Learning About Diffusion at Two Levels: Agent-based Micro-scale and Equation-based Macro-scale

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Abstract

Diffusion is a crucial phenomenon in many fields of science and engineering, and it is known to be difficult for students to learn and understand. Ideally, students should understand (1) the macro-level patterns of concentration change including Fick's laws which describe these patterns quantitatively, (2) the micro-level random-walk mechanism of diffusing particles, and (3) how these two levels of description are related, i.e. how the macro emerges from the micro. We describe agent-based models (ABMs) of diffusion designed to help students accomplish these learning goals and report the outcomes of implementing them in a university materials science course. The results indicate that the ABM activities helped students understand the micro-level processes of diffusion compared with students from the previous year, but that gaps remained in their understanding of the macro-level patterns of diffusion and the connection between the levels. We conclude with a brief description of our re-designed learning activities to improve outcomes in future years.

1. Introduction

1.1 Diffusion as emergent process and "levels confusions"

Atomic-scale diffusion is a critical physical behavior in the field of materials science as well as many other areas of science and engineering. Diffusion is also well documented in education literature as difficult to understand, especially when the main mode of instruction is lecture-based as opposed to inquiry-based [1]–[3]. One difficulty stems from "levels confusion" [4] in which a person attributes properties of the macro-level to the micro-level or vice versa. For example, traffic jams emerge from collection of cars in transit, and, surprisingly, they move in the opposite direction of the cars. People can be confused by this, thinking "the cars move forwards, how can the jam move backwards?", but this fails to recognize that the micro-level (cars) is different from the macro-level (the jam). Specifically for diffusion, "levels confusion" can manifest as believing atoms deterministically move from areas of high concentration to areas of low concentration [5], when in reality, *individual* atoms move (approximately) randomly. The macro-level change in concentration emerges from the statistical distribution of random atomic trajectories. Ideally, materials science students should understand the micro-level process of diffusion, the macro-level dynamics of how concentration changes in space and time, and how these two levels are related. This study reports on the outcomes of students after they engaged in activities designed by the authors to support learning these three aspects of diffusion.

1.2 Background on Diffusion and Fick's Law

Diffusion arises from random movement of particles at the micro-level. A common way to model this random movement is to imagine particles occupying spaces on a grid and randomly hopping to a neighboring site each time step, as depicted in Figure 1.

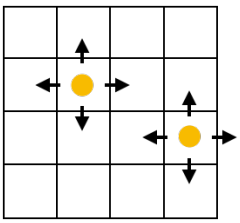


Figure 1: depiction of random walk diffusion.

At the macro-level, diffusion is observed as changes in concentration and is classically modeled by Fick's laws. Figure 2 shows a discretized concentration profile with the *number* of atoms at each *x*-position in a hypothetical grid (one can acquire the concentration at each *x*-position by dividing the number of atoms by the discrete volume). For this example, we assume that each particle has a 50% chance of jumping in the *x*-direction each time step, with an equal chance of going in either direction. The curved black arrows with numbers in Figure 2a show the average number of particles that will hop in each direction. In Figure 2b, the blue dotted lines with numbers and arrows above them show the average *net* number of particles that will pass through these lines each time step, known as the *flux* (in three dimensions, flux has units *#/cm²/second*). To demonstrate, four particles will pass through the line between *x*=1 and *x*=2, but the *net flux is zero*, because two particles are going in each direction and cancel each other—they are simply exchanged. The flux at each *x*-position is determined by the slope of the concentration profile, because this is proportional to the imbalance of particles jumping from either side of the dotted line. This relatively simple observation is known as Fick's 1st law and, when all quantities are taken to be continuous, is written mathematically as $J = -D\,\frac{\partial c}{\partial x}$, where J is flux, c is concentration, x is position and D is a constant known as the diffusion constant, which quantifies the jump frequency.

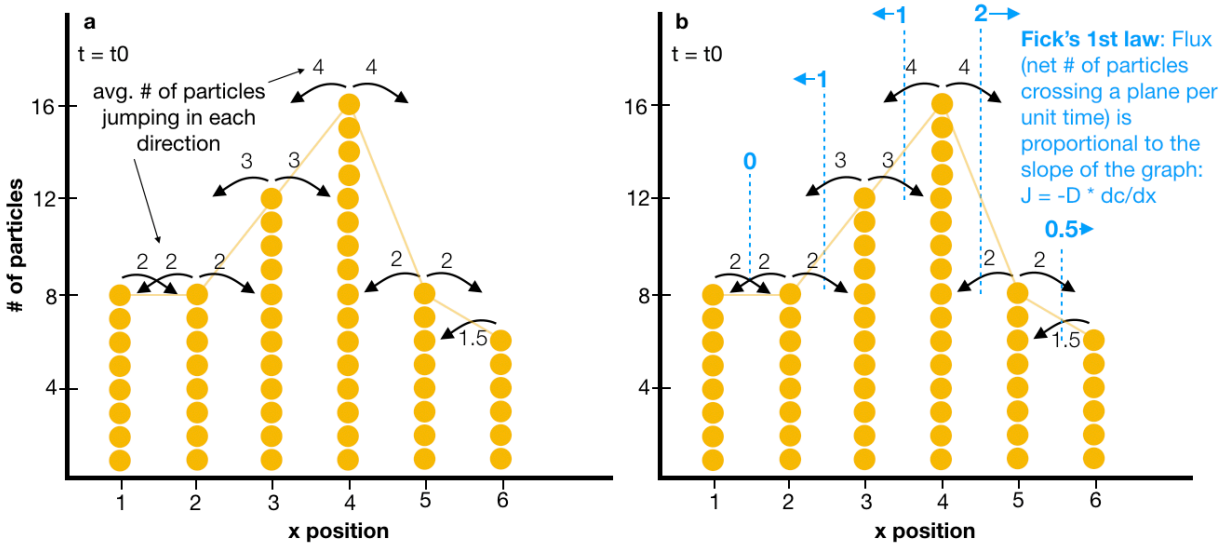


Figure 2: (a) A discretized concentration profile showing number of atoms at each x position. The curved black arrows show the number of atoms jumping in each direction per time step (assuming particles have a 25% of jumping in each direction). (b) Depiction of Fick's 1st law: blue numbers with arrows indicate the flux of particles through that blue dotted line.

