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From Integrated Rate Laws to Integrating Rate Laws: Computation as a Conceptual Catalyst

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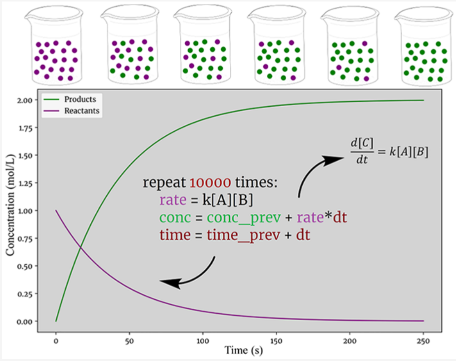

ABSTRACT: When learning chemistry, students must learn to extract chemical information from mathematical expressions. However, chemistry students' exposure to mathematics often comes primarily from pure mathematics courses, which can lead to knowledge fragmentation and potentially hinder their ability to use mathematics in chemistry. This study examines how computation can affect students' blending of cognitive resources and their framing of mathematics in a chemical context. How students analytically and numerically interpret mathematical expressions in chemistry are examined through 14 individual clinical interviews with undergraduate chemistry students. The analysis was done by performing a thematic analysis of the interviews through a theoretical lens provided by the blended processing framework. This analysis reveals that computation and iterative thinking might serve as a catalyst for conceptual understanding and blending of cognitive resources. These findings suggest that we should evaluate how computational approaches could be leveraged to give students a better understanding of both mathematical models and the chemical concepts illustrated through these models.

KEYWORDS: *chemical education research, undergraduate, physical chemistry, kinetics, computational chemistry, mathematics*

■ INTRODUCTION

Chemistry is often called "The Central Science" because it has a central role in both mathematics and other natural sciences. Chemistry is important for a multitude of disciplines, and several disciplines are important for chemistry. This means that a chemist routinely deals with concepts from disciplines like mathematics, physics, and biology, in addition to concepts from chemistry. Consequently, problem-solving in chemistry requires the use of a multitude of visual and symbolic models and representations.[1−4]

Many students struggle to combine these different concepts and tools when studying chemistry. For example, in chemical kinetics, rate laws can be understood both as a model describing the change of concentration in a reaction as well as an equation that can be solved with certain mathematical methods. In order to understand and use rate laws, students must thus draw on conceptual knowledge from both chemistry and mathematics. But inferring chemical information from a mathematical expression is not a trivial task.

Researchers have shown that students who learn mathematics in a purely mathematical context may later interpret mathematical expressions as purely mathematical entities, even when those expressions encode disciplinary meaning.[5,6] That students compartmentalize knowledge and fail to draw connections between mathematics and natural sciences is well-known from previous studies.[7−9] However, this framing can affect which cognitive resources they draw on when interpreting mathematical models chemically, leading students to perform symbolic manipulations without managing to infer significant chemical content from the models.

One way students can connect the mathematical domain with the chemistry domain is by using programming and computation.[10] Computers present a different way of representing and thinking about both chemistry and mathematics, and this may affect how students think about certain problems and concepts in these subjects.[11,12]

Although researchers have studied how students understand mathematics in a chemistry context,[13] there is comparatively little systematic research on how students use programming and numerical methods to explore chemical models. This lack of empirical research represents a gap in the research literature. This paper will therefore examine how scientific computing can act as a catalyst for helping students understand mathematical models in chemistry.

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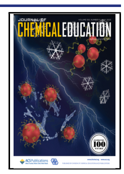

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Literature Review and Background

Researchers have long been interested in understanding the ways students use mathematics to reason and solve problems in various scientific disciplines. One of the primary results of this research is that students often experience knowledge fragmentation when combining mathematical knowledge with disciplinary knowledge, making it difficult for them to draw connections between the two.[14−16] These disconnects seem to be especially prevalent in physics and chemistry, where mathematics is a critical part of understanding within the disciplines. One reason for this disconnect is that physics and chemistry students use mathematics in a different way than mathematicians do.[17] For instance, inferring scientific meaning from mathematics requires a different understanding and skillset than symbolically manipulating a mathematical equation.[18−22]

Mathematics in Science

Town, Bain, Rodrigues, and collaborators[16] recently conducted a major study investigating how students integrate mathematics and chemistry knowledge. Their project produced several articles and a book on mathematical understanding in chemistry.[13] Key findings from this project included the following:[23]

- Students perform better on algorithmic problems than on conceptual problems.
- Mathematics is framed and used differently by chemists than by mathematicians.
- Students have difficulty interpreting mathematical representations as models. The mathematical representations are interpreted as algebraic/symbolic entities instead.

Related to these findings is the fact that students often manipulate mathematical variables without considering what they represent.[26,27] Similar results can also be found in the physics education research literature,[6,26−28] where researchers have found that the ways students frame mathematical problems can significantly affect their problem-solving practice and understanding. For example, when students frame a problem purely as an exercise in symbol manipulation, it can suppress their understanding of the underlying mathematical and physical or chemical concepts.[27] Based on these results, researchers have argued that the cognitive resources that are available for students in a particular context depend heavily on student framing.[29] This study builds on these results by expanding the learning context to include programming and computation.

Computation in Science and Mathematics

Ideas of how computers can affect learning in mathematics were introduced as early as the 1960s by mathematician Seymour Papert.[11] His idea was to utilize computers to make mathematical concepts tangible for children. A growing accessibility of computers and an exponential increase in computer power have made these ideas increasingly relevant in the past 30 years.

Studies on reasoning and learning in mathematics through computation show that programming can improve interdisciplinary cognitive skills and learning in mathematics.[12,30−33] Other studies extend these results to natural science as well, by showing that computation can be used to learn and understand physics.[28,34−37] Although research on how students may understand chemistry through programming is lacking at the moment, there are some recent publications that show how programming can be integrated into the chemistry curriculum.[10]

Chemical Kinetics

Rate laws are an ideal subject for studying how students understand mathematics in a chemistry context because they are relatively simple mathematical models that convey chemical information. There is also a strong existing research base on student understanding of chemical rate laws.[23,38,39] For example, researchers have found that students tend to not draw connections between rate laws and *integrated* rate laws, framing them as distinct entities with minimal or no connection to each other.[38] Students may thus interpret "integrated rate laws" purely as mathematical entities, not conceptually as an integrated differential equation where an expression for *change* in a system is integrated to get an expression for a *state* of the system. This exemplifies the knowledge fragmentation described above.

Other aspects of chemical kinetics and students' understanding of rates has also been studied in detail.[40] One important finding is that students often conflate ideas from chemical kinetics and chemical equilibrium.[41−45] Students also find it difficult to define the term rate.[44,46,47] In addition, the dynamic and temporal aspects of reaction rates have been reported as a possible source of alternative conceptions. For instance, students might misunderstand instantaneous change as a change from the initial state to the final state.[48,49] Some students also encounter great difficulty characterizing how the reaction rate changes during a reaction. This means that we might benefit from exposing students to additional representations of reaction rates, especially representations that show the temporal and dynamic aspects of rate laws. Although several researchers have studied how rate laws are understood as mathematical models with different frameworks and in different contexts, no such research has been done on numerical computation and programming. This study will thus address how students may use computation to make sense of mathematical chemical models. The main hypothesis is that scientific computing can help bridge the conceptual gap between chemistry and mathematics.

Theoretical Framework

To understand how students draw on cognitive elements from different disciplines to construct meaning, the *blended processing* framework[23] is used in this study. This framework is a theory originally proposed by Fauconnier and Turner[50,51] in the field of cognitive linguistics. Blended processing describes how collections of cognitive structures blend and integrate to form meaningful or conflicting units. This theory conceptualizes concepts as consisting of collections of cognitive elements, which are activated in specific contexts. Large collections of such elements form a *mental space* from which individuals can draw and combine specific components.[52] For instance, when solving a stoichiometric problem, a student needs to combine their knowledge of algebra, arithmetic, and significant figures with their knowledge of reaction equations and stoichiometric relations between products and reactants. The former are elements from a mathematical mental space, and the latter are elements from a chemical mental space. These connections may, in turn, allow students to construct new meanings and understandings.[23] They are often illustrated using blending diagrams, such as that shown in Figure 1. This model of student cognition will be used to analyze and illustrate how students connect cognitive elements from different mental spaces.

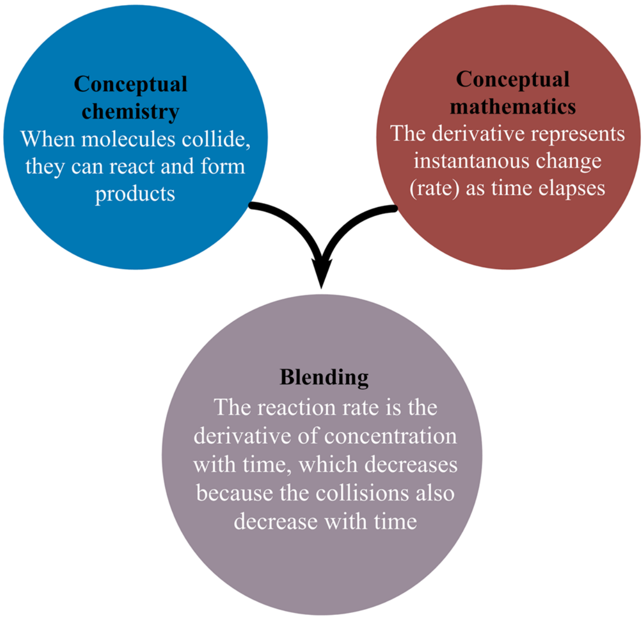

Figure 1. Illustration of a possible outcome of conceptual blending. Distinct sets of cognitive resources are modeled as forming different mental spaces. Conceptual blending involves combining resources from two or more mental spaces to form new meaning. Here, resources from chemistry are used together with the mathematical concept of rate to construct an understanding of how reaction rate depends on molecular collisions over time. Knowledge of collision theory from chemistry is combined with a conceptual understanding of the derivative from mathematics to explain how the derivative represents reaction rate and how it depends on molecular collisions.

The blended processing framework is well suited for describing interdisciplinary concepts in chemistry. For example, Bain et al.[8] use this framework to analyze problem-solving in chemical kinetics, identifying when and how different mental spaces from chemistry and mathematics are blended together. An example of a blending process is illustrated in Figure 1. Here, we see how concepts from chemistry and mathematics blend to create new meaning.

Fauconnier and Turner describe mental spaces as small conceptual packets that are constructed as we think and talk. Blending occurs when input from two mental spaces is projected upon a third space.[53] In the example from Bain et al. which is illustrated above, meaning, which is both stored in the brain and constructed in the moment, from mathematics and chemistry is combined to give rise to new meaning. We can use these mental spaces to model how students combine thought and language to construct new meaning across disciplines, addressing the problem with compartmentalization, or "disciplinary siloing" of ideas.[38]

The blending of cognitive elements and mental spaces has also been studied in physics education.[27,52,54−60] However, there is a gap in the literature around how scientific computing can contribute to the blending of resources in chemistry learning. This study therefore uses the blended processing framework, together with perspectives from previous literature on blending of mathematics and chemistry or physics, to study how students make sense of mathematical models in chemistry. Our research questions are as follows:

1. How do students use elements from different mental spaces when solving a problem involving mathematics and chemistry?
2. How do programming and computations contribute to the ways students make sense of mathematics in chemistry?

METHODS

Data collection for this project took place at the University of Oslo (UiO) in Norway. At UiO, rate laws are covered in general chemistry in the first semester, and more thoroughly in physical chemistry in the third semester. Chemistry students at the University of Oslo also take a course in programming for chemists in the first semester, which covers general programming with Python, numerical methods, and how to explore chemistry and chemical models with programming. Solving rate laws numerically is part of the course. Although most participants in the project were chemistry majors, two of the participants were from the Material Science program. Students from this program have a more general programming course in the first semester, where rate laws are not covered explicitly, although the methods required to solve them are.

Data collection for this study used a cognitive clinical interview methodology.[61] Clinical interviews have seen frequent use in science education research, especially in studies where researchers aim to probe a student's thinking to better understand the cognitive mechanisms behind their reasoning.[62,63] In the present study, these interviews required students to solve several problems from chemistry related to rate laws. In the first part of the interview, students were first asked to define and give examples of rate laws. This was followed up by a question about the relation between the change in concentration (that is, the rate laws) and the concentration itself. In this step, the students had to explain what the derivative meant in this context, and what it meant conceptually to integrate the rate laws. Next, they were asked how to determine the concentration from a rate law.

In the second part of the interview, students were introduced to a Python (3.9) code where three rate laws were integrated for the reaction $H_2(g) + I_2(g) \rightarrow 2HI(g)$ at high temperature, as shown in Figure 2. The students were

```
for i in range(N-1):
    HIder = k*H[i]*I[i]
    Hder = -0.5*HIder
    Ider = Hder
    HI[i+1] = HI[i] + HIder*dt
    H[i+1] = H[i] + Hder*dt
    I[i+1] = I[i] + Ider*dt
    t[i+1] = t[i] + dt
```

Figure 2. Integration loop for the reaction $H_2(g) + I_2(g) \rightarrow 2HI(g)$ at high temperature, as provided to interviewees.

asked to explain what the code represents. The reaction was simplified as irreversible to make the conceptual information clearer, even though the reaction is reversible. The code showed only the loop, where the rate laws were defined, and the integration was done with the simple Euler method.

In the code above, the declaration of variables is implicitly done in the lines above the ones shown. This code begins with a for-loop, essentially repeating the lines below the first line N

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J. Chem. Educ. 2023, 100, 1739−1750

− 1 times. HI, H, I and t are arrays, which are a kind of mathematical lists in Python. The arrays are filled with values as the loop progresses. The variable i is a counter which is used as an index for the arrays, denoting where to put the values that are calculated at each iteration in the loop.

Data collection proceeded over two stages. First, 3 pilot interviews were conducted with preservice teachers specializing in chemistry. The questions in these interviews were more open-ended, which lead the students into a memory exercise rather than an exercise in problem-solving and conceptual understanding. The interview protocol was therefore adjusted to contain for example specific rate laws and complete or semicomplete program code. Finally, chemistry students from the bachelor and master programs at the University of Oslo (UiO) were recruited for subsequent interviews. Eleven bachelor students volunteered for the main interviews; all interviews were conducted individually to provide sufficient time and room for individual reasoning and reflection, and all participating students were awarded a gift card. Every student had participated in at least one course covering rate laws.

Audio and video for all 14 interviews were recorded and transcribed. The transcribed video recordings were then anonymized using pseudonyms, after which they were deductively coded and analyzed by the first author using Nvivo 12. The main codes were decided a priori, but some codes were added throughout the coding process. The codes were chosen as descriptions of possible mental spaces (like conceptual chemistry and procedural mathematics). These mental spaces are based on our experience with teaching, as well as previous research.[5] The main spaces we identified was conceptual chemistry, programming, conceptual mathematics and procedural mathematics.

To properly distinguish between codes, criteria for the different mental spaces were established. For example, using terms from a specific discipline, like "concentration", does not necessarily imply that the students are using resources from a conceptual chemistry space. To qualify as conceptual chemistry, the students needed to use resources from chemistry as an explanation or a description of a chemical phenomenon. These resources can be at the micro level, like using the concept of molecular collisions to describe reaction rate, or at the macro level, for example referring to reaction equations, discussing how reactants and products depend on each other, or stating the fact that the concentration of different species change as time passes.

The procedural mathematics mental space and the conceptual mathematics space are two distinct, but related spaces. The procedural mathematics space represents resources that students use to do algorithmic problems without relating the symbols to what the mathematics really means. On the other side, the conceptual mathematics space represents resources connected to an understanding of what mathematical symbols and operators mean (like the derivative representing instantaneous change). That students can do procedural mathematics without actually understanding what the equations and solutions mean are shown in several studies.[5,17] This provides theoretical justification for treating these two spaces as separate.

The interviews were approved by the Norwegian Center for Research Data. Identifying data like e-mails and names were encrypted and stored on a secure device separate from the interview recordings. These data were only available to the first author. Every participant signed a consent form describing their participation and how the data is stored and used.

The data were coded three times by the first author in the space of a year to ensure the internal stability of the codes. After these three rounds of coding, a second researcher coded about 60% of the data. The researcher was instructed to code the data in such a way that codes were mutually exclusive.

The data were then unitized to ensure that the same segments were coded by both researchers. In this process, we identified segments that were coded by one researcher but not the other. Those segments were anonymized, which means that they were marked as coded, without showing the actual code. These segments were then coded by the researcher that did not code the segments in the first place. This resulted in a data set where every coded segment was coded by both researchers.

The resulting inter-rater agreement was then measured by Cohen's kappa, which takes into account the possibility of agreement by chance. This resulted in $P(\text{observed}) = 0.73$ and $P(\text{chance}) = 0.14$, which gives a kappa of $\kappa = 0.68$. This shows a substantial agreement even before discussing the codes.[64] The inter-rater analysis was done in MAXQDA Analytics Pro 2022.

After calculating an initial kappa, the first author and external researcher met to discuss the code thoroughly through a negotiated agreement process.[65] This resulted in perfect agreement ($\kappa = 1.00$) and further refinement of the codes. Through this discussion, both researchers realized the need for one additional code reflecting the process where students infer concepts from chemistry from computer code (P+CC). This code was applied to a few segments during the negotiated agreement process. Table 1 shows the final codes and one example of each code from the data.

After the initial rounds of coding, a thematic analysis was done to examine whether we could find recurring themes in how students reasoned about problems in different contexts.[66] For example, it was examined whether certain parts of the problem-solving process contained more of specific codes than others. In this analysis, a priori codes were used as models of cognitive resources, collating codes into themes describing patterns in student reasoning. In this process, a theoretical relationship between expressed language and cognitive resources was assumed. Thus, the thematic analysis was done at the latent level, identifying possible underlying conceptualizations of the semantic content of the data.

Patterns in situations where blending did or did not occur were identified through the codes and cognitive mechanisms behind these patterns were theorized. These themes were grounded in the blended processing framework and the hypothesis that computation might help students blend. The themes were finally reviewed and renamed after a thorough analysis of the coding scheme and the whole data set.

■ RESULTS

Overview

Through this analysis, three main themes related to conceptual blending and computation were identified, based on recurring patterns of student reasoning documented in the interviews:

1. Procedural mathematics does not facilitate blending.
2. Students who interpret computer code tend to blend resources from different mental spaces.

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Table 1. Coding Scheme with Descriptions of Each Theme and Examples from the Data Material

Code	Description	Example from the Data
		Mental Spaces
PM (Procedural Mathematics)	Remembering of formulas (static) and/or algorithmic symbol manipulation (dynamic), e.g., integrating with integration rules.	"I remember there was some stuff from mathematics. That we multiplied with *e* to the power of something."
CM (Conceptual Mathematics)	Describing what a mathematical expression means, e.g., understanding the derivative as describing change.	"That is what the integral is − the area under the graph."
CC (Conceptual Chemistry)	Using chemistry knowledge to solve a problem, or describing a chemical system, e.g., talking about collisions of molecules or change in concentration as a system evolves.	"I'm thinking that [the change of] HI starts a bit slow. Then it increases exponentially until we reach a maximal reaction rate. Then it will increase more slowly because we are getting fewer and fewer reactants."
P (Programming)	Describing programming structures and syntax.	"This is a for-loop. Which will run for all... From 0 to N minus 2 [...]. It's an iterator."
		Blending of Resources
CM+CC	Inferring chemical concepts from a mathematical expression or the other way around. Using mathematics to understand chemistry.	[Answering what the derivative in the rate laws mean, i.e., connecting the definition of the derivative with its chemical meaning in a particular context] "That means the change in time, the change in concentration with time."
P+CM	Inferring mathematical concepts from programming.	[Explaining code] "You have the derivative too, then you multiply by dt. So that means you have actually divided it, and then you multiply by dt again. So, you get the integrated form, then."
P+CC	Inferring chemical concepts from programming.	[Explaining code] "I think that this is the derived concentration of hydrogen iodide. It is the rate law."
CC+P+CM	Inferring chemical and mathematical concepts from programming. Moving back and forth between different mental spaces.	"We start by defining starting conditions: concentrations and time and so on. We also use these initial conditions to calculate the new values. In the future. And they are based on the rate laws with respect to a certain reactant. They can depend on each other."

3. Blending and dynamic reasoning is facilitated through iterative thinking.

Segments illustrating the first theme are dominated by the code PM (procedural mathematics) with little or no relation to other codes. This occurs in the data when students are trying to manipulate the rate laws using analytical mathematics. Data illustrating the second theme are dominated by a mix of codes, indicating that students are switching between mental spaces and using cognitive resources from different domains to make sense of different problems. The third theme provides a potential mechanism behind this blending process, suggesting that the stepwise, iterative nature of a computational approach helps to facilitate blending.

These three themes will now be unpacked, illustrating each with examples from the data corpus. Note that interviews were conducted in Norwegian, so the parts of the transcription shown in this article have been translated from Norwegian to English.

Theme 1: Procedural Mathematical Knowledge Does Not Facilitate Blending

When students used elements from a procedural mathematical mental space, there were little evidence of conceptual blending. For instance, when faced with the task of finding or sketching the concentration from a rate law of the form $\frac{d[A]}{dt} = -k[A]$, nearly every student was trying to do the symbolic manipulations necessary to integrate the law, without explaining what the integral meant mathematically and chemically. This trend could mean that students use procedural mathematics as a "go-to" strategy when faced with a mathematical problem. This in turn hindered them from inferring any chemical information about the system. For example, when John was asked how we can determine different rate laws, he replies:

> ***John:*** *[...] if it is the zeroth, first, or second law, then we can integrate these general rate laws into the integrated versions. And if it turns out to be correct with the concentration... Develops linearly, or something. I cannot quite find the words. So, we get a linear function. Ehm. Which shows the concentration. Well, I even remember the formulas, but I cannot "place it".*
>
> ***Interviewer:*** *But I can hear that you remember a lot here. If you—just write down any rate law.*
>
> ***John:*** *Yes, we have ln(k) is equal to [pause]. Hmmm. Irritating. I have flash cards on them, but it is been a long time since I've made them.*

In his response to the question on how we can determine rate laws, John immediately tries to remember the integrated versions of the rate laws. In doing so, he bypasses answering the question on how we can determine rate laws (which must be done experimentally). He is thus describing the formulas and symbols used in certain rate laws without explaining what they mean. It can therefore be inferred that John does not move between spaces or blend resources from different spaces while solving the mathematical problem. He remembers some formulas, as well as some elements of an integrated rate law (the natural logarithm), but he does not infer chemical information from them.

After a discussion about what the rate laws mean, John is asked to find the concentration given a rate law. In response, he tries to integrate the rate laws while also occasionally trying to recall them from his previous chemistry classes. He thus

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J. Chem. Educ. 2023, 100, 1739−1750

remains in a procedural mathematical mental space throughout the process.

Surprisingly, without being asked directly about it, and without being aware of the theoretical framework of the study, John proceeds to explain how blending of resources is hard and contextually dependent:

> ***John:*** *We are very dependent on certain contexts to apply what we have learned. I often notice that when I work in parallel with different subjects, where I realize in a subject that I—"here I can use a thing from another subject". It can be difficult for me to apply what I have learned from one subject to another. For it is so apparently, on the surface, different.*

This shows us that students can also be aware of the problems they face when trying to combine knowledge from different disciplines. In some cases, students were able to integrate the rate laws analytically; however, even in these cases, blending did not occur. For example, one interviewee, Amelia, successfully managed to integrate the rate law analytically without errors. This success may have been due to her stronger background in mathematics than the other students. However, here again, we see that she does not infer significant chemical information from the integrated rate laws either during or after the process of integration. For example, here is how Amelia approached the integration task:

> ***Amelia:*** *It [the rate law] must be integrated! And then there will be, no, sorry. [long pause] How is it possible to forget basic math?! [thinking]. There will be separation of variables, then. And then there will be k, dt, and then there will be integration. We need to separate variables, and then integrate. So, it will be ln. Okay, it is like that. Let us see. k becomes 0. Also, it becomes ln here, ln A_0, and then kt, kt_0, of course assume that one is zero, for there is no point in using it. [...] So, if we want the concentration, then we can take this over there. We can also take the exponential. [...] Then you can maybe write this first. That was it. Also [laughter], if I'm doing something wrong, it is because I do not see it [...].*

We see here that Amelia goes back and forth with symbols and rules but makes no mention of the chemical information in the rate laws while she is in the process. Even after she has successfully integrated the rate law, she makes little attempt to interpret it, rather opting to try to remember the graphs representing concentrations for different rate laws:

> ***Amelia:*** *I do not remember exactly how it [the concentration as a function of time] looks like, but exponential functions are kind of curved and exponentially growing and so forth.*

Based on this example, we can see that Amelia still does not infer chemical information from the rate laws, even though she clearly knows how to integrate them. Thus, like John, Amelia seems to be drawing exclusively from a procedural mathematical mental space, exhibiting little evidence of blending. Several other students exhibited similar behaviors, focusing on mathematics to the exclusion of conceptual chemical knowledge or interpretation.

That students do not automatically blend resources when in a procedural mathematics space is in alignment with what is shown in other studies involving mathematics in chemistry.[16] In addition, the fact that students use procedural mathematics as a "go-to" strategy when faced with mathematical problems in chemistry is an important result from this analysis. Thus, we can see that chemical concepts are not automatically used by students when solving a problem from chemistry involving a lot of symbolic manipulations and interpretations.

This result show that chemistry educators need to make special care in the design of teaching activities where mathematical procedures are used and conceptual chemical and/or mathematical knowledge is the goal. We will now look at how designing a mathematical problem through code can affect the use of different mental spaces.

Theme 2: Students Who Interpret Computer Code Tend to Blend Resources from Different Mental Spaces

From our discussion of theme 1 it is apparent that students did not blend automatically when drawing on resources from a procedural mathematical mental space. When using resources from a procedural mathematical space, the students' reasoning about mathematical models in chemistry tended to be static and dominated by rules and algebraic operations. But when they were exposed to scientific computing, a shift was observed: students began to blend resources in a more dynamic way.

As an example, we saw previously that John was automatically using resources from a procedural mathematical mental space when first introduced to the rate laws, shifting between trying to integrate the rate laws and remembering the integrated rate laws from chemistry class. However, when asked to explain the code that integrates the rate laws numerically in the second part of the interview, he begins to exhibit signs of conceptual blending: inferring chemical information from mathematics and the computer code itself and vice versa. For instance, when asked about how he would solve the equations numerically, he replied:

> ***John:*** *We start by defining starting conditions: concentrations and time and so on. I usually make lists that are empty. We also use these initial conditions to calculate the new values. Ehm. Forward in time, in a way. Ehm. And they are based on the different rate laws with respect to a certain reactant. It must preferably contain the other concentrations as well. They can depend on each other. Ehm. Find the new concentrations. Save it in lists and then loop it back and use the current values as starting conditions for the next round of Euler's method. Which is then saved again, and then plot it.*

By explaining how to use lists and loops to numerically find the new concentrations of products and reactants as the reaction unfolds, John is drawing upon knowledge from different disciplines. Thus, when he explains the code that integrates the rate law numerically, he shows a higher degree of blending and dynamic reasoning than when he tried to symbolically solve the rate law. Instead of trying to remember integration rules or the integrated rate laws as static entities, he starts to reason and draw conclusions about different processes drawn from different mental spaces. For example, he uses his knowledge of the iterative integration process ("We also use these initial conditions to calculate new values", programming mental space) in combination with what the rate laws represent ("And they are based on the different rate laws", conceptual chemistry space). Furthermore, as predicted by the conceptual blending framework, this blending is producing new, emergent meaning.

Amelia, who successfully solved the rate law analytically, has never seen a numerical solution of rate laws before. Despite this, she also manages to infer quite a lot of chemical and mathematical information from the code:

Amelia: Then I assume this here is the concentration of H. It says HI there, and H there and I there, but also because it says half. And we have two here [pointing to 2HI in the chemical equation], we also have one there [pointing to H_2 in the chemical equation] We also assume the same for iodide, because that is exactly it, it is half of the product [...].

[...]

Amelia: it uses the equation there [points to HIder in the code and then the rate laws that are written on a piece of paper]. And dt must be defined somewhere. In other words: It takes the previous one, that is, what was determined by the rate law, here. It also adds the new [value of the] rate law multiplied by delta t, dt. So, it builds up every time, sort of accumulating, in the new list HI.

[...]

Amelia: What Euler's method does is integrate it [the rate law], or approximate it [the integral]. Because what you find is the concentration when you integrate it. So, this is the concentration [points to HI [i + 1] in the code].

In the first quote, Amelia explains the lines where the rate laws are defined in the code by using her knowledge of stoichiometry from the chemical equations to interpret the code. She points out that the code "says half" and "have two here", which lead her to assume that the code represents concentrations of H_2, I_2, and HI. This is an example of knowledge emerging from blending knowledge from the programming space and conceptual chemistry space (P+CC). In the second quote, she proceeds to explain how we use rate laws to determine the change in concentration, and then add this change every time step. We also see from the third quote that she views this iterative process as a way of integrating the rate laws, which draws on knowledge from the conceptual mathematics space (CM). From the different mental spaces, Amelia constructs a new meaning of the rate laws as dynamic entities that we can integrate to find the concentration with time (CC+P+CM). This is similar to the example of blending that we saw with John.

Another student, Chris, claimed to know the integration rules and how to use them in a mathematical context, but when presented with the problem of solving rate laws, he struggled to explain or understand what integrating meant. Like John and Amelia, he used mostly resources from a procedural mathematics space for the first 15 min of the interview. However, when presented with computer code, he too began to blend elements of mathematical and chemical knowledge:

Chris: [...] And then we have how the concentration evolves. Let us see. This means that the next concentration, that is, the next value for the concentration, numerically, is given by the initial value of HI, which is calculated. [...] Then we add the change in concentration for HI after a very short period of time, or after a change in time. And the same thing happens below, as for those above. For H, the same thing happens, that you take the starting concentration and add the change in the concentration, over time. And the same for iodine. [...] Then you loop it.

Here, Chris blends knowledge from conceptual chemistry of what the rate laws mean ("how the concentration evolves") with his mathematical knowledge of the numerical method ("the next value for the concentration, numerically, is given by the initial value of HI"). This blending process seems to be mediated by the way the code represents the problem as an iterative process, as discussed in the next section.

These examples show that the computational task facilitated conceptual blending, allowing students to infer important chemical and mathematical concepts through computer code. We saw previously that students tended to focus on symbolic manipulations when approaching the problem analytically, hindering chemical information to be inferred from the mathematical models. One possible reason for this is that most rules of integration and differentiation are not directly related to the definitions of their respective mathematical concepts. When students use these rules, their focus can shift toward "plug-and-chug" strategies to get the "right answer". Integrating a function does not necessarily mean that they understand what that function or integrated function means. Simple numerical methods, on the other hand, are based on the very definition of mathematical concepts. As such, it might be easier to infer what different mathematical concepts mean in a chemical context.

