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Right but Wrong: How Students' Mechanistic Reasoning and Conceptual Understandings Shift when Designing Agent-Based Models Using Data

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Abstract: When learning about scientific phenomena, students are expected to *mechanistically* explain how underlying interactions produce the observable phenomenon and *conceptually* connect the observed phenomenon to canonical scientific knowledge. This paper investigates how tight integration of the complementary processes of designing and refining computational models using real-world data can support students in developing mechanistic and canonically accurate explanations of diffusion. Specifically, we examine two types of shifts in how students explain diffusion as they create and refine computational models using real-world data: a shift towards mechanistic reasoning and a shift from non-canonical to canonical explanations. We present descriptive statistics for the whole class, as well as three student work examples to illustrate these two shifts as 6th grade students engage in an eight-day unit on the diffusion of ink in hot and cold water. Our findings show that (1) students develop mechanistic explanations as they build agent-based models, (2) students' mechanistic reasoning can co-exist with non-canonical explanations, and (3) students shift their thinking toward canonical explanations after comparing their models against data. These findings could inform the design of modeling tools that support learners in both expressing a diverse range of mechanistic explanations of scientific phenomena and aligning those explanations with canonical science.

Keywords: Diffusion, Comprehension, Computer Simulation, Thinking, Education

Introduction

Developing scientific explanations is a complex skill that involves both describing a phenomenon and explaining its underlying mechanisms. When learning about scientific phenomena, students are often expected to develop explanations that both *conceptually* connect the observed phenomenon to canonical scientific knowledge and *mechanistically* explain how underlying interactions produce the observable phenomenon.

Engaging in mechanistic reasoning is a powerful scientific practice that allows one to make predictions and theorize about phenomena (Machamer et al., 2000; Salmon, 1978). Mechanistic explanations identify the underlying, often unobservable entities that give rise to a phenomenon and specify the sequence of events, from input to output, that produce the phenomenon (Louca et al., 2011; Machamer et al., 2000; Perkins & Grotzer, 2000; Springer & Keil, 1991).

In the past decade, science education reforms (National Research Council, 2012; NGSS Lead States, 2013) have called for integrating mechanistic reasoning as a crosscutting concept into science instruction and encouraging students to construct and apply mechanistic accounts. One way to support students in developing mechanistic explanations is to engage them in creating and refining computational, agent-based models (henceforth "ABM"; Dickes et al., 2016; Löhner et al., 2005; Louca & Zacharia, 2008; Fuhrmann et al., 2018; Wilensky, 2003; Wilkerson et al., 2015a; Xiang & Passmore, 2015). Much of this work has shown how designing computational ABM supports engaging in mechanistic reasoning as learners encode properties and behaviors for individual agents and observe the aggregate outcomes from their interactions. Computational agent-based modeling can also scaffold students' developing a canonical understanding of scientific phenomena (e.g., Wilkerson et al., 2015b).

However, in traditional science classes, computational models are primarily used to confirm a theory rather than as an inquiry tool. Students use or manipulate a canonically accurate model that scientists or curriculum designers have developed over many years. Perhaps because developing adequate programming expertise with modeling tools can be challenging, students are rarely given opportunities to construct models to test their own ideas. As a result, students do not get to engage in iterative model building that is often informed by data analysis (Blikstein, 2014; Fuhrmann, et al., 2014; Krajcik & Merritt, 2012).

Empirical data analysis plays a crucial role in professional modeling practice. Scientists use data to construct, refine or decide between possible models (Passmore et al., 2009; Nersessian, 2002) and to assess the adequacy of a given model by the degree to which that model explains the data (Passmore & Svoboda, 2012). However, model-based learning in science classrooms typically separates modeling and data-based practices (Blikstein et al., 2016; Fuhrmann et al., 2018), with physical experimentation and data collection being largely disconnected from theory building and model design.

Integrating real-world data into the computational modeling process provides learning opportunities that do not arise when students focus on models alone. The Bifocal Modeling framework (Blikstein, 2014) suggests integrating real-world data collection and analysis with computational modeling to enable real-time comparisons of simulated and real-world data. Juxtaposing real-world data and modeling enables students to notice and attend to discrepancies between models and data, making noise, uncertainty, and intrinsic differences between them as issues for discussion (Blikstein et al., 2016; Fuhrmann et al., 2018). Integrating real-world data and analysis into computational modeling can also scaffold students in developing canonical understanding of scientific phenomena (Blikstein, 2014; Fuhrmann, et al., 2014). To date, however, few computational modeling platforms support learners in both *constructing* models or theories of scientific phenomena and *comparing* those models to real-world data to refine and validate them, and few studies have examined how moving between these activities might support the side-by-side development of mechanistic explanations and alignment of those explanations with canonical descriptions of phenomena. As computational modeling and data-based investigations continue to gain traction in the classroom (e.g., Arastoopour Irgens et al., 2020; Conlin et al., 2020; Sengupta et al., 2013; Fuhrmann & Blikstein, 2017), it is important to understand how integrated modeling experiences that incorporate data might shape these important aspects of science learning in concert.

This paper aims to explore how iteratively designing models and refining them based on real-world data can support students in developing mechanistic and canonically accurate accounts of diffusion. We show how this process of *designing* ABM supports shifts in student thinking towards mechanistic, sometimes non-canonical explanations while *comparing* those models against real-world data supports shifts towards canonically accurate explanations. To make this argument, we draw on data from 16 sixth-grade students in a science class engaging in an eight-day unit about diffusion using MoDa (Eloy et al., 2022; Fuhrmann et al., 2022; Wagh et al., 2022). MoDa is a domain-specific, block- and agent-based computer modeling environment. It is one of a growing number of tools that introduce students to computational modeling of scientific phenomena through a modular toolkit of domain-specific procedures (e.g., Sengupta et al., 2013; Hutchins et al., 2020). Over the course of the unit, students collected and analyzed experimental data and designed paper and computational models to investigate and explain why ink spreads at a different rate in hot and cold water. We are guided in this work by the following research question: How do students' mechanistic reasoning and conceptual understandings shift as they design ABM of diffusion using real-world data?

We argue that our findings bear both theoretical and practical implications. We document the occurrence of mechanistic reasoning before canonical conceptual understanding of diffusion, adding to literature that explores the potential independence of these forms of learning (Russ et al. 2008; Wilkerson et al., 2015). In particular, we document developments in students' mechanistic reasoning as they build and refine agent-based computational models, shifting their reasoning toward canonical norms as they compare those models to real-world data. By suggesting the mediating effects of different curricular elements on these forms of learning—model-building supporting mechanistic reasoning and data validation supporting canonical understanding—we also see this paper as informing design and facilitation practices for model-based science learning. Finally, the emergence of these findings in a typical school setting, run autonomously by the classroom teacher without extensive researcher support, suggests their potential to impact real-world teaching and learning.

