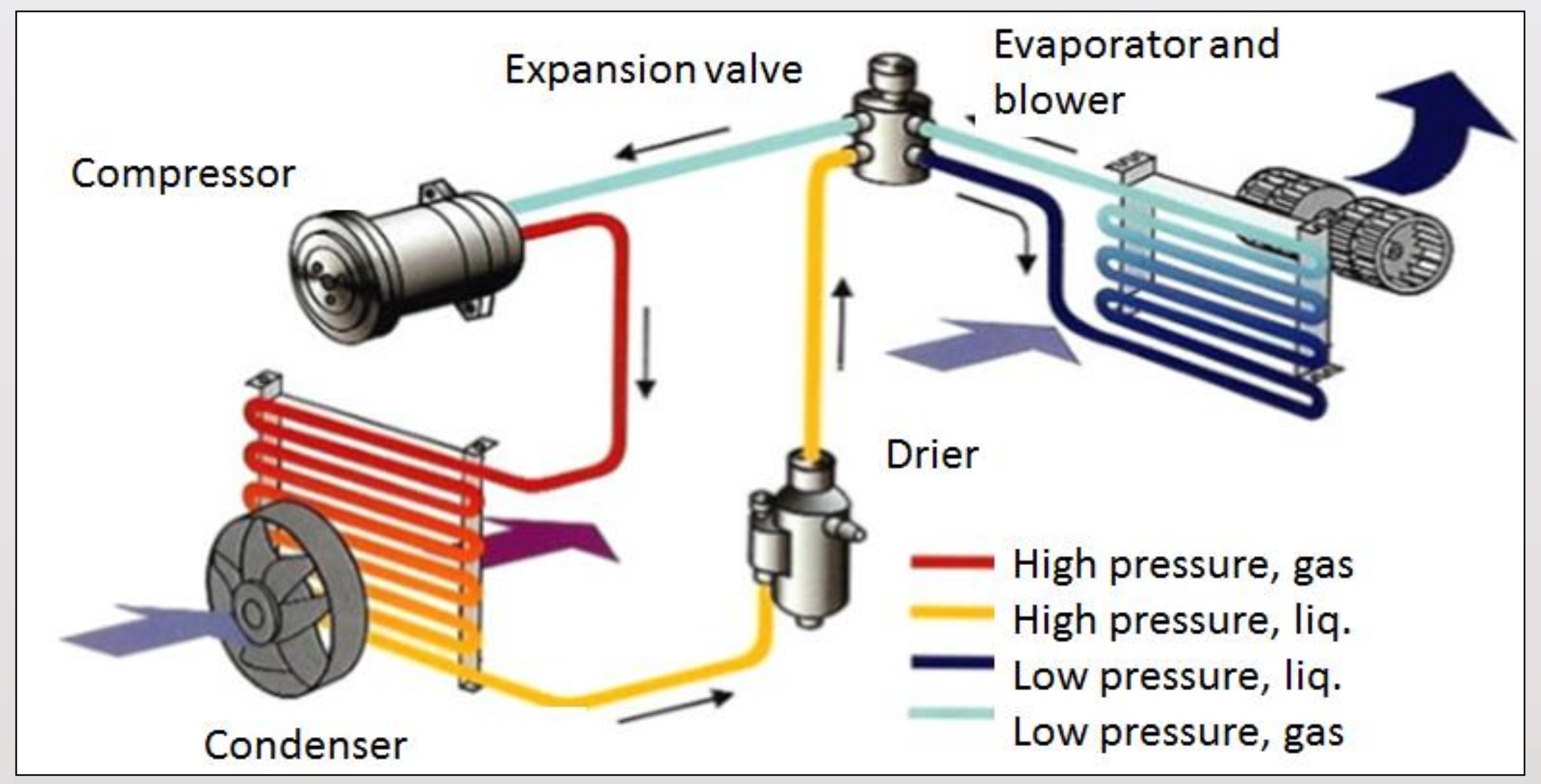


Figure 1- Designing an air conditioning system requires understanding of thermodynamic concepts. (http://www.jemservice.co.uk/aircondiag.png)

Objective

Create a framework for illustrating thermodynamic concepts.