The main argument here is that the programming task led to blending of resources from different mental spaces, whereas the task of finding the concentration did not necessarily lead to blending. It is therefore important to address the different natures of the main tasks. The first task of finding the concentration from the rate laws was framed as a productive task where students had to come up with a solution themselves. In the second task, the students were asked to interpret an already existing solution, which is a responsive task. These two tasks are quite different, and one can argue that the first task will automatically lead students into trying to remember solutions or try to solve the problem using rules and algorithms.

Nevertheless, even though some students managed to solve the integral fully or partially, we did not see any attempts to make sense of the integral and infer any chemical information from it. We also prompted several students to dive into their chemical knowledge by asking them to construct diagrams showing the concentration as a function of time. Even then, several students did not use much of their chemical knowledge, instead opting to remember how the graphs looked like or how the function would look like from the rate laws. For example, by asking Freya to sketch a graph for the concentration as a function of time given the rate law $v = k[A]$, she replied:

Freya: I think it should increase. Because the change in A... Or it goes down. I think I remember rate laws as either graphs that increases or graphs that decreases. But I am always confused of that is on the y- or x-axis. Over time the concentration of C will increase. So just a straight line going up. Or a bit like a second order [function]... But I'll say a straight line going up.

We can see that no conceptual chemical concepts are used as part of the argument, other than what the student has seen before in chemistry class. She mainly uses mathematical arguments to infer how the reaction unfolds, without thinking about when or how the reaction ends or reaches equilibrium. Here, chemical arguments, like collision theory or merely discussing the relation between products and reactants, could be used to discuss how the reaction would unfold.

Despite the differences of the two tasks, it could be argued that even if the students were shown a complete calculation of an integrated rate law from the beginning, they would not interpret the process as time-dependent and dynamic, and thus, they would not blend resources from different mental spaces. We saw that even when given multiple opportunities to include arguments from chemistry in their reasoning, most

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J. Chem. Educ. 2023, 100, 1739−1750

students failed to do so. They framed the first task mainly as a remembering task or as a task where they needed to solve a mathematical, not chemical, problem. When they were shown the computer code, they instead framed the task as both a programming task, a mathematical task and a chemistry task. A reason for this will further be examined when we proceed to unpack the third theme of the analysis.

Theme 3: Blending and Dynamic Reasoning Is Facilitated through Iterative Thinking

In the previous section, it was argued that computation helped to facilitate a shift from a static, recall-based approach to rate laws toward a more dynamic, blending-based approach. However, the question remains: what is it about computation that facilitates this shift? Based on the data collected, we argue that a key element may be the *iterative* approach that underlies numerical methods, in which the next state of a system is equal to a previous state plus a change in that state, given by the rate laws. This way of reasoning was shown in the examples presented in the previous section. However, other students made this element even clearer in their interviews. For example, both Freya and Ada used iterative thinking to describe the rate laws and how the concentration evolves with time:

> ***Freya:*** *Oh yes. Plus. We also add what we assume is in a way the extra that you get over time. And we get that by iterating it over time, HIder, yes, multiplied by dt.*

Freya makes the iterative process explicit by using the verb *iterate*. She explains the process as "adding the extra you get over time", which she clearly knows is the variable *HIder* in the code, which again represents the rate law. The temporal aspect of the iteration process is also explicitly remarked by Freya: "We get that by iterating it over time". The integration process is thus now interpreted as a dynamic way of evolving the system in time, instead of a static process of moving symbols around in accordance with certain rules.

Ada provides another example of this:

> ***Ada:*** *[...] So here it is defined what HI looks like, and it is as you wrote there [she points at the given rate law]: k times H times I. [...] We also define H and I, just so that we have some values to put in here [points to the concentration of H_2 and I_2 in the rate law]. And once we have defined the first value, then we can go to other values, as we do here. [...] And we do that for HI, for the product, as we have the original value of the product plus a change. We also have the reactants. What happens now is change. It is the original value plus an amount of change, and the same with the other reactant. We also see what happens with the change. [...] And it depends on these, here [points at H[i] and I[i]]. And what happens next is. That is the first thing that happens. And that is the change, and here's the final value [points at HI[i + 1]].*

Here, Ada points out that we need an initial value of the system. We can then use this value and the rate law, which represents a change in the system (conceptual chemistry), to calculate the next concentration of the chemical species (conceptual mathematics). This is another example of how the integration is performed stepwise through time instead of symbolically.

Both Freya and Ada explain how we add a change in concentration every time step. In these explanations they use resources from mathematics, programming and chemistry. These resources are combined to produce new meanings, as illustrated in Figure 3. The iterative approach seems to help the students to interpret symbols as chemical entities by

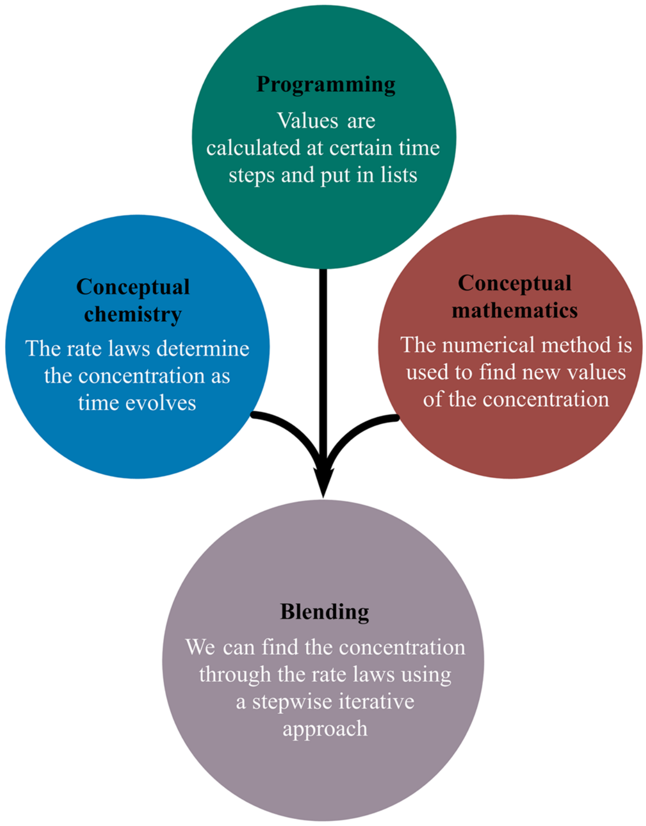

Figure 3. Freya and Ada's problem solving provide examples of new meaning emerging from the blending of knowledge from different mental spaces mediated through a programming mental space.

introducing a temporal, dynamic element to the problem-solving. This dynamic element, where integration is a sum of changes in a system, shifts the students' focus from mathematical rules to conceptual understanding of integration as a sum of states over time. This allows for easier connections between the mathematical model and the dynamic chemical phenomenon.

The iterative approach is also described *explicitly* by some students. For instance, when asked how he would solve the rate laws, Thor sketches a program that uses Euler's method without trying to solve them analytically first. When asked about what he understands by using a numerical solution, he describes the iterative approach explicitly:

> ***Thor:*** *It is kind of, because what I'm thinking, sort of, is that every time that goes by, a little bit more hydrogen and a little bit more iodine is used to form more hydrogen iodide, and thus it is—let us say it is per second, then, then it means that the next second, then there will be less hydrogen and iodine present to react. And thus, less hydrogen iodine will be formed. And that is the [mental] picture I feel the calculation helps me with at least. It divides the process into small moments that make it very easy to understand what is happening second by second.*

Thor describes the numerical integration as an iterative process of "small moments" where a change in concentration happens. He uses this iterative way of solving rate laws as a way of understanding how the system evolves with time. Thus, he

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J. Chem. Educ. 2023, 100, 1739−1750

interprets the rate laws dynamically, in contrast to the symbolic, static interpretation associated with the symbolic integration that was shown earlier. This kind of iterative thinking described by Thor, and exemplified by Freya and Ada, seems to facilitate the blending of different resources. We can say that this numerical, iterative approach catalyzes the blending of resources from different mental spaces.

