Connecting the "chemistry triplet" through co-designing computational models with teachers: a case study on calorimetry

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Abstract

The physical processes underlying many chemistry concepts are imperceptible. As a result, teachers must help students learn core chemistry concepts by connecting particulate, macroscopic, and symbolic representations, commonly known as "the chemistry triplet." Research has shown that teachers can demonstrate the connections between these representations using computational models. However, there are few chemistry models available to teachers and the existing ones are often not modifiable to suit different learners' needs. We present a design study examining how a teacher co-created a virtual calorimetry lab with a computational expert. Our findings show that leading the co-design process of the model enabled the teacher to connect conceptual explanations to physical lab activities and to all three representations in the chemistry triplet.

1. Introduction

The chemistry education literature suggests that students must master the "*chemistry triplet*" [e.g., 2-5] (Figure 1), a prevalent metaphor connecting the multiple representations of chemical phenomena: (1) particulate, (2) experiential, and (3) symbolic [12, 13]. Understanding each of these representations gives meaning to verbal explanations, lab activities, calculations, and molecular simulations. Research shows that expert chemists are able to fluidly move between these three representations, while most students have difficulty connecting them even after mastering symbolic representations [2, 3, 7].

Although many teachers strive to teach the triplet and incorporate activities with each representation, they find it difficult to demonstrate the connections between them [e.g., 2, 12]. Prior research has shown that computational modeling can help students connect the triplet by

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exposing how numerous interactions at the particulate level may lead to the emergence of observable phenomena at the experiential level (e.g., [6, 11, 17, 18]). Further, computational experiments with statistical methods can help students demystify symbolic representations (e.g., specific heat formula) (e.g., [14]). However, there are few computational models readily available for teachers, especially ones that allow teachers to modify or customize them for their students' needs. Therefore, teachers often find themselves adjusting their lesson plans according to available models or simulations.

To address this issue, we engaged high school science teachers in a month-long summer professional development (PD) experience for designing high school STEM units that incorporate computational thinking and modeling. The PD engaged the teachers in a *co-design process* to develop computational components and models that were specifically tailored to their teaching goals. Prior work has shown that co-design experiences can increase teacher agency and result in higher-quality curricular materials [14]. In this study, we investigate how positioning teachers as co-designers of computational models with modeling experts may affect teachers' goals and curricular design practices.

Specifically, we present a detailed ethnographic account of how a high school chemistry teacher, K (pseudonym), co-designed a brand-new calorimetry sandbox model as a virtual lab in an Energy in Chemical Reactions unit with other computational activities. Using data from co-design discussion excerpts, teacher interviews, email exchanges, and artifacts (e.g., screenshots, sketches), we investigate: *(1) How did the co-designing experience of a computational model impact K's teaching goals and unit planning? (2) How did co-designing a computational model address difficulties K experienced when teaching with the chemistry triplet?*

2. Methods

2.1. Participants & Settings: We address our research questions using ethnographic data collected during a 4-week summer professional development (PD) program. The PD positioned eight high school teachers and six computational researchers as co-designers of brand-new science curricular units involving tightly integrated computational thinking activities. The first four days involved workshops on computational practices and tools. The remaining three weeks focused on co-design. From Tuesday to Thursday, co-design teams worked in-person on computational models and lessons for their units. On Fridays and Mondays, teachers worked from home and emailed researchers as needed.

2.2. Data collection: We framed the co-design sessions as naturally occurring collaborations between teachers and computational experts, not as interventions. Therefore, we sought to collect extensive ethnographic data [9, 10, 19] in order to document teachers' co-design practices. We audio recorded each co-design group meeting, wrote research memos, and saved correspondences between teachers and experts. We also collected design materials created by teachers (e.g., sketches, computational models) and documented changes over time. Lastly, we conducted exit interviews with each teacher at the end of the PD and end of the school year.

2.3. Data analysis: We analyzed K's co-design experience in three stages. First, we transcribed the audio recordings and matched them with non-verbal data. Then, we divided the transcripts into self-consistent fragments. We collaboratively coded [1, 8] each fragment according to the coding scheme presented in Table 2. Finally, we re-constructed a final set of data fragments as a narrative that represents K's co-design practices. Below, we present a shortened version of our findings due to space constraints. See Tables 1-3 for detailed data fragments.

3. Findings

K has 10+ years of experience as a high school teacher at a predominantly African American selective-enrollment school in a major U.S. city. She teaches both honors chemistry and AP chemistry, with the former being a prerequisite for the latter.

