Teaching Molecules How to React: Middle School Students' Learning through Computational Modeling of Chemical Reactions Using M.M.M Platform

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מלמדים מולקולות להגיב: למידת תלמידי חט״ב דרך מידול ממוחשב של תגובות כימיות עם פלטפורמת חומר.רב.בתנועה

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Abstract

The particulate model of matter is a foundational idea that describes and explains many phenomena in chemistry and physics. However, chemical reactions are usually taught as a detached event, disregarding the multiple interactions between molecules, the dynamic nature of the process, and the underlying mechanism. Thus, many students think that substances are joined together, modified, or transformed into products in a one-step process. To this goal, we designed and developed the MMM-React, based on a framework that supports computational modeling with a complex systems perspective. It enables the construction of a variety of models in chemistry and physics with a small set of computational blocks, making a clear separation between properties, actions, and interactions of different kinds of entities. The study uses mixed methods with 60 middle-school students in a pretest-intervention-posttest design. Findings demonstrated a significant increase in students' conceptual understanding, specifically in concepts related to micro-level, the particulate model, and in system components related to emergence. Analysis of students' discourse during interacting with MMM-React shows how the design of the separate computational blocks supported in viewing chemical reactions as parallel events occurring among many molecules with the necessary condition of collisions, after which breaking and forming bonds occur.

Keywords: Modeling, chemistry education, computational thinking, block-based programming, chemical reaction.

מילות מפתח: מידול, הוראת הכימיה, חשיבה מיחשובית, תכנות מבוסס-בלוקים, תגובות כימיות.

Introduction

The particulate model of matter is a foundational idea in chemistry and physics that describes and explains many scientific phenomena. It explains physical changes such as an increase of pressure inside a balloon when one inflates it or chemical reactions as endlessly moving molecules that collide with each other and with the container wall. However, chemical reactions are usually taught as a detached event. They are presented in symbolic forms such as A + B → C, highlighting the type and amounts of the reactants and products. This representation disregards the multiple parallel interactions of the many molecules, the dynamic and probabilistic nature of the process, and the underlying mechanism by which the product molecules are formed. Indeed, it has been found that students do not relate chemical reactions to the particulate model of matter, they miss the underlying process of collisions between particles, and possibly breaking and forming bonds (Garcia & Taber, 2009). They think that substances are joined together, modified, or transformed into products in a one-step process (Andersson, 1986; Johnson, 2000; Sevian & Talanquer, 2014; Yan & Talanquer, 2015).

To address these challenges in learning chemistry and physics, we have designed and developed the MMM platform (Levy et al., 2018). MMM is based on a framework that supports computational modeling of systemic phenomena in chemistry and physics with a complex systems perspective (Bar-Yam, 2003), via a unified perspective of the mathematical and computational basis of many systems in these domains (Saba et al., 2021). It enables the construction of a wide variety of models of systems, in which the micro-level objects are coded with a small set of computational blocks, and the macro-level objects are drawn in. Applying computational modeling to chemical reactions, the MMM-React design supports students in decomposing the process into the probabilistic actions of moving, colliding, breaking and forming bonds. Moreover, the learning design involves modeling various chemical reactions with the same building blocks, supporting students in generating patterns and abstracting the principles underlying reactions, such as the similarities between different reaction types: synthesis reactions, decomposition reactions, or combustion. When observing the visual model, students recognize that chemical reactions involve interactions between numerous particles that are in constant motion and collide with one another. This promotes their mechanistic reasoning (understanding the processes that underlie cause-effect relationships; Russ et al., 2008) of a system's behavior as emerging from the interactions between its constituent entities through a complexity perspective.

This paper presents an investigation with sixty middle school students, their interactions with the programming platform and their learning. The main research question is: How can engaging students in modeling and block-based programming of chemical reactions through a complexity approach and the unified view of MMM-React support their related mechanistic understanding and abstraction of principles?

The Learning Environment

With the MMM platform, students program models of systems in chemistry and physics with a block-based interface (Levy et al., 2018). MMM-React integrates agent-based modeling using NetLogo (Wilensky, 1999) to create a basic model and NetTango (Horn et al., 2020) to integrate it with a block-based interface. The chemistry learning environment, MMM-React, also includes an activity guide on physical and chemical changes, the process underlying a chemical reaction and types of chemical reactions.

To model chemical reactions, students define the participating molecules. Each kind of molecule (named a group) has a separate coding space. Coding is done by dragging blocks into one of three cavities: properties (e.g., shape), actions (e.g., move forward), and interactions (e.g., if meeting another molecule then collide). The blocks that signify a chemical reaction, that is breaking and producing molecules, are 'remove ball' and 'add ball' respectively (Figure 1). Students then run the model and observe the system as it changes. They can add visualizations to highlight particular objects or events in the model as well as measurement devices.

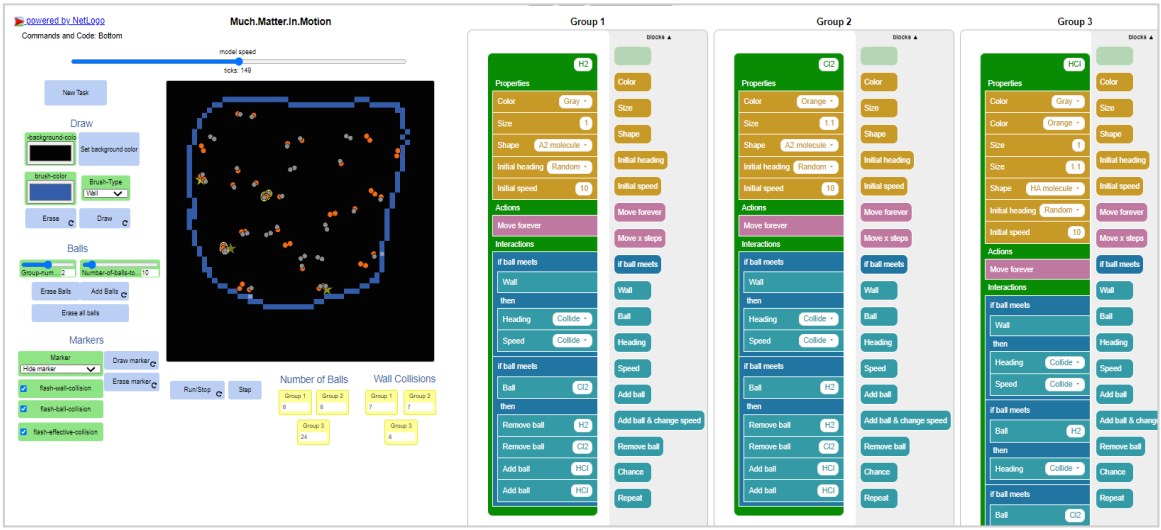

Figure 1. MMM-React interface, an example of an HCl (hydrochloric acid) production reaction. Painting and visualization tools are on the left side of the interface, and block-based coding is on the right side, with each type of molecule having its own coding space.

Methods

The study was framed as a pretest-intervention-posttest design. Participants are 60 middle school science students from two medium-high socioeconomic schools. One 9th grade class ($N = 23$) from one school, and two 8th grade classes ($N = 37$) from the other. The three classes studied four double-period lessons (8 hours total) in which they learned with the same learning environment. The sessions were co-taught by the teachers and the first author. Data collection tools included identical pre- and posttest interviews, questionnaires, students' filled activity worksheets, an audio-recorder, and a screen-capture software. The questionnaires were composed of 12 multiple-choice and open answers relating to chemical reactions – physical/chemical change, the particulate model, micro- and macro-level of reactions, one drawing task, one computational thinking question, and one transfer question. Six items were used in previous research (e.g., Zhang & Linn, 2013) and six constructed in-house and piloted. Students' answers to the items were coded as correct or incorrect. The drawing task was coded for including actions (breaking/forming bonds, movement), the number of steps described, and mass conservation. A paired-samples *t*-test was conducted to compare the effect of the intervention (pretest vs. posttest) on students' scores – overall conceptual learning, by concept and by system thinking. The quantitative analysis was followed by qualitative analysis of students' work with the MMM-React learning unit using their videos.

Findings

Quantitative analysis. An independent-samples t-test showed that no statistically significant difference between groups in the pretest, $t(58) = 1.424$, $p = .160$. Analysis of the pre- and posttest questionnaires shows a statistically significant increase, $t(59) = 24.162$, $p < .001$, $d = 3.12$. To determine what typifies the impact of the learning unit, the answers were analyzed by concept and by system thinking (Table 1).

Table 1. Conceptual learning by concept and by system component: pretest and posttest mean scores ($N = 60$)

	Learning object (# of items)	Pretest *M (SD)*	Posttest *M (SD)*
Total		39 (12)	69 (14) ***
Conceptual learning	Physical / chemical change (5)	58 (16)	62 (17)
	Reaction product as new substance (5)	52 (18)	55 (20)
	Particulate model (3)	33 (18)	48 (25) **
	Reactants/products atomic structure (5)	38 (15)	57 (18) ***
	Bond breaking / formation (8)	49 (20)	63 (24) ***
	Random motion (3)	21 (12)	63 (21) ***
System thinking	Macro (6)	54 (19)	57 (20)
	Micro (6)	38 (18)	65 (24) ***
	Micro-Macro (3)	38 (12)	57 (13) ***
	Emergence (5)	38 (14)	53 (18) ***
	Interactions (6)	52 (19)	63 (23) *
	Randomness (3)	21 (12)	63 (21) ***

Note: $^{**}p < 0.01$; $^{***}p = 0.000$

Data of learning by concept and by system component show that learning with the MMM-React unit was most effective where the learning concepts are related to the micro level. Thus, there was a significant learning of concepts such as *bond breaking / formation,* however, no significant improvement in items related to the *macro level*, such as *physical / chemical change*. In addition, there was a significant learning in concepts related to the *particulate model*, and in system components related to *micro-macro* and *emergence*.

Quantitative analysis. One case study is presented to show how a pair of students, Ori and Darya (pseudonyms), works with the MMM-React modeling platform. At the time of the conference, more case studies will be presented. To show the shift in their understanding, we present their pre- and posttest drawings of water production, and a few episodes from their video. Students' drawings, their coding actions and especially their conversations provide windows into their learning about central concepts related to chemical reactions. They also show how the platform's design provides access to discussion about these concepts: the molecular structure of reactants and products, maintaining the identity of atoms in a chemical reaction, the underlying process of a reaction, stoichiometry, molecules' endless motion, and mass conservation.

Pretest. Before the activity, the average scores of Ori and Darya's was ~ 40%. Ori's drawing of a chemical reaction was partly correct: he viewed chemical reactions as joining moving atoms; however, he illustrated the reactants as separate atoms, ignoring the step of bond breaking. He also started his drawing incorrectly from three atoms only, probably since he knew in advance that only these atoms compose a water molecule. This means that he knew about the

mass conservation, although he did not know how to keep it. Darya wrote that she does not know how to draw water production.

Working with MMM-React. In the following, we describe Ori and Darya while they were coding the reaction of $H_2+Cl_2 \rightarrow 2HCl$. When defining the reactants and products, Darya did not know how to color the product. She watches Ori dragging the blocks into the scripting area (Figure 3),

Darya: Why do you color them [the atoms] red and white?
Ori: you always have two reds and two whites. They do not change; they just join in a different way.
Darya: I understand, they are not being changed, they just join differently.
Ori: It is like taking the twins Yafit and Eden. Once they were in the same classroom, and now they are in separate classrooms, but they are still sisters [having the same characteristics].

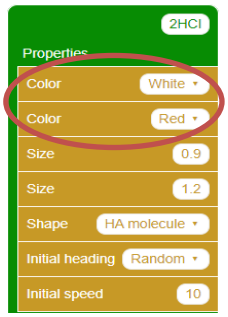

Figure 3

This conversation demonstrates how the MMM-React supports students in understanding an important point: during a reaction, atoms are *rearranged* to form chemical bonds; the atoms themselves are not modified or transformed, but rather they retain their atomic identity.

Next, Ori drags the "Move-forever" block into the scripting area (Figure 4).

Darya: The molecules moved until they join?
Ori: Even after that. Molecules always move, this is one of the rules of the molecules. It is like you and Alona… oops we met! And now we will move together, forever.
Darya: And if we separate?
Ori: You will not separate. The only thing that will separate you is a chemical reaction.

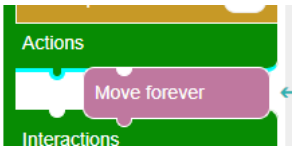

Figure 4

This quote emphasizes the importance of setting the "Action" block. It makes students aware of the endless movement of atoms.

Ori drags the "Remove-ball" block into the scripting and fills "H2" (Figure 5),

Darya: Why?
Ori: Why remove a ball? Because we need to have a balance between the numbers of the atoms, there is always the same number of balls, if you add a ball then you have to remove a ball.

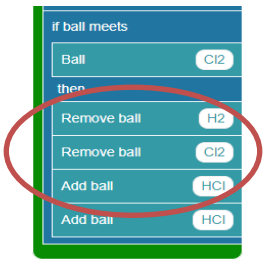

Figure 5

By an intuitive and simple action of adding and removing, we see how the MMM-React assists students in understanding the law of mass conservation and the related balancing of a reaction.

Ori and Darya run the simulation and observe.

Ori: So, the product is 2HCl. We put two molecules, we got two molecules. And why did we add two [blocks of Add-balls]?
Darya: because we need to [according to the activity worksheet]

Ori: But why? We added two because we removed two. After all, we always need to have 30 [balls]. Lets' say we [four friends] are in an escape room. You can choose who will go out, but you have to choose who will get inside, should be someone else.
Darya: Say, I'm going out, but Ella comes in
Ori: Yes, there are always four in the room.

Here again, we see how using the blocks prompted Ori and Darya to realize that the number of atoms should be balanced.

Posttest. After the activity, Ori and Darya's average scores were ~80%, about twice their pretest scores. Ori's drawing improved – he started from two molecules rather than three separate atoms in the pretest and included the steps of breaking and forming bonds while conserving the mass in the reaction. Darya also learned the steps of a chemical reaction and attended to keeping the number of atoms of each type the same.

Discussion and Conclusions

This paper describes how science middle school students, who worked with the MMM-React, part of a learning environment that integrates computational modeling with a complex systems perspective and a unified view of systems, shifted from viewing chemical reactions as a single-step attachment of molecules to mechanistic reasoning of a sequence of interactions between molecules.

The design of the interface, that separates between properties, actions, and interactions addresses the main difficulties in understanding chemical reactions. By defining the participating molecules and setting the *properties* of each of them, students understand that atoms are rearranged and conserved. By setting the *actions*, students refer to the constant motion of particles in the particulate model they have previously studied. By coding the *interactions* students realize that the process is a sequence of steps that logically build upon each other: in order to create new bonds, the existing bonds should first be broken, and this happens only after collisions between the molecules. Finally, running their models enables students to observe the emergent nature of chemical reactions. Applying this sequence of steps to other types of reactions will enable students to generate a common pattern for the mechanism of a chemical reaction.

Contribution to the teaching and learning of science. Learning with MMM-React enables to interact with chemical reactions in a way that overcomes two persistent hurdles that have been highlighted by several leading chemistry education researchers: (1) chemical reactions *based on the particulate model* involving interaction between numerous particles that are in constant motion and collide with one another; (2) a chemical reaction is a process in which atoms are *rearranged* into different combinations of molecules.

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