Molecular-level computer simulations have been created to illustrate the connection between molecular behavior and macroscopic properties. These simulations aim to provide learners with a more robust framework with which to reason about thermodynamics. Six troublesome concepts have been identified, including:

- Work
- c_V vs. c_P
- Reversibility
- Reaction rate vs. equilibrium
- Phase equilibrium
- Hypothetical paths

Virtual Learning

University enrollment is increasing and conventional teaching methods are struggling to adapt to larger class sizes. The level of student-teacher interaction is decreasing and it is difficult to offer the same level of hands-on laboratory learning to larger groups.

Virtual laboratory simulations offer interactive learning to larger audiences than do conventional laboratory activities. Bucknell University and University of Colorado have created and are using online thermodynamics simulations in their university courses. (http://phet.colorado.edu/en/research)

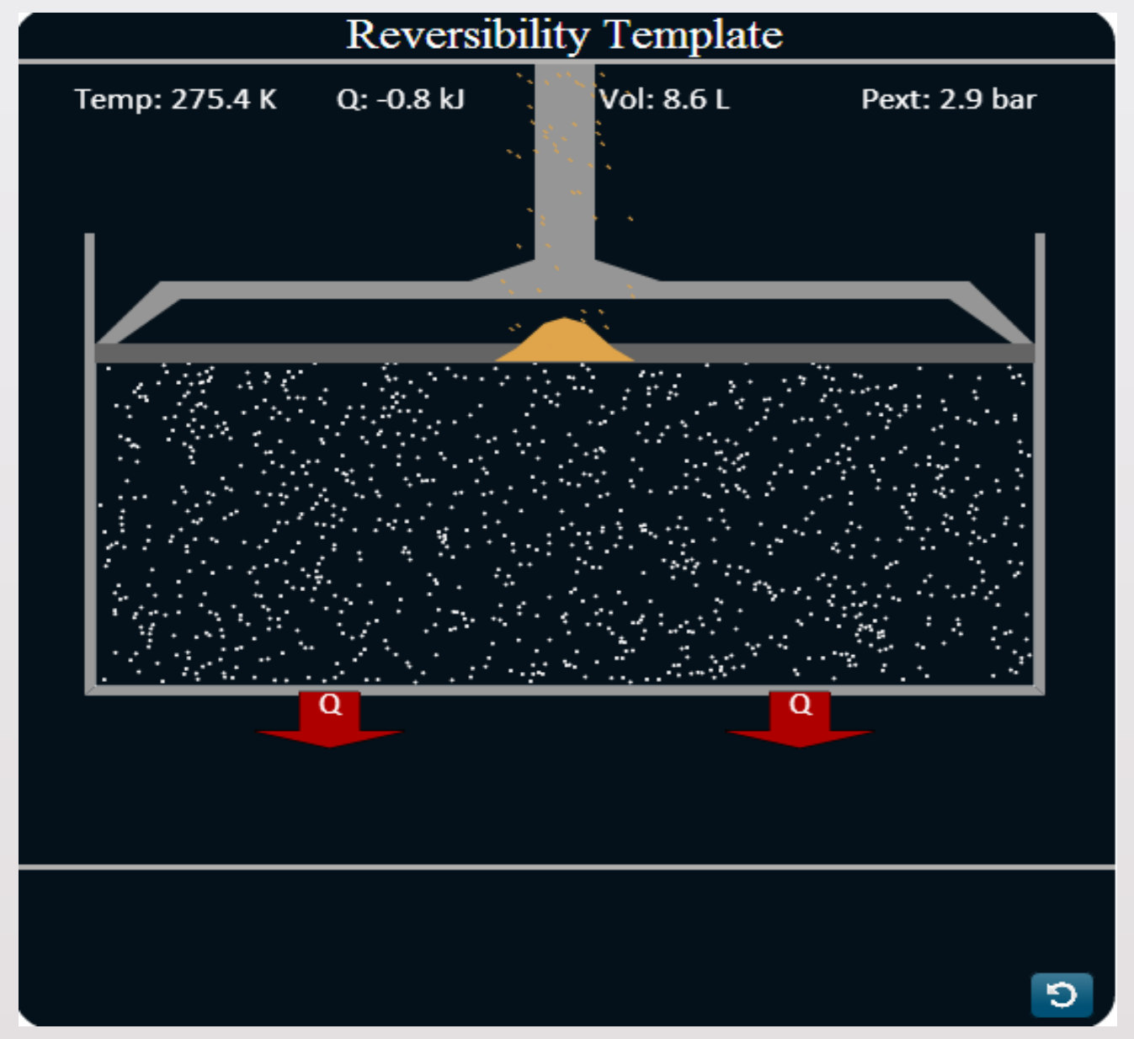
Virtual laboratories are used currently in a senior level unit operations class to give students a process engineering opportunity at minimal cost.

(http://cbee.oregonstate.edu/education/VirtualCVD/)

Threshold Concepts

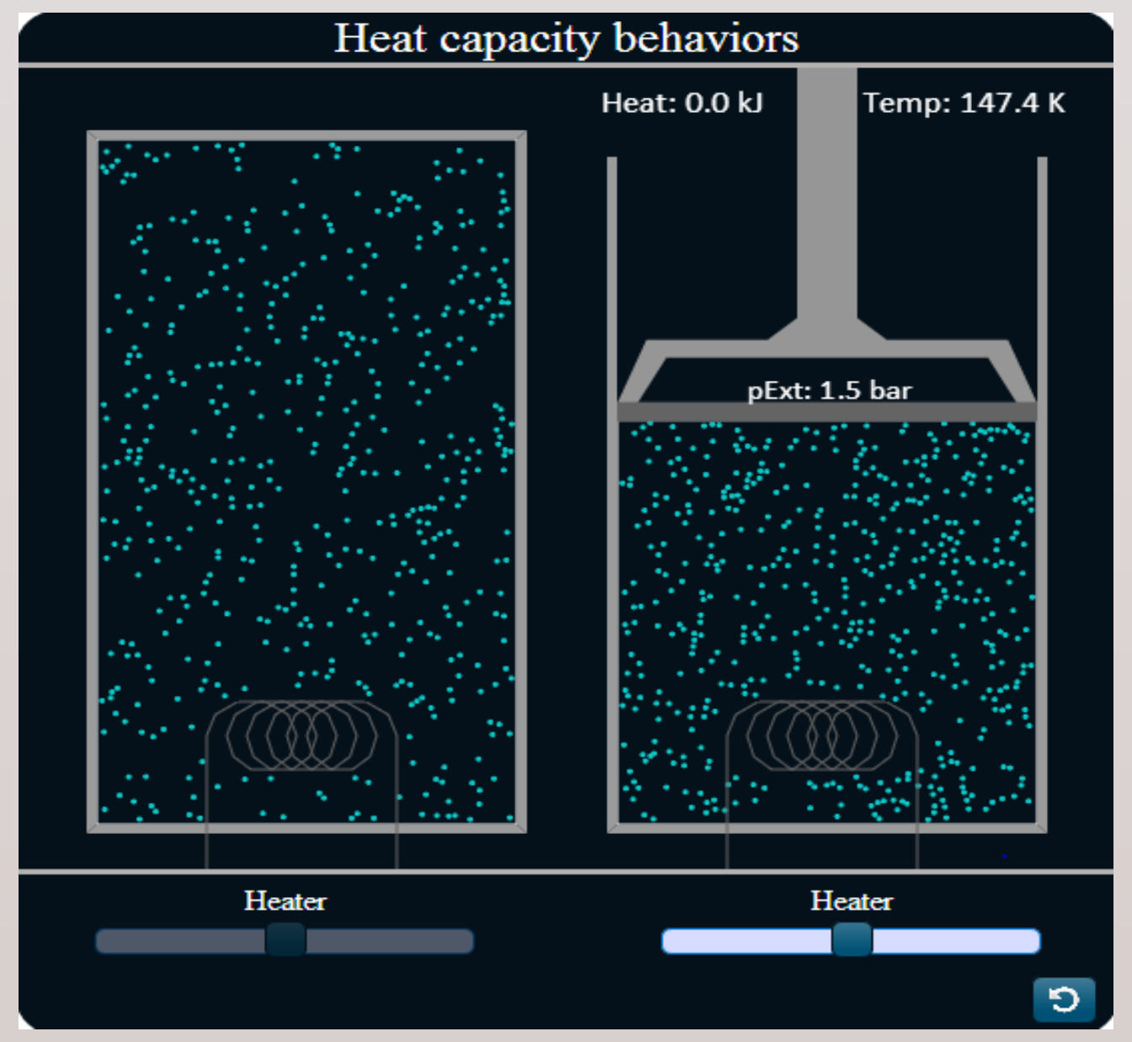
Threshold concepts are troublesome topics that once understood, lead to a deeper understanding of topic. We identified six threshold concepts to address and scenes from those simulations are seen below.

Reversibility: Learners compress a container with weighted blocks. The blocks get smaller until they are represented by sand, or infinitely small changes in driving force. Learners can see the amount of work added approach the amount of work recovered, grounding the differences between reversible and irreversible processes.



$$\Delta S_{sys} = 0$$

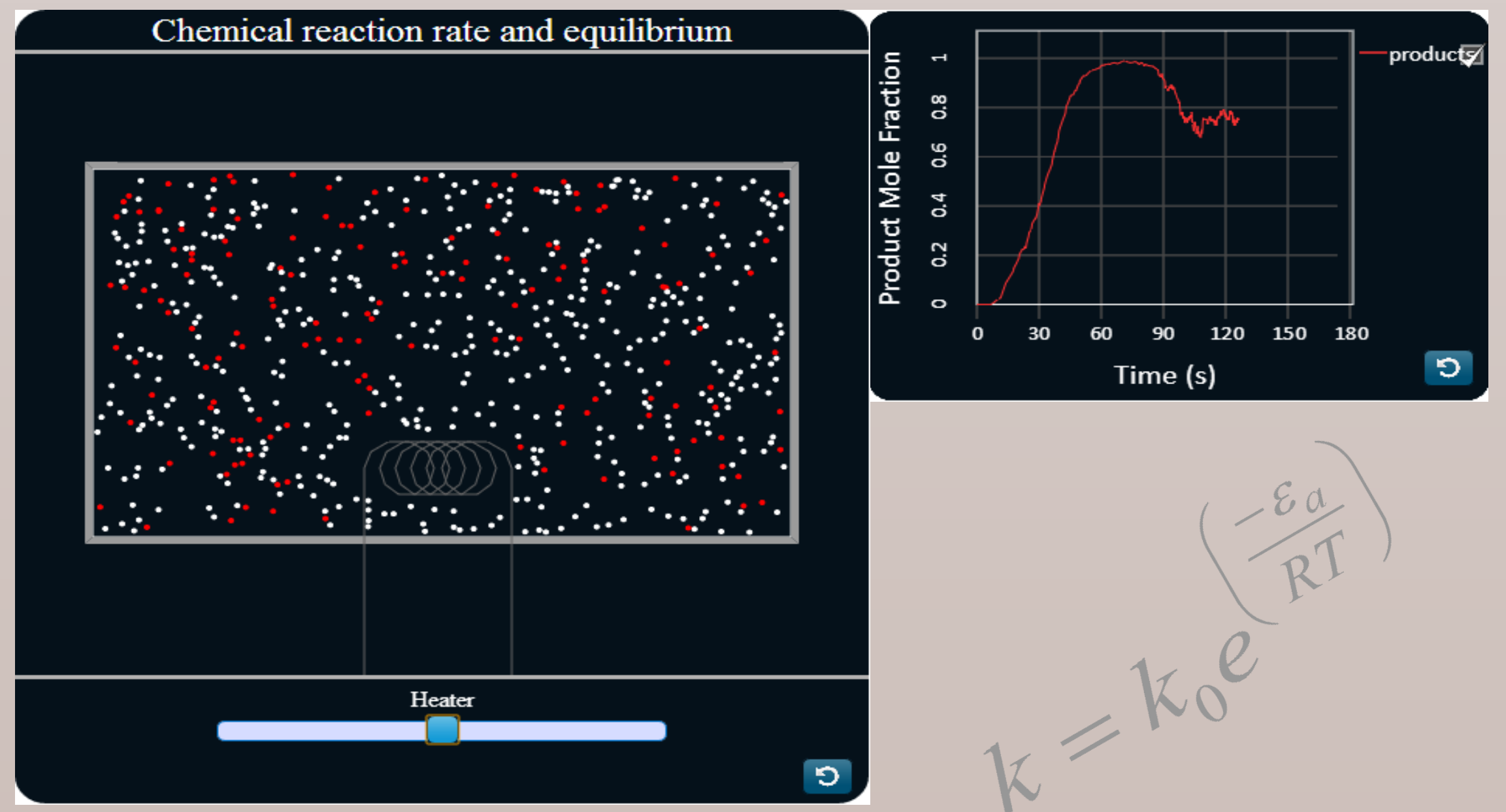
c_V vs. c_P: The distinction between heat capacity of constant volume and constant pressure is explored. Learners are given a constant volume container and constant pressure container. They are asked to heat the systems to the same temperature and compare the values of energy required.



$$c_V = \frac{3}{2}R$$

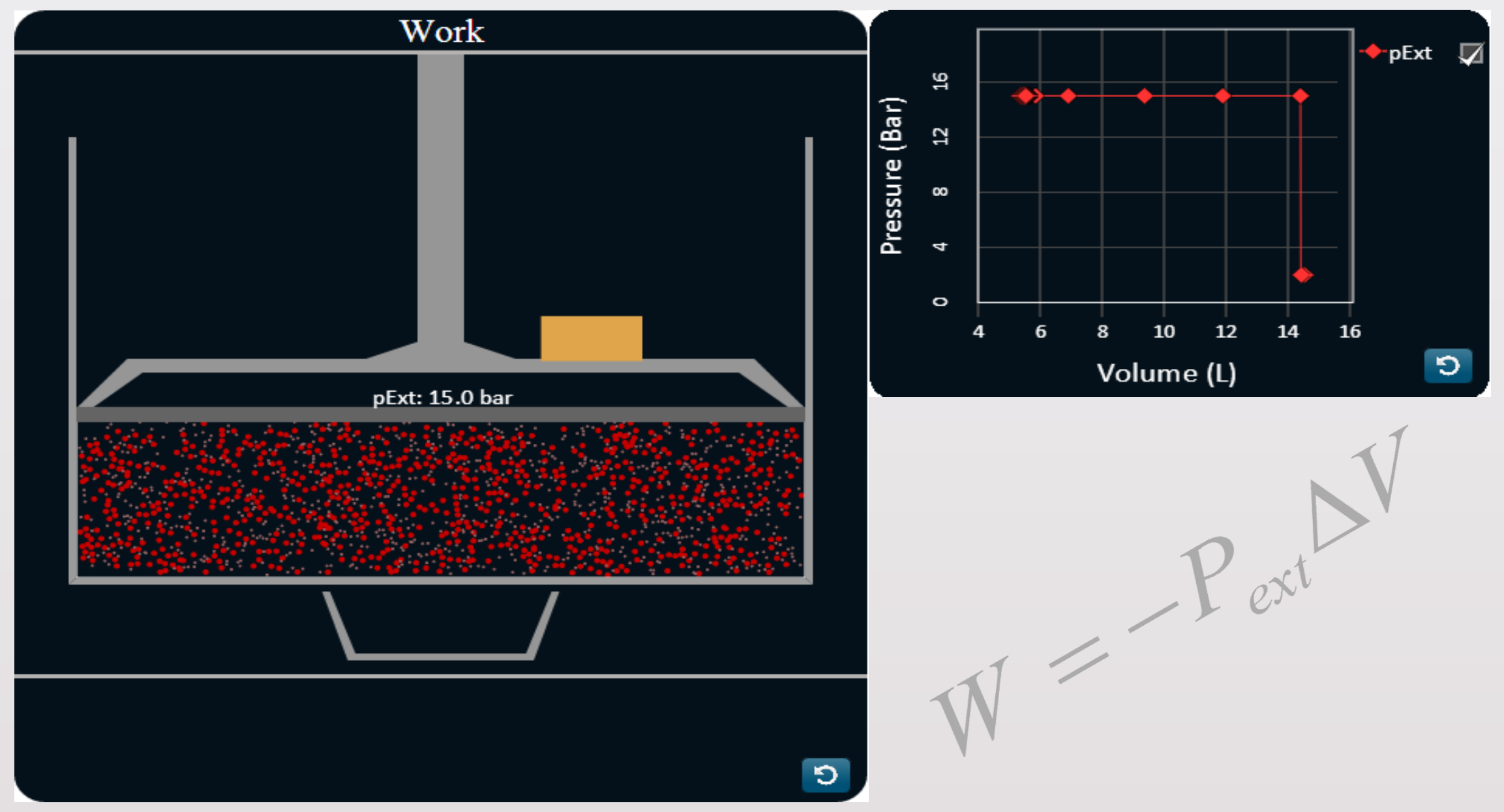
$$c_P = \frac{5}{2}R$$

Chemical reaction rate and equilibrium: The rate of a reversible reaction is measured at different temperatures. Chemical equilibrium is then examined and learners explore how temperature effects both rate and equilibrium.



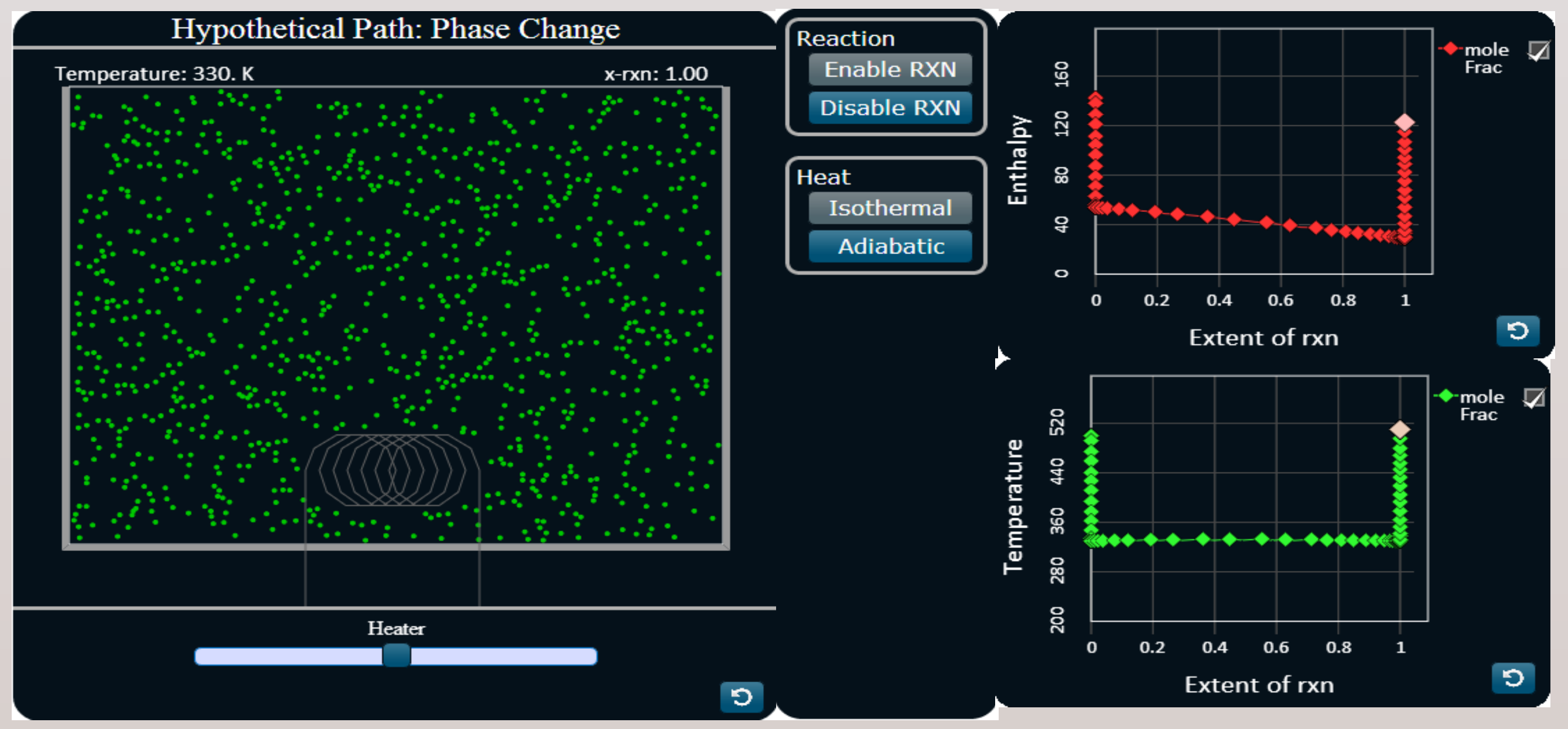
$$k = k_0 e^{\left(\frac{-\varepsilon_a}{RT}\right)}$$

Work: The origin of work is presented as the result of simple Newtonian mechanics. Learners see that momentum transfer from a piston to the molecules leads to a system energy change. They are then able to compress and expand a system under different external pressures to visibly see the amount of work.

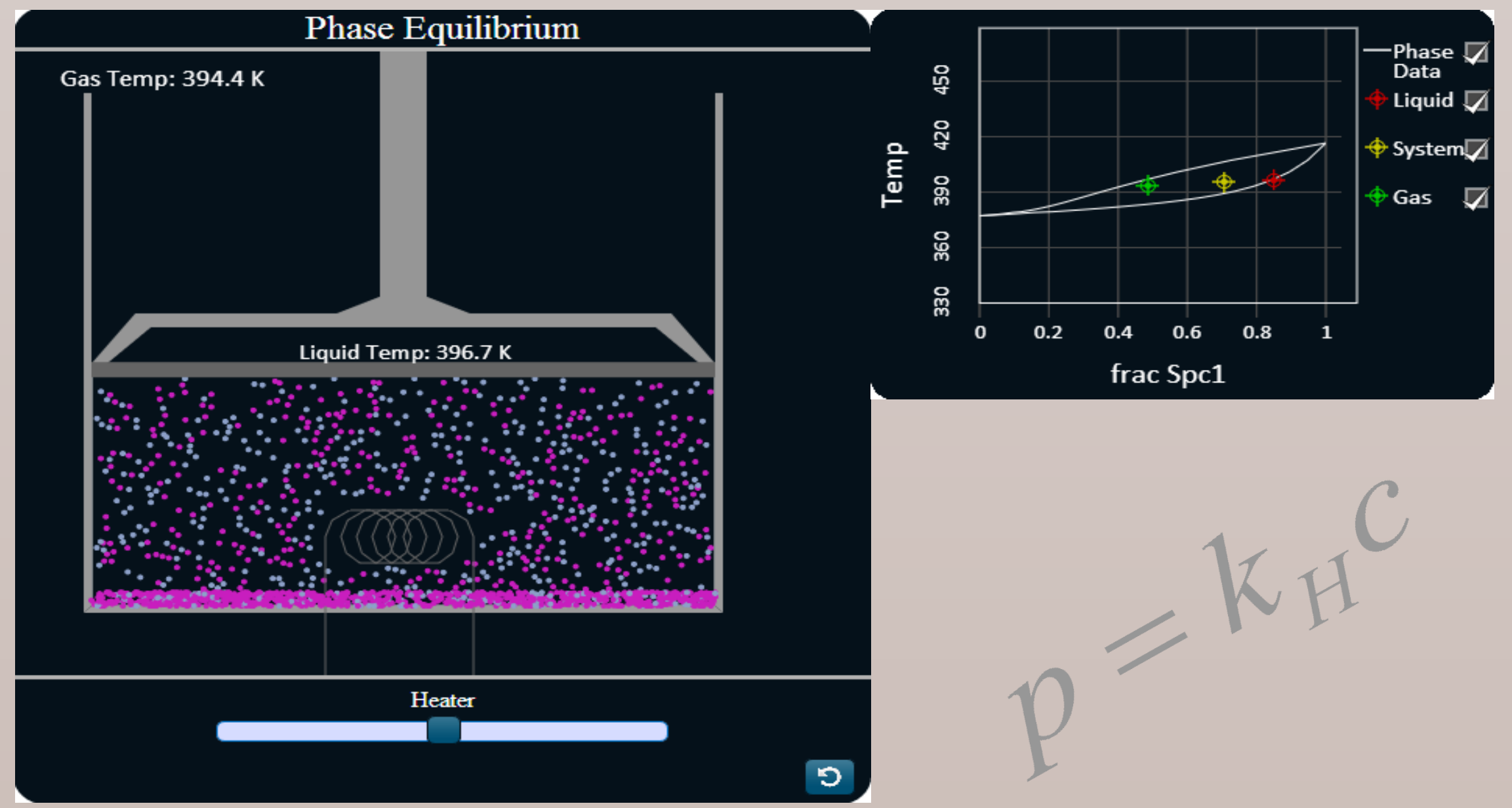


$$W = -P_{ext}\Delta V$$

Hypothetical paths: Hypothetical paths are essential to calculating macroscopic properties such as enthalpy, entropy and internal energy. This simulation allows learners to perform a reaction at a temperature with an unknown enthalpy of reaction (Δh_{rxn}). The learners are then able to create a hypothetical pathway to calculate the Δh_{rxn} and system enthalpy change.



Phase equilibrium: Multi-component, multi-phase systems are explored giving learners the ability to change the temperature and pressure of a system. Learners can see in real time how it affects a system's tie line and the compositions of the gas and liquid phase and the overall system.



$$p = k_H c$$

Usability Study

Eight participants who have completed engineering thermodynamics courses at Oregon State University were recruited to complete a simulation and answer questions about the experience. The interview responses were transcribed and analyzed. These provided feedback on the strengths and weaknesses of the simulations.

Students mentioned visual learning and student-simulation interaction as benefits of using the simulations. All of the students recommended the simulations be used in thermodynamics courses.

"Thermo is very hard to understand… It is hard to express with picture but with this simulation it turns the concepts into visuals. This simulation helped me understand how the thermodynamic concept works very well." -ChE Senior

"The interactive aspect of… real early on in the simulation when I could drag down the bar and see how the momentum was transferred to the molecules… that was really cool." -ME Senior

Implementation

The simulations are created using HTML, CSS, and JavaScript, and are available on the web. The physics are computed using Newtonian behavior, and thermodynamic gas properties emerge from the ensemble behavior.

The simulation is displayed using the HTML <canvas> tag, which allows for hardware accelerated rendering. Each simulation is defined by a data file, which describes each scene and the associated text. The simulation platform interprets the data and displays the physical setup.

What's Next?

The simulations will be integrated into thermodynamics classes in the School of Chemical, Biological, & Environmental Engineering through the AIChE Concept Warehouse. The Concept Warehouse presents the students with online questions and allows the instructor to instantly see student responses.

Simulations' effectiveness will be analyzed by comparing current student performance on Concept Warehouse questions against performance from past years.

Through Concept Warehouse, the simulations will be made available to thermodynamics instructors at other universities.

Acknowledgements

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