Background

To ground this work, we first explore the role of mechanistic reasoning in scientific explanations as a component of science learning. Next, we briefly survey the literature on learners' canonical and non-canonical ideas about diffusion, the target phenomenon in this study. Finally, we review varied approaches to create environments that support learners in developing scientific explanations. This background review lays the foundation for MoDa, the educational environment used in this study, and our analytical foci in evaluating students' work with it.

Mechanistic Reasoning as a Component of Science Learning

Mechanistic reasoning is a core form of explanation in science education. It involves accounting for the factors and relationships underlying a phenomenon (Russ et al., 2008; Kris et al. 2019; Louca et al., 2011; Machamer et al., 2000; Perkins & Grotzer, 2000; Russ et al., 2008; Springer & Keil, 1991). Existing frameworks focus on different aspects of mechanistic reasoning (e.g., Hmelo-Silver & Pfeffer, 2004; Russ et al., 2008; van Mil et al., 2013). The Russ et al.'s (2008) framework that we draw on in this paper identifies important structural elements of scientific accounts. According to Russ and colleagues, students engaging in mechanistic knowledge building ask questions about their observations and figure out explanations for the "how" and "why," and not only the "what," of a scientific phenomenon. The focus on mechanisms breaks up the original explanation-seeking "why question" into a series of smaller questions about the causal process. For example, what are the participating entities, and what are their relevant properties? How are the entities and their interactions organized? And what factors could prevent or modify the outcome? In wondering about and formulating answers to these questions, students move beyond the more simplistic descriptive work of observation toward a more causal account of the phenomenon.

Proposing a framework one level up from that of Russ et al. (2008) and building on others' work, Krist and colleagues (2019) emphasize "thinking across scalar levels" as a primary epistemic heuristic in mechanistic reasoning. Explaining a phenomenon by identifying the underlying causes involves thinking at least one scalar level below the observable level of the target phenomenon. For example, identifying that there is a non-visible entity (e.g., water is composed of molecules), is an essential step in reasoning about mechanism (Schwarz et al., 2009).

In the next section, we explore another type of explanation used in science learning specifically when learning about diffusion.

Canonical and Non-canonical Explanations as Components of Science Learning

Students can generate a range of explanations to account for scientific phenomena, many of which differ from those generally accepted by the scientific community. Depending on the theoretical alignments, these non-canonical ideas are also called "misconceptions" (Fisher, 1985; Odom, 1995), "inadequate conceptions," "alternative conceptions" (Astolfi, 1999), "epistemological resources/personal epistemologies" (Hammer & Elby, 2002), and "naive thinking" (Inagaki & Hatano, 2006). This paper aligns with the view that it is essential to offer students opportunities to explore their non-canonical ideas, using them as epistemological resources to connect to the accepted canonical explanations (Hammer & Elby, 2002).

In this paper, we focus specifically on diffusion as a foundational mechanism widely used in many fields, including chemistry, biology, and physics (Friedler et al., 1987). It explains many processes, such as molecular transportation within cells, gas exchange and circulation, water and electrolyte balance, and osmosis. The canonical definition for diffusion is the net movement of any substance from a region of higher concentration to a region of lower concentration as the result of individual molecules or atoms moving or bouncing off one another during the course of Brownian motion. Although diffusion is a key concept in science curricula (NGSS Lead States, 2013), it has been challenging for high school and college students (Friedler et al., 1987; Meir et al., 2005; Odom, 1995; Sanger et al., 2001; Westbrook & Marek, 1991; Zuckerman, 1994). For example, students often anthropomorphize particles, explaining diffusion as the result of a "desire" or "drive" by the particles to reach equilibrium rather than recognizing the constant presence of Brownian motion (Friedler et al., 1987; Meir et al., 2005; Odom, 1995; Sanger et al., 2001; Zuckerman, 1994). Dynamic equilibrium – the end state of diffusion in which particles' movement continues – presents similar challenges, with learners often describing that particles reach equilibrium and then stop moving (Friedler et al., 1987; Meir et al., 2005; Odom, 1995; Sanger et al., 2001; Zuckerman, 1994). In the following section, we review varied approaches to support learners in developing explanations.

Integrating Modeling and Data Analysis for Science Learning

Integrating real-world data into the modeling process provides learning opportunities that do not arise when students focus on models alone. For example, exploring and making sense of real-world data might encourage students to explore more deeply the underlying features of a phenomenon (Schwarz et al., 2013). Similarly, real-world data can help students evaluate models as they decide how well a model aligns with the data, and what conclusions are justified by the data (Holmes et al., 2015). One such learning approach is the Bifocal Modeling framework (Blikstein, 2014; Blikstein et al., 2016; Fuhrmann et al., 2014, 2018). It engages students both in conducting experiments and collecting data and in designing computational models to explain scientific phenomena (Figure 1). In particular, Bifocal Modeling emphasizes comparisons of simulated and experimental data. Through such comparative work, students come to notice similarities and discrepancies between the physical experiment and their model of it, iteratively revising their model to reduce these discrepancies and align with a canonical explanation of the scientific phenomenon. Activities designed according to this framework can develop students' conceptual understanding and meta-modeling competencies (Blikstein, 2014; Fuhrmann et al., 2018).

Bifocal Modeling is just one example of a collection of approaches that integrate multiple modes, or aspects, of scientific modeling in service of more sophisticated student understandings. For example, Chiu, et al. (2015) describes how what they describe as "augmented virtual labs" that combine virtual and physical demonstrations of the same scientific phenomena supported students' construction of explanations and refinement of alternative ideas. Other studies such as Bielik, et al. (2021) and Wilkerson, et al. (2015) highlight how constructing and exploring models across multiple media (e.g. drawing, animation, agent-based modeling, systems modeling) can support complementary aspects of modeling. Those studies, however, focused on the construction of explanations. We build on this work by studying the co-development of mechanistic reasoning and conceptual understanding through the sustained comparison of students' models to real-world data.

Our current work extends these studies of integrated modeling approaches in three ways. First, many studies and platforms that emphasize integrated approaches make use of *pre-built* simulations, rather than allowing students to build and test their *own* models. Building their own models within MoDa allows students to express and explore the variety of different understandings of a phenomenon that they may bring to a science classroom. Additionally, MoDa enables students to compare their own models side by side with visualizations of real-world data so students can refine and validate their models. Such data-based validation is built into MoDa rather than leaving such integration to external curricular materials. Finally, this study represents an experienced teacher's use of these integrative tools and frameworks in a relatively autonomous, classroom context, e.g., the instruction was not heavily supported by researcher intervention. Similar studies of computational modeling platforms were conducted in lab settings or in intensive workshops run by researchers (Bielik et al., 2021 and Wilkerson, et al.). Our research context - a typical middle school classroom run by the classroom teacher with minimal researcher support - adds to the growing body of work (Farris et al., 2019; Pierson et al., 2020) that works to extend researcher-dependent interventions by evaluating classroom feasibility.

[Insert Figure 1 and caption here]

Methods & Materials

MoDa: An Environment that Integrates Agent-based Modeling and Visualizations of Real-world Data

Building on prior research that developed and evaluated domain-specific computational modeling platforms (e.g., Wilkerson et al., 2015), MoDa is a web-based environment that combines creating computational models using domain-specific code blocks with visualizations of real-world data (Eloy et al., 2022; Fuhrmann et al., 2022; Wagh et al., 2022). MoDa allows students to build models using domain-specific code blocks (Wilkerson et al., 2015), and then compare their model outputs with visualizations of real-world data from similar phenomena (Eloy et al., 2022; Fuhrmann et al., 2022; Wagh et al., 2022). This design enables students to work with domain-specific code blocks that align with the learning domain (in this case “diffusion”), and a variety of common ideas they have about how phenomena within that domain work. For example, in modeling the diffusion of ink in water, students could use a canonical “bounce” or a non-canonical “attach” or “erase” block to model particle interactions. By then comparing their computer modeling results with video or quantitative data that reflect the phenomenon in real life, students can validate their models and make changes. For example, when modeling the non-canonical "attach" particle interaction, which was drawn from previous work on students’ extended studies of diffusion (Fuhrmann et al., 2022), students often notice that the simulated molecules form clumps that contrast with what they see in the video data, leading them away from this non-canonical theory of diffusion. A core idea of the Bifocal Modeling framework (Blikstein., 2014), on which the platform is built, is for students to test their ideas by comparing simulations of those ideas against real-world data. Taking the traditional Bifocal Modeling one step further, MoDa embeds data visualization within the computational modeling environment itself rather than leaving such integration to supplementary curricular activities.

MoDa consists of A) a modeling environment and B) a real-world data area (Figure 2). The modeling environment includes: 1) a coding area where students can drag and drop domain-specific blocks built on Google's Blockly library; 2) a simulation area (built on top of the NetLogo engine, Wilensky, 1999b) in which students can see the result of their code and control different variables in the simulation, such as temperature; and 3) data visualizations that illustrate the modeling results in graphs. Figure 3 details the available domain-specific blocks - organized into categories of general properties, actions, and control mechanisms - available for programming models of diffusion.

This paper describes a study in which the unit on ink diffusion in water was implemented in two 6th-grade classes. Two videos, generated by the research team - of ink spreading in hot and in cold water - were included in MoDa as real-world data, reflecting a common classroom demonstration of diffusion (Dou et al., 2013) that was already in use by our collaborating teachers given its simplicity and accessibility.

[Insert Figure 2 and caption here]

[Insert Figure 3 and caption here]

Participants

The study took place in an independent college preparatory day school in California with students from two 6th-grade science classes. White students comprise 74% of the student population, while two or more races account for 18%, Asian or Pacific Islander students represent 5%, Hispanic students constitute 2%, and Black students make up 1%. The student-teacher ratio is 5:1. Across the two classes, there were 18 students in total, however only 16 consented to participate in this study (eight girls, six boys, and two non-binary students). The science teacher had been part of this project for 1.5 years and participated in professional development and co-design sessions with the project team.

Instructional Sequence

The unit occurred over eight class periods and included activities to explore ink diffusing in hot and cold water (Figure 4). Similar to Bielik et al. (2021) and Wilkerson et al. (2015), students explored the target phenomenon in multiple media, using paper modeling and ABM. In our design, however, students validated their models against real-world data tightly integrated within the platform, throughout the unit as opposed to treating external video data as a starting point for their modeling work. Throughout the sequence, students were instructed to focus on how the drop of ink in clear water gradually colored the water, and how this related to heat and the interaction of molecules. The instructional sequence was implemented independently by the classroom teacher with minimal researcher support.

The class met twice a week. To introduce the topic of diffusion, the teacher placed lavender oil on tissue paper and asked students to raise their hands when they smelled the oil. The class had a brief discussion of the spatial dimensions of the scent's movement through the room. They then followed the sequence described in Figure 4. They conducted an experiment comparing the rate of ink spread in hot and cold water. They ran the experiment three times at each water temperature and recorded their data. They then analyzed the data collaboratively and individually drew paper models to explain the difference in the rate of ink spread across the two conditions. Students were then introduced to MoDa through four challenges that focused on different programming blocks. Students then worked in pairs to draw another paper model of their explanation before collaborative coding computational models to explain their observations and comparing their models to the video data. Students shared their paper and computational models with the class to get feedback from their peers and teacher. On the last day, students discussed the validity of their model and watched a video that described the canonical explanation for diffusion.

[Insert Figure 4 and caption here]

Data Sources

In this manuscript, we draw on analysis of five sources of student data (bolded and italicized in Figure 4's timeline):

1. Students' responses to open-ended questions on the pre-survey about how and why ink diffuses in water (Day 1) (see Appendix A for questions).
2. Students' drawn models of the experiment (Day 2). Two students were absent on this day and did not produce individual drawings.
3. Students' pair drawings after first working in MoDa (Day 5).
4. Students' model share-outs in pairs as they presented their computer models to their classmates (Day 7). By analyzing students' descriptions of these models, not the models themselves, we focus on student utterances rather than the language of the coding environment.
5. Student responses to open-ended questions on the post-survey about how and why ink diffuses in water.

Collectively, these five data sources represented diverse modalities, including student utterances and drawings. We acknowledge limitations of using and comparing across these data sources. For example, drawings could prompt more attention to the spatial organization of depicted elements compared to post-test open-ended questions on which students use only words. Similarly, when analyzing student utterances, it can be challenging to separate students' ideas from their (re)statements of the teacher's explanation. Nonetheless, these five data sources provide a window into how students' mechanistic reasoning and conceptual understanding of diffusion developed over the course of the unit. Narrowing our analysis to only the most similar data forms (e.g., only the survey questions or drawings) would give a more limited view of students' learning trajectories.

Data Analysis

Our data include both individual- and pair-level data. Of our five data points, three are at the individual level, while two were at a pair level. In order to respect variation between students in a pair, we treat the individual as the level of analysis and assign pair-level data to each student in that pair. We acknowledge that in ascribing pair-level data to each individual, this approach would potentially misattribute one student's learning to their partner (overestimation). However, the alternatives - either dropping the two pair-level data points or combining individual data for a pair-wise level of analysis - give limited view of the learning trajectories and blur distinctions between students in a pair, respectively.

Preliminary review of students' data suggested they were exhibiting mechanistically detailed but non-canonical explanations for diffusion (Russ et al., 2008; Wilkerson et al., 2015). We document the occurrence of mechanistic reasoning before the canonical conceptual understanding of diffusion, adding to literature that explores the potential independence of these forms of learning. In order to understand the impacts of specific features of the tool and curriculum on these distinct elements of reasoning, we used separate coding rubrics for mechanistic reasoning and canonical understanding, as detailed below.

Mechanistic Reasoning

In coding whether a specific explanation had elements of mechanistic reasoning, we used a modified version of Russ et al.'s (2008) framework (Table 1). We followed Krist et al.'s (2019) practice of omitting Russ et al.'s (2008) first two code categories since the activity prompts already describe both the target phenomenon ("In which does it spread faster?") and the experimental setup ("A drop of ink is placed in a glass of hot water and a glass of cold water"). Additionally, Russ et al.'s "chaining" code focuses on the time dimension, similar to how a storyboard presents events chronologically. Krist et al.'s "linking" code emphasizes movement across multiple levels, from microscopic entities to macroscopic aggregate phenomena. Since we did not want to focus on time or scale, we created a new code, "causality," in place of and closely related to Krist et al.'s (2019) "linking" and Russ et al.'s (2008) "chaining." "Causality" is the highest level of mechanistic reasoning in our rubric and is defined as reasoning about how individual entities, along with their properties and interactions, give rise to the aggregate phenomenon. See Table 1 for the full list of codes, their definitions, and examples.

[Insert Table 1 and title here]

Two researchers independently coded each data source, achieving at least a 91% match rate on a training set, by data source, and at least a 87% match on the remaining data. The score for work completed by pairs of students (i.e., pair drawings and model presentations) was attributed to both students of the pair.

Canonical Understanding of Diffusion

To code whether students' understanding of diffusion connected to canonical descriptions, we coded their written or verbal explanations. We take these explanations as a proxy for their understanding of the phenomenon at the time, acknowledging that we cannot characterize understanding directly or completely. To code student explanations, we chose not to use an existing framework (She, 2004; Stains & Sevian, 2015; Westbrook & Marek, 1991) because such frameworks predominantly include some level of mechanistic reasoning. To code for conceptual understanding independently of mechanistic reasoning, we coded the above data sources using grounded coding (Corbin & Strauss, 2014). Two researchers independently pulled out keywords from students' responses, drawings, and model descriptions to characterize their explanations at each point in the instructional sequence (Table 2). Through iterative coding, these keywords were clustered into two components: 1) those describing particle interaction and 2) those describing the effect of temperature. This distinction was made because, oftentimes, student responses would exhibit a canonical understanding of one component of diffusion while maintaining a non-canonical understanding of the other component (e.g., "When the water is heated up, the water molecules move faster [canonical effect of temperature], therefore attracting the ink particles more [non-canonical particle interaction]"). Each response was then collaboratively coded to mark a canonical or non-canonical explanation of diffusion. Responses lacking one component were deemed canonical so long as the represented component was accurate. Non-canonical responses were those in which either of the present component(s) was incorrect. Responses of "I don't know" or lacking both components were coded as "no explanation."

[Insert Table 2 and title here]

Examples Selection

Based on the results of the above coding and analysis, three example students were selected for closer narrative description of 1) the mechanistic explanations they developed as they engaged with agent-based computational models and 2) how mechanistic explanations co-existed with non-canonical theories and eventually shifted toward canonical science. Selection criteria included data density (i.e., no absences), frequent utterances, and clear demonstration of shifts in both variables of interest (i.e., mechanistic reasoning and understanding of diffusion). Students are referred to by pseudonyms.

Results

To answer our research questions, we share the results of students' developing mechanistic reasoning and characterize their developing conceptual understanding of diffusion. Below, we share aggregated, whole-class frequencies and select narrative descriptions to illustrate how developments in the two dimensions of explanations of diffusion are linked to elements of the computational modeling platform and surrounding curriculum as students progress through the unit.

Result #1: Students develop mechanistic explanations as they build agent-based models

Our first finding indicates that students' mechanistic reasoning developed as they built agent-based models. Across the instructional sequence, more students exhibited mechanistic reasoning (Figure 5a), and they consistently mentioned a greater number of mechanistic reasoning elements (Figure 5b). From the first to last day of the instructional sequence, the number of students using mechanistic reasoning grew dramatically from two students out of 16 (12.5%) on the pre-survey to 16 out of 16 students (100%) on Day 7 and 68.7% on the post-survey (Figure 5a). We noticed especially large increases from the pre-survey to Day 2, when students drew paper models, and from Day 2 to Day 5, when students started using MoDa. We infer from these results that, over the course of the unit, students began thinking about diffusion at a mechanistic level.

[Insert Figure 5 and caption here]

Result #2: Students' mechanistic reasoning co-exists with non-canonical explanations

Considering the below learning trajectories together (Figure 6) suggests that students' mechanistic reasoning co-exist with non-canonical theories. Furthermore, students' mechanistic reasoning and conceptual understanding of diffusion did not develop in parallel but were instead slightly staggered, with students proposing mechanistic explanations with non-canonical explanations before proposing canonically-aligned explanations. As the unit progressed, the distribution of students' explanations shifted from no explanation or non-canonical (split evenly on the pre-unit survey) to a prevalence of canonical explanations (Figure 6). On Day 5, 37.5% of students (6 out of 16 students) provided a canonical explanation for diffusion, and on Day 7, 43.7 % of students (7 out of 16 students) provided a canonical explanation of diffusion. In the post-unit survey, 62.5% of students (10 out of 16 students) explained diffusion in a way that was scientifically accurate (Figure 6). In addition, some non-canonical explanations persisted, while some students who offered at least some explanation on Day 5 (regardless of accuracy) offered no explanation on the post-survey.

[Insert Figure 6 and caption here]

Data shows that from the pre-survey to Day 2, over four times more students included mechanistic reasoning in their explanations for diffusion, but none of those responses included a canonical explanation of the phenomenon. By Day 5, all but two students included causal mechanisms for diffusion, but the majority of students still submitted non-canonical explanations. It could be that the physical experiment, paper model and the introduction to the MoDa environment prompted students to think about causal mechanisms. However, they might still have been exploring various theories to explain diffusion without figuring out what is the canonical explanation.

Result #3: Students shift from non-canonical to canonical explanations after testing theories and refining their models against the data

Breaking down student explanations of diffusion into component pieces - particle interactions and the effect of temperature - indicates that their understanding of these components did not develop concurrently, rather they seemed to progress somewhat autonomously. Canonical explanations for the effect of temperature - namely that particles move faster at higher temperatures and slower at a low temperature - appeared on Day 2 and were more prevalent on the post-survey (Figure 7a). Canonical explanations of particle interactions - that they bounce off each other - appeared first at Day 5 and were shared by slightly less than half the students on the post-unit survey (Figure 7b). Only after students spent significant time testing different theories within that environment and comparing them to the video data (days between day 2 and 7 in Figure 7) did students start to shift away from non-canonical theories and converge on the canonical explanation.

[Insert Figure 7 and caption here]

Illustrative Examples

To provide a clearer illustration of how students developed explanations that include both mechanistic reasoning and non-canonical elements, we next present narratives of three students' work. These instances also show how comparing their mechanistic, non-canonical theories against data helped shift students' thinking toward the canonical theory of diffusion.