Below, we first detail how the co-design experience impacted K's teaching goals and unit plan (RQ1) in Sections 3.1-3.4 using data from the PD (e.g., co-design session, emails, screenshots of model). Then, we describe how co-designing a model addresses the chemistry triplet (RQ2) in Sections 3.5 and 3.6, using data from her exit interviews.

3.1. K was hesitant to work on the calorimetry unit because she could not find computational models online. She was unsure how to incorporate computing into her unit: “I was looking at virtual calorimetry things [online] and, umm, I don't know how computational any of that would be?” Her co-design partner, P, encouraged her, saying “I like the idea of picking a challenge,” so they decided to start working on a calorimetry model.

3.2. K wanted her virtual calorimetry lab to fit her existing unit structure. K’s unit addressed a common student misconception she observed with her students: “[they think] energy is required to break bonds,” noting that “we have to shake that out of them.” Therefore, her unit started with a naturally occurring phenomenon (spontaneous combustion of mulch), proceeded with lab activities, and culminated in mathematical applications. She explained:

> “The whole point of the unit is for them to understand that there's various oxygen breathing critters that are going through the process of cellular respiration and to ultimately go through and calculate the fact that there's ultimately energy released in the overall reaction.”

3.3 K and P struggled to find an existing computational model. Over the next few days, K and P worked on potential ideas for computational calorimetry activities. K also searched for existing calorimetry simulations online. She found a few that were not useful:

> “It's really not worth it. I mean, it's nice to see there's a ton of these out there. Basically, any calorimetry [simulation] is the same garbage, pictures, and then you like ‘*choose this*’ and ‘*you put this in.*’ It's so pointless.”

Because of this, P suggested creating their own model. “We can start creating a model the way you want it to be, from scratch. Then we can start designing the learning activities around it.”

3.4. K drew on her specific and detailed teaching goals to lead the co-design process of the model. The next time K and P met, they started designing a brand-new computational model. K shared her goals, and P encouraged her to sketch out the model, which resulted in the first prototype of the model (Figure 2). Using K's sketch and existing models of particulate motion, K & P discussed the particle representation in the calorimetry sandbox model in detail before creating the model.

From then on, K worked on the curricular materials of her unit while P worked on creating a simple version of the calorimetry sandbox using the NetLogo agent-based modeling environment [15]. They shared their progress and ideas with each other regularly during the PD and the following school year, resulting in the development of the calorimetry sandbox model detailed in Figure 3.

<u>3.5. K designed the computational model for the chemistry triplet.</u> During her post-PD interview, K explained that she wanted to create the calorimetry sandbox to help students understand symbolic, particulate, and experiential representations:

> "P is building the calorimetry simulation, which is huge because one of my hesitations for ever including calorimetry was students wind up doing this calculation and they're like '*I don't even know what that means'*."

Second, in response to the question "What do you anticipate would be beneficial for students?" she stated:

> "Seeing things on a microscopic level is very helpful because, "energy is required to break a bond," Why? But they start to see a simulation of these particles banging to that particle and here's what happens. Look! This one slows down and this one does this. And they're like, "*Oh, okay!*" [...] if they see that kind of thing on the microscopic scale and a simulation, it'll make so much more sense when they're going back and applying it on the macroscopic scale."

<u>3.6. K believed that the calorimetry sandbox model addressed her teaching goals by connecting her physical lab with energy calculations.</u> We conducted another interview with K at the end of

the school year to document her reasoning and whether her ideas had changed. In response to "How do you think computational models might help in teaching?" she stated:

> "We built the model so that [students] can see, '*Oh here's why I'm going to choose this material. This is why I need a Styrofoam cup,*' and not a tin or a glass beaker because I want that energy state contained. If they understand that, the whole concept of calorimetry is going to make more sense, rather than just "*I'm dumping stuff into a coffee cup because the lady told me*," which is really what a calorimetry lab winds up."

Further, K mentioned how important this model was to ensure her honors chemistry students understand why they do specific calculations and the concepts at a higher level:

> "Having taught calorimetry before to honors chem students, there's a bunch of calculations involved and the kids don't understand what any of them mean."

The following year, K participated in the PD again, this time as a returning teacher. During a panel discussion with the returning teachers, one of the new teachers asked her about how co-designing with computational experts was different from finding existing models online:

> "I have a lesson that I love, and I already have designed a lab that I love, and someone helped me design a simulation for me that specifically goes with my unit. So, it makes a perfect story to help kids understand exactly what is going on, so I don't have to adjust to an out of the box simulation."

She added: "It has little idiosyncrasies that I want kids to see or that I want kids to be able to manipulate that I couldn't in a PHET model."

