Putting the Taxonomy into Practice: Investigating Students' Learning of Chemistry with Integrated Computational Thinking Activities

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Abstract

Integration of computational thinking (CT) practices in high school mathematics and science curricula has gained momentum after the publication of Weintrop et al.'s taxonomy of CT practices in science and mathematics (CT-STEM). We designed a high school chemistry unit on ideal gas laws aligned with the CT-STEM taxonomy. Two teachers taught this unit to a total of 121 high school regular chemistry students over the course of ten class periods. Our preliminary findings demonstrate significant increases in students' achievement after learning the content with tightly-integrated CT activities. We present an overview of our unit, the description of an example code-first CT activity, and the results of our quantitative analysis.

1. Introduction

Learning researchers and funding bodies focus increasing attention on the domain of computational thinking (CT) as adoption in schools increase. In the 2018 fiscal year only, The National Science Foundation awarded upwards of 50 million dollars for STEM+Computing projects [1]. With so many resources flowing into CT in the classroom, it is more important than ever for stake holders to ensure that research translates into effective learning environments for students.

The academic literature refers to CT in a number of ways, including the ways of thinking regularly employed by computer scientists [2] and the ways of thinking required to instruct a computer to accomplish a set of goals [3]. We employ a more concrete articulation put forth by Weintrop et al. [4] that defines CT in terms of the practices of computing experts. Wilensky et al. [5] argue that the value of CT is not realized in standalone modules like an after-school program or a computer science course, but rather drives achievement when made an integral part of students' everyday science and mathematics learning. For example, rather than teach a separate

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CT course, a high school chemistry teacher could replace a traditional unit on gas laws with a unit that embeds CT within it. In such a unit, students could create computational models, conduct experiments with gas molecules, and use data practices to construct an understanding of pressure not as an abstract equation, but in terms of the frequency and energy that particles impact their container. Such CT-embedded units promote richer scientific learning and better align with the knowledge and skills of scientists and mathematicians [4, 6, 7].

Despite the attention CT has garnered for its capacity to foster achievements in science and mathematics, few units or curriculum-level designs exist that embed CT. We contribute a novel and effective unit design to serve as an exemplar for researchers and practitioners in the design of future embedded curricula.

2. Background

Before the popularization of the term computational thinking, Wilensky and colleagues developed several gas laws units for high school chemistry that used similar ideas [8, 9]. Gas laws were chosen because temperature, pressure, and the laws that describe their relationships are recognized as challenging for students and led to a multitude of misconceptions [10]. At school, the study of these relationships often encompasses memorization of the equation $PV = nRT$, where students answer questions about what happens to one variable when another is changed [11]. In one such unit, titled Connected Chemistry 1 (CC1, [12]), students ran prefabricated computational models to observe the relationship between gas particle behaviors and key variables like the temperature and pressure. At the completion of the unit, students were able to form multi-level explanations of the chemical system; they were able to smoothly transition between micro, macro, and symbolic representations of gaseous matter.

Weintrop et al.'s Computational Thinking in Science and Math (CT-STEM) taxonomy (Figure 1) was later developed within the Center for Connected Learning and Computer-Based modeling (CCL) to formalize an actionable definition of computational thinking, allowing for curricula like the CC1, which already included many CT practices, to be revised to employ the full spectrum of CT in STEM practices (what we call CT-ifying the unit). This taxonomy operationalizes Wilensky et al.'s [5] argument for embedding computational thinking in science and mathematics learning and defines four strands of computational thinking practices: data, modeling & simulation, computational problem solving, systems thinking. Each category contains computational practices employed by contemporary scientists and mathematicians, which serve as guidelines for activities and tools teachers should build into their curricula. The taxonomy is also intended to function as a design framework for embedded CT-STEM learning environments. However, further work is required to translate these CT practices into well-defined design arguments for empirical testing.