Example #1: A mechanistic "barrier" theory: On day 2 of the unit, students individually drew models on paper to explain their ideas about diffusion, prompted by the instructions to "Zoom in on what is happening that causes the ink to move about. Make sure to add labels and arrows to clearly communicate your ideas.” Uma created the drawings and explanations in Figure 8:

[Insert Figure 8 and caption here]

In this instance, despite being in the early stages of the learning sequence, Uma provided a mechanistic explanation for the non-canonical "barrier theory" of diffusion. In her drawing and explanation of the experiment, she focused mainly on the water, identifying entities (“water atoms”), their properties (“hotter,” “mass,” “resistance”), their spatial organization (see drawing), and reasoned about the relationship between cause and effect. She related the temperature of water to the ink’s ability to spread and reasoned that cold water “atoms” formed a barrier that prevented the color from spreading while hot water “atoms” separated from each other, allowing the color to spread. Though her explanation of particle interaction was non-canonical, her mechanistic explanation was highly detailed. On day 5, after working with her partner in MoDa, Uma drew an even more detailed mechanistic explanation for the non-canonical “barrier” theory (Figure 9):

[Insert Figure 9 and caption here]

In this example, in addition to the water particles, Uma identified ink particles. She also drew lines between particles, and explained that “in cold water, particle[s] attach to catch other [particles] and get higher density making them heavier.” She reasoned about the causal relationship between temperature and particle movement (line 4), maintaining a highly mechanistic, non-canonical explanation for diffusion (the “barrier” theory). On the post-survey, Uma did provide a canonical explanation (“the ink particles move in random direction from high concentration to low concentration” and “The particles move slower in cold and faster in hot”), though we don’t know specifically what prompted her shift in reasoning.

Example #2: A mechanistic attach theory refuted by video data: On Day 5 after being engaged with MoDa for two days, Quora and her partner collaboratively drew a detailed mechanistic explanation for the "attach" theory of diffusion (Figure 10).

[Insert Figure 10 and caption here]

Quora and her partner identified underlying entities ("water particles" and "ink particles"), their properties ("move faster," "move much slower"), and reasoned about the relationship between cause and effect between temperature and movement (line 1 for hot temperature, line 2 for cold temperature.) Though their explanation for the effect of temperature was canonical, they maintained the idea that particles interact by "pick[ing] up" or attaching to one another (in the drawing). Thus, they presented a detailed mechanistic account of a non-canonical theory.

Later, when presenting their code to the class, Quora described how she and her partner refuted the non-canonical "attached" theory to settled on the canonical "bounce-off" theory:

Quora: It did not work because we realized that in the model there were clumps that
were not what we saw in real life and the video.
We decided that this was the wrong model and we decided to design the
"bounce off" model. If particles are moving slowly they will hit each other slowly so
ink will sink to the bottom of the container, and it is similar in the video when we look
at cold water.
We compared the model with the video, and it looks the same. Let's start with
low temperatures. It resembles the video, look how ink goes slow and sinks down.

In this context, as Quora compared their original "attach" model with the video data and the class experiment (line 3, 5), they identified discrepancies between their model and the video ("we realized that in the model there were clumps"). The inconsistencies caused them to realize that their model was inaccurate and shift their explanation for particle interaction to the canonical “bounce off” theory.

Example #3: A mechanistic “attach/freeze” explanation refuted by video data: On day 5, after engaging with MoDa for a duration of two days, Jade and Joy collaboratively drew a model that offered a detailed mechanism for non-canonical “attach/freeze” explanation of diffusion (Figure 11).

[Insert Figure 11 and caption here]

Jade and Joy demonstrated mechanistic reasoning as they identified entities (“ink molecules,” “water molecules”), their properties (“warm” and “cold”), their activities (“spread[ing],” “attached,” “freeze,” “interact”), and speculated on causation (“cold molecules freeze, but warm water does not?”). Though they proposed a few particle interactions (“attached,” “freeze,” “interact”), none were the canonical “bounce-off” interaction, and they did not yet seem to understand how temperature affects the speed of particle movement. Although they offered a detailed mechanistic explanation, it was not yet aligned with canonical explanations of diffusion.

When they presented their computational model to the class on day seven, Jade and Joy explained how the comparison of their model to the video (on day 6) advanced their thinking and ultimately lead them to the canonical explanation:

Joy: We played the video, we saw that particles fall dramatically and modeling that was kind of hard. I was trying to add blocks [code blocks] to see what each block is doing, but we also looked at the video to see if it matched the model or not. We did trial and error, adding a block and checking the video, and again.
Teacher: This is what scientists do when they design models. They are trying to run the model and looking at the video [data] and testing, running the model in cold temperature to match the video [data].
Joy: … We wanted to move the water particles and spread them more, then bounce the particles so they will spread more. Move things to bounce off them. In cold water, it's

the exact same thing, but all particles move slower. Ink particles moving and spreading slower.

Jade and Joy took a self-described "trial and error" process of adjusting their model based on comparison with the video (line 3-4). Eventually, they decided a purely "bounce off" model gave them the closest match to the video and described how it worked for both hot and cold water (line 9). By comparing their computational model to the video data, Jade and Joy achieved an explanation that was both mechanistic and aligned with canonical understanding.

Summary of findings

Students' explanations of diffusion shifted throughout the instructional sequence from no explanation or non-canonical (split evenly on the pre-unit survey) to a prevalence of canonical explanations. Examining the above learning trajectories together (Figure 5) suggests that students' mechanistic reasoning and conceptual understanding of diffusion *did not develop in parallel*. Mechanistic reasoning surfaced as students engaged with the level of the causal explanation (i.e., a particle level in the case of diffusion) and often co-existed with wrong, non-canonical ideas. Canonical understanding developed as students compared their modeled mechanistic explanations against real-world data.

Discussion

Mechanistic reasoning and canonical understanding do not develop in parallel

Over the course of an eight-day unit on diffusion, 6th-grade students' mechanistic reasoning both progressed and co-existed with non-canonical explanations. At the beginning of the instructional unit, 6th grade students did not explain causal mechanisms for diffusion. After being introduced to the MoDa agent-based environment, they began providing more mechanistic explanations. Echoing previous work (e.g., Fuhrmann et al., 2018; Fuhrmann et al., 2022a; Fuhrmann et al., 2022b), engagement with a block-based environment that enabled students to describe the creation of particles (entities), their properties, and activities, resulted in explanations of diffusion that included these micro-level, causal mechanisms.

Surprisingly, mechanistic reasoning did not immediately direct students to canonical explanations. As students generated mechanistic explanations of how ink particles spread in cold and hot water, the mechanisms they initially expressed were largely non-canonical. The shift to a canonical explanation mainly occurred when students validated their computational models with the experimental data, often facilitated by the teacher during class presentations. As students compared their designed models with video of the diffusion experiment, they often noticed discrepancies that prompted them to rethink their explanations and re-design their models to better resemble the real-world data. We note that this trend organically emerged in a science class taught by a teacher experienced with computational modeling rather than through researcher intervention. While the role of discrepancies in developing thinking in this way is not new (Fuhrmann et al., 2018), the integration of video data into the modeling platform itself likely facilitated and elevated such comparisons. Moreover, echoing tenets of the conceptual change literature (Smith III et al., 1994), these findings underscore the efficacy of the activity design - including the modeling platform, the curriculum activities, and teacher facilitation - in surfacing the range of students' non-canonical explanations, in this case, about diffusion (Friedler et al., 1987; Meir et al., 2005; Odom, 1995; Sanger et al., 2001; Zuckerman, 1994). We position our findings as aligned with existing literature such as that on learning progressions covering a range of topics (Merritt & Krajcik, 2013; Johnson & Tymms, 2011; Hadenfeldt et al., 2014).

In the course of a computational modeling unit exploring diffusion, students' explanations seem to traverse a two-dimensional space defined by axes of mechanistic reasoning and canonical understanding (Figure 12). Students typically began with non-mechanistic, non-canonical explanations (see Figure 12, bottom left) eventually transitioning to mechanistic, canonical explanations (see Figure 12, top right), sometimes by way of mechanistic, but non-canonical explanations (see Figure 12, top left). This co-existence of mechanistic reasoning and non-canonical explanations reinforces the notion that mechanistic reasoning is a function of an argument's structure rather than its content (Krist et al., 2019; Russ et al., 2008). Interestingly, few students exhibited canonical explanations with non-mechanistic reasoning (see Figure 12, bottom right). We posit, and support with the above data, that: 1) modeling experiences (whether on paper or in a computer model) drove the development of students' mechanistic reasoning, and 2) comparing their own models with the video data in MoDa together with teachers' use of the designed curriculum shifted students' conceptual explanations from non-canonical to canonical.

[Insert Figure 12 and caption here]

Implications for educational design and practice

This study holds several implications for teachers and educational designers. First, despite its limited block library, MoDa accommodated students' diverse ideas. As "a tool to think with" (Papert, 1980), MoDa's block library, in conjunction with the accompanying curriculum, encouraged students to articulate and explore various non-canonical explanations for diffusion. Related work on computational modeling, including our own (Wagh, A., & Wilensky, U., 2018; Wilkerson et al., 2015), has typically provided students with programming blocks designed around canonical ideas in science. Based on the findings presented above, we suggest the value of including blocks that enable students to express their own ideas, including non-canonical ones, as a crucial step in learning science; being able to engage in modeling in ways that are more epistemically authentic to professional practice in developing their mechanistic reasoning and conceptual understanding of scientific phenomena through computational modeling.

Second, the design of the MoDa's modeling area alongside real-world data provided students with direct access to data for reference, enabling them to compare their models with empirical evidence embedded in MoDa. Students' validation of their models based on data offers opportunities for refining non-canonical models and transitioning toward canonical explanations, as both the aggregate data and vignettes above illustrate.

Furthermore, we note that these findings emerged within a middle school classroom run by the teacher, rather than in extended workshops or one-on-one settings run by researchers. Thus, appropriate curriculum design and expert facilitation can foster advanced disciplinary sense-making in everyday classroom settings.

Lastly, the development of mechanistic reasoning alongside non-canonical explanations appears to be closely associated with MoDa's capabilities and underscores the importance of offering authentic modeling experiences. This study highlights the need for a deeper level of disciplinary sense-making, encompassing not only access to data but also considering the overall unit design including facilitation, time management, elements of UI/UX, the curricular activities, and the support of exceptional teachers. Modeling plays a central role in this comprehensive design. The documented correspondences between developing mechanistic reasoning and conceptual understanding - linked to explanatory mechanism and data-based validation, respectively - could inform the design and teaching of other, non-computational modeling instructional materials within science classrooms.

Limitations

We note the role of the instructional unit's diverse media in prompting and capturing students' developing skills and understanding. Our five data sources included three different media: typed responses to open-end pre/post-survey questions, models drawn with pen and pencil on paper, and verbal descriptions of block-based coding models. We suspect that the text-based typed responses in particular may have made it harder for students to enter detail or description that the drawings and verbal presentations better supported (see, from Day 7 to the post-test, the decrease in mechanistic reasoning (Figure 4a) and the decrease in students offering any explanation of diffusion (Figure 5). We interpret these findings as suggesting the strengths of particular media - in this case, paper models and verbal presentations - for eliciting more detailed explanations from students. Finally, we applied the same two coding rubrics to all three data types.

Based on the implications above, we may have underestimated students' reasoning or understanding at the time-points that used text-based responses (pre- and post-unit survey). Further analysis that leverages deeper conceptual mapping techniques (e.g., as in Moreira et al., 2019 or Macrie-Shuck & Talanquer, 2020) could offer deeper insight into the structure and nature of students' explanations, versus our intention to examine this development as intertwined interactions with the specific features of tools and data-based comparisons. We also note the relative prevalence of text-based activities and assessments within educational resources more generally and echo calls to streamline the collection and assessment of richer media such as drawings and verbal explanations that may more fully capture students' learning.

Finally, we acknowledge that not all the students demonstrated a canonical understanding of diffusion by the end of the unit (10 out of 16 demonstrated a canonical understanding at post-test). However, we maintain that incorporating non-canonical ideas into science instruction and environments, as MoDa does, is essential as it: 1) surfaces students' prior knowledge and possible sources of confusion, allowing educators to mediate the learners' knowledge building; and 2) allows students to experience how scientists work and how scientific models are generated and validated. We also acknowledge that giving time for students to explore non-canonical ideas can be a new dynamic for teachers, who may need support in learning how to scaffold their students' reasoning toward canonical understanding.

Conclusions

This study of 6th grade students' work in a computational modeling unit on diffusion both described whole class shifts in mechanistic reasoning and conceptual understanding across the instructional sequence and offered three illustrative examples of student work to trace those shifts to elements of the instructional unit and modeling environment. We found that students' mechanistic reasoning co-existed with non canonical theories. In particular, students' explanations took on more mechanistic elements as they used the agent-based modeling environment. Separately, their explanations shifted from none given or non-canonical to canonical as they used the modeling environment to simulate non-canonical theories, compared them to experimental video data, and revised their models to resolve discrepancies. Implications for model-based design and curriculum include the necessity of exploring non-canonical theories to surface students' diverse ideas about a phenomenon and of integrating comparison with real-world data to connect those ideas with canonical science.

Data Availability Statement

The data that support the findings of this study are not publically available so as to protect the identity of the participants involved.

References

Ackermann, E. (1996). Perspective-taking and object construction. In *Constructionism in Practice: Designing, Thinking, and Learning in a Digital World*. Lawrence Erlbaum Associates.

Arastoopour Irgens, G., Dabholkar, S., Bain, C., Woods, P., Hall, K., Swanson, H., Horn, M., & Wilensky, U. (2020). Modeling and measuring high school students' computational thinking practices in science. *Journal of Science Education and Technology*, *29*, 137–161.

Astolfi, J. P. (1999). El tratamiento didáctico de los obstáculos epistemológicos. *Revista Educación y Pedagogía*, *25*, 149–171.

Blikstein, P. (2014). Bifocal modeling: Promoting authentic scientific inquiry through exploring and comparing real and ideal systems linked in real-time. In *Playful user interfaces* (pp. 317–352). Springer.

Blikstein, P., Fuhrmann, T., & Salehi, S. (2016). Using the bifocal modeling framework to resolve "Discrepant Events" between physical experiments and virtual models in biology. Journal of Science Education and Technology, 25(4), 513–526. https://doi.org/10.1007/s10956-016-9623-7 [PDF].

Bielik, T., Fonio, E., Feinerman, O., Duncan, R. G., & Levy, S. T. (2021). Working together: Integrating computational modeling approaches to investigate complex phenomena. Journal of Science Education and Technology, 30, 40-57.

Conlin, L., Hutchins, N., Grover, S., & Biswas, G. (2020). *"Doing Physics" and "Doing Code": Students' Framing During Computational Modeling in Physics*. International Conference of the Learning Sciences.

Corbin, J., & Strauss, A. (2014). Basics of qualitative research: Techniques and procedures for developing grounded theory, 4th edn Sage Publications. *Thousand Oaks*.

Craver, C. F. (2007). *Explaining the brain: Mechanisms and the mosaic unity of neuroscience*. Clarendon Press.

Darden, L. (2006). *Reasoning in biological discoveries: Essays on mechanisms, interfield relations, and anomaly resolution*. Cambridge University Press.

Dickes, A. C., Sengupta, P., Farris, A. V., & Basu, S. (2016). Development of mechanistic reasoning and multilevel explanations of ecology in third grade using agent‐based models. *Science Education*, *100*(4), 734–776.

Eloy, A., Wolf, J., Fuhrmann, T., Bumbacher, E., Wilkerson, M. H., & Blikstein, P. (2022). MoDa: Designing an integrated platform for computational modeling & data analysis for sustained investigations in science classrooms. *Proceedings of the 2022 Annual Meeting of the International Society for the Learning Sciences (ISLS 2022)*, Hiroshima, Japan.

Farris, A. V., Dickes, A. C., & Sengupta, P. (2019). Learning to interpret measurement and motion in fourth grade computational modeling. Science & Education, 28, 927-956.

Fisher, K. M. (1985). A misconception in biology: Amino acids and translation. *Journal of Research in Science Teaching*, *22*(1), 53–62.

Friedler, Y., Amir, R., & Tamir, P. (1987). High school students' difficulties in understanding osmosis. *International Journal of Science Education*, *9*(5), 541–551.

Fuhrmann, T. Blikstein, P. (2017). Complex Bifocal model Labs in a Science Class: Combining Computer Models and Real World Data in a Diffusion Unit. Paper will be presented at the Annual Meeting of the American Educational Research Association (AERA), San Antonio, TX, USA.

Fuhrmann, T., Fernandez, C., Blikstein, P., & de Deus Lopes, R. (2022). "Can Molecules

Change their Color?” Exploring Students' Non-Canonical Ideas while Programming a Model of Diffusion. Proceedings of the 2022 Annual Meeting of the International Society for the Learning Sciences (ISLS 2022), Hiroshima, Japan.

Fuhrmann, T., Salehi, S., & Blikstein, P. (2014). A Tale of Two Worlds: Using bifocal modeling to find and resolve “Discrepant Events” between physical experiments and virtual models in Biology. *Proceedings of the 2014 Annual Meeting of the International Society of the Learning Sciences (ISLS)*. International Conference of the Learning Sciences, Boulder, CO.

Fuhrmann, T., Schneider, B., & Blikstein, P. (2018). Should students design or interact with models? Using the Bifocal Modelling Framework to investigate model construction in high school science. *International Journal of Science Education*, *40*(8), 867–893.

Fuhrmann, T., Wagh, A., Eloy, A., Wolf, J., Bumbacher, E., Wilkerson, M. H., & Blikstein, P. (2022). Infect, Attach or Bounce off?: Linking Real Data and Computational Models to Make Sense of the Mechanisms of Diffusion. *Proceedings of the 2022 Annual Meeting of the International Society for the Learning Sciences (ISLS 2022)*, Hiroshima, Japan.

Gabel, D. (1999). Improving teaching and learning through chemistry education research: A look to the future. *Journal of Chemical Education*, *76*(4), 548.

Gilbert, J. K., & Treagust, D. F. (2009). *Multiple representations in chemical education* (Vol. 4). Springer.

Hadenfeldt, J. C., Liu, X., & Neumann, K. (2014). Framing students’ progression in understanding matter: a review of previous research. Studies in Science Education, 50(2), 181-208.

Hammer, D., & Elby, A. (2002). On the form of a personal epistemology. *Personal*

Epistemology: The Psychology of Beliefs about Knowledge and Knowing, *169190*.

Holmes, N. G., Wieman, C. E., & Bonn, D. A. (2015). Teaching critical thinking. *Proceedings of the National Academy of Sciences*, *112*(36), 11199–11204.

Hutchins, N. M., Biswas, G., Zhang, N., Snyder, C., Lédeczi, Á., & Maróti, M. (2020). Domain-specific modeling languages in computer-based learning environments: A systematic approach to support science learning through computational modeling. International Journal of Artificial Intelligence in Education, 30, 537-580.

Inagaki, K., & Hatano, G. (2006). Young children's conception of the biological world. *Current Directions in Psychological Science*, *15*(4), 177–181.

Johnson, P., & Tymms, P. (2011). The emergence of a learning progression in middle school chemistry. Journal of Research in Science Teaching, 48(8), 849-877.

Johnstone, A. H. (1982). Macro and microchemistry. *Chemistry in Britain*, *18*(6), 409–410.

Johnstone, A. H. (2000). Teaching of chemistry-logical or psychological? *Chemistry Education Research and Practice*, *1*(1), 9–15.

Krist, C., Schwarz, C. V., & Reiser, B. J. (2019). Identifying essential epistemic heuristics for guiding mechanistic reasoning in science learning. *Journal of the Learning Sciences*, *28*(2), 160–205.

Levy, S. T., & Wilensky, U. (2009a). Crossing levels and representations: The Connected Chemistry (CC1) curriculum. *Journal of Science Education and Technology*, *18*, 224–242.

Levy, S. T., & Wilensky, U. (2009b). Students' learning with the connected chemistry (CC1) curriculum: Navigating the complexities of the particulate world. *Journal of Science Education and Technology*, *18*(3), 243–254.

Levy, S. T., & Wilensky, U. (2010). *Mining Students' Actions for Understanding of Complex*

Systems: Students' Explorations of Gas Models in the Connected Chemistry Curriculum. Annual Meeting of American Educational Research Association, Denver, Colorado.

Löhner, S., van Joolingen, W. R., Savelsbergh, E. R., & van Hout-Wolters, B. (2005). Students' reasoning during modeling in an inquiry learning environment. *Computers in Human Behavior*, *21*(3), 441–461.

Louca, L. T., & Zacharia, Z. C. (2008). The use of computer‐based programming environments as computer modeling tools in early science education: The cases of textual and graphical program languages. *International Journal of Science Education*, *30*(3), 287–323.

Louca, L. T., Zacharia, Z. C., & Constantinou, C. P. (2011). In Quest of productive modeling‐based learning discourse in elementary school science. *Journal of Research in Science Teaching*, *48*(8), 919–951.

Machamer, P., Darden, L., & Craver, C. F. (2000). Thinking about mechanisms. *Philosophy of Science*, *67*(1), 1–25.