Fick's 2nd law describes how concentration will change over time. Figure 3a retains the blue numbers indicating flux from Figure 2b and adds green numbers indicating how many atoms will be gained or lost at each *x*-position. The change in number of atoms is simply the sum of the atoms entering or leaving that *x*-position, i.e. the flux on either side. For example, at *x*=2, the flux on the left is zero and the flux on the right is -1 (1 to the left). So, the number of atoms at *x*=2 will increase by 1 at the next time step. At *x*=3, the number of atoms will not change despite the non-zero flux on either side, because the fluxes are equal and thus cancel. In general, if the fluxes on either side of an *x*-position are the same, then the concentration profile will have zero curvature; if they are unequal, the concentration profile will have non-zero curvature. Thus, the change in concentration at a given *x*-position is proportional to the curvature of the concentration profile at that point. This is known as Fick's 2nd law, and when all quantities are taken to be continuous, is written mathematically as the partial differential equation $\frac{\partial c}{\partial t} = D\,\frac{\partial^2 c}{\partial x^2}$, where c is concentration, t is time, x is position and D is the diffusion constant.

It is perhaps worth noting this approach to explain Fick's laws was developed after the course reported on in this study. The students did not have Fick's laws explained this way.

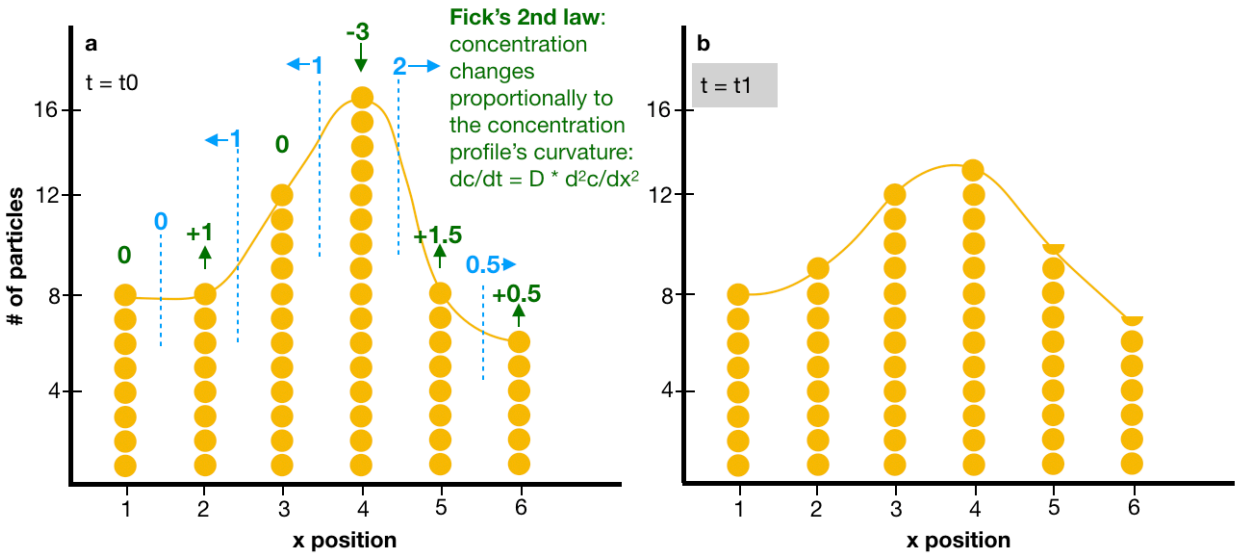


Figure 3: (a) Depiction of Fick's 2nd law: blue numbers with arrows are the same as in Figure 2b. Green numbers indicate how the number of particles at each x position will change in the next time step. This number is determined by the flux in and out of that x position, i.e. the blue numbers on either side of the x position. (b) What the concentration profile will look like at the next time step.

1.3 "Restructurations" of Knowledge for Understanding Emergence

Traditionally, diffusion in materials science is taught by derivation of Fick's Laws which do not foreground the emergent nature of diffusion. Fick's Laws describe how macro-scale concentration changes in time with no direct reference to atoms. Students are capable of using rote understanding of the equations to solve for the evolution of diffusion behavior for simple,

analytical systems, but often have difficulty extending the concepts or describing diffusional behavior at the atomic and molecular scale.

In contrast to equation-based models such as Fick's Laws, Agent-based modeling (ABM) is a computational paradigm in which individual agents are programmed to have certain behaviors with the goal of understanding how macro-level patterns or properties of the system emerge from the simple agent behaviors. In materials science, the "agents" are most likely to be atoms or molecules, and of course, materials scientists already use this type of modeling in such techniques as molecular dynamics and Monte-Carlo methods (we will use ABM to refer to all such methods). However, these techniques are usually seen as advanced calculation methods, not as primary representations of phenomena with powerful learning properties.

A change in how knowledge is represented can have powerful effects on learning. For example, when Europe still used Roman numerals, long division and multiplication were so difficult that most people had to take such problems to professional "calculatores" [6]. Now that we use Hindu-Arabic numerals, elementary school children routinely learn long division and multiplication. Wilensky and Papert [7] termed this type of change in representational form a "restructuration" of knowledge and argued that computational, agent-based representations could have equally dramatic benefits for understanding complex phenomena, because they foreground how macro-level properties emerge from micro-level rules.

Several groups have investigated the use of ABM to help students learn about emergent phenomena in materials science [8] and related subjects of chemistry [9], [10] and physics [11]. This study investigates the use of ABM for learning about diffusion as the first step in a design-based research process [12] to create an effective diffusion curriculum for materials science students.