We contribute to the effort towards a design framework for CT-embedded curricula with a novel and empirically validated unit design for teaching gas laws in a high school chemistry course. Our unit takes the original CC1 unit as its starting point but adds new activities to foreground computational problem solving practices. In addition, we build on the three decades of constructionist Connected Chemistry studies, which themselves were precursors to the current CT in STEM research agenda [8, 9, 12, 13, 14, 15, 16]. Our unit, called "Connected Chemistry 2019 (CC'19)", incorporates CT by (1) the authentic use of programming with the NetTango blocks-based interface to NetLogo [17, 18], (2) agent-based modeling with NetLogo [19], (3) data analysis with CODAP [20], and (4) hands-on physical experiments.

Our primary investigation targets two questions: (1) *Do the students' understandings of the relationship between micro-level particulate behavior and macro-level properties (e.g., temperature, pressure) change after completing CC'19?* (2) *Does the CC'19 unit yield a statistically significant increase in students' chemistry content achievement?*

3. The Connected Chemistry 2019 CT-embedded curricular unit

CC'19 consists of six lessons that were implemented over eight class periods. Each lesson contains CT activities tightly integrated with the chemistry content, hands-on experiments, and class discussions. The design of the lessons is heavily influenced by the CC1 unit [12], which itself tightly integrated many CT practices into content learning activities. The main difference between the two is that we foregrounded computational-problem solving practices in CC'19. We provide a general overview of the unit in Table 1. A public version of CC'19 is accessible via https://ct-stem.northwestern.edu/curricula/unit/.

A full review of the CC'19 lessons is beyond the scope of the current manuscript. Here, we present the first lesson as an example to illustrate (1) the novel aspects of CC'19 over its predecessors, and (2) how we addressed a major design challenge of incorporating CT practices as intended by Wilensky et al. and Weintrop et al.

As a whole, we designed the introductory lesson of the CC'19 unit with a pedagogical objective, a CT objective, and a content-learning objective. Pedagogically, we wanted to bootstrap the rich ideas that students bring into the classroom prior to instruction [21, 22]. As CT, we wanted to promote computational problem-solving practices by designing a code-first learning environment [23] in which students can use blocks-based programming to construct computational models of gas particles. In order to promote chemistry learning, we wanted these activities to build towards the main assumptions of the Kinetic Molecular Theory (KMT) because we wanted them to be able to explain how gas pressure, a macro-level property, emerges from numerous gas particles interaction with each other and the container.

To achieve our pedagogical objective, we designed a beginning activity in which the students explored an air duster can as a simple real-world object that has a fixed volume and only gas particles inside. The students hypothesized about what happens when the valve is pressed and presented their hypotheses by drawing sketches. The teachers projected the students' sketches and conducted whole-class discussions on the students' ideas.

To achieve our CT objective, we designed a three-step scaffolded approach. The students first used a static modeling toolkit that resembled the sketching activity. They constructed a computer model by adding stationary walls, removable walls, green particles, and orange particles. Second, they used a NetTango blocks-based programming environment to develop a small-scale model of gas particles. Lastly, they loaded their static air duster models into the NetTango environment to see whether their air-duster model behaved as they anticipated. This process allowed them to design and construct a computational model to test their initial hypotheses.

Designing a code-first activity for KMT was challenging because we assumed no prior programming experience. A traditional approach would require students to use some very difficult computational constructs such as variables, vector calculations, and collision detection. To overcome these obstacles, we designed a new approach to blocks-based programming that we call *phenomenological programming* [24]. Our programming blocks provide procedural templates such as *each particle*, *moves* and *bounces* that can be modified with phenomenologically transparent statements [21, 25] such as spinning for the *moves block*, and *like a balloon* for the *bounces block* (Figure 2b). Each statement embeds simple assumptions about gas particles. For example, when hitting a wall, a billiard ball would not lose any energy, while a balloon would lose some energy. This way, students quickly start programming particles without the challenging task of converting their intuitive understanding of gas-particles to formal computer-code.

4. Methodology

<u>4.1. Participants & Settings:</u> This study took place in Spring 2019. Two teachers and a total of 121 tenth and eleventh grade chemistry students at a U.S. Midwest public high school participated (Table 2). The implementation lasted a total of 10 class periods over the course of 8 days. The students used ChromeBooks to access the lessons.