One important reason that the computer code facilitates blending is that it is very explicit. That is, it represents chemistry and mathematics in a less abstract way than standard mathematical notation. For instance, every variable name can be equated to a specific chemical entity. In addition, mathematical operations in computer code are often easy to interpret, as they mostly consist of simple arithmetic. Even algorithms for numerical integration consist only of addition and multiplication. As such, when students read the code, they managed to understand their chemical content, and from this, blend different resources. In this way, we argue that code can activate and prime different mental spaces, which makes them readily accessible for blending.

Another reason that computer code can facilitate blending, is that it can serve as an iterative representation of dynamic, temporal phenomena. For example, a code where concentration is increasing in discrete time steps contains more information about the dynamic nature of kinetics than an integrated rate law does. A for-loop representing a numerical method prompts the discussion of a dynamic phenomenon. As such, it is not the code itself that directly facilitates blending. It is merely used as a representation that emphasizes the dynamic and iterative nature of kinetics. Thus, it is the *interpretation* of the numerical method which is *represented* by the code that facilitates blending.

■ CONCLUSION AND IMPLICATIONS

The data and analysis presented here show that students do not tend to blend chemistry knowledge with mathematical knowledge when working procedurally with symbolic entities from mathematics. However, interpreting an iterative numerical solution helps the students to foreground the dynamic and time-dependent nature of reaction kinetics. In this process, students are more likely to engage in conceptual blending and thereby construct new emergent understandings. This blending process is facilitated through iterative thinking mediated by programming code. The code serves as a representation of the numerical method, making it easier for students to interpret reaction kinetics as dynamic and stimulating students to interpret both the chemical and mathematical aspects of the problem.

The numerical approach introduces a more dynamic, temporal way of solving a mathematical problem, and this makes the inference of the chemical dynamics of the system more accessible. When exposed to a numerical approach, the students also shifted their mindsets from static remembering to dynamic reasoning. They used their knowledge of programming, mathematics, and chemistry in a blended mental space, trying to make sense of the problem, instead of remembering and "getting it correct". Thus, the students were more invested in understanding and *integrating* the rate laws (iteratively) instead of remembering what the *integrated* rate laws look like. This gives us an answer to the second research question on how a computational approach might contribute to the understanding of mathematics in a chemistry context. The fact that a stepwise iterative solution facilitated both blending of resources and reinforced the understanding of mathematical models as dynamic entities is also in alignment with research in physics education.[52,67]

Using iterative approaches to mathematical models in chemistry can also be a way to address the problems students have with interpreting the dynamic, temporal aspect of rate laws, as addressed in the literature review section. When both the mathematics and the chemical system are described as evolving with time, it might also be easier for students to understand the connections between the mathematical model and the chemical system it represents, which previous research has regarded as problematic for many students.[12,17,23−25,28]

Bain et al. state that we can help students view mathematical expressions as less abstract by making the connection between the mathematical model and what it represents explicit.[8] Their findings suggest that this can be done by making theoretical connections explicit or by partaking in laboratory work. Based on the findings from this study, we argue that computation and numerical methods can serve a similar role. When students use programming to explore models, every step and connection between chemistry and mathematics is explicit.

We do not claim that analytical methods are of no importance in chemistry. A solid understanding of symbolic mathematics is required to make sense of mathematical models. But we might ask ourselves whether the traditional emphasis on analytical methods and symbolic manipulation is the best approach if the goal is to help students to better understand the relation between mathematical and chemical concepts. With the computer as a powerful tool that is readily available to most students, we have a new opportunity to evaluate the way we teach mathematics in chemistry. Also, it can help us understand how we can leverage students' mathematical knowledge to help them make sense of important concepts in chemistry.

There is of course a danger of introducing a new discipline or element of a discipline to students. If computation is introduced as a separate discipline (for example, through decontextualized computer science courses), students may fail to blend resources from the computational space with resources from other spaces. A computational education for chemists should therefore be grounded in chemical problems in such a way that we help students to integrate computation, science, and mathematics. This way of programming can be called *scientific programming*, which is an interdisciplinary approach to programming in a scientific context.[68]

Another implication of this study is that chemistry instructors should be wary of static or fragmented treatments of analytic approaches to chemistry. For example, some textbooks may present one subchapter concerning "rate laws", then another subchapter on "integrated rate laws", without much connection between the two. This conceptual separation might be due to the complexity of integration rules and to save the students the burden of *remembering* the derivations, but this approach may inadvertently hinder blending and understanding of what mathematics contributes to chemistry. Without "hiding" the mathematics, we suggest that one could instead implement a numerical approach, with the possible effects on student reasoning shown in this article. More research on the effect of the implementation of numerical methods and computations in different contexts in chemistry would be a great addition to the educational literature.

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J. Chem. Educ. 2023, 100, 1739−1750

We suggest that the static framing observed in this study may come from how chemistry is traditionally taught, rather than from chemistry students simply failing to make certain conceptual connections. Redish and Kuo refer to this problem as "students having difficulty in translating the way symbology is used to make meaning differently in math and science classes".[17] In other words, math in science is not the same as math in math,[17] which we should take into account when designing courses and educational programs. Introducing our students to calculus through a mathematics course does not automatically imply that they get a good understanding of how to use calculus in chemistry. We must help them bridge these understandings, either by making mathematics courses for chemists, or by taking time to bridge the gap between mathematics courses *in* our chemistry courses. Either way, we cannot always blame the students for not understanding math in science automatically.

LIMITATIONS

The small number of participants ($N = 14$) means we cannot generalize causal relations between iterative thinking and blending of resources in a general population of chemistry students. Although we can suggest potential mechanisms and causal relations in our population of students, which can then be followed up on by later studies. We examined how including a computational component affected how the students made sense of certain chemical models. Further studies are needed to examine different mathematical chemical models and different populations of students.

All students in this study had a background including a course in programming, either scientific programming in general or programming for chemists. Students without this background might struggle to understand numerical solutions of rate laws like those discussed above, which might hinder their ability to infer mathematical or chemical information from the code.

It is worth noting that the mental spaces used as a model for describing the blending processes are theoretical constructs which are grounded in both the data from this study and in the literature describing student difficulties with combining resources from different disciplines ("disciplinary siloing"[38]). It may help to describe the cognitive mechanisms behind these phenomena, but it is nevertheless important to keep in mind the limitations of the model. It does not represent specific parts in the brain, nor are there sharp borders between the mental spaces. The spaces might be interpreted as available cognitive and linguistic resources either stored in the brain or constructed in the moment in an interconnected discourse and can be used as a model to understand the dynamic construction of meaning.

Lastly, we have previously addressed that the two tasks of finding the concentration from the rate laws and interpreting a computer code that had already solved the integrals, are different. Therefore, we encourage future research to further explore different task designs when comparing analytical and computational approaches to a mathematical problem in chemistry.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.2c00881.

Interview Protocol: Questions guiding the interview with possible follow-up questions (PDF) (DOCX)

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Notes

The authors declare no competing financial interest.

Webpage with course material for a first-year course in programming for chemists (in Norwegian, but Google Chrome can provide a good translation): https://andreasdh.github.io/programmering-i-kjemi/docs/intro.html.

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REFERENCES

(1) Corradi, D.; Elen, J.; Clarebout, G. Understanding and Enhancing the Use of Multiple External Representations in Chemistry Education. *J. Sci. Educ. Technol.* **2012**, *21* (6), 780−795.