4. Significance

Our findings suggest that K wanted to connect the chemistry triplet for her calorimetry unit but she could not figure out how. The co-design experience helped her achieve her teaching goals through designing a virtual calorimetry lab that fit her unit perfectly, even when it came to "little idiosyncrasies" that she wanted her students to notice.

Furthermore, K's calorimetry sandbox model is a novel contribution to chemistry education literature. As she herself remarked during the initial co-design sessions, she tried extensively to search for a similar model, but she could not find any. Thus, K's calorimetry unit, which is published online, is a significant contribution because it includes multiple computational thinking activities that can help students connect the chemistry triplet.

Overall, this work suggests that computational models are powerful for learning complex concepts across representational levels, yet existing computational models may not address teachers' needs and challenges. Increasing co-design opportunities may help more teachers achieve their goals and result in higher quality curriculum and computational models that other teachers can adopt or further modify to address their own goals.

6. Acknowledgements

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8. Appendix: Figures

Figure 1: The Chemistry Triplet (taken from Treagust et al. [13])

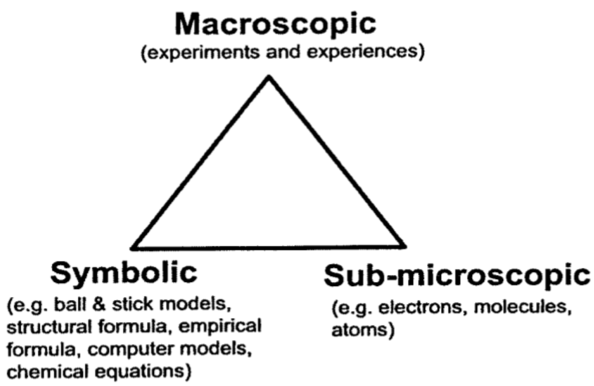


Figure 2: K's sketch of the calorimetry sandbox model with a cleaned version for readability