<u>4.2. Data collection:</u> All students took a chemistry content test before and after the implementation (see Table 3). This test included a total of ten questions. First eight questions were multiple-choice. The ninth question required an open-ended verbal answer. The last question was a sketching task.

<u>4.3. Data analysis:</u> In this paper, we focus on the quantitative analysis of the pre and post-test data because our analysis of the students' sketches is still in progress. We graded the first eight questions by marking the correct answers as one (1) and the wrong answers as a zero (0). We graded the ninth question over a scale between 0 to 2 based using a scoring rubric (see Table 4). We blinded the students' answers, combined them in one column, and ordered them randomly so

that graders did not know whether an answer was from a pre or post-test. The first two authors graded all 182 student responses. We measured the inter-rater agreement by calculating the inter-class correlation coefficient (shortly ICC [26]) and found it to be 0.8376, an outcome considered as a good level of agreement. We averaged the two authors' grades to reach a final score. In addition, an independent scorer graded a randomly selected 20% of the data. We found the ICC between the authors' and the independent scorers' grades as 0.815. We analyzed the students' pre and post-test scores using *the paired-samples t-test* and *the cohen's d effect size* statistical measures. We dropped the columns with missing data because we collected enough paired data for statistical analysis (n = 91).

5. Results

We found that the difference between the students' pre-test scores (M_{pre}=4.77, SD_{pre}= 1.59) and post-test scores (M_{post}=6.02, SD_{post}= 1.97) was statistically significant; $t(90) = -6.10$, $p < 0.001$. We found a medium effect size (d = 0.696).

In addition, we observed a meaningful positive change in the students' verbal explanations (Table 5). Their pre-test answers were often short and lacked sophistication. They either did not mention the particulate nature of gas at all, or when they did, there were misconceptions such as "*if the car is moving, the tires are moving, and the molecules in them are moving, which heats it up*". The concept of particles hitting the walls of the tire was virtually missing. In the post-test, many students formed answers based on a particulate understanding of the gases, kinetic energy, and impacts with the walls of the container.

6. Conclusions and future work

Computational thinking (CT) has been receiving great attention from researchers, policy makers, and educators. One of the promising arguments for CT is that it can boost students' learning of science and mathematics when tightly integrated with content [4]. Even though prior constructionist research indicates the plausibility of this argument [11, 23, 27], more empirical studies are needed. In this paper, we presented our preliminary findings from an implementation of the Connected Chemistry 2019 CT-embedded high school unit. We found a statistically significant increase in the students' content test scores. We also found that the students' verbal explanations of a complex gas-laws related problem improved significantly. We argue that the meaningful increase in student achievement is a good indicator for embedding CT practices as an integral part of the everyday STEM classroom.

7. References

[1] The National Science Foundation (2019, March 18). Retrieved from https://www.nsf.gov/about/budget/

[2] Wing, J. M. (2006). Computational thinking. Communications of the ACM, 49(3), 33-35.

[3] Nardelli, E. (2019). Do we really need computational thinking? Communications of the ACM, 62(2), 32-35.

[4] Weintrop, D., Beheshti, E., Horn, M., Orton, K., Jona, K., Trouille, L., & Wilensky, U. (2016). Defining computational thinking for mathematics and science classrooms. Journal of Science Education and Technology, 25(1), 127-147.

[5] Wilensky, U., Brady, C. E., & Horn, M. S. (2014). Fostering computational literacy in science classrooms. Communications of the ACM, 57(8), 24-28.

[6] Guzdial, M. (1994). Software-realized scaffolding to facilitate programming for science learning. Interactive learning environments, 4(1), 001-044.

[7] Eisenberg, M. (2003). Mindstuff: Educational technology beyond the computer. Convergence, 9(2), 29-53.

[8] Wilensky, U. (1999a). GasLab—An extensible modeling toolkit for connecting micro-and macro-properties of gases. In *Modeling and simulation in science and mathematics education* (pp. 151-178). Springer, New York, NY.

[9] Wilensky, U., Levy, S. T., & Novak, M. (2004). Connected Chemistry curriculum. http://ccl.northwestern.edu/curriculum/chemistry/. