How Can Computational Modeling Help Students Shift Their Ideas Towards Scientifically Accurate Explanations?

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Abstract: This paper explores how MoDa, an integrated computational modeling and data environment, enabled students to express their ideas about diffusion and shift them toward canonical ideas. Drawing on data from an 8-day unit with two 6th-grade science classes, we analyze students' utterances in presentations, drawings, and written responses to document their diverse ideas about diffusion We present three case studies to illustrate how engaging with computational modeling in MoDa and the unit around it enabled students to shift from non-canonical ideas towards more canonical explanations of diffusion. In particular, we identify three factors that helped in shifting students' ideas: the availability of code blocks to represent a diverse range of ideas including non-canonical ones, consistent access to video data of the phenomenon, and model presentations to the whole class. The paper illustrates how a computational modeling tool and curriculum can make students' diverse ideas visible and shift them toward canonical explanations.

Introduction

Scientists tightly integrate computational modeling and real-world data analysis; they develop and evaluate multiple theories to explain a phenomenon before converging on a single explanatory account (Chandrasekharan & Nersessian, 2002; MacLeod & Nersessian, 2013; Nersessian, 2002). Similarly, in science education, students come to the classroom with diverse ideas to account for how the world works (Rosebery et al., 2005; Smith III et al., 1994). Computational modeling tools can surface students' diverse ideas and make them available for exploration and critique (Linn and Hsi, 2000; Wilkerson, Gravel and Macrander, 2013; Sengupta, Dickes and Farris, 2021). However, computational modeling environments have largely been used in science education to confirm canonical ideas rather than for students to explore multiple, possibly non-canonical theories. Hence, little time is spent allowing them to design explanatory models or showing them the evidence for the model. Moreover, integrating real-world data into the modeling process provides learning opportunities that do not arise when students focus on models alone (Bumbacher et al., 2018). However, opportunities for students to explore and analyze real-world data and to design computational models based on evidence remain largely disconnected. Existing work that integrates computational modeling and data analysis relies on curricular activities outside the modeling environment to link the two (Blikstein et al., 2014; Blikstein et al., 2016; Fuhrmann et al., 2014).

This paper investigates how MoDa (Eloy et al., 2022; Fuhrmann et al., 2022; Wagh et al., 2022), a computational, block- and agent-based modeling environment that integrates model design and real-world data analysis, enabled students to express and refine their thinking about diffusion. Drawing on an 8-day computational agent-based modeling unit on diffusion with two 6th grade science classes, we analyze students' utterances in presentations, their drawings, and their written responses. We illustrate three different non-canonical ideas that students expressed while designing a MoDa model for diffusion and trace how these ideas shift over time. In particular, we identify three features of the MoDa unit - the availability of code blocks to represent a diverse range of ideas including non-canonical ones, consistent access to data through the modeling activity, and whole class model presentations - as contributing to shifts in students' thinking toward canonical explanations of diffusion. Our findings suggest the value of integrated modeling and data analysis activities for both surfacing students' diverse ideas and shifting them towards scientifically accurate explanations.

Theoretical background

We first briefly review the literature on computational modeling, focusing on domain-specific block-based modeling in particular and how it has been incorporated into science classrooms. We then contextualize this study within work that emphasizes the link between data use and scientific model construction.

Block-based, computational, agent-based modeling

Designing computer models combines the advantages of traditional modeling with computational literacy, opening new possibilities for inquiry-based learning (White & Frederiksen, 1998). Agent-based computational modeling environments, in particular, simulate the actions and interactions of autonomous agents (e.g., individual organisms, particles, molecules) in order to understand the behavior of a system. Domain-specific block-based programming environments provide students with a limited library of blocks related to the target phenomenon (Wilkerson et al., 2015) and significantly lower the threshold for students to program and test their theories about scientific phenomena (Hutchins et al., 2020; Repenning, 2017). The domain-specific nature of programming can align with students' existing ways of thinking and provide a language to articulate their scientific ideas (e.g., Aslan et al., 2020). It also supports students' developing conceptual understanding and mechanistic reasoning (Wagh & Wilensky, 2018). In the last two decades, innovations in agent-based, and domain-specific, block-based computational modeling technologies have enabled learners to create their own models using visual and block-based (as opposed to script-based) programming in environments such as NetTango (Horn et al., 2014), Deltatick (Wilkerson-Jerde et al., 2015), ViMap (Sengupta et al., 2021), and Much.Matter.in.Motion (Saba et al., 2021).