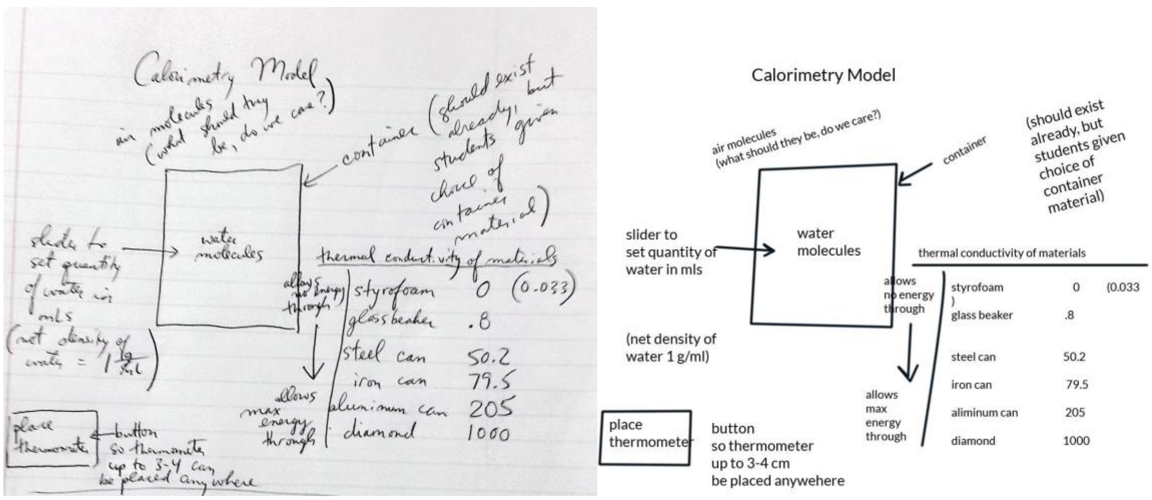
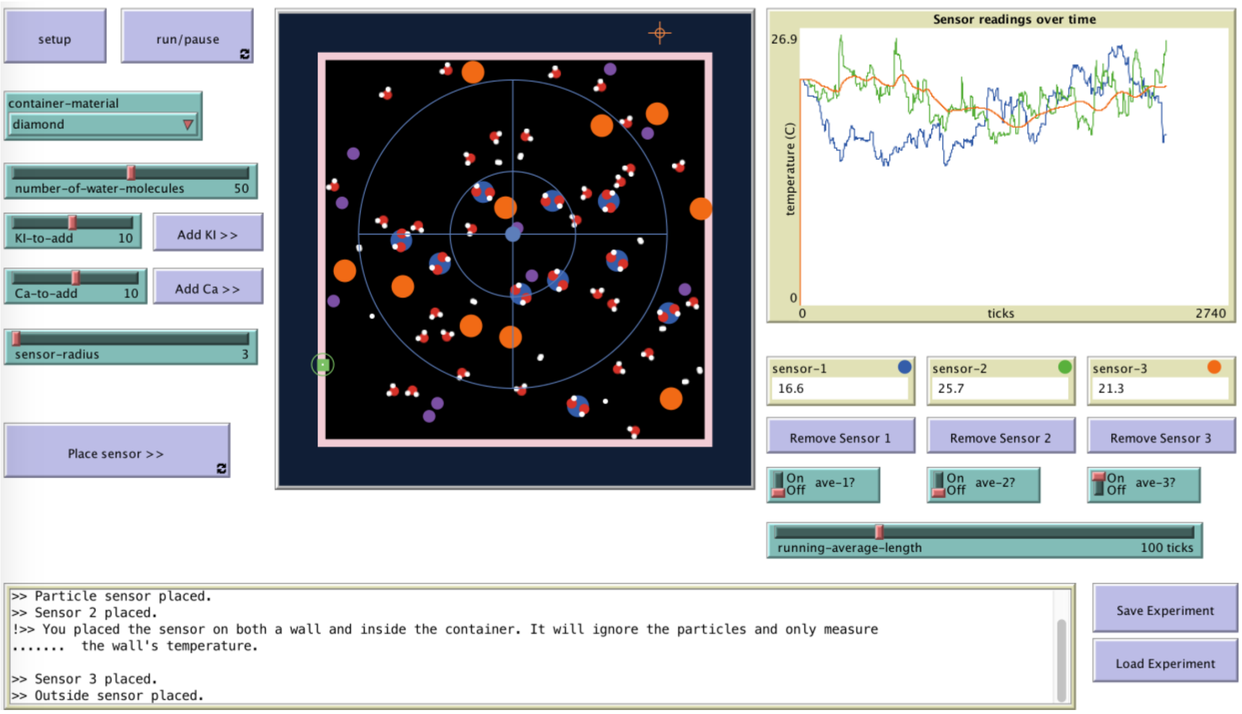
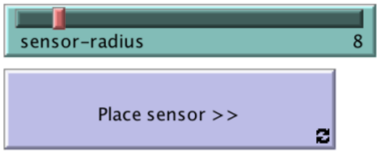
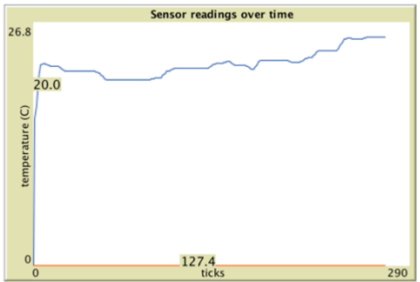
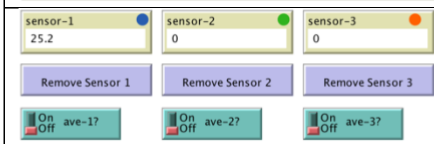
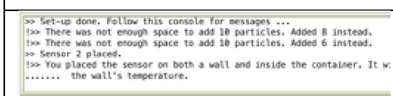
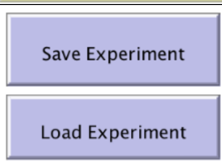


Figure 3: The calorimetry sandbox model created by K and her co-design partner (with explanation table below)



Interface element	**Purpose/function**
setup	<u>Setup button</u>: This button clears everything in the model with the exception of sensors, resets the ticks counter, creates the container walls, and creates water molecules on random locations. It does not change the values of the parameters.
run/pause	<u>Run/pause button</u>: This button runs the model when it is not or stops it when it is already running. When the model is running, the particles move around and interact with each other according the kinetic molecular theory of gases.
container-material: diamond (styrofoam, glass, steel, iron, aluminum, diamond)	<u>Container material chooser</u>: This chooser allows the user to change the material of the container when the setup button is clicked. The available options are: styrofoam, glass, steel, iron, aluminum, and diamond. The materials are sorted in terms of heat conductivity, with styrofoam being the least conductive and diamond being the most. Each material option is represented with a different container color. For example, diamond is light red, steel is dark gray, and styrofoam is white.
number-of-water-molecules 50	<u>Container material chooser</u>: This slider allows the user to change the number of water molecules created in the model when the setup button is clicked. Each of these molecules are placed in random locations within the container and given random directions. However, they are given the same kinetic energy.
KI-to-add 10; Add KI >>; Ca-to-add 10; Add Ca >>	<u>Add KI & Add Ca buttons</u>: These buttons and the sliders next to them allow the user to add either KI molecules or Ca molecules to the simulation. They will be placed in random directions. If there is not enough empty space to place the chosen number of particles, the model will print a warning message in the console.