1.4 Research Questions

We investigated the following research questions:

After using both Fick's laws and an agent-based computational model:

1. How did students reason about changes in macro-level concentration profiles, and did they use Fick's laws for this reasoning?
2. Did students understand the micro-level random-walk mechanism underlying diffusion?
3. How did students understand the relationship between the micro- and macro-level descriptions, specifically in terms of the ABM (which models diffusion at the micro-level from which the macro-level concentration profiles emerge) and Fick's 2nd law (which describes macro-level concentration profile dynamics directly)?

We also discuss implications of our results and how we intend to re-design our learning activities to enhance learning of all these levels.

2. Methodology

2.1 Setting and Participants

The study was conducted in a sophomore-level materials science course taught by the second author of the paper in 2019. The course is the third materials science course for majors after an introductory survey course and a course on chemical thermodynamics. The class consisted of 20 students, 15 of whom presented as male and 5 as female. Seventeen of the students consented to have their coursework analyzed for this research, and five of those were also interviewed. An additional four students from the previous year's course in 2018 were interviewed for comparison. Institutional review board approval was obtained to perform research with students, and no incentives were provided for study participants.

2.2 Design Based Research

This study reports on the first stage of a design-based research process to produce and study an intervention for helping students understand diffusion. Educational design research seeks both to create practical interventions to improve learning and to develop theory explaining why those interventions work; the process is iterative with successive cycles of design and analysis aimed at refining both the intervention and theory [12]. The core of the intervention for this study consisted in the students interacting with and extending two ABMs co-designed by the authors of this paper. The ABMs and activities are described further in the next section. This study is rooted in design-based research in that the object of study—student understanding of diffusion—was directly mediated by our newly designed ABM activities, and the future work resulting from our findings will aim to refine our designs and then to implement and study them again.

2.3 Agent-based Models and Learning Activities to "Restructurate" Diffusion Knowledge

The materials science course in which the study took place traditionally starts the unit on diffusion by introducing Fick's laws. Random walk behavior is discussed, because it is involved in deriving Fick's laws, but only briefly. After Fick's 2nd law has been derived, several materials-relevant solutions are demonstrated for various initial/boundary conditions but without derivation, because the analytical methods used to solve Fick's 2nd law are too advanced for most students in the course. In the focal classroom of this study, this traditional sequence was maintained, and then after the unit on Fick's laws, the students engaged in learning activities using ABMs written in NetLogo [13] to investigate how concentration profiles emerge from atoms moving in random walks.

The ABMs were intended to "restructurate" diffusion knowledge. To give a sense of why these models could be a restructuration, Figure 4 shows Fick's 2nd Law, the classic differential equation used to model random-walk diffusion in one dimension, along with four solutions to it for four different initial/boundary conditions. The approaches used to solve each scenario require mathematical approaches outside the core mathematics sequence, and without this background, students struggle to see how these solutions are related to both Fick's 2nd Law and the physical conditions they model.

$$\left(\frac{\partial c}{\partial t}\right) = D\left(\frac{\partial^2 c}{\partial x^2}\right) \qquad \text{Fick's 2nd Law}$$

$$c(x,t) = \bar{c} + \beta(0) sin\left(\frac{\pi x}{l}\right) \exp\left(-\frac{Dt\pi^2}{l^2}\right) \qquad \text{Sinusoidal initial condition}$$

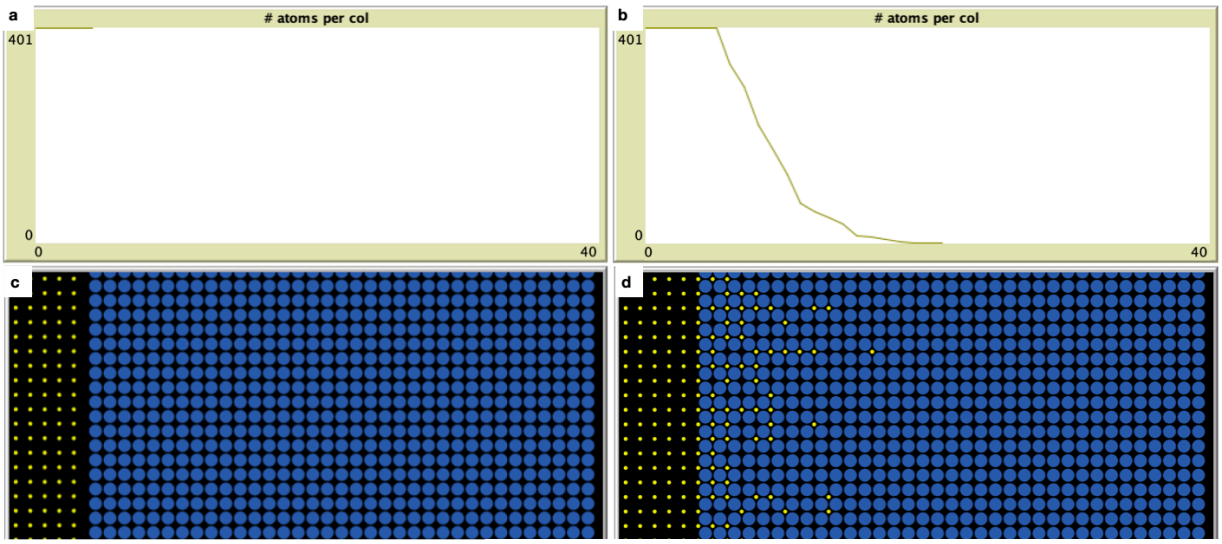
$$c(x,t) = \frac{4c_o}{\pi} sin\left(\frac{\pi x}{h}\right) \exp\left(-\frac{Dt\pi^2}{h^2}\right) \qquad \text{Diffusion out of a slab}$$

$$C = \frac{M}{2\sqrt{\pi Dt}} \exp\left(\frac{-x^2}{4Dt}\right) \qquad \text{Thin film tracer diffusion}$$

$$\frac{c_s - c(x,t)}{c_s - c_o} = \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \qquad \text{Constant surface concentration}$$

Figure 4: Fick's 2nd law, the classic differential equation for modeling diffusion along with four solutions to various initial conditions.

In contrast, Figure 5 shows screenshots of the ABM the class used to model a carburization process (carbon diffusion into iron). The blue circles represent the atoms of the material being diffused into (e.g., iron, the solvent) and the yellow circles represent the diffusing atoms (e.g., carbon, the solute). Above this "atomistic" view is a graph of the number of atoms per column in the simulation—essentially a concentration profile. The bottom-left pane shows the main code



e

```
to go
  ask d-atoms [random-walk]
  set-constant-left-surface-concentration
  tick
end

to random-walk
  let neighbor one-of neighbors4
  if [not any? d-atoms-here] of neighbor[
    move-to neighbor
  ]
end
```

Figure 5: An ABM of diffusion. In (c) and (d), the blue and yellow circles represent iron atoms and diffusing carbon atoms to give a micro-level picture of carbon atoms diffusing through an iron lattice. (c) shows the initial condition before any diffusion and (d) shows after some diffusion has occurred. (a) and (b) show concentration profiles associated with the micro-level views below them. This version of the model has a constant surface concentration on the left surface to model a carburization process, the same situation that the last equation in Figure 4 describes. (e) shows the core NetLogo code of the model.

for this model to run. The code "asks" the diffusing atoms to pick a neighboring interstitial site, and then if it is unoccupied, to move to it. This process is repeated at each subsequent time step in the calculation. In contrast to the differential equation, analyzing different starting conditions does not obscure the fact that the atoms always behave the same way. Instead, learners can simply change the initial distribution of yellow atoms and then run the exact same code.

Students in this study first explored an ABM of random walk behavior in which they numerically found the relationship between time and the root-mean-square distance of random walkers in 1 and 2 dimensions. They then explored the ABM shown in Figure 5 to learn about the emergence of concentration profiles from random-walk behavior. They analyzed the code of the ABM to learn how random-walk is modeled and explored the resulting behavior under various initial conditions.

2.4 Data Collection and Analysis

The study used mixed-methods [14] involving students' written answers from an exam, followed by interviews to both confirm/disconfirm and complement the findings from the exam data. We analyzed seventeen students' written responses to exam questions on (1) the macro-level dynamics of concentration profiles, (2) the micro-level atomic processes, and (3) the relationship between assumptions in Fick's laws to assumptions in computational atomistic agent-based models.

To gain deeper insight into their reasoning, we selected five students who exemplified different answer types on the exam questions and conducted interviews in which they re-did the exam questions while "thinking aloud" and explaining their answers in the style of a clinical interview [15]. In this type of interview, questions are prepared in advance to probe different aspects of the subject's thinking, but the interviewer is free to improvise follow-up questions to clarify and further probe the subject's thought processes. The students were interviewed two to three months after they finished the course. For comparison, we also interviewed four students from the previous year of the course who did not use the NetLogo model. These students were selected at random from a group of about ten students from the previous year's course who consented to be interviewed.

3. Results

The results section is organized in the same order as the exam question we analyzed. The students were asked to consider the following decarburization process: A 1 cm thick slab of ferrite (α-iron) with an initial carbon content of 0.06 atomic% is held at 700 °C in a vacuum (meaning the surface concentration is always zero on both sides of the slab). They were then asked various questions about this system, discussed in the following sub-sections. It should be noted that students were allowed to bring one page of notes to the exam, but not during the follow up interviews.

3.1 Macro-level Dynamics of Concentration Profiles

In this section we investigate our first research question: how did students reason about changes in macro-level concentration profiles, and did they use Fick's laws for this reasoning?

3.1.1 The Exam Question and Numerical Results

Students were asked on the exam to sketch three carbon concentration profiles of the system at three different times: prior to any decarburization and then at two different times after appreciable decarburization. Figure 6 shows the exact question that students saw with an example of a student answer coded as fully correct.

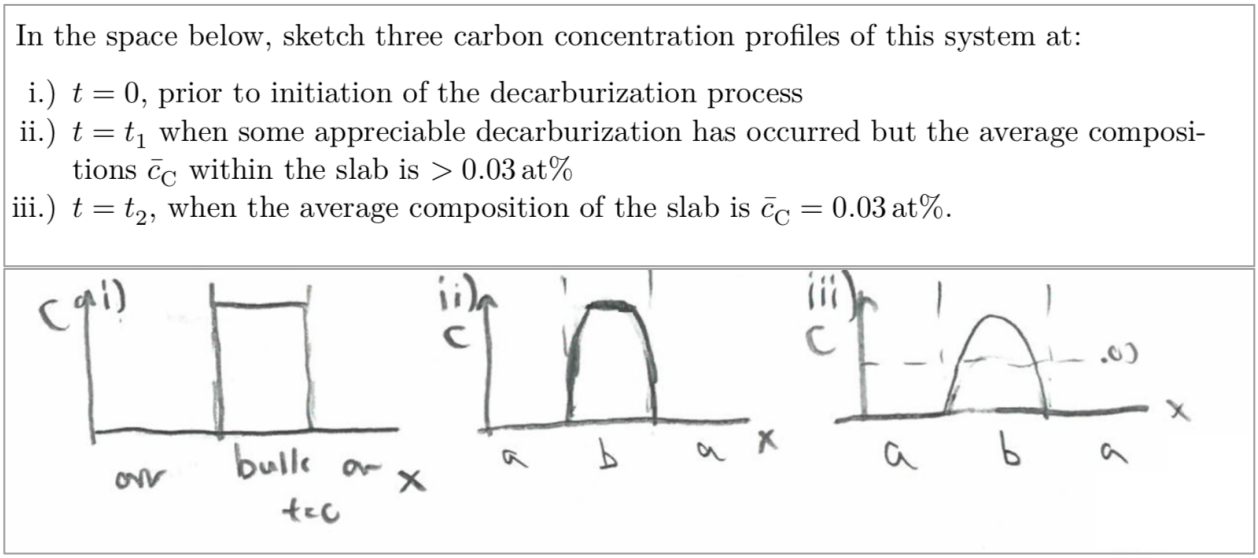


Figure 6: Top: the question that students were asked on the exam to draw concentration profiles. Bottom: an example student answer that was coded as fully correct.

Most of the students were generally correct on the exam, but this was not very valuable for revealing the students' thought processes since they were allowed a sheet of notes. It is likely that many students had the solution to Fick's 2nd law and the accompanying concentration profile for this situation on their note sheet. However, one interesting feature of the exam solutions did suggest something about student thinking: only nine of the seventeen students drew graphs with the correct curvature everywhere. If students were using Fick's 2nd law to reason about the curvature of the graph, they would conclude that the curvature should always be negative (downwards) in this situation once decarburization starts. Figure 7 shows an example of a student who sketched the correct general trend for this concentration profile over time, but incorrectly flipped the curvature near the interface of the system.

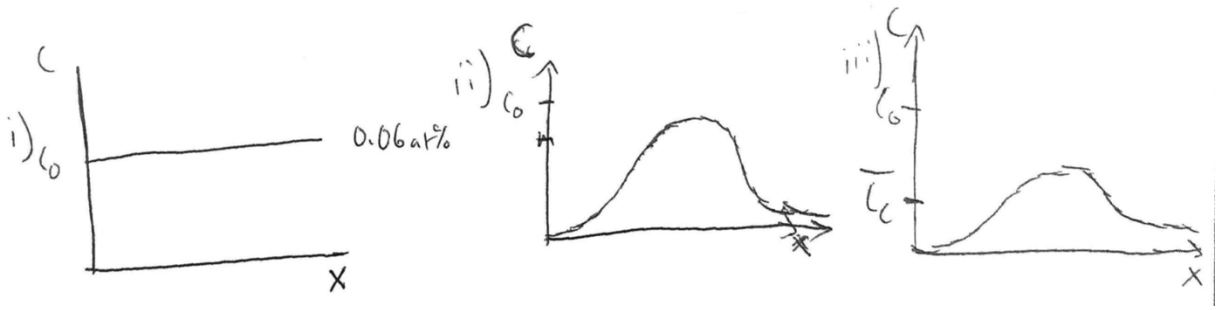


Figure 7: Sketch of concentration profiles that are generally correct but have the wrong curvature near the boundaries.

3.1.2 Why Did Students Fail to Draw the Correct Curvature Everywhere?

Of the five students interviewed from the current version of the course (in 2019), three drew concentration profiles on the exam with correct curvature everywhere and two did not. In contrast, only one of the five drew concentration profiles with the correct curvature everywhere during the follow-up interviews. This student was the only one to reason about the curvature of the graphs by considering the governing behavior of Fick's 2nd law, and even he only did so after follow-up questions. Most of the five students used a combination of simply remembering the shapes of the curves for the problem and reasoning about the general shape from boundary conditions.

One student, Peter, drew the correct general shape of the concentration profiles on both the exam and in the interview, but the curvature was slightly wrong on both. His sketches from the interview are shown in Figure 8. The general progression is correct, but the curvature incorrectly turns concave up near the interface for both the second and third graphs.

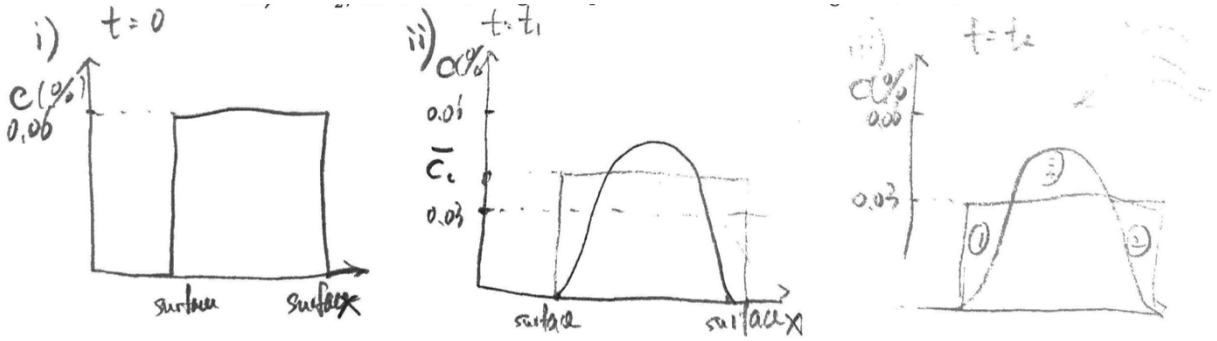


Figure 8: Peter's concentration profile sketches from the interview. The general shape is correct, but the curvature incorrectly turns concave up near the interface in the second and third sketches. The rectangles overlapping the profile in the second and third sketches are to estimate the average concentration level.

When Peter drew the second graph, he seemed to reason about the boundary conditions to produce the general shape:

> Peter: So, at $t=t_1$. So, here surface concentration is still kept at a constant. So, outside the surface is still zero. But it should look something like this (drawing) 2nd graph. So, like, if you're closer to the surface, there should be a larger portion of carbon atoms diffusing out of the material itself than those caught in the middle. So, it's this, like, damping effect.

He identified that the graph should always be zero just outside the boundary, and that the general shape is produced because "if you're closer to the surface, there should be a larger portion of carbon atoms diffusing out the material." This is solid reasoning, but when asked about the shape of the curve, he said he drew it from memory:

> Interviewer: Why is it curved the way that you drew it?
>
> Peter: You mean like the shape of the curve?
>
> Interviewer: The shape of the profile yeah, why is it shaped that way?
>
> Peter: (long pause) So like--actually this is from memory, that when we ran through the computational exercise in the class, there was like this damping effect from the exponential term. (authors note: he is probably referring to the exponential term in the "diffusion out of a slab" equation in Figure 4)

Here Peter claims that he simply remembered the shape of the curve from class as opposed to reasoning about it. When the interviewer specifically asked about the curvature of the graph, it became clear Peter was not considering it:

> Interviewer: So maybe this (your graph) is just from memory, but here it's concave down, and then it looks like at the very edge you drew it sort of concave up. Was that intentional? Or is that just…
>
> Peter. Oh, I didn't—I don't think that was intentional.

From this final exchange, it is clear that Peter did not specifically consider the curvature of the graphs and did not use Fick's 2nd law to reason about it. The small region of upwards curvature he drew at the interface could be due to prior experience with Gaussian distributions.

The one student from the five who did use Fick's 2nd law to think about the curvature, Parker, started out by just remembering the shapes of profiles. As soon as the interviewer told him that he was going to repeat the last question from the midterm he said:

> Parker: So, it's the decarburization…which was the draining plate problem…it starts out as that (drew a flat line) and then the average compositions goes down…but it becomes like an upside-down parabola.

He went on to draw the sketches in Figure 9, which have the correct direction of curvature on all regions of the graph.

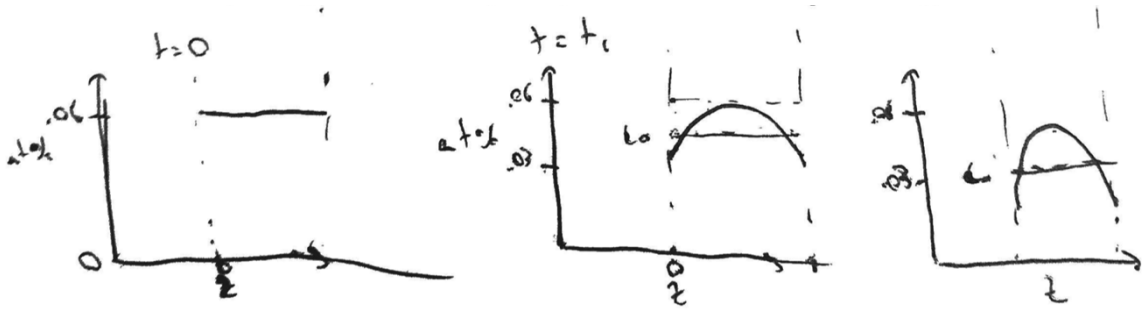


Figure 9: Parker's sketches of the concentration profile over time. The direction of curvature is correct: concave down everywhere for the second and third graphs.

When the interviewer asked Parker if the concentration profile will always have that shape for this problem, he said "yeah concave down, I think." The interviewer then asked if anything could change the curvature of the profile. In the following exchange, Parker gives an intuitive explanation which the interviewer provides a counter example to. Then, after saying he remembers the correct shape from class, Parker finally realizes he can use Fick's 2nd law to explain the curvature:

> Interviewer: Is there anything that could change the curvature of that profile?
>
> Parker: Physically it makes sense [that] it would be always concave down, because it's going to be a higher concentration farther from the interface.
>
> Interviewer: You could have a higher concentration curved like this (Figure 10), and it's still higher concentration further from the interface.
>
> 
>
> **Figure 10:** the interviewer's sketch of profile that is higher concertation further from the interface, but not always concave down.
>
> Parker: Um, yeah, I guess that is true. Is there anything I could change [to change the curvature]? (long pause) I don't know if I have an answer.
>
> Interviewer: That's fine.
>
> Parker: I mean, I'm pretty sure. I remember from the class that it's like this (pointing to his graph in Figure 9). But I don't necessarily have [a reason]—oh, well, maybe—because Fick's first law is—yeah. So, his second law is the second integral of—its basically the curvature concavity. The second integral is equal to the change in composition over time. So, this (Figure 10) is concave up. So, it would be gaining [concentration]… That's not really the case (in what I drew), because it's draining. [and therefore, the curvature does always need to be concave down]

Parker eventually uses Fick's 2nd law to conclude that the curvature he drew (always concave down) is correct. However, he initially did not use Fick's 2nd law to draw his concentration profiles, and none of the other students used Fick's 2nd law to reason about the curvature (except for one from the previous year).

3.1.3 Discussion of Macro-level findings

Only about half of the students drew concentration profiles with the fully correct curvature on the exam. Of the five students interviewed, three drew correct curvature on the exam, but only one did in the follow-up interview (about two months after the exam). This student was also the only one of the five to use Fick's 2nd law to reason about the curvature, and even he only did so after some prompting. These results suggest that most students did not become proficient at reasoning about concentration profile dynamics using ideas of curvature and Fick's 2nd law.

3.2 Micro-level Random Walk Process

In this section, we investigate our second research question: Did students understand the micro-level random-walk mechanism underlying diffusion?

3.2.1 The Exam Question and Numerical Results

Students were asked on the exam to write pseudo-code that could model the decarburization process at an atomistic level. They were told to assume that there was already code to initialize the system with atoms on a grid. The NetLogo model that the students worked with during the course (Figure 5 above) modeled a carburization process in which atoms do a random walk on a square lattice and one edge of the model is held at a constant concentration of atoms by removing all atoms on that edge on each time step and repopulating the edge-sites with a probability proportional to the surface concentration. The pseudo-code students had to write on the exam question was essentially the same except that atoms had to be removed when they reached the edge without any repopulating of atoms.

Here is an example of a student's pseudo-code that was marked correct:

> -At each tick (timestep), ask each carbon atom to move to one of its four neighbors randomly, as long as there isn't already an atom there.
> -If any carbon atom is outside the boundaries of the slab, kill the carbon atom
> -Move to the next tick

This student correctly defined a random walk as an atom moving to one of its four neighbors randomly (four because they were told to assume a 2D square lattice) and also identified how to remove carbon atoms from the system to model decarburization. Fifteen of the seventeen exams we analyzed showed answers similar to this one.

Two of fifteen students wrote pseudo-code in which the atoms move deterministically towards the surface. For example, one such student wrote:

> At each tick, move carbon atoms one empty interstitial site towards the surface.
> If the carbon atom reaches the surface, it should stay out

The two students with this type of answer are displaying a classic misconception about diffusion: thinking that particles deterministically move from areas of high concentration to low concentration.

None of the students interviewed from the 2019 course displayed the "deterministic atom" misconception, but two of the four students who took the course the previous year did (they had not used the NetLogo model). The relevant section of one of these interviews is detailed in the next subsection to shed light on the thinking process that leads to this misconception.

3.2.2 Thinking Process Behind the "Deterministic Atom" Misconception

At the time of the interview, Kim was a third-year undergraduate student in materials science. At the beginning of the interview she sketched a 2D lattice of the system shown in Figure 11. The open circles represent iron atoms and the closed circles represented interstitial carbon atoms. After she sketched the lattice, the interviewer asked her to pick an atom and draw the path that it might travel as it diffused. She drew the arrows in Figure 11 while answering the following:

> Kim: Okay. Well, I guess since the concentration is zero, this one, I would say will go this way. Or like this one might go that way (she drew the arrows in Figure 11 while saying this).
>
> Interviewer: Okay, why is that?
>
> Kim: Because they tend to move in the like—as the concentration gradient, like—if it's higher concentration here, and then they would go this way to like even it out.
>
> Interviewer: Okay, so you're saying--So that's the path that it would follow. So [it would] just move in that direction until it exited the material?
>
> Kim: Um or--Yeah. Or it would move from like, the area of higher concentration towards the area of lower concentration.

In this interview exchange, Kim states that individual atoms will move deterministically in the direction of lower concentration to "even it out." This is a classic example of "levels confusion" as discussed in Section 1.1. Later in the interview when asked to write pseudo-code, she demonstrated that she knew the atoms should move randomly but did not give up on the idea that they should move in a certain direction and was not sure how to reconcile those ideas. The following exchange occurred when the interviewer asked Kim how individual atoms would move when she started writing her pseudo-code:

Figure 11: Kim's sketch of the lattice. Open circles are iron atoms and filled in circles are carbon atoms. The two circled carbon atoms with arrows are her indication of how they might diffuse.

> Kim: Wouldn't it just randomly move around kind of like—hmm—Yeah, I actually just, I don't really understand how carbon—like a single carbon atom—would know which direction to go.
>
> Interviewer: You can start with what you were just saying
>
> Kim: Like, [it would] randomly go and it would just like, hop around to different interstitial sites, I guess.

> Interviewer: Okay. Does that make sense to you that that's what would happen?
>
> Kim: Yeah. That makes sense to me. I just don't know how it would go in a certain direction.

Kim remembered that the atoms should move randomly, but also seems to think that they have to move in a specific direction to exit the material. It became clear later in the interview that this was because she continued to think that individual atoms will move down the concentration gradient. As discussed in the introduction, atoms are equally likely to move in any direction in random walk diffusion. The reason that concentration gradients even out over time is that there are simply more atoms in the high concentration area available to randomly wander over to the lower concentration area than vice versa, and eventually the whole system becomes fully randomly mixed.

3.2.3 Discussion of Micro-level findings

It is encouraging that fifteen of the seventeen students correctly defined a random walk in their pseudo-code, especially because two of the four students interviewed from the previous year's course struggled with reconciling their memory of atoms moving randomly with their intuition that atoms must move down the concentration profile. This suggests that our NetLogo learning activities helped the students understand that atoms truly move randomly and not deterministically down the concentration gradient.

3.3 Relating the Representations at Different Levels

In this section, we investigate our third research question: how did students understand the relationship between the micro- and macro-level descriptions, specifically in terms of the ABM and Fick's 2nd law? At the end of the interview, students were asked about the connection between Fick's 2nd law and the ABM of diffusion. The interviewer used slightly different wording in each interview, but the question was always along these lines:

> Interviewer: There are these two different ways of describing diffusion in this question that you've used: the differential equation and an agent-based model. What's, the relationship between those? Like how do you think about: What's the relationship between them? What are the pros and cons of each? What are the strengths and weaknesses of each?

Nothing in the learning activities in the course specifically asked students to compare the representations. The results for each of the five interviews are summarized.

3.3.1 Peter's Response

Peter answered that the two representations are different ways of describing the same phenomenon each with their own advantages:

> Peter: I think of them as this—as two different ways to describe the same phenomenon. To me, there isn't much of a difference. But I think this agent-based model is more like--I think it helps with like visualization, like at an atomic scale, what is happening. This (Fick's law) is more like at the macro scale, like you can draw the concentration profile, like, just by reading the curve. If you want to do that in agent-based model, you literally have to count each like, how many carbons there are in one column in NetLogo. So, this is more, this (Fick's law) is like a general overview. This (the ABM) is like more individual specific for me.

Peter's response is concise, and he identifies one advantage for each representation: the ABM helps with visualization of the micro-level process while Fick's 2nd law can be faster for generating concentration profiles. We would add that the ABM helps with conceptualizing the phenomenon as well, not just visualizing it.

3.3.2 Parker's Response

Parker answered the question in terms of probabilistic and ideal behavior:

> Parker: What is the relationship? Well, I think—Fick's second is like the mathematical relationship to show it (diffusion)…if you did an infinite number of agent-based modeling experiments, and then average them all up, you get, like the mathematical equation of Fick's second. So—because the agent-based modeling is just showing how, when you sort of have these things like random walk—like probabilistically it tends to go towards, like, approach this behavior, this mathematical model more and more….Fick's 2nd law is important because it's the mathematical model that describes what the ideal behavior is, but then the agent-based model is strong, because you can see how that behavior arises from these sort of, like things from random walk, and like, the probability of which one—of like how—the probability of each jump that it will take.

Parker understood Fick's 2nd law to be the ideal behavior (i.e., one that is sufficiently large that all noise averages out) while the ABM shows how that behavior arises probabilistically from random walk behavior.

3.3.3 James's Response

James saw the NetLogo model as a way to improve conceptual understanding, but not as a rigorous model of diffusion like Fick's 2nd Law:

> James: I see the NetLogo [model]—or like any simulation—as a way to try to wrap your head around conceptually what's going on, but I don't see it as a rigorous model of diffusion. I think that most models are highlighting one specific aspect that they want the person to kind of wrap their head around. So, in this case, it's like random walk behavior, what does that look like? But it sacrifices, other things like, it's not necessarily realistic in terms of the diffusion…it targets one part of the model and says, "Okay, we're gonna try to do this really accurately", and kind of says everything else is of secondary importance, whereas Fick's second [law] is like a universal truth, that like, is always true. But…it (Fick's 2nd law) just has a very specific application, I guess—like, or it can get—it can be complicated to solve completely in a lot of circumstances. But like, It's not wrong. It's correct.
>
> Interviewer: Are there cases where it's (Fick's 2nd law) not? Where it's not correct?

> James: Probably, I would imagine, so. I don't know. Usually when you hear the term "law", you kind of assume generality, especially in science—but I don't know. I don't know enough about diffusion to say one way or the other confidently.

James, viewed the ABM as good for increasing conceptual understanding but didn't view it as a rigorous model. Based on his last comment, it seems his understanding of Fick's 2nd Law as rigorous comes partially from the word "law" in the title. He did not seem to understand that Fick's 2nd Law is derived from the random walk behavior directly modeled in the ABM.

3.3.4 Allen's Response

Allen did not understand the connection between the two representations:

> Allen: I don't know. I mean, this one we're assuming random walk diffusion. And we're also assuming that like, every time step, like every atom moves, they all move like just as frequently as each other. Not sure how that relates to this. (pause) Yeah, I just don't really know.
>
> Interviewer: Okay. But they are modeling the same thing at the end of the day, or not?
>
> Allen: I mean, I would say yes, but I just—I don't really know how they're related.

Allen's explicit statement that he didn't understand the connection between the levels is confirmed by an earlier statement in his interview. After writing correct pseudo-code of the micro-level process, he was unsure if his code would produce the same concentration profiles he had sketched earlier.

3.3.5 Tom's response

Tom and the interviewer had a long exchange on this question. Tom first described that Fick's 2nd law relates changes in concentration with distance to changes in concentration over time. Then he tried to relate this to the atomic behavior in the ABM, but didn't come up with an explanation that satisfied him, concluding:

> Tom: Yeah, I'm not too sure about comparing those two models.

3.3.6 Discussion of Relating Representations at Different Levels

There was a wide range in responses about the relationship between the agent-based and differential equation representations. Peter and Parker both seemed to understand that the two represent the same thing and were aware of advantages of each. James viewed Fick's 2nd Law as the rigorous model and the ABM as not rigorous but still useful to learn conceptually about diffusion. Finally, Allen and Tom felt they did not know how the representations were related. These mixed results imply that our next iteration of the learning activities should explicitly address the connection between the various representations that students use to help students understand that the macro-level behavior described in Fick's Laws emerges directly from the micro-level behavior programmed in the ABM.

4. General Discussion

4.1 Summary of Findings

To summarize our findings: (1) regarding our first research question, most students did not use Fick's 2nd law or ideas of curvature to reason about concentration profiles (the macro-level), even though they were taught Fick's 2nd law in the course (2) regarding our second research question, most students understood the micro-level random walk mechanism; encouragingly, only 2 of 17 students from the current class displayed the "deterministic atom" misconception compared to 2 of 4 students interviewed from the previous year's class and (3) regarding our third research question about the relationship between the micro- and macro-level descriptions, students displayed a variety of understandings (or lack thereof) about the relationship between the ABM and Fick's 2nd law. These findings suggest that exploring the agent-based representation helped students better grasp the micro-level random walk behavior of diffusion. However, many students still struggled with connecting both the ABM to the differential equation representation in Fick's laws and from Fick's laws to the graphical representation of concentration profiles. Future work (discussed below) will attempt to improve these two outcomes.

4.2 Limitations

There are several limitations to the current study. First our claim that engaging with the ABM led fewer students to exhibit the "deterministic atom" misconception is based on a comparison between 17 students from the study year with only four students from the previous year. Additionally, the students from the previous year were interviewed more than a year after they took the course, compared to the students from the study year who were interviewed only 2-3 months after they took the course. On the other hand, the older students were exposed to diffusion again in later courses. This is an ongoing study and additional data from future years will address these limitations.

4.3 Future Work

Based on the findings reported here, we re-designed the learning activities to increase student understanding of (1) the connection between the micro-level and macro-level of diffusion and (2) the dynamics of the macro-level as described by Fick's laws. Specifically, instead of starting the diffusion unit with Fick's laws, we start with student explorations of the ABM representation, including both the micro-level rules and how concentration profiles change over time. Then, instead of the professor deriving Fick's laws in lecture, students derive Fick's laws in a scaffolded activity, similar to our explanation in Section 1.2, which emphasizes the connection between atomic random-walk behavior and changes in the concentration profile. After this activity, students watch a video lecture with a formal derivation of Fick's laws. We believe that these changes will succeed in helping students connect between the micro-level and macro-level, because they will actively and explicitly derive the macro-level description (Fick's laws) directly from the micro-level behavior. In contrast, the students reported on in this paper were presented with the two levels in reverse (first Fick's laws and then the ABM activities), and it was largely left up to the students to make the connection between the levels. Similarly, we think students

will better understand the dynamics of the macro-level by informally deriving Fick's laws themselves before being shown a formal derivation. Results of this re-design will be reported in future publication.

4.4 Closing Remarks

This study reported on the first iteration of a design-based research project to develop a unit for learning about diffusion at both the micro and macro levels using computational agent-based modeling representations, the traditional differential equation representations (Fick's laws), and accompanying graphical representations. Our findings suggest that the agent-based representation helped students understand the micro-level process of diffusion better, but the current curriculum structure and learning activities leave room for improvement in helping students understand the connection between all the representations of diffusion.

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