One design tradeoff of relatively small block libraries is the more limited opportunities for students to explore non-canonical ideas. In some cases, students are asked to use or manipulate a model from existing blocks that only present "canonical" scientific explanations of phenomena. Students miss the opportunity to engage in iterative model building: to articulate and test out an initial idea, identify its limitations, and try out different ideas and explanations. We study the intentional inclusion of non-canonical blocks in MoDa's block library to study the implications surfacing and understanding students' ideas about scientific phenomena.

Using data to design models

Modeling and data practices are tightly intertwined in professional scientific work (Nersessian, 2002). Scientists use data from real world phenomena to both design and validate computational models to build explanatory theories about those phenomena. However, model-based learning approaches in the science classroom predominantly focus on model-based and data-based practices separately (Bumbacher et al., 2018). The Bifocal Modeling framework (Blikstein et al. 2016; Fuhrmann et al., 2014) suggests integrating real-world data collection with computational modeling to enable real-time comparisons of simulated and real data. Juxtaposing data and modeling enables students to notice and attend to discrepancies between models and data, bringing noise, uncertainty, and intrinsic differences between them (Blikstein et al., 2016; Gouvea & Wagh, 2018). Such comparisons create new learning opportunities, enabling students to develop conceptual understanding and meta-modeling competences (Blikstein, 2014; Fuhrmann et al., 2018), deeply explore the underlying features of a phenomenon (Schwarz et al., 2013), and make decisions based on data to think critically and evaluate models (Holmes et al., 2015). Besides designing classroom activities that enable and emphasize this integration, learning environments can also highlight for students the links between real-world data and computational modeling (e.g., Bumbacher et al., 2018). Without available tools, it is difficult to engage students in the explicit coordination of computational models and real-world data for theory building and to study the types and conditions of learning that arise from comparing real-world data and computational models.

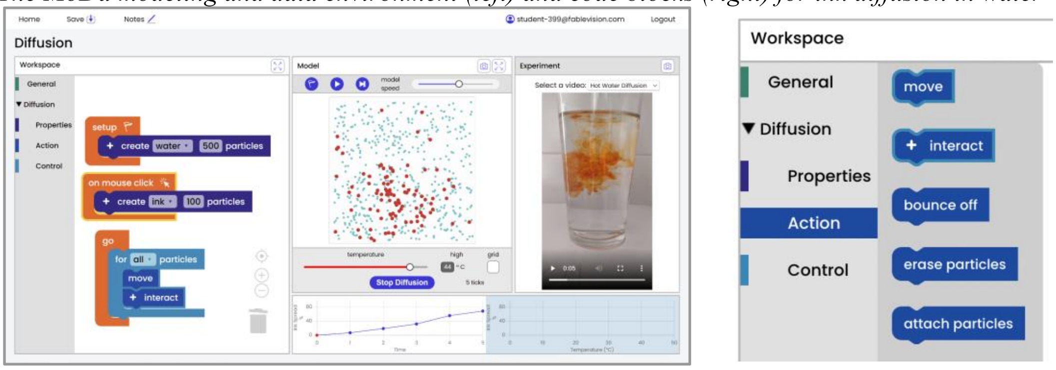
Building on these research traditions of integrating data and modeling, we explore two research questions: (1) How do students use a block- and agent-based computational modeling environment to express their initial ideas about diffusion? (2) How do students' ideas about diffusion shift over the course of the unit?

