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DEVELOPMENT OF INTERACTIVE VIRTUAL LABORATORIES TO HELP STUDENTS LEARN DIFFICULT CONCEPTS IN THERMODYNAMICS

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INTRODUCTION

Virtual laboratories are receiving attention as an alternative way to engage students and promote learning as technology becomes more integrated into classroom instruction.^[1] Physics educators at the University of Colorado have developed a set of virtual laboratories they call PhETs that allow students to explore representations of physics phenomena, some of which are impossible to view in a laboratory environment.^[2] The PhET simulations are designed to allow students to construct their own understanding of physics and are useful as a part of learning activities in class.^[3] PhET simulations are open ended, so learning activities need to guide, but not constrain, students using them. Research on this type of virtual laboratory has shown that it significantly improves learning.^[4,5]

We have designed the Interactive Virtual Laboratories (IVLs) to target important engineering concepts, similar to what PhETs provide for physics education. However, unlike PhETs, the Interactive Virtual Laboratories are explicitly scaffolded. They are not open-ended sandbox environments, although they do allow some level of experimentation. Instead, students are guided by prompts and must answer numerical and discussion questions to proceed. Students are expected to interact with the simulations in intentional ways to gain understanding and answer questions. The approach taken in designing them was to target a specific thermodynamics threshold concept in each simulation.

Meyer and Land^[6] introduced threshold concept theory as a way to view learning and curricular progression. They

describe threshold concepts as concepts critical for understanding a topic. Without this understanding, a learner cannot progress. Their definition of threshold concepts differ from



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“core concepts,” or conceptual building blocks that progress understanding of a subject, by specifying four main features of threshold concepts: transformative, irreversible, integrative, and troublesome. Threshold concepts are transformative because they create a significant shift in how learners perceive subjects on a fundamental level, sometimes even leading to a transformation of personal identity. They are irreversible because learners are unlikely to forget their shifted perspectives after crossing a threshold. They are integrative because they expose the previously hidden interrelatedness of subject knowledge. Finally, they are troublesome in that they are conceptually difficult for students to learn, often yielding counterintuitive or unexpected results. In engineering, there is recent attention to curriculum development based on identifying threshold concepts,^[7] but we must also be aware that many instruction approaches do not fundamentally reform faulty student assumptions.^[8] We propose that threshold concept theory is a useful framework for identifying topics for Interactive Virtual Laboratories, and Interactive Virtual Laboratories are useful tools for enabling students to learn threshold concepts.

We identified a broadly defined set of threshold concepts for the Interactive Virtual Laboratories that range from misconceptions of first principles to capabilities needed to solve problems. These threshold concepts include understanding hypothetical paths, the difference between reaction rate and equilibrium, the difference between constant pressure and constant volume heat capacities, the conditions necessary for a reversible process, and the mechanism through which pressure-volume work adds energy to a system. The last two threshold concepts are the focus of the current study. We chose these threshold concepts based on information from three sources. First, we analyzed student written responses to conceptual questions using a database system, leading to an identification of common misunderstandings.^[9,10] Second, we referenced the literature on misconceptions in chemical engineering and physics as a basis to confirm our identification of threshold concepts. Third, we used the last author’s domain knowledge and twenty years of experience teaching thermodynamics to identify threshold concepts.

Elby^[11] examined reasons why physics students often study in unproductive ways, such as focusing on memorizing equations and solution algorithms, rather than gaining a deep understanding of physics. He surveyed 106 college physics students, asking how they study for class in order to do well in the course. Furthermore, he asked them to compare their study methods with how they would study if they were only interested in learning physics deeply, without grade pressure. He found that many students use rote-based study methods because they believe it will help them on exams, even when they are aware that they are not learning the material in a way useful for real-life application. In developing the Interactive Virtual Laboratories, we took a highly conceptual approach.

To correctly answer problems, specifically discussion questions, students must use conceptual understanding to synthesize data. A rote understanding leads to incorrect numerical answers and poor discussion answers.

Two research questions are addressed in this study:

- (i) *How does the way students engage with the simulations affect how they comprehend the targeted threshold concept: Do they complete the simulations with a singular focus on equations and variables, or do they use a more conceptual approach by solving problems using the information depicted in the simulation display and graphs?*
- (ii) *How do students perceive the simulations: Do they view them as useful learning tools, and what recommendations do they make for them?*

INTERACTIVE VIRTUAL LABORATORIES

The Interactive Virtual Laboratories are a series of two-dimensional simulations designed to address targeted threshold concepts. They are available for instructors to use through the AIChE Concept Warehouse website (<http://cw.edudiv.org/>). They were developed following design principles for educational multimedia. We used Mayer’s^[12] approach involving cognitive load theory, which asserts that students have a maximum information processing capability. Excess information overloads the student’s learning channels and reduces information processing. We also incorporated the findings of Scalise *et al.*^[13] from a synthesis of the results of 79 studies of virtual laboratories to find best practices for virtual laboratory design, including an emphasis on focal points rather than step-by-step instructions, basing design to minimize cognitive load, and introducing scaffolding with fading. Finally, we kept in mind the design principles suggested by Mayer and Moreno^[14]:

- **Multiple representation principle:** *Explanations in the form of a combination of words and pictures are more effective than words or pictures alone.*
- **Contiguity principle:** *Simultaneous presentation of words and pictures works better than presentation in succession.*
- **Spatial contiguity principle:** *Closer proximities of text and image enhance the learning outcome.*
- **Personalization effect:** *Deeper learning can be achieved by conversational style text rather than formal style text.*

The IVLs are written in JavaScript and HTML for easy incorporation into student laptops and web browsers. They make use of the HTML5 Canvas element to draw two-dimensional objects for simulating molecular behavior. Each simulation depicts ideal gas molecules as perfectly elastic spheres. Individual labs consist of examining the effect of different processes on the molecules, such as compressing

or heating them, while performing numerical computations and answering discussion questions. Each individual simulation targets a single threshold concept and adheres to a scaffolded design following the predict-observe-explain technique proposed by Gunstone and Champagne.^[15] Before interacting with the simulation, students are asked to predict what will happen if they make a change, such as raising the temperature or increasing pressure. Students then perform and observe the virtual experiment and, afterwards, explain if their prediction was accurate and what effects the change had using information present in the simulations. The goal of the simulations is to allow students to describe molecular and macroscopic thermodynamic phenomena in terms of the underlying physical behavior using conceptual knowledge. In real experiments, students cannot see molecular interactions,

and their understanding often becomes abstract and removed, existing only in the form of equations. The Interactive Virtual Laboratories allow students to see how molecular interaction gives rise to the phenomena described by mathematical equations. This paper focuses on how students use two IVLs, one based around the thermodynamics threshold concept of pressure-volume work and the other on that of reversibility.

1. **Pv Work.** Work is an abstract concept, and it is often difficult for students to understand how the act of doing work on a system adds energy. Intuitively, students may understand that compressing a gas causes it to undergo an increase in temperature, or a 'heating up'. The purpose of the work simulation is to give students a physical model explaining why doing work on a gaseous system adds or removes energy from a physical and molecular perspective, ultimately showing students that work adds energy through

an exchange of momentum and kinetic energy between a system and its surroundings. Students develop the understanding that a moving, perfectly elastic sphere colliding with a wall moving towards it rebounds with a speed greater than if the wall had been stationary. By using this simulation, students can apply their knowledge of elastic collisions to thermodynamic work.

The simulation uses a progressive understanding approach to assist conceptual learning. It first introduces students to the idea of Pv work in the context of a single molecule. The molecule is represented by a single sphere in a closed container as shown in Figure 1. The molecular speed is shown every time the molecule collides with a wall. Students are allowed to move the upper wall of the container by clicking and dragging a

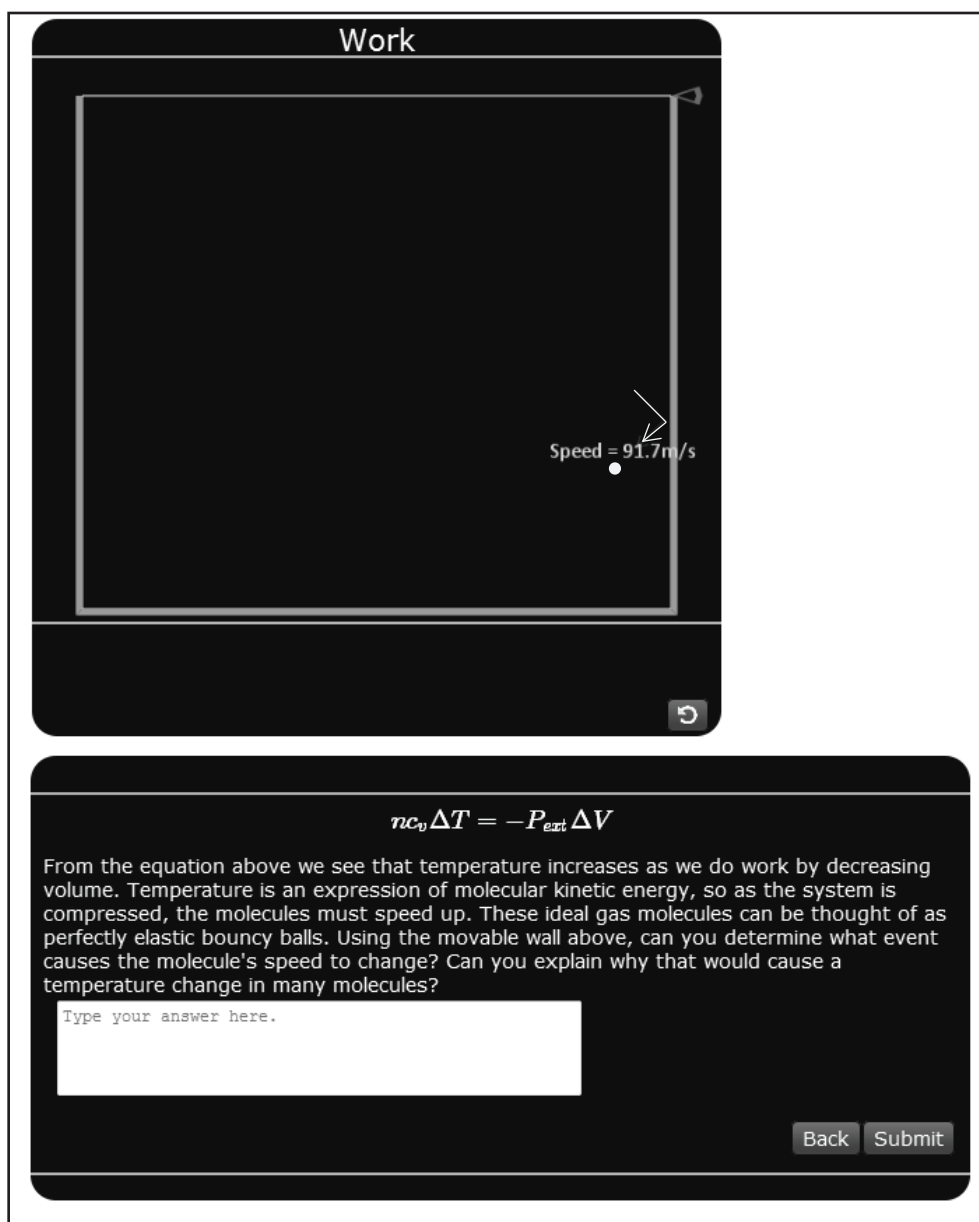


Figure 1. Screenshot of the single molecule in a closed container. The top wall can be moved by clicking and dragging the arrow to the right of the container. The molecule speed is displayed with every wall collision and changes when colliding with a moving wall.