McCauley, R. N. (2007). Reduction: Models of cross-scientific relations and their implications for the psychology-neuroscience interface. In *Philosophy of psychology and cognitive science* (pp. 105–158). Elsevier.

Meir, E., Perry, J., Stal, D., Maruca, S., & Klopfer, E. (2005). How effective are simulated molecular-level experiments for teaching diffusion and osmosis? *Cell Biology Education*, *4*(3), 235–248.

Merritt, J., & Krajcik, J. (2013). Learning progression developed to support students in building a particle model of matter. In *Concepts of matter in science education* (pp. 11–45). Springer.

National Research Council. (2012). *A framework for K-12 science education: Practices, crosscutting concepts, and core ideas*. National Academies Press.

NGSS Lead States. (2013). *Next generation science standards: For states, by states*. The National Academy Press.

Odom, A. L. (1995). Secondary & college biology students' misconceptions about diffusion & osmosis. *The American Biology Teacher*, 409–415.

Papert, S. A. (1980). *Mindstorms: Children, computers, and powerful ideas*. Basic Books.

Perkins, D. N., & Grotzer, T. A. (2000). *Models and Moves: Focusing on Dimensions of Causal Complexity To Achieve Deeper Scientific Understanding.*

Pierson, A. E., Brady, C. E., & Clark, D. B. (2020). Balancing the environment: Computational models as interactive participants in a STEM classroom. Journal of Science Education and Technology, 29, 101-119.

Russ, R. S., Scherr, R. E., Hammer, D., & Mikeska, J. (2008). Recognizing mechanistic reasoning in student scientific inquiry: A framework for discourse analysis developed from philosophy of science. *Science Education*, *92*(3), 499–525.

Salmon, W. (1978). Why ask, "Why?"? An inquiry concerning scientific explanation. *Proceedings and Addresses of the American Philosophical Association*, *51*, 683–705.

Samon, S., & Levy, S. T. (2017). Micro–macro compatibility: When does a complex systems approach strongly benefit science learning? *Science Education*, *101*(6), 985–1014.

Sanger, M. J., Brecheisen, D. M., & Hynek, B. M. (2001). Can computer animations affect college biology students' conceptions about diffusion & osmosis? *The American Biology Teacher*, 104–109.

Schwarz, C. V., Akcaoglu, M., Ke, L., & Zhan, L. (2013). *Fifth grade students' engagement in modeling practice across content areas: What epistemologies in practice change* *over time and how*. Annual Meeting of the American Educational Research Association, San Francisco, CA.

Sengupta, P., Kinnebrew, J. S., Basu, S., Biswas, G., & Clark, D. (2013). Integrating computational thinking with K-12 science education using agent-based computation: A theoretical framework. *Education and Information Technologies*, *18*, 351–380.

She, H.-C. (2004). Facilitating changes in ninth grade students' understanding of dissolution and diffusion through DSLM instruction. *Research in Science Education*, *34*(4), 503–525.

Smith III, J. P., DiSessa, A. A., & Roschelle, J. (1994). Misconceptions reconceived: A constructivist analysis of knowledge in transition. *The Journal of the Learning Sciences*, *3*(2), 115–163.

Springer, K., & Keil, F. C. (1991). Early differentiation of causal mechanisms appropriate to biological and nonbiological kinds. *Child Development*, *62*(4), 767–781.

Stains, M., & Sevian, H. (2015). Uncovering implicit assumptions: A large-scale study on students' mental models of diffusion. *Research in Science Education*, *45*(6), 807–840.

Taber, K. S. (2013). Revisiting the chemistry triplet: Drawing upon the nature of chemical knowledge and the psychology of learning to inform chemistry education. *Chemistry Education Research and Practice*, *14*(2), 156–168.

Talanquer, V. (2011). Macro, submicro, and symbolic: The many faces of the chemistry "triplet." *International Journal of Science Education*, *33*(2), 179–195.

Wagh, A., & Wilensky, U. (2018). EvoBuild: A quickstart toolkit for programming agent-based models of evolutionary processes. Journal of Science Education and Technology, 27(2), 131-146.

Wagh, A., Fuhrmann, T., Eloy, A. A. da S., Wolf, J., Bumbacher, E., Blikstein, P., &

Wilkerson, M. H. (2022). MoDa: Designing a Tool to Interweave Computational Modeling with Real-world Data Analysis for Science Learning in Middle School. In Proceedings of Interaction Design and Children, 206–211.

Westbrook, S. L., & Marek, E. A. (1991). A cross-age study of student understanding of the concept of diffusion. *Journal of Research in Science Teaching*, *28*(8), 649–660.

Wilensky, U. (1999a). *GasLab: An extensible modeling toolkit for exploring micro-and macro-views of gasses. Computer Modeling and Simulation in Science Education*.

Wilensky, U. (1999b). NetLogo (and NetLogo user manual). *Center for Connected Learning and Computer-Based Modeling, Northwestern University. Http://Ccl. Northwestern. Edu/Netlogo*.

Wilensky, U. (2003). Statistical mechanics for secondary school: The GasLab multi-agent modeling toolkit. *International Journal of Computers for Mathematical Learning*, *8*, 1–41.

Wilkerson, M. H., Gravel, B. E., & Macrander, C. A. (2015). Exploring shifts in middle school learners' modeling activity while generating drawings, animations, and computational simulations of molecular diffusion. *Journal of Science Education and Technology*, *24*(2), 396–415.

Wilkerson, M. H., Wagh, A., & Wilensky, U. (2015). Balancing curricular and pedagogical needs in computational construction kits: Lessons from the DeltaTick project. *Science Education*, *99*(3), 465–499.

Wright, C., & Bechtel, W. (2007). Mechanisms and psychological explanation. In *Philosophy of psychology and cognitive science* (pp. 31–79). Elsevier.

Xiang, L., & Passmore, C. (2015). A framework for model-based inquiry through agent-based programming. *Journal of Science Education and Technology*, *24*(2), 311–329.

Zuckerman, J. T. (1994). Problem solver's conceptions about osmosis. *The American Biology Teacher*, 22–25.

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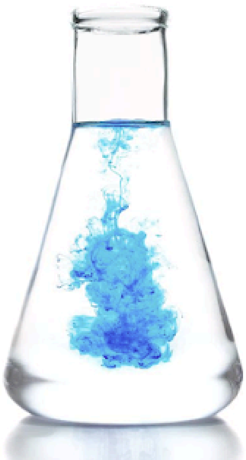
Appendix A. Pre- and Post-test Open-ended Questions

1. Imagine you put a drop of ink or food coloring in a glass of water; after some time, it will spread all through the water. How does the ink make its way through the water?



Your answer

2. Imagine you have a glass with hot water and another with cold water. In which glass would the ink spread faster?

- ◯ It will spread faster in cold water.
- ◯ It will spread equally fast in both glasses.
- ◯ It will spread faster in warm water.
- ◯ It will not spread in either glass
- ◯ I don't know.

3. Explain your answer to the previous question.

Your answer