	Sensor radius slider and Place sensor button: This slider allows the user to choose how large of a sensor they would like to place within the model. Once they choose the appropriate size, they can click the button and move their mouse cursor over the model view itself to place the sensor. The user can place a sensor as large as 50-units, which would almost completely cover the whole container, or as little as 1 unit. The user can place the sensors anywhere inside the container, anywhere on the container walls, or anywhere outside the container. The user can only place 3 containers in total.
	Sensor readings over time plot: This plot will show the change in temperature values reported by the sensor over time (measured in terms of ticks). Each sensor is shown with a different color (blue, green, red).
	Individual sensor controls: These controls show the last temperature value reported by each sensor, allows the user to remove any of the sensors, and allows them to choose whether they would like to plot the last instant reading or plot the running average of the readings of a given sensor.
	Running average length slider: This slider allows the user to choose the amount of time (in terms of ticks) that should be used to calculate the running average of the sensors.
	The console: This console shows messages about critical events in the model such as where a sensor is placed, how many particles added, etc.
	Save & Load experiment buttons: These buttons allow the user to save their current experimental setup (including the number of particles, the location of the particles, the kinetic energy of the particles, the placement of the sensors, and the visualization settings) and also allows them to load a previously saved experimental setup.

8. Appendix: Tables

Table 1. The structure of K's calorimetry unit

	Lesson	Content	Example student activities
1	Phenomenon Introduction	Spontaneous combustion. Thinking about decomposition on the microscopic level.	Students will watch two separate videos of mulch or compost piles spontaneously combusting. They will answer questions such as: "Describe what you believe is happening on a microscopic level to cause compost to spontaneously combust." and "Where is the energy coming from to cause the fire?
2	Chemistry Lab	Breaking ionic bonds	Students will dissolve five different ionic compounds in water to observe and measure the temperature difference before and after dissolving. Students will also observe how changing variables such as the amount of ionic compound used or the amount of water the ionic compound is dissolved in affects the temperature change.
3	Conceptual Modeling	Ionic compound breaking in water	Students will create sketch models.
4	Computational Chemistry Lab	Endothermic reactions	Students will utilize a simulation that shows the dissolving of an ionic compound in water. Students will create sketch models of ionic compounds.
5	Conceptual Modeling	Transfer of energy when a compound separates into ions in water.	Students will reflect on the previous lesson and create sketch models of the bonds breaking.
6	Modeling Bond Formation	Exothermic reactions	Students will observe two different synthesis reactions that release heat so students can observe that bond formation is exothermic. Students will model bond formation including the PE/KE of the system/surroundings before and after.
7	Calculating energy transfer	The specific heat formula	Students will analyze a pre-compiled set of experimental data table for heating water in terms of dependent variables, independent variables, and the temperature change (ΔT). Students will calculate the specific heat for mercury based on a pre-compiled set of experimental data table.
8	Computational Chemistry Lab	Introduction to calorimetry Exothermic reactions	Students will utilize a physical calorimeter to measure the energy released in an exothermic reaction when solid calcium metal is added to water. Students will use the virtual calorimetry lab to replicate the physical experiment.
9	Conceptual Modeling	Modeling endothermic reactions	Students will utilize a physical calorimeter to measure the energy released in an endothermic reaction. Students will use paper cut-outs of the atoms involved in the chemical reaction.

			Students will use the virtual calorimetry lab to replicate the physical experiment.
10	Conceptual Modeling	Modeling a chemical reaction by counting the number of bonds made vs broken	Students will be guided through modeling a full chemical reaction by counting the number of bonds that must be broken versus the number of bonds formed in order to determine if the overall reaction is likely endothermic or exothermic.