Materials & methods

MoDa: The modeling and data environment

The block- and agent-based, domain-specific computational modeling environment used in this study is MoDa (Eloy et al., 2022; Fuhrmann et al., 2022; Wagh et al., 2022), which was designed for middle school students and teachers to use in science classrooms. MoDa combines computational models using domain-specific code blocks (Wilkerson-Jerde et al., 2015) with the Bifocal Modeling framework, in which learners compare their computational models with real-world data (Blikstein, 2014; Fuhrmann et al., 2018). MoDa consists of a modeling area (built using Google's Blockly library), in which students can drag and drop blocks to program agent-based models that run on the NetLogo engine (Wilensky, 1999). It also includes a real-world data area with videos serving as visual data. In the unit described in this paper, this area includes two videos of ink spreading in hot and in cold water (Figure 1, left). The simulation area includes phenomenon-relevant parameters (e.g., temperature) that students can adjust to evaluate their models. The code library includes blocks for the canonical explanation (i.e., the "bounce off" block that changes heading on collision) of diffusion and typical non-canonical student explanations such as “attach” that makes two particles stick together and “erase” that deletes a particle (Figure 1, right).

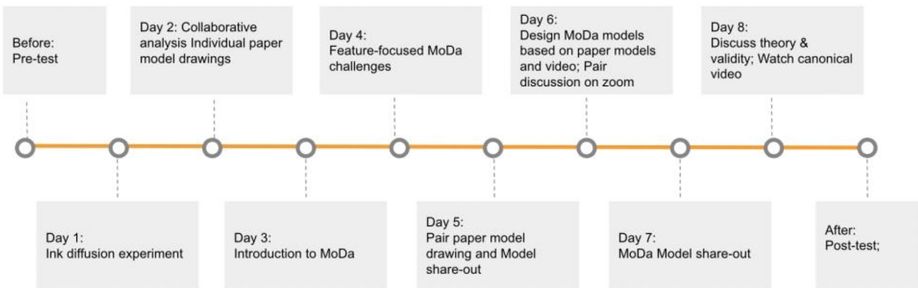
Figure 1
The MoDa modeling and data environment (left) and code blocks (right) for ink diffusion in water



Participants, settings, and instructional sequence

Participants were 6th grade students in a private school in California. Across two classes with the same teacher, 16 students consented to participate (8 girls, 6 boys, and 2 non-binary students). They conducted a diffusion experiment to compare the rate of ink spread in hot and cold water and drew paper models to explain the difference in the rate of spread across the two conditions. Students used MoDa to program computational models to explain their observations and shared both their models with the class for feedback. On the last day, students discussed the validity of their models and watched a video of the canonical explanation for diffusion. All names are pseudonyms. The science teacher has been part of this project for 2 years and participated in professional development and co-design sessions with the project team. The unit occurred over eight class periods and included activities to explore ink diffusing in hot and cold water (Figure 2). Although diffusion is an important concept in science curricula (NGSS, 2013), it can be challenging for students to learn. 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 bouncing off one another during the course of Brownian motion. Diffusion occurs faster at higher temperatures because temperature is expressed, molecularly, through an increase in Brownian motion. The science classes did not meet every day of the week, so a few days passed between days of the instructional sequence.

Figure 2
The diffusion unit’s instructional sequence



Data sources and analysis

To identify students’ different explanations for diffusion, we analyze videos of students designing MoDa models (Day 6) and of students presenting their models to their classmates (Day 7). We then trace these explanations back to their origins in earlier data sources (pre-test responses and drawings on Days 2 and 5, respectively) and to their conclusions in students’ post-test responses to construct progressions of students’ explanations through the unit. We marked moments in which students either changed or articulated having changed their explanations and we identified what factors contributed to the shift. This analysis was done independently by the first author and two other co-authors. The above data sources were coded using grounded coding (Corbin & Strauss, 2014) to identify factors that led to students’ shifts. We construct three cases that typify both the non-canonical ideas that students shared and their trajectory toward a shift to a canonical understanding of diffusion.

Results

Our analysis revealed that students were able to express a range of ideas to explain how diffusion works through their computational models. In total, we identified nine kinds of explanations about diffusion expressed in code. We identified three factors that played a key role in shifting student thinking towards more canonical explanations: the availability of domain-specific blocks to model non-canonical ideas, consistent access to the phenomenon through the video data within MoDa, and model presentations to the whole class. Below, we illustrate three initial non-canonical ideas that students expressed while designing a MoDa model for diffusion: the barrier model, the attach model, and the density model. For each idea, we present examples of how students stated, drew, and coded it in MoDa, and how their ideas shifted towards the canonical explanation.

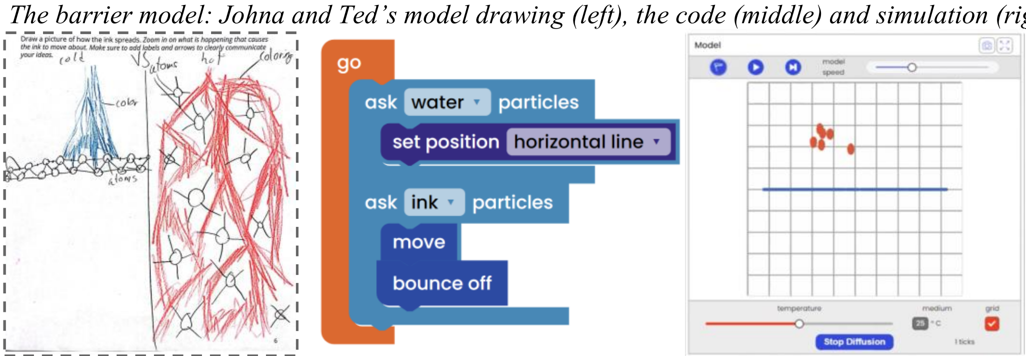
The barrier model

In their first non-canonical model, Johana and Ted had cold water particles create a barrier or border that blocks the ink particles from spreading throughout the glass (Figure 3, left). By the time they created the pair drawing on Day 5, Johana and Ted had expressed the canonical effect of temperature on ink and water particles ("When the water or ink molecules are warm, they move/spread faster. When they are cold, they move/spread slower.") but maintained a non-canonical explanation of particle interaction. While creating their MoDa model on Day 6, Johana and Ted coded the barrier model.

Ted: We need to fix that horizontal line thing.
Johana: Is it supposed to be like a barrier or something?
Ted: Yes, I bet it can still pass it through.
Johana: If we make it so they have to bounce off, then it won't be able to pass through it.

In creating their barrier model, Johana and Ted included the canonical "bounce off" particle interaction to prevent the ink particles from passing through their water barrier (Figure 3, middle). By adding drops of ink above this water "barrier," the students kept the ink at the top of the simulated beaker (Figure 3, right).

Figure 3
The barrier model: Johna and Ted's model drawing (left), the code (middle) and simulation (right).



After a few more revisions to their code, primarily focused on the ink particles' movement, Johana recognized an important discrepancy between their simulation and the video data.

Johana: Even if we get this to work, if the border is on the top, it won't let the ink go to the bottom, right? And doesn't, every time when we see it [in the video], it comes down towards the bottom? Maybe here, let me try something. [...] So, our initial idea was to create a border at the middle, then we realized that even if we programmed that, we would have to program them to bounce off, right?
Instructor: Yes
Johana: So they would be staying at the top, and that is not what it looks like in the actual thing [the video].
Instructor: Oh so you revised your model.
Johana: So now I am more, leaning towards the bounce off model.

In the whole classroom model presentation on Day 7, Johana and Ted had not yet finalized their code but emphasized that *"we had a border [barrier] and we are going to take that away. So it's just they are bouncing off* *of each other and, again, if something is moving quickly and it bounces off, it is going to travel further. If something is moving slowly, and even if it bounces off, it is not going to travel as far."* They explained the reduced spread in cold water solely as a result of temperature, in line with canonical science.

The density model

Introducing the variable of weight to the system, Miguel expressed the idea that hot water particles were lighter than cold water particles. As early as his Day 2 drawing, he explained that *"The ink in the cold just sank to the bottom of the glass. It might have lower density, so there is more space for the ink. It might have been the only place it could move into."* In his drawings (Figure 4, left), Miguel's "density theory" implies pockets of heavier, more densely packed cold water particles, where ink has minimal open paths ("places") to spread. In contrast, he understood hot water to be uniformly less dense, allowing the ink to diffuse everywhere throughout the glass.

Figure 4
The density model: Miguel and Wade's model drawing (left), code (middle) and experiment (right).

On Day 5, when Miguel and Wade coded their density model, they created more water particles for the cold water condition and fewer particles for the hot water condition (Figure 4, middle). In Day 6 pair drawing, they created a density model, but after a discussion with the teacher, Miguel decided to test his dense theory by using the scale in the classroom (Figure 4, right). When he learned that the hot and cold water beakers weighed the same, Miguel balled up his paper model and threw it in the trash (note the wrinkle lines in Figure 4). Still, he maintained the density theory going into the Day 6 computational model presentations.

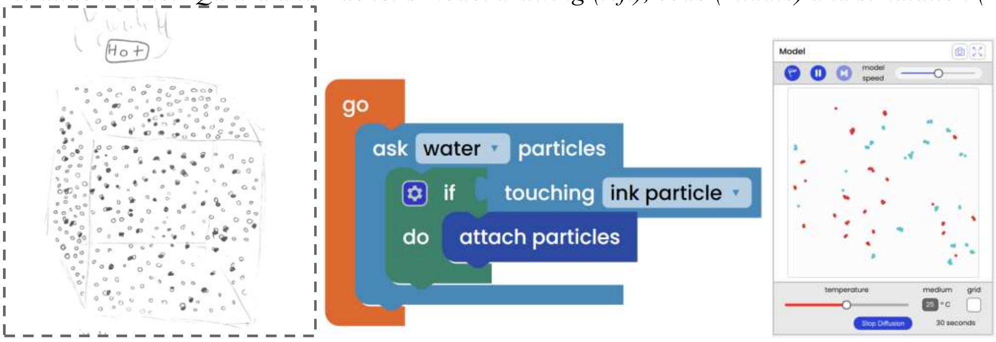
> *Miguel: First set it to 203 [particles]… this right now is hot water ... I basically modeled density by the amount of water particles on the grid… I know hot water has a lower density than cold water, so there are less particles to model a lower density.*
> *Instructor: (plays simulation and video; class notes discrepancies) How can we model the cold water diffusion?*
> *Miguel: Set water particles to 500.*
> *Instructor: (plays simulation and video; class compares) ... What are you thinking about density based on what we just saw? (7 second pause) Did you notice a huge difference between hot and cold when you changed the density?*
> *Miguel: Uhh, yeah, it… one seemed… I don't know, not really.*
> *Instructor: I didn't either! I didn't notice too much of a difference, and I think that's really important information. What about anyone else? (solicits individual students for reactions)*

After the whole-class presentation comparing the fit between his hot and cold models with the other students' presentations and the corresponding videos, Miguel started to doubt his density theory ("I don't know, not really."). By the post-test, Miguel expressed the canonical theory for diffusion that *"since particles move faster in hot water, they will bounce off more things in a certain amount of time."* Wade, Miguel's partner who joined class remotely for the Day 6 model presentations, maintained the density theory through the post-test, explaining the difference between cold and hot water diffusion as "*cold has density, hot has air bubbles*."

The attach model

Qahira expressed the attach theory, the idea that the ink spreads in water because the particles "pick up" or stick to one another. Though Qahira didn't articulate the attach model on her pre-test or Day 2 drawing, she clearly expressed it in her Day 5 pair drawing with Rachel (Figure 5, left), which she captioned *"In the hot water the water particles move faster, as they move they pick up the ink particles around them spreading the ink faster. In the cold water the water particles move much slower than in the hot water so they pick up the ink and spread them much slower."* She then coded this model on Day 6 using the "attach particles" block (Figure 5, middle), which made the particles clump together (Figure 5, right).

Figure 5
The attach model: Qahira and Rachel's model drawing (left), code (middle) and simulation (right)



As Qahira and Rachel stated while presenting their model on Day 7, they eventually changed their minds about the attach model.

Qahira: We realized that ink particles attached more than one ink particle to the water particles and making clumps and moving around like that. That wasn't really what we saw at all in the video. And, therefore, comparing real life with the model, we were able to figure out that one was not the right one.
Instructor: Explain your thinking about this bounce off.
Qahira: Well, our thinking was, if the particles of water are moving slowly in the cold water, they're not gonna hit the ink particles as fast. Therefore the ink particles have time to fall to the bottom and then, like, so, yeah. It will kind of look good, I guess, in the model, similar to what the water does in hot water and cold water [in the video].

By coding their non-canonical attach theory and comparing the simulation to the video data, the students realized their theory wasn't accurately capturing the diffusion phenomenon. Qahira noticed a better fit between her simulation and the video when using the bounce off model. She maintained this canonical understanding through the post-survey, where she explained *"the hotter the water, the faster the water particles move. When the ink and water particles collide, they bounce off of each other."*

Discussion

Our findings highlight three key points. First, students brought a diverse range of ideas about the mechanisms underlying ink diffusion in water, some of them canonical and some of them not. Although limited in number, *the collection of domain-specific blocks available in MoDa* enabled students to express these diverse theories and test them by creating a diverse set of models. In contrast to the drawn paper models, which students completed before modeling their theories in MoDa, the dynamism of computer models seemed to prompt students to refine their non-canonical models in ways not afforded by drawing static models. Consistent with the literature on model-based learning, students began to shift away from non-canonical theories once they saw how those theories played out in action. Also consistent with conceptual change research (Smith III et al., 1994), students may have been more willing to change their ideas away from non-canonical explanations after seeing why those ideas don't function in the way they expect, in contrast to simply seeing why a canonical theory works. Second, *students' consistent access to video data* of the ink-in-water experiment within the modeling environment seemed crucial to their evolving theories of diffusion. Aligned with our previous work (Fuhrmann et al., 2018), comparing their models with experimental data highlighted discrepancies between the data and models, leading students to shift towards other, canonical explanations. For all students presented in this paper, the lack of alignment between the video data and their coded model (e.g., the simulated barrier blocking ink in ways that did not occur in the video, particles clumping in the attach simulation and not in the video data) led to a shift in student explanations towards canonical ideas.

Finally, *computationally representing their theories in code to the whole class* turned students' ideas into concrete artifacts available for consideration and critique by the class community. Computational models can serve as critical artifacts for sense making at the level of the classroom (Wilkerson et al., 2017). In presenting to the whole class, students shared their own ideas and listened to other students' ideas. The models presented by students in these whole class presentations led to students shifting their explanations and revising their models to reflect canonical ideas. Though not a focus of this analysis, we suspect the concrete yet dynamic representation of students' thinking afforded by MoDa also enabled the teacher to guide both individual and whole-class instruction toward disciplinary norms. Further work is needed to validate this assumption.

Conclusions

To conclude, MoDa and the unit described in this paper was used by these classes as an inquiry tool that enabled students to express, explore, and develop their ideas about a scientific phenomenon. Acknowledging students' existing ideas early on in the unit through the design of blocks in MoDa and accompanying activities supported students in developing a range of models including non-canonical models. Having access to real-world data to notice discrepancies through comparison with the model as well as presenting their ideas and computational models to the whole class supported students in iteratively refining their models to represent a more canonical explanation of diffusion.

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