(2) Farida, I.; Helsy, I.; Fitriani, I.; Ramdhani, M. A. Learning Material of Chemistry in High School Using Multiple Representations. *IOP Conf. Ser. Mater. Sci. Eng.* **2018**, *288*, 012078.

(3) *Multiple Representations in Chemical Education*; Gilbert, J. K.; Treagust, D., Eds.; Gilbert, E. J. K., Series Ed.; Models and Modeling in Science Education; Springer Netherlands: Dordrecht, 2009; Vol. *4*. DOI: 10.1007/978-1-4020-8872-8.

(4) Madden, S. P.; Jones, L. L.; Rahm, J. The Role of Multiple Representations in the Understanding of Ideal Gas Problems. *Chem. Educ Res. Pr.* **2011**, *12* (3), 283−293.

(5) Jones, S. R. What Education Research Related to Calculus Derivatives and Integrals Implies for Chemistry Instruction and Learning. In *It's Just Math: Research on Students' Understanding of Chemistry and Mathematics*; ACS Symposium Series; American Chemical Society: Washington, DC, 2019; Vol. *1316*, pp 187−212. DOI: 10.1021/bk-2019-1316.ch012.

(6) Sherin, B. L. How Students Understand Physics Equations. *Cogn. Instr.* **2001**, *19* (4), 479−541.

(7) Elby, A. Helping Physics Students Learn How to Learn. *Am. J. Phys.* **2001**, *69* (S1), S54−S64.

(8) Bain, K.; Rodriguez, J.-M. G.; Moon, A.; Towns, M. H. The Characterization of Cognitive Processes Involved in Chemical Kinetics Using a Blended Processing Framework. *Chem. Educ. Res. Pract.* **2018**, *19* (2), 617−628.

(9) Redish, E. F.; Saul, J. M.; Steinberg, R. N. Student Expectations in Introductory Physics. *Am. J. Phys.* **1998**, *66* (3), 212−224.

(10) Ringer McDonald, A.; Nash, J. A. *Teaching Programming Across the Chemistry Curriculum*; American Chemical Society: Washington, DC, 2021.

(11) Papert, S. *Mindstorms: Children, Computers, and Powerful Ideas*, 2nd ed.; Basic Books: New York, 1993.

https://doi.org/10.1021/acs.jchemed.2c00881
J. Chem. Educ. 2023, 100, 1739−1750

(12) Sand, O. P.; Lockwood, E.; Caballero, M. D.; Mørken, K. Three Cases That Demonstrate How Students Connect the Domains of Mathematics and Computing. *J. Math. Behav.* **2022**, *67*, 100955.
(13) *It's Just Math: Research on Students' Understanding of Chemistry and Mathematics*; ACS Symposium Series; American Chemical Society: Washington, DC, 2019; Vol. *1316*. DOI: 10.1021/bk-2019-1316.
(14) Hammer, D. Misconceptions or P-Prims: How May Alternative Perspectives of Cognitive Structure Influence Instructional Perceptions and Intentions? *THE JOURNAL OF THE LEARNING SCIENCES* **1996**, *5*, 97−127.
(15) Hammer, D. More than Misconceptions: Multiple Perspectives on Student Knowledge and Reasoning, and an Appropriate Role for Education Research. *Am. J. Phys.* **1996**, *64* (10), 1316−1325.
(16) Towns, M. H.; Bain, K.; Rodriguez, J.-M. G. In *It's Just Math: Research on Students' Understanding of Chemistry and Mathematics*; ACS Symposium Series; American Chemical Society: Washington, DC, 2019; Vol. *1316*. DOI: 10.1021/bk-2019-1316.
(17) Redish, E. F.; Kuo, E. Language of Physics, Language of Math: Disciplinary Culture and Dynamic Epistemology. *Sci. Educ.* **2015**, *24* (5), 561−590.
(18) Caballero, M. D.; Wilcox, B. R.; Doughty, L.; Pollock, S. J. Unpacking Students' Use of Mathematics in Upper-Division Physics: Where Do We Go from Here? *Eur. J. Phys.* **2015**, *36* (6), 065004.
(19) Smith, T. I.; Thompson, J. R.; Mountcastle, D. B. Student Understanding of Taylor Series Expansions in Statistical Mechanics. *Phys. Rev. Spec. Top. - Phys. Educ. Res.* **2013**, *9* (2), 020110.
(20) Pepper, R. E.; Chasteen, S. V.; Pollock, S. J.; Perkins, K. K. Observations on Student Difficulties with Mathematics in Upper-Division Electricity and Magnetism. *Phys. Rev. Spec. Top. - Phys. Educ. Res.* **2012**, *8* (1), 010111.
(21) Smith, T.; Thompson, J.; Mountcastle, D. Addressing Student Difficulties with Statistical Mechanics: The Boltzmann Factor. *AIP Conf. Proc.* **2010**, *1289*, 305−308.
(22) Loverude, M. Student Understanding of Basic Probability Concepts in an Upper-Division Thermal Physics Course. *AIP Conf. Proc.* **2009**, *1179*, 189−192.
(23) Bain, K.; Rodriguez, J. M. G.; Towns, M. H. Chemistry and Mathematics: Research and Frameworks to Explore Student Reasoning. *J. Chem. Educ.* **2019**, *96* (10), 2086−2096.
(24) White, P.; Mitchelmore, M. Conceptual Knowledge in Introductory Calculus. *J. Res. Math. Educ.* **1996**, *27* (1), 79−95.
(25) Habiddin, H.; Page, E. M. Examining Students' Ability to Solve Algorithmic and Pictorial Style Questions in Chemical Kinetics. *Int. J. Sci. Math. Educ.* **2021**, *19* (1), 65−85.
(26) Tuminaro, J.; Redish, E. F. Elements of a Cognitive Model of Physics Problem Solving: Epistemic Games. *Phys. Rev. Spec. Top. - Phys. Educ. Res.* **2007**, *3* (2), 020101.
(27) Bing, T. J.; Redish, E. F. Epistemic Complexity and the Journeyman-Expert Transition. *Phys. Rev. Spec. Top. - Phys. Educ. Res.* **2012**, *8* (1), 010105.
(28) Sand, O. P.; Odden, T. O. B.; Lindstrøm, C.; Caballero, M. D. How Computation Can Facilitate Sensemaking about Physics: A Case Study. In *2018 Physics Education Research Conference Proceedings*; American Association of Physics Teachers: Washington, DC, 2019. DOI: 10.1119/perc.2018.pr.Sand.
(29) Hammer, D.; Elby, A.; Scherr, R. E.; Redish, E. F. Resources, Framing, and Transfer. In *Transfer of Learning from a Modern Multidisciplinary Perspective*; IAP: Greenwich, CT, 2005; pp 89−119.
(30) Psycharis, S.; Kallia, M. The Effects of Computer Programming on High School Students' Reasoning Skills and Mathematical Self-Efficacy and Problem Solving. *Instr. Sci.* **2017**, *45* (5), 583−602.
(31) Goldenberg, E. P.; Carter, C. J. Programming as a Language for Young Children to Express and Explore Mathematics in School. *Br. J. Educ. Technol.* **2021**, *52* (3), 969−985.
(32) Benton, L.; Saunders, P.; Kalas, I.; Hoyles, C.; Noss, R. Designing for Learning Mathematics through Programming: A Case Study of Pupils Engaging with Place Value. *Int. J. Child-Comput. Interact.* **2018**, *16*, 68−76.
(33) Sand, O. P.; Lockwood, E.; Caballero, M. D.; Mørken, K. Students' Development of a Logarithm Function in Python Using Taylor Expansions: A Teaching Design Case Study. *Digit. Exp. Math. Educ.* **2022**, *8* (2), 213−255.
(34) Ferrarelli, P.; Iocchi, L. Learning Newtonian Physics through Programming Robot Experiments. *Technol. Knowl. Learn.* **2021**, *26* (4), 789−824.
(35) Svensson, K.; Eriksson, U.; Pendrill, A.-M. Programming and Its Affordances for Physics Education: A Social Semiotic and Variation Theory Approach to Learning Physics. *Phys. Rev. Phys. Educ. Res.* **2020**, *16* (1), 010127.
(36) Lin, Y.-T.; Wang, M.-T.; Wu, C.-C. Design and Implementation of Interdisciplinary STEM Instruction: Teaching Programming by Computational Physics. *Asia-Pac. Educ. Res.* **2019**, *28* (1), 77−91.
(37) Sherin, B.; diSessa, A. A.; Hammer, D. Dynaturtle Revisited: Learning Physics Through Collaborative Design of a Computer Model. *Interact. Learn. Environ.* **1993**, *3* (2), 91−118.
(38) Rodriguez, J.-M. G.; Bain, K.; Towns, M. H. The Role of Epistemology and Epistemic Games in Mediating the Use of Mathematics in Chemistry: Implications for Mathematics Instruction and Research on Undergraduate Mathematics Education. *Int. J. Res. Undergrad. Math. Educ.* **2020**, *6* (2), 279−301.
(39) Bain, K.; Rodriguez, J.-M. G.; Towns, M. H. Investigating Student Understanding of Rate Constants: When Is a Constant "Constant"? *J. Chem. Educ.* **2019**, *96* (8), 1571−1577.
(40) Bain, K.; Towns, M. H. A Review of Research on the Teaching and Learning of Chemical Kinetics. *Chem. Educ. Res. Pract.* **2016**, *17* (2), 246−262.
(41) Voska, K. W.; Heikkinen, H. W. Identification and Analysis of Student Conceptions Used to Solve Chemical Equilibrium Problems. *J. Res. Sci. Teach.* **2000**, *37* (2), 160−176.
(42) Kousathana, M.; Tsaparlis, G. Students' Errors in Solving Numerical Chemical-Equilibrium Problems. *Chem. Educ Res. Pr.* **2002**, *3* (1), 5−17.
(43) Van Driel, J. H. Students' Corpuscular Conceptions in the Context of Chemical Equilibrium and Chemical Kinetics. *Chem. Educ. Res. Pract.* **2002**, *3* (2), 201−213.
(44) Cakmakci, G. Identifying Alternative Conceptions of Chemical Kinetics among Secondary School and Undergraduate Students in Turkey. *J. Chem. Educ.* **2010**, *87* (4), 449−455.
(45) Turányi, T.; Tóth, Z. Hungarian University Students' Misunderstandings in Thermodynamics and Chemical Kinetics. *Chem. Educ. Res. Pract.* **2013**, *14* (1), 105−116.
(46) Kırık, Ö. T.; Boz, Y. Cooperative Learning Instruction for Conceptual Change in the Concepts of Chemical Kinetics. *Chem. Educ. Res. Pract.* **2012**, *13* (3), 221−236.
(47) Cakmakci, G.; Leach, J.; Donnelly, J. Students' Ideas about Reaction Rate and Its Relationship with Concentration or Pressure. *Int. J. Sci. Educ.* **2006**, *28* (15), 1795−1815.
(48) Kolomuç, A.; Tekin, S. Chemistry Teachers' Misconceptions Concerning Concept of Chemical Reaction Rate. *Int. J. Phys. Chem. Educ.* **2011**, *3* (2), 84−101.
(49) Çalik, M.; Kolomuç, A.; Karagölge, Z. The Effect of Conceptual Change Pedagogy on Students' Conceptions of Rate of Reaction. *J. Sci. Educ. Technol.* **2010**, *19* (5), 422−433.
(50) Fauconnier, G.; Turner, M. *Way We Think: Conceptual Blending and the Mind's Hidden Complexities*; Basic Books, 2002.
(51) Coulson, S.; Oakley, T. Blending Basics (Linguistic Aspects of Conceptual Blending Theory and Conceptual Integration). *Cogn. Linguist.* **2001**, *11*, 175−196.
(52) Odden, T. O. B. How Conceptual Blends Support Sensemaking: A Case Study from Introductory Physics. *Sci. Educ.* **2021**, *105* (5), 989−1012.
(53) Fauconnier, G.; Turner, M. Conceptual Integration Networks. *Cogn. Sci.* **1998**, *22* (2), 133−187.
(54) Hu, D.; Rebello, N. S. Understanding Student Use of Differentials in Physics Integration Problems. *Phys. Rev. Spec. Top. - Phys. Educ. Res.* **2013**, *9* (2), 020108.