Table 2. The simplified coding scheme used for data reduction

Code	RQs	Rationale	Example excerpts and non-verbal data
Chemistry Triplet	RQ2	Determining the role of the chemistry triplet in K's co-design process	**[EX9]** "one of my hesitations for ever including calorimetry was students wind up doing this calculation and they're like [imitating students] "*I don't even know what that means.*" And so if they had the simulation first and they develop an understanding of "*Oh, here's what's going on and here's what I'm actually measuring, that's why I'm using that number in that equation.*" I want them to go into the calorimetry lab with all of that understanding, so, then all their numbers are just going to make sense" **[EX12]** "And having taught calorimetry before to honors chem students, the first issue is, there's a bunch of calculations involved and the kids don't understand what any of them mean. This formula, you know, $Q = m * c * \Delta T$, I'm changing T and they plug in numbers and they don't have a clue what they just calculated." **Excerpt from the Unit Overview written by K:** This unit starts by addressing a common student misconception: that energy is released when bonds break. The first lab focuses on bonds breaking where students will discover that energy is actually required for bonds to break. Students are then provided with a microscopic view of the bonds breaking process so they can explain why energy is absorbed rather than released when bonds break. An exothermic synthesis reaction is demonstrated for students next so they understand that energy is released when bonds form. Students put the two concepts of bond breaking and bond forming together in order to explain overall chemical reactions as endothermic or exothermic. Calorimetry will be employed to measure the energy absorbed or released in a chemical reaction. Students will utilize a calorimetry simulation prior to completing the actual lab so they fully understand what is occurring on a microscopic scale throughout the process and why they are being asked to perform certain calculations to calculate energy.
Teaching Goals	RQ1 RQ2	Understanding how K's teaching goals informed her co-design process	**[EX2]** "Yeah, well, the big misconception is something I mentioned before, which is that students often come in thinking that energy is released when a bond breaks. They've been told somewhere in science history that, you know, energy is stored in bonds. They've just been told that blanket statement. And therefore, if a bond breaks, energy is released and we have to shake that out of them." **Screenshots from the videos used by K to introduce spontaneous combustion of mulch in Lesson 1:** 

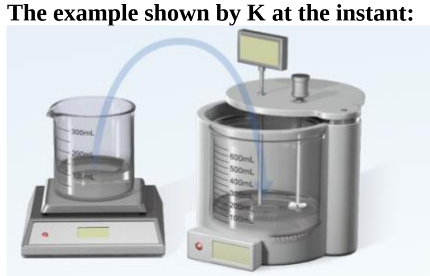
Unit Planning	RQ1	Triangulating, as best as possible, the ideal unit image K may have had in her mind during the co-design process	**[EX14]** "It's different because the simulations I'm using are ones that I've specifically designed. In other words, I have some lab that I do that I think is a really great lab that is a big part of one of my units. Sometimes we'll do labs with kids that last like two weeks because we make them go through multiple trials and really get at the idea of error analysis. The simulations that have been designed for me are to my specifications, so I don't have to take an out-of-the-box PHET simulation and design a lesson around it."
Computational modeling	RQ1 RQ2	Investigating how K's perception of computational models as a teacher may have informed her co-design process	**[EX5]** "K: Just to give an idea of how we're saying that there's basically just garbage out there. What is out there is things that look like this *(pointing towards her computer screen showing another simulation)*. **P:** Send me the link for this one, too. **K:** Well, I mean, it's really not worth it. I mean, it's nice to see there's a ton of these out there. Basically any calorimetry is the same garbage with pictures and then you like "choose this" and "you put this in" and it's just like, it's so pointless." --- **The example shown by K at the instant:** 

Table 3. Extended excerpts from K's co-design sessions (as cited in the manuscript).

Excerpt #	**Raw Data**
EX1	**K:** I was looking at virtual calorimetry things [online] and, umm, I don't know how computational any of that would be? Because, I really wanted [students] to be able to see "*Why?"[...]* "*Why do I want a styrofoam cup and not a- not a glass beaker?*" And you know what I mean? Like, *[imitating a student:]* "*Why does that matter?*" And like just the concepts of heat loss so they understand your basic coffee cup calorimeter and why. Why that setup is the setup that would be used, as opposed to just tossing some stuff in a beaker. **Co-design [P]artner:** The gas laws [content] is there. Like, taking the pieces and adopting for you should be rather straightforward. **K:** Oh, yeah. **P:** But I also like the idea of picking a challenge. **K:** The challenge is something like it is not there yet.
EX2	**K:** Yeah, well, the big misconception is something I mentioned before, which is that students often come in thinking that that energy is released when a bond breaks. They've been told somewhere in science history that, you know, energy is stored in bonds. They've just been told that blanket statement. And therefore, if a bond breaks, energy is released and we have to shake that out of them.

EX3	**K:** I'll just talk you through [the unit]. It starts off with, umm, they watch a couple of videos of a compost heap, spontaneously combusting. And so, they watch this occurring in two different instances, two different videos of basically compost or mulch just catching on fire from nowhere. **P:** Oh! **K:** And so the entire question that we're asking is, well, "*How did that happen? Obviously, that's some kind of energy, like, where did that come from?*" Right? So the entire gist or the whole point of the unit is for them to understand that there's various oxygen breathing critters that are going through the process of cellular respiration and to ultimately go through and calculate, by the very end of the unit, which takes like 6-7 weeks, they calculate the fact that there's ultimately energy released in the overall reaction. They do that based on finding the enthalpy from looking at all the bonds broken versus all the bonds made and you know, average bond enthalpies, and all that. So, that's beginning to the end. In the middle, the way it goes through, is they start with, umm, putting a whole bunch of ionic compounds into water. And we have systematically chosen them so that we only have provided the endothermic ones. We don't want them to see the exothermic ones because we want them to go through and see "*Okay, every time I put one of these things in water, temperature goes down. What's going on?*"
EX4	**K:** So, it's got, umm, you just start it and it's got the hydrogen and oxygen molecules. And then it says add some energy to break one of the molecular bonds. So, just this this miraculous energy just floats in. Whoo! Yellow energy balls, which is like, "*Okay, what is that?*" It's kind of strange because it's like "*What is that supposed to be?*" So that bothers me because I'm like "Okay, what? What are your energy balls exactly?"
EX5	**P:** So, I think for you, we can start creating a model the way you want it to be, from scratch. Then we can start designing the learning activities around it. **K:** Just to give an idea of how we're saying that there's basically just garbage out there. What is out there is things that look like this *(pointing towards her computer screen showing another simulation)*. **P:** Send me the link for this one, too. **K:** Well, I mean, it's really not worth it. I mean, it's nice to see there's a ton of these out there. Basically any calorimetry is the same garbage with pictures and then you like "choose this" and "you put this in" and it's just like, it's so pointless. **P:** It's actually worse than doing the [lab physically]. **K:** No, I agree. But I mean, that's what they all look like like that. And that's all I've seen. At least I haven't. I haven't looked at tons. Beyond you know ... **[A]nother Teacher:** Is that what the [PHET] one looks like, too? **K:** No, not even, if you go to [Anonymous webpage], **A:** Oh, I just thought it was [Anonymous]. **K:** It's just heating thermo and I don't think it's any calorimetry. It just takes you to any heat and thermodynamics thing they have and I don't believe there's anything technically calorimetry.
EX6	**K:** Maybe there could even be some kind of a choice of container or something like that. You know, it's like, if they did it in a glass beaker or something like that, there would be energy loss through the bottom of the glass beaker, right? Because that's going to allow for the transfer of energy through the glass more so than styrofoam.

	Like, we want to contain that heat and measure the heat that was, you know, essentially released from from those bonds being formed, and the fact that, you know, all this energy was released, and if they didn't have those containers, all the energies, or at least some of the energy is going to be lost. And so, "Why are you choosing this container?" Right? So that would be the kind of thing that we could build into the sim. And then they would have to verify their choice of "I'm using styrofoam because of this." **P:** I like it a lot and we can really make it innovative. It's more like a sandbox, in the sense that, like, they can actually design it themselves, or they could place the molecules, they could place sensors, like they can construct it, construct an experimental setup in the sandbox and save it, and then run that experiment again and again, if they want to. **K:** So, I'm just gonna start sketching? **P:** Yeah, draw on paper.
EX7	**P:** I don't understand this. Breaking [bonds], I understand. If [a particle] hits [the other] hard enough, [the bond] breaks. How does it form? **K:** Same thing. **P:** If it's coming slowly enough? **K:** No, I mean, when a bond is formed, it has to do with several things. It does have to be fast enough again. So, in other words, the molecules of the atoms have to smash into each other hard, but technically they also have to be in the correct orientation. So, orientation plays a role. That is another thing that we don't really discuss on the honors level, it is an AP thing. **P:** Then I'll probably implement it as a chance. **K:** The correct orientation, fast enough, um what else? Yeah, and not just fast enough but also hard enough because, you know, the force at which they collide with each other.
EX8	**P:** A lot of conceptual work... **K:** Yeah. We do a ton of that before we throw math at them because we really want them to have an understanding of what all the math means. Because, if you just throw the math at them they just, you know, they plug and chug but they don't they don't get it. So...
EX9	**[I]nterviewer:** What is the science content or topic that you've focused on and have you taught this topic before? **K:** The broad topic is having students understand the energy that is either absorbed or released in an overall chemical reaction and why? By breaking that chemical reaction down into steps of breaking and then making bonds. And we have students go about it by modeling and in a qualitative approach. And then after they develop that understanding, then they look at a more quantitative approach to the entire thing. And [my co-design partner] is building the calorimetry simulation, which is huge because one of my hesitations for ever including calorimetry was students wind up doing this calculation and they're like [imitating students] "*I don't even know what that means.*" And so if they had the simulation first and they develop an understanding of "*Oh, here's what's going on and here's what I'm actually measuring, that's why I'm using that number in that equation.*" I want them to go into the calorimetry lab with all of that understanding, so, then all their numbers are just going to make sense. I hope so. (laughs).

	I: Okay. In your unit, what do you anticipate will be beneficial for your students? **K:** Um well always seeing things on a microscopic level is VERY helpful because, okay, fine, “energy is required to break a bond.” Why? But they start to see a simulation of these particles banging to that particle and here's what happens, and look, this one slows down and this one does this. And they're like, “oh, okay”. And so they can accept it much more easily when they can see it. I mean, even if it's just a simulation, they can now take that and go back and apply to the macro scale. And I feel like it's going to be the same thing with calorimetry, whereas if they see that kind of thing on the microscopic scale and a simulation, it'll make so much more sense when they're going back and applying it on the macroscopic scale.
EX10	**P:** You couldn't use the final version of the calorimetry model but how do you think computational models might help in this process, compared to traditional ways of teaching? **K:** In terms of calorimetry specifically, just doing a lab, they still don’t understand what's going on. Um, because they're basically just putting some chemicals in a cup and sticking a thermometer in it and take measurements and they don't understand why. “Why am I giving them a Styrofoam cup?” Right? So, that’s why we built the model. That model is meant to be the intro to doing an actual calorimetry lab. Basically, it's supposed to be the model and then that's like the planning aspect of it so they can see, “*oh here's why. I'm going to choose this material. This is why I need a Styrofoam cup*” and not a tin or a glass beaker even because I want that, you know, energy state contained in that. If they understand that, the whole concept of calorimetry is going to make more sense, rather than just [imitating students] “*oh, dumping stuff into a coffee cup because the lady told me*”, which is really what a calorimetry lab winds up being if they don't understand what's supposed to be happening inside that cup.
EX11	**P:** You couldn't use the final version of the calorimetry model but how do you think computational models might help in this process, compared to traditional ways of teaching? **K:** In terms of calorimetry specifically, just doing a lab, they still don’t understand what's going on. Um, because they're basically just putting some chemicals in a cup and sticking a thermometer in it and take measurements and they don't understand why. “Why am I giving them a Styrofoam cup?” Right? So, that’s why we built the model. That model is meant to be the intro to doing an actual calorimetry lab. Basically, it's supposed to be the model and then that's like the planning aspect of it so they can see, “*oh here's why. I'm going to choose this material. This is why I need a Styrofoam cup*” and not a tin or a glass beaker even because I want that, you know, energy state contained in that. If they understand that, the whole concept of calorimetry is going to make more sense, rather than just [imitating students] “*oh, dumping stuff into a coffee cup because the lady told me*”, which is really what a calorimetry lab winds up being if they don't understand what's supposed to be happening inside that cup.
EX12	**K:** And having taught calorimetry before to honors chem students, the first issue is, there's a bunch of calculations involved and the kids don't understand what any of them mean. This formula, you know, $Q = m * c * \Delta T$, I'm changing T and they plug in numbers and they don't have a clue what they just calculated. [...]They have no idea. And frankly, last year, I felt very similar about the AP students and their understanding of calorimetry that they were basically just plugging and chugging a bunch of numbers and didn't really get it. And I thought “You know what? We need to integrate this into our honors chem energy unit” so that all these

	calculations when they're doing them later, at a higher level, they actually get it because I never want students to be just calculating a bunch of numbers like it's supposed to mean something.
EX14	**New Teacher:** Well, I have a follow up question. I have used [Anonymous] simulations for the last 15-20 years, I have made dozens and dozens of labs with critical thinking questions based on each simulation. Then, how is this different from using this like any other simulation that's out there? **K:** It's different because the simulations I'm using are ones that I've specifically designed. In other words, I have some lab that I do that I think is a really great lab that is a big part of one of my units. Sometimes we'll do labs with kids that last like two weeks because we make them go through multiple trials and really get at the idea of error analysis. The simulations that have been designed for me are to my specifications, so I don't have to take an out-of-the-box [Anonymous] simulation and design a lesson around it. I have a lesson that I love that I already have designed the lab that I already love and someone helped me design a simulation for me that specifically goes with my unit. So, it makes a perfect story to help kids understand exactly what is going on, so I don't have to adjust to an out of the box simulation. It's been created for me and it's just any little tweak that I want to make, [my co-design partner] made it. And you know that's what makes it so great. It is little idiosyncrasies that I want kids to see or that I want kids to be able to manipulate that I couldn't in a [PHET] model. It can be done.