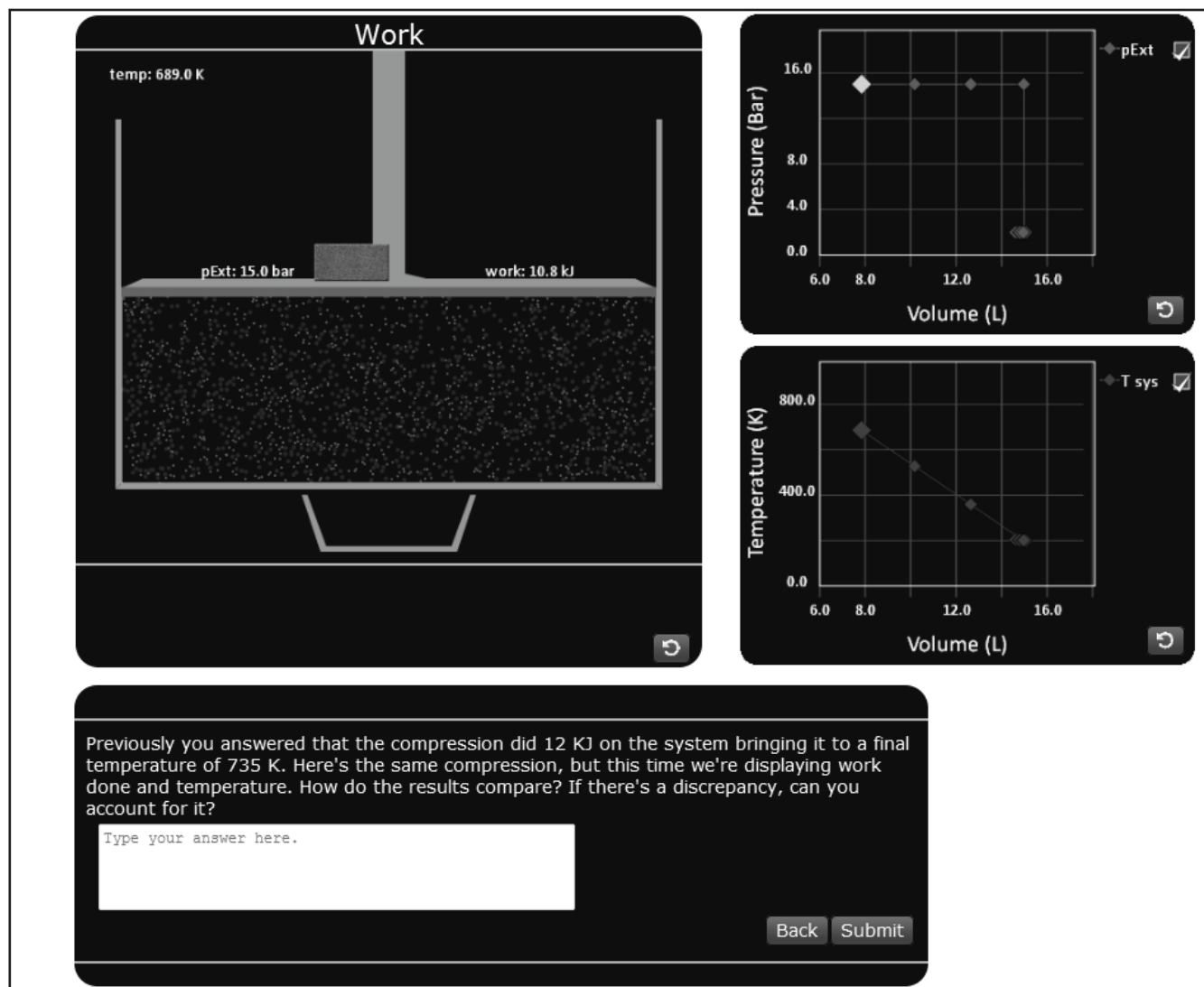


Figure 2. Screenshot of the compression process with temperature and work displayed. Pv and Tv graphs are to the right of the system.

slider. When students move the wall so that it is approaching the molecule when they collide, the molecule speeds up through an exchange of momentum. Students are then asked to explain how the temperature relates to the molecular kinetic energy and why an increase in molecular speed leads to an increase in system temperature when many molecules are present.

The simulation then progresses to a more complicated system with more molecules, as seen in Figure 2. Students are asked to compress and expand the system while performing numerical computations to calculate values of work and temperature change. By applying knowledge gained from the single molecule section of the simulation, students can see how the molecular speed distribution changes as the system is compressed. Molecules that collide with the compressing wall speed up first before distributing their kinetic energy to the other molecules as the system reaches equilibrium.

Students can also see why expanding against a lower pressure leads to a much smaller temperature change than the preceding compression.

2. **Reversibility.** The purpose of the reversibility simulation is to give students a physical model to show the difference between reversible and irreversible processes. Often, students assume real processes can be approximated as reversible when such an assumption is inappropriate. The simulation goal is to show students the conditions necessary for a system to be reversible and help students see when assumptions of reversibility are appropriate. Similar to the Pv Work simulation, the Reversibility simulation takes a progressive understanding approach and primarily consists of a series of isothermal piston and cylinder assembly systems. Students are asked to compress and expand the system between two different states several times. Each time they perform the process, they do it in a greater number of steps. Ultimately, students are expected

