Development of Interactive Virtual Laboratories to Help Students Learn Difficult Concepts in Thermodynamics

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Abstract
In this project, we explore the use of threshold concept theory as a design basis for development of Interactive Virtual Laboratories in thermodynamics. Thermodynamics is a difficult subject for chemical and biological engineering students to master. One reason for the difficulty is the diverse and challenging set of threshold concepts that they must coherently synthesize and be able to apply in a diverse range of contexts. Based on our experience and from reports in the literature, we have identified a set of threshold concepts we propose are critical for mastery of thermodynamics. To help students better learn these concepts, we have been developing Interactive Virtual Laboratories. This paper describes the development and initial investigation of two such laboratories. They are available for instructors to use through the AIChe Concept Warehouse website (http://cw.edudiv.org/).

The Interactive Virtual Laboratories are a series of two-dimensional simulations designed to address the targeted threshold concepts. The design of these laboratories is based on allowing students to see and explore alternative representations of the phenomena that they are learning. They allow inquiry-based, scaffolded activity, and each has several activities that provide multiple representations. These activities guide students to perform virtual experiments, and also to place the virtual experiments in the context of the concepts that they are learning. They explain concepts in a way that is less abstract and more intuitive to students by providing a dynamic representation of phenomena at a molecular level. Students are expected to answer numerical questions and, whenever possible, predict and explain the effects of macroscopic changes (i.e., pressure, temperature, composition, energy) based on observations of molecular properties.

In the study reported in this paper, we investigate how students experience the laboratories and whether the students perceive the simulations are beneficial towards learning. The two interactive virtual laboratories studied address the concepts of \(P_v\) work and reversible processes. Eight participants took part in the clinical study outside of the engineering classroom. All students had previously taken a thermodynamics course and had access to a thermodynamics textbook and the internet as they completed the laboratory. A “think aloud” protocol was used where students were audio recorded as they verbally described their actions in completing the laboratory. The transcribed audio recordings together with video recordings of the computer screen on which they worked were analyzed. After completing the laboratory, a semi-structured interview asked participants about their perceptions of the simulation’s effectiveness, their previous thermodynamics experience, and a brief assessment of what they learned. All interviews were transcribed for analysis.

The participants generally responded positively to the simulations. Seven out of eight students explicitly stated that the dynamic simulations helped them visualize and engage with the processes more than they could with the static depictions in books or lecture. However, some difficulties were observed, including interacting with the interface and understanding specifically what a question was asking. One participant found the interactivity to be unintuitive. We also noticed a relation between how the participants framed knowledge and their approach to
completing the laboratory. Students who activated more sophisticated frames typically completed the simulation more quickly and accurately than those with more naive frames. Students who did not do as well tended to focus on trying to identify equations they had used in the past, even going so far as to use them in an unsuitable context. On the other hand, students who completed the simulations accurately and more quickly appeared to integrate what they were seeing on the screen with their foundational conceptual knowledge to form new understanding.

**Introduction**

Virtual laboratories are receiving attention as an alternative way to engage students and promote learning as technology becomes more integrated into classroom instruction. 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. 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. 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.

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 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 ‘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, but we must also be aware that many instruction approaches do not fundamentally reform faulty student assumptions. 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. 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 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 while developing the IVLs. We used Mayer’s 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. 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:

- **Multiple representation principle**: Explanation 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\(^1\). 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. The IVLs can currently be accessed online via the AIChE Concept Warehouse (cw.edudiv.org). 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 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 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.

**Figure 3.** A one-step compression process.

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. 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.

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.

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 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 lab. An interviewer observed participants while completing the simulation. Students had access to a chemical engineering thermodynamics textbook, *Engineering and Chemical Thermodynamics*\textsuperscript{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 can be found in the tables of Appendix A, 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 delta U over dt plus delta of kinetic energy over t plus delta 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\textsuperscript{17}. More investigation is warranted.

\textbf{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:

\begin{quote}
“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.”
\end{quote}

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

\begin{quote}
“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.”
\end{quote}

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:

\begin{quote}
“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.”
\end{quote}

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/).

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References


### Appendix A – Example Quotations

Table A1. All quotes were taken from the single molecule simulation where students were asked to explain how doing work increases the temperature and molecular kinetic energy of a system. Students moved the slider to see how doing work adds energy to a system.

<table>
<thead>
<tr>
<th>Student</th>
<th>Quote</th>
<th>Notes</th>
</tr>
</thead>
</table>
| Alfred  | “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.”

“If 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.” | | |
| Beverly | “I guess, um, when I think about the ideal gas law because […] so perfectly elastic means that no energy is lost when it collides, so if there are more collisions, I feel like the collisions are what cause there to be pressure in the system, so it would make sense that there are more collisions because if it is a smaller space, then your pressure will increase, but I guess they’re asking you more about why the speed changes.”

“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?”

“When the molecule collides with the walls, the speed will increase, and when there is a smaller space, there are more collisions.” | Beverly notices the molecules speed up when colliding with the moving wall at the end, but describes temperature as a result of “collisions.” |
| Carl    | “Energy of the system is delta U over dt plus delta of kinetic energy over t plus delta of potential energy over time, and that’s equal to heat plus work. And this is an adiabatic process, so heat is zero.”

“I’m trying to find out how the temperature or, uh, changing the volume is relevant with changing the speed of a molecule because that is what I need to answer. Since the equation is n times Cv times delta T is equal to negative external pressure times change in volume. Well, uh, as the volume decreases, that means the change in volume gets larger and larger as the closed system gets compressed, and the change in volume compared to the initial pressure gets bigger, and the negative external pressure is constant and n and Cv are constant, so temperature must be changed to apply the equation, so that’s why temperature increases as the closed system gets compressed more and more.”

“Since n, Cv, and negative external pressure are constant, delta T must | The balance Carl uses is for an open system. The kinetic energy he refers to is the macroscopic kinetic energy of the system, not the molecular kinetic |
be increasing as the closed system gets compressed more (delta V increases).”

“Since energy is conservative, so if the kinetic energy gets larger, potential energy must be lowered to maintain that balance of energy, so as the closed system gets more compressed by external pressure, so volume decreases. That means the height of the closed system goes down, therefore the potential energy goes down, and the energy balance must be applied, so kinetic energy has to go up. Therefore speed of molecules must go up as the closed system gets more compressed. However, each molecule is super tiny, so I don’t think this matters. I’m not sure about this.”

| David  | “I want to see something. So it’s just a transfer of momentum from the piston head that’s coming down.” |
|        | “Momentum is transferred from piston head to molecule.” |

Carl does not talk about the effects of the wall collision. Instead, he focuses exclusively on equations. Before commenting on momentum transfer, David experiments with the slider and finds that the molecule does not speed up when the volume changes, only when the molecule hits the wall.
Table A2. Student responses to the final conceptual question: “Describe the mechanism for how work adds energy to a system.”

<table>
<thead>
<tr>
<th>Student</th>
<th>Quote</th>
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<tr>
<td>Alfred</td>
<td>“Yeah basically, on a molecular level. As you push a wall, for example, you’re, the wall is moving, so it has a kinetic energy which transfers elastically to the molecules. So as those hit back, they speed up when you're compressing them, because they're going in the opposite direction. That causes the temperature to go up”</td>
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<td>Beverly</td>
<td>“I guess, if adding energy in the form of work, um, and it’s an adiabatic system, then maybe the temperature can’t dissipate, so it is higher in the end. I don’t know.”</td>
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<tr>
<td>Carl</td>
<td>“Uh. Yeah. So. Well. Energy is always conserved. However what I noticed was... wait. What am I doing? OK. So once you put some work to the system and when you trying to do some work to the surrounding, they get different values. But energy is always conservative, just the work.”</td>
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<tr>
<td>David</td>
<td>“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.”</td>
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<tr>
<td>Elaine</td>
<td>“I’m thinking about how I would calculate the work. I’m thinking work equals P dV, integral P dV”</td>
<td>The only person who uses the differential definition of work.</td>
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<td>“And you went from, this little graph, I can tell we went from twelve liters to six liters, so V one equals twelve and V two equals six. And the pressure should be, it’s a constant pressure applied, um, at three point, oh, four bars.”</td>
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<td>“So now I’m going to take the integral. So P is constant, so it comes out, and we have the integral of dV from V one to V two. Which would be, that would be…”</td>
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<td>Frank</td>
<td>“Estimate the value of work, well, work, I’m just going to look in the book real quick for that work equation, pretty sure it’s like P delta V.”</td>
<td>Frank looks up the correct equation in the book.</td>
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<td>“Alright, we’ve got work, we’ve got all kinds of work, so I’m going to rock the P equals, no, work is equal to P times delta V. So it says external pressure is equal to four bar, and the volume change was […] eleven minus six times four is twenty.”</td>
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<td>George</td>
<td>“It looks like the work is negative integral of P dV, P being the external pressure. And in this case, the external pressure consists of contribution from both the block and the atmosphere.”</td>
<td>George looks up the correct equation in the book.</td>
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<td>“P external would actually be four bar, and then change in volume, that is about eleven point six to five point nine”</td>
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<tr>
<td>Henry</td>
<td>“We have heat leaving. And we have a change of two, uh, bar.”</td>
<td>Henry initially uses the equation for reversible work.</td>
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<td>“Are students supposed to guess if this is ideal or non-ideal? Or, um, reversible or non-reversible, that is what I mean.”</td>
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<td>“And this is isothermic (sic)? OK. Work is right here. We started at two bar. We had a q leave.”</td>
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Table A4. Student responses to the final conceptual question: “What conditions are necessary for a process to be reversible?”

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<td>Elaine</td>
<td>“Um. A reversible process. Yeah. Oh yeah. It would be if the same amount of work is added, put onto the system, and the system does the same amount of work.”</td>
<td>Unclear if she did not fully understand the question.</td>
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<tr>
<td>Frank</td>
<td>“I mean just adding infinitesimally small amounts of pressure or mass to a system can make it reversible, because you can take little bits off. And yeah.” “To be reversible means you can go back to its original state, whereas say you have a, like the one block putting it on and then putting it back, or taking it off. You lose some energy compared to a reversible process where you can get back to your state that you were originally from.”</td>
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<tr>
<td>George</td>
<td>“Uh. I think um. That your, you are taking, you are adding and taking away the mass, um. By a little amount at a time, so that the system is releasing the heat. Same amount as work, like they reach that equilibrium pretty quickly. As you take that incremental amount of work, and that's why that makes a reversible process. Otherwise if you were adding a block and removing a block, that's a big change at a time, I think the system don't have time to reach that equilibrium state.”</td>
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<td>Henry</td>
<td>“Yeah. That was a final question on there, too. Well you can't have a reversible one, but incremental increases in pressure were worked onto the system in infinitely small amounts, would be the only way to get it reversible. But you would need an infinite amount of time to do that.”</td>
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**Student Feedback**

**Table A5.** General feedback on the $P_v$ work simulation.

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<th>Student</th>
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<td>Alfred</td>
<td>“My general impressions. The simulation, I thought it was pretty neat to see in real time. I feel like in some ways though, you can just illustrate the printers. But unless it's the second time seeing it. Because I first learned it by looking at pictures in the book. When I see it moving, all I think back is to that picture I had seen in the book earlier, you know, where it draws the path. Or unless you're like, Dr Chang draws out the, in our notes. But I've seen the path.”&lt;br&gt;“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. So that was helpful, yeah.”&lt;br&gt;“Were there any features that I particularly liked. I'm trying to think back. Just like things moving, you get to play with it a little bit, that was pretty cool.”&lt;br&gt;“The layout is nice. I mean you've got the, all your choices. I think it might be beneficial to your team to match what the person is doing with their auto-responses, to put a number on each page, or a number on each question, and then, or like a letter designation on each answer, since it's kind of unclear. So I don't have to say, oh yeah I'm choosing choice, and CP delta T equals minus P external delta V, I would just be like choice C. or the third choice.”</td>
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<td>Carl</td>
<td>“Uh, it wasn't really understandable. Like, thermodynamic concept is really hard to understand for the whole thing, because, well. One because it's hard to express on the picture or video, but this simulation helped me out, helped me out a lot to understand by making the concept visualize, like a movie things. So actually, I took thermodynamic before, but this simulation helped me understand how the thermodynamic concept works, really well. So this is a really great tool for teaching the people who don't know anything about thermodynamics. And in the future this will be a lot helpful for the other concept of thermodynamics such as fugacity, Gibbs energy, entropy, some other concepts, too.”&lt;br&gt;“Features? Uh because, especially the [attend?] of simulation, I had to drag the mouse to move, to put the blocks on the piston. So by, I actually tried to, by, by I used the mouse to drag the mouse and to see the behavior of how the piston, I don't know, how the temperature changes, pressure changes, work, the amount of work, energy, it helped me out to understand more, because I actually did it by myself by</td>
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dragging the mouse along. And I think it would be helpful for the other concepts, fugacity, Raoult’s Law?, Gibbs energy, entropy, something like that. I actually liked the dragging the mouse and moving around, because you actually experiencing something, not just listening, looking in the video or something.”

“By reading the book, and listening to the lecture in the professor's course, a lot of, OK some people might listen, but some people might get bored, not get interested as much as before. So this I think, this simulation tool is also useful for making people pay attention, make them interested about the real fundamentals of thermodynamic. So yeah. Definitely this is a good tool for people who will be taking the course.”

David “Well, one thing, the charts had bars and liters. But then on the simulation itself, the diagram with the piston and the molecules, the diagram was in kilojoules, not bar liters. So there's the mismatch of units kind of threw me off a little bit. Which I should be on top of, but nonetheless, it was a little bit, it added some confusion.”

“I liked how simple it was, because you had the simulation, the plot to the right, and then the text to the bottom. That was a good setup. I thought it was clean, and it was nice that you don't have to scroll down a whole bunch, or scroll to the right or the left to see everything, like you do on some simulations.”

“It was easy to use just because there's a one way track and it didn't stop you if your input values didn't line up exactly with what theirs where. Or the simulation wanted you to put in.”

“Um. One part was when I had to read the area under the pressure volume graph and it asked me for a number and I wasn't sure if my number had to be, I guess I knew it didn't have to be that close, but I didn't want it to be way off what the computer had. But it was kind of difficult to read the chart, because I knew it looked about like it was 15 bar, but it would have been 16, maybe 14 and a half.”

“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.”
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<th>Student</th>
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| Elaine  | “General impression. I liked... let's see. Overall I think I enjoyed the simulation because it does put an image in your mind about like... the concept, or like mostly your, mostly you're just exposed to equations. In classrooms. And so it helps to put an image to an equation. Like what does actually putting a constant pressure on something look like, and how does that, look. And so... I like the simulations because they help put that image to concepts.”  
“I really liked the graph to the side. That, I mean you can see the little dots moving around, but you can't really tell the pressure buildup, so having that graph to the side is helpful.”  
“Um. It's easy to use. There... I think it's easy because it's simple. Like there's no other, oh like what's this button, what's this button? It's like what you need is presented on the page.”  
“I would say the simulation definitely improved my understanding. Did you ask about understanding or learning? ... Yeah. Just again like seeing that image, what are these variables look like, how do they behave with each other? It's important for me to connect the ideas.” |       |
| Frank   | “I thought it was really awesome. The PV diagram... the PV diagram paired with the actual simulation really helps you visualize what's actually going on in the system. So that really helped me figure out what I needed to do. It kind of helped me remember some things from thermo.”  
“I like the questions, actually. I like how it's not throwing it all on you at once. It's kind of a step process where they ask you to you know, put the weight on, what do you think, put the weight off, what do you think. It's not just question after question. It makes you go through the entire thing and actually think about what, what is going on in the system.”  
“Um. Maybe like a help button or something. If you get stuck, it kind of hurts when you're just stuck and then you just want to quit. Whereas if there was maybe hints or something. I mean maybe something to help you along the way, and that would definitely make the experience much more enjoyable. Make it last longer, you know. Instead of getting frustrated and just quitting. So other than that, everything was pretty good.”  
“Um. I remember one problem that I had was trying to take the block |       |
off. You can't really take the block off, you have to push the back button. But in the other simulation, you could definitely take the block off. I don't know if I just mis-clicked or something, but yeah. In the first one, you couldn't take a block off, but when there was 2 blocks you could take both the blocks off. “

“It was definitely easy to use. It's pretty straightforward though. Put a block on, put a block off. I mean, maybe confusion of where the block goes, but I mean, anywhere you drop the block, it'll go to where it needs to go, basically. So there's no real like, gimmicky, you don't run into problems or anything. Again with the sand, adding that to get the specified 4 bar, I could maybe see a problem with that, but I mean it, the pressure does change slowly enough to where you can catch it and find it at 4 bar, or 2 bar, or whatever it asks you to get it at. so. Other than that, the simulation ran pretty well.”

George

“I was uh. I thought it's pretty cool. Like the way that, the way that piston moves, and the way that the plot was showing how the system is behaving. That gives students an understanding of what kind of process is going on. I was kind of nervous. But like I really thought it was exciting for student to learn this way because I think running through the simulation like this for different concepts would be really helpful for them, at least as I was going through, like this is one of the easier concepts in thermodynamics. But like I mean, not being able to use them over the year, so I don't really remember exactly how it works, so able to look at this process, I thought gave me a chance to, if not learn from scratch, but to pick up what I learned before.”

“Um. I... uh. Like I sort of mentioned, like the pressure versus volume graph on the side was pretty neat. And I also liked how the, you can see the molecules are molecules are moving, it's like I think the microscopic level that's really hard for students to understand visually. And yeah.”

“I don't know if it was me not being careful enough, at the beginning, or the simulations warning. But I was really confused in the beginning. 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.”

Henry

“It seemed straightforward, I knew what it was asking for. I didn't seem too rushed, not that there was a time limit on anything, so. Most of the information or the questions I would have about the system were
answered. All the relevant information.”

“It was simple. I mean there wasn't too much that could go wrong. It didn't seem like there was any way to mess the system up.”

“You got your point across, but there might be additional stuff. In this case, you had only a isothermic, but you could have one where it's not isothermic, where it's adiabatic. Or one with non ideal gases, which would be also beneficial.”

“It seemed straightforward and easy to use.”