(55) Kuo, E.; Hull, M. M.; Gupta, A.; Elby, A. How Students Blend Conceptual and Formal Mathematical Reasoning in Solving Physics Problems: Conceptual and Formal Mathematical Reasoning. *Sci. Educ.* **2013**, *97* (1), 32−57.

(56) van den Eynde, S. *Blending of Mathematics and Physics: Undergraduate Students' Reasoning in the Context of the Heat Equation*. Ph.D. dissertation, University of Groningen, 2021. DOI: 10.33612/diss.177955315.

(57) Van den Eynde, S.; Schermerhorn, B. P.; Deprez, J.; Goedhart, M.; Thompson, J. R.; De Cock, M. Dynamic Conceptual Blending Analysis to Model Student Reasoning Processes While Integrating Mathematics and Physics: A Case Study in the Context of the Heat Equation. *Phys. Rev. Phys. Educ. Res.* **2020**, *16* (1), 010114.

(58) Van den Eynde, S.; Goedhart, M.; Deprez, J.; De Cock, M. Role of Graphs in Blending Physical and Mathematical Meaning of Partial Derivatives in the Context of the Heat Equation. *Int. J. Sci. Math. Educ.* **2023**, *21*, 25−47.

(59) Gregorcic, B.; Haglund, J. Conceptual Blending as an Interpretive Lens for Student Engagement with Technology: Exploring Celestial Motion on an Interactive Whiteboard. *Res. Sci. Educ.* **2021**, *51* (2), 235−275.

(60) Close, H. G.; Scherr, R. E. Enacting Conceptual Metaphor through Blending: Learning Activities Embodying the Substance Metaphor for Energy. *Int. J. Sci. Educ.* **2015**, *37* (5−6), 839−866.

(61) Ginsburg, H. The Clinical Interview in Psychological Research on Mathematical Thinking: Aims, Rationales, Techniques. *Learn. Math.* **1981**, *1* (3), 4−11.

(62) Russ, R.; Lee, V.; Sherin, B. Framing in Cognitive Clinical Interviews about Intuitive Science Knowledge: Dynamic Student Understandings of the Discourse Interaction. *Sci. Educ.* **2012**, *96*, 573−599.

(63) Posner, G. J.; Gertzog, W. A. The Clinical Interview and the Measurement of Conceptual Change. *Sci. Educ.* **1982**, *66* (2), 195−209.

(64) McHugh, M. L. Interrater Reliability: The Kappa Statistic. *Biochem. Medica* **2012**, *22* (3), 276−282.

(65) Watts, F. M.; Finkenstaedt-Quinn, S. A. The Current State of Methods for Establishing Reliability in Qualitative Chemistry Education Research Articles. *Chem. Educ. Res. Pract.* **2021**, *22* (3), 565−578.

(66) Braun, V.; Clarke, V. Using Thematic Analysis in Psychology. *Qual. Res. Psychol.* **2006**, *3* (2), 77−101.

(67) Sherin, B. L. *The Symbolic Basis of Physical Intuition: A Study of Two Symbol Systems in Physics Instruction*. Ph.D. dissertation, University of California, Berkeley, 1996.

(68) Denning, P. J.; Tedre, M. Computational Thinking: A Disciplinary Perspective. *Inform. Educ.* **2021**, *20* (3), 361−390.