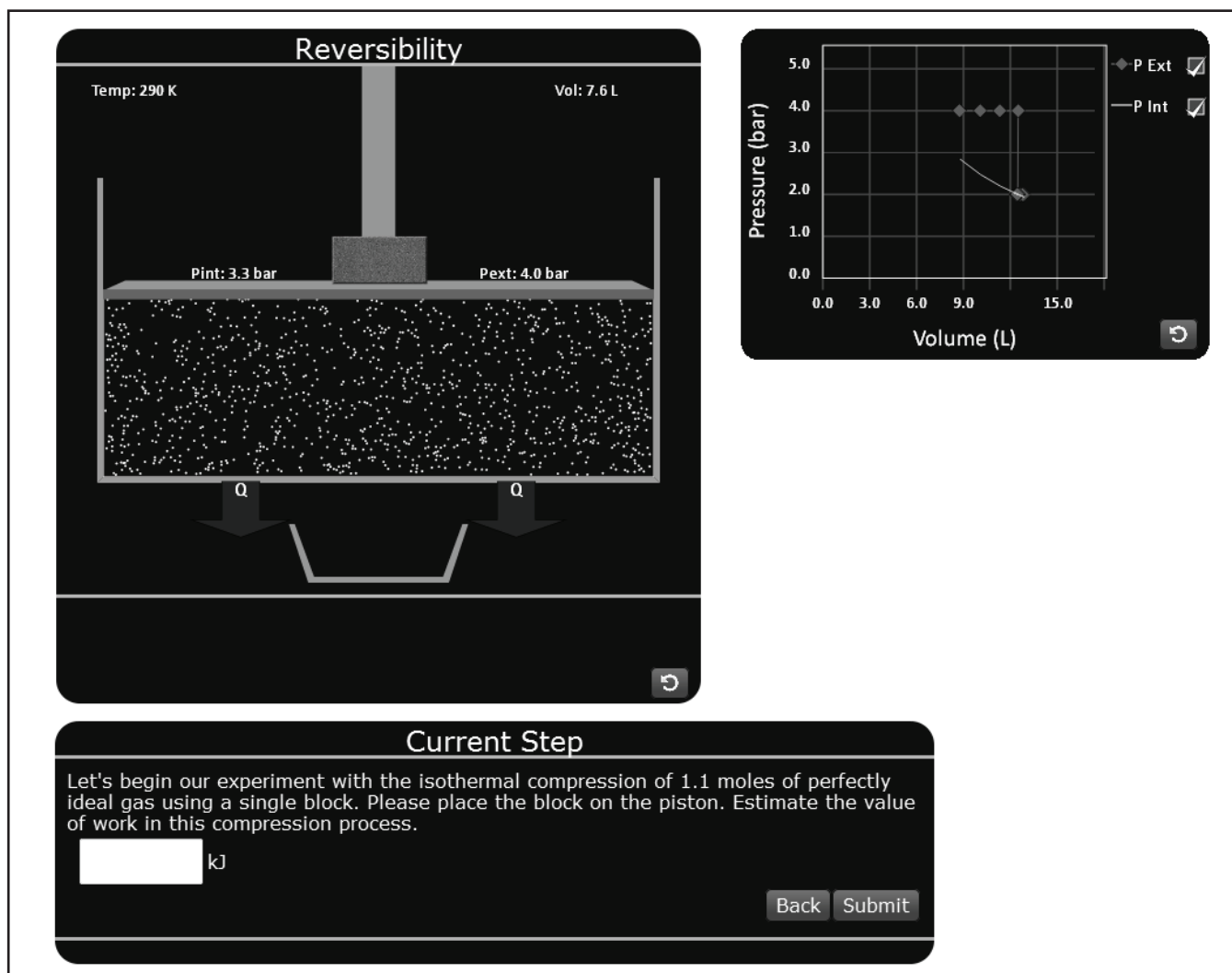


Figure 3. A one-step compression process.

to see that a system must always be in equilibrium with its surroundings for a process to be reversible, meaning only differential changes in input are allowed. Another result is that a process approaches reversibility as it is performed in a greater number of steps with smaller step size.

The simulation starts with a compression process in a single step, as shown in Figure 3. Students are asked to compress an ideal gas system by placing a single block on a piston and allow it to come to rest. Students then expand the piston by removing the block. Students are able to see that the process is irreversible, as the amount of work done on the system initially is not what is gotten out during expansion.

Next, students compress the system using two steps instead of one, and the same is repeated for expansion. Students are expected to see that it requires less work to compress the system to the same final state in two steps than in a single step under constant pressure. They are also expected to see that more work is done by the system when it expands in multiple steps.

Students then perform one more compression and expansion. However, this time they are given very small grains of mass to place on the piston as shown in Figure 4 (following page). This process is supposed to be approximately reversible, as the amount of work required to compress the system is equal to the work done when the system expands. Students are expected to see that the process approaches reversibility as the number of steps increase and the changes in input become infinitesimal.

The Reversibility simulation shows that reversible processes must always be in a state of equilibrium and therefore require an infinite number of infinitesimally small steps to complete.

METHODS

Eight individuals took part in the study described in this paper: four third-year students and four fourth-year students. Seven of the eight students were undergraduates in chemical engineering while one was an undergraduate in mechanical

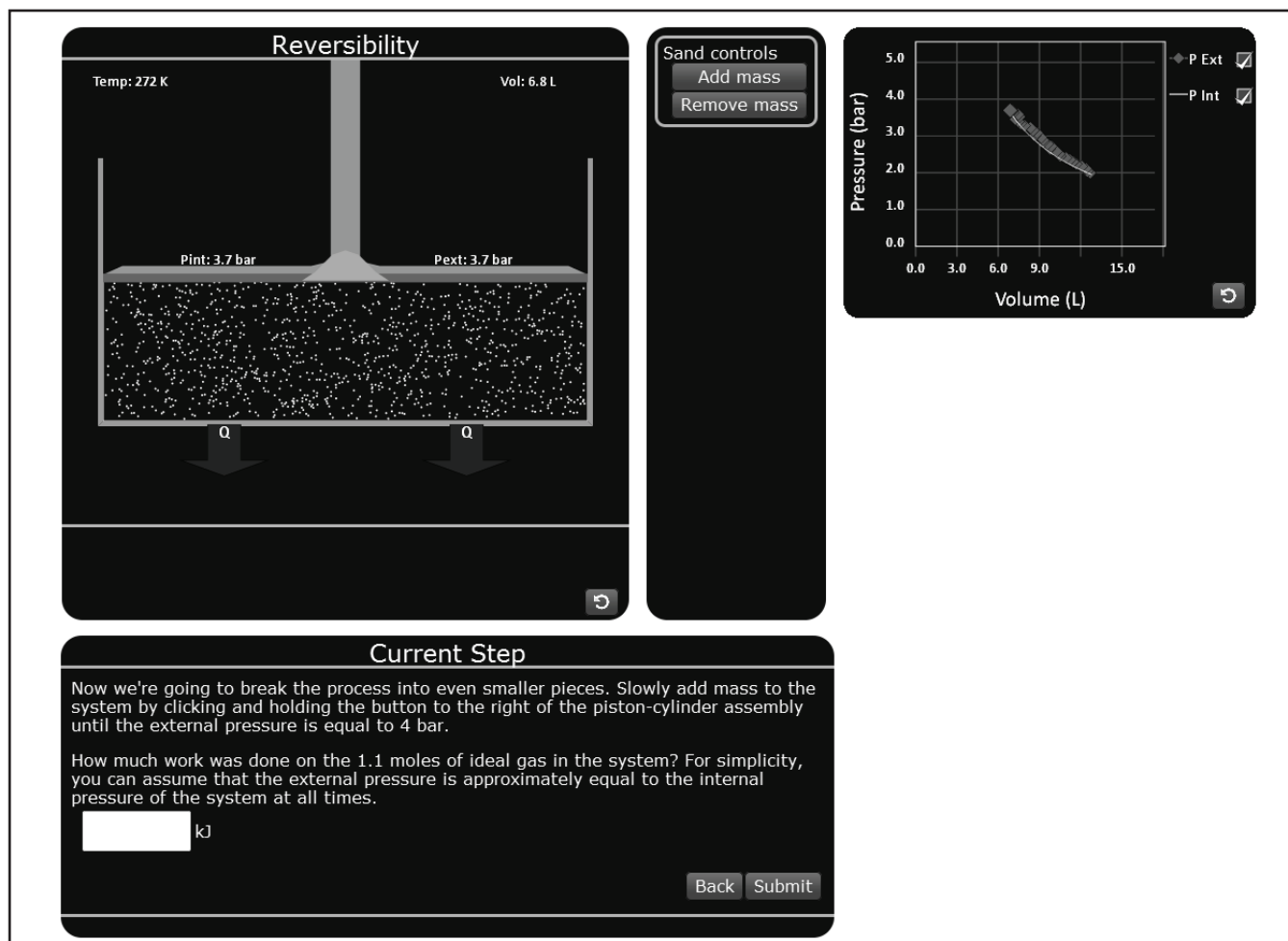


Figure 4. An approximately reversible compression using differential sand elements. Sand is placed on or removed from the piston using the buttons to the right of the piston.

engineering at the time of the study. All had taken at least one undergraduate course in engineering thermodynamics. The study was approved by the IRB and all students signed informed consent forms.

Participants completed either the Work or Reversibility IVL. An interviewer observed participants while completing the simulation. Students had access to a chemical engineering thermodynamics textbook, *Engineering and Chemical Thermodynamics*,^[16] and the internet while completing the simulations. We used video screen capture technology to record the screen and audiotape the students working on the simulation. We used a “think aloud” protocol where students verbally described their actions and thought processes while working. Interviewers did not answer any questions directly related to the topics covered in the simulations. However, they did answer general questions about the simulations and interview process as well as asking participants to explain their actions if unclear. Students who ran into difficulties with a question and were unable to answer it were told to make a guess and continue.

After completing the simulation, students were asked a series of questions assessing how well they understood the material and asking for feedback on the simulation design. The interviewer first asked for general impressions and feedback for the simulation in addition to asking what the participant thought was the main point of the simulation. The interviewer asked the students questions about their thoughts on the simulation: the usability, usefulness for learning, and ways they might be incorporated into classes. Interviewers also asked students to compare their performance and learning in two different chemical engineering thermodynamics classes, one that uses a traditional lecture-based format and one that incorporates technology-assisted active learning pedagogies. Finally, interviewers asked a conceptual question relating directly to the main purpose of the simulation. On Work, students were asked to describe the mechanism through which Pv work adds energy to a system. On Reversibility, students were asked what conditions are necessary for a process to be reversible.

To answer the first research question about how students engage with the Interactive Virtual Laboratories, we examined the recordings of students completing the simulations as well as the transcribed post-simulation interviews. We looked specifically at the section of the simulation where the main conceptual idea was introduced to see if the student gained a conceptual understanding of the physical phenomenon. We also tried to see how the student went about making sense of the information. We compared these data to how the student answered the conceptual question at the end of the interview to see if the student retained the information if they understood it at first or if they managed to make sense of it later if they did not.

To answer the second research question about student perceptions of Interactive Virtual Laboratories, we analyzed the transcribed post-simulation interviews. We looked specifically for statements where the participant indicated a feature of the simulations that was particularly useful or confusing. We also looked for suggestions made by the students to help improve the simulations.

RESULTS

The approach students took to complete the simulations can be generally divided into two distinct groups: equation-based and concept-based. The IVLs were designed to elicit a concept-based approach in students. The reasons some students used an equation-based approach and its effect on their learning when using the simulations is of particular interest to us. In general, students who used a concept-based approach focused largely on the physical phenomena being modeled by the simulations and used the data generated by the simulation to formulate explanations during the discussion questions. On the other hand, students who used an equation-based approach focused on finding an equation that mathematically relates variables while answering the discussion questions, often without noticeably giving attention to the pertinent physical phenomena. Of course, none of the students used an approach that was solely concept-based or equation-based. Some participants switched approaches depending on the question being asked; others switched from equation-based to concept-based when they found that the former was not sufficient to complete the simulation satisfactorily.

In the following explorations of simulation use, we use select quotations to illustrate student thinking and reasoning. Additional quotes are presented in Appendix A of reference 17, which provide insight into how students engaged with the most conceptual portions of the simulation, along with additional feedback and suggestions for simulation improvements.

PV WORK

Perhaps the most illustrative example of the contrasting equation-based and concept-based methods is the different ways Alfred, David, Beverly, and Carl completed the single

molecule simulation on Pv Work. The single molecule simulation allows students to experiment with a single molecule in a closed container and shows them that work adds or removes energy from a system through an exchange of momentum and molecular kinetic energy. The purpose is to give students a way to figure out for themselves what causes the energy and temperature to change, instead of making them guess using abstract ideas about molecular kinetics.

Alfred

Alfred's approach to the single molecule was highly concept-based. He noticed that the molecule speeds up when it collides with the wall, as shown in the following quotation:

"Oh, it's when it hits the moving wall. That's what will cause it to speed up because when the wall's moving, it smacks into it [...] and when I don't move the wall, the thing doesn't change speed because all of the collisions are perfectly elastic. That makes sense."

From this statement, we can see that Alfred notices that the molecular speed only changes when the molecule collides with a moving wall. A stationary wall does not lead to a change. Alfred also explains how this information can be applied to the temperature change in a system of many molecules:

"It causes a temperature change in many molecules because it increases the average speed of all the molecules distributed inside the container when they all hit the slowly approaching wall."

Alfred also answered the final conceptual question during the interview correctly, indicating that he was able to use the simulation to understand the main threshold concept.

David

David, similar to Alfred, also used a concept-based approach when completing the single molecule simulation. He noticed how momentum was transferred during the collision with the moving wall. He responded to the final conceptual question as follows:

"So when you change the volume, that's doing work. And so that is introducing momentum that is transferred to the molecules which adds kinetic energy which gives them a higher internal energy, which then changes the internal temperature."

This response indicates that David understood the threshold concept and related it to the simulation.

Beverly

In distinct contrast to Alfred and David, Beverly used a largely equation-based approach when completing the single molecule simulation. In this example, we can see that she focuses on the ideal gas law in a situation when its use is inappropriate:

"Well it speeds up when you have a smaller space, so does the ideal gas law matter? Is that what they're trying to talk about?"

She states that the molecule's speed increases as the volume is decreased. However, this is not necessarily the case. She does not comment on the fact that the molecule only speeds up during a collision with the moving wall. If the volume decreases without the molecule making contact, then the molecular speed stays constant. Beverly did attempt to take a concept-based approach after she became aware that the ideal gas law could not provide a sufficient explanation:

"When the molecule collides with the walls, the speed will increase, and when there is a smaller space, there are more collisions."

Unfortunately, she confused the temperature dependency on molecular kinetic energy with a dependency on "number of collisions." During the final conceptual question, Beverly attempted to give an answer before withdrawing it, stating that she did not know.

Carl

Carl took a solely equation-based approach to the single molecule simulation, unlike Alfred and David who successfully took a concept-based approach, and Beverly who tried a concept-based approach unsuccessfully. He attempted to explain the phenomena using an open-system energy balance:

"Energy of the system is ΔU over dt plus Δ of kinetic energy over t plus Δ of potential energy over time, and that's equal to heat plus work. And this is an adiabatic process, so heat is zero."

Carl does not take into account that he is not using an open system. He also confuses the macroscopic kinetic energy term in the balance with molecular kinetic energy. Similar to Beverly, Carl realizes that his reasoning is insufficient to explain what causes a temperature change and says that he does not know the answer. He also provided an incorrect answer during the final conceptual question.

We cannot determine what exactly causes students to take one of the two general approaches, but it appears to depend largely on the student's predisposition. Student orientations are fairly robust; students who customarily take an equation-based approach will continue to do so when completing the IVLs unless something forces them to take a concept-based approach. However, Beverly and Carl show that students who take a largely equation-based approach are not rewarded. Instead, the IVLs force a conflict in these students. They try to generate an explanation but realize that they are incapable of understanding the threshold concept, as demonstrated by Beverly and Carl's lack of confidence when answering conceptual questions. In addition, the IVLs do, as is seen with Alfred and David, reward students who take a concept-based approach by helping them understand difficult threshold concepts. This information shows that to be fully successful, the IVLs should better address those students who take equation-based methods.

REVERSIBILITY

Student approaches also differed in the reversibility simulation. However, three out of the four students were able to answer the final conceptual question correctly. The approaches taken by Elaine, Frank, George, and Henry during the Reversibility simulation were less distinct from one another than the students who completed the Work simulation, so closely examining each student is less helpful here. Instead, we will briefly go over what type of approach each student took and then compare it to how they answered the final conceptual question.

Elaine

While doing the simulation, Elaine was the only person to use the differential definition for work without looking in the textbook. In this way, she was the only one to take a concept-based approach from the start of the simulation. However, she was also the only participant to incorrectly answer the final conceptual question. Her answer may have been due to some confusion, as instead of describing the conditions necessary for a reversible process to take place, she simply gave the definition of a reversible process.

Frank, George, and Henry

Frank, George, and Henry all initially used equation-based approaches. All three looked in the book to find an applicable equation for the single-step compression process. While Frank and George correctly used the equation to find work done under constant pressure, Henry used the equation for reversible work. However, after seeing the two-step process, Henry realized he had made a mistake and went back to use the correct equation. After completing the simulation, all three were able to correctly answer the final conceptual question. The fact that all three understood the threshold concept covered in the simulation shows that they were able to use a concept-based approach to synthesize the physical information, at least when answering discussion questions.

DISCUSSION

After seeing some of the ways students approached the simulations, we need to consider why the Reversibility simulation is more effective in explaining the threshold concepts than the Pv Work simulation. One explanation is based on the freedom granted by each of the simulations. The Work simulation uses minimal scaffolding during the single molecule simulation. Students are allowed to experiment with the container and molecule and are expected to answer a discussion question. However, they are only required to hit the molecule once before proceeding to the next question. Students are supposed to create their own understanding when this is happening. The prompt also does not thoroughly explain molecular kinetic theory, so students may not fully understand that the gaseous system temperature is a function of the average molecular kinetic energy. On the other hand,

the Reversibility simulation is highly structured. The students cannot interact with the simulation more than was intended; they can only place or remove mass from the piston. The progressively more complicated processes also act as checks for students who have answered incorrectly. As was seen with Henry, someone who treats the single-step process as reversible will realize his mistake when he sees that the two-step process must be different.

This simulation data appears to show that the most effective simulations for teaching threshold concepts are those that are highly scaffolded and provide progressively more complex systems. These design elements keep students from straying too far from the desired threshold concept while also giving students a way to compare their answers from previous questions to new situations and see how they compare. However, this assertion is based on limited data and is different than what other researchers have suggested.^[18] More investigation is warranted.

STUDENT FEEDBACK

Student feedback to the simulations was generally positive. One common element of feedback was that students found the dynamic representation of molecules and thermodynamic phenomena to be more useful than the static depiction found in books. In fact, Beverly was the only participant who did not state that she found the dynamic molecules and plots useful for helping visualize the system. For example, Alfred said:

“Actually, you know what helps, is actually seeing it moving, I can see which way the path is moving so that kind of guides me along better. Because drawing the path is one thing, but seeing where it starts and ends is also another thing.”

David also provided the following comment in response to being asked if he thought the simulations would help people do well in class:

“It definitely wouldn’t hold them back. It would, to have a simulation like that, it would have a lot of students including me just understand what’s going on. And even if that doesn’t help me get a better grade on a test or whatever, at least that tells me what I’m doing, like why am I even bothering with this equation.”

Some students also made suggestions for improving the simulations. Frank suggested a button that would give students hints when they are stuck. Henry suggested adding more variety to the systems present in the Reversibility simulation such as including a non-ideal gas or adiabatic systems along with the isothermal ones.

Finally, George had some difficulty understanding what he was asked to do in the Reversibility simulation:

“I guess I took the question as, I wasn’t really aware that was a block in the beginning. And I thought it asked me to choose a value of blocks that work them, by a block, and put them on to the simulation. Other than that I think it’s great.”

Essentially, he did not understand that to place the block on the piston, he had to physically click and drag the block. George’s example reinforces the importance of using precise wording when providing instructions to prevent any confusion that may arise from differing interpretations.

SUMMARY

This study examined student engagement and feedback from eight participants using two different Interactive Virtual Laboratories to learn threshold concepts. Student approaches to interacting with and completing the simulations can be roughly divided into two groups: concept-based and equation-based. Students who used a concept-based approach on the simulations were very successful at understanding and explaining the key threshold concept in both the Pv Work and Reversibility simulations. Students who instead used an equation-based approach were forced into a state of conflict during the conceptual simulation sections, as they realized that they could not successfully engage in the simulations using this approach. Participants who completed the Pv Work simulation with an equation-based approach became cognizant of their lack of conceptual understanding but did not change their approach. However, participants who completed the Reversibility simulation switched to a concept-based approach when presented with increasingly complicated thermodynamic systems. Comparisons between the Pv Work and Reversibility simulations suggest that IVLs are most successful when using a highly scaffolded design along with a series of increasingly complex systems to ease the student into comprehension. Additionally, student feedback to the simulations was largely positive. Students particularly liked how the IVLs provide a visual and dynamic representation of the abstract thermodynamic systems. Some student suggestions for simulation improvements include adding buttons for additional hints and assistance as well as adding more complexity to the systems, such as including non-ideal gases or switching between adiabatic and isothermal systems. The IVLs are available for instructors to use through the *AIChE Concept Warehouse* website (<<http://cw.edudiv.org/>>).

ACKNOWLEDGMENTS

The authors gratefully acknowledge support from the National Science Foundation under the grant TUES 1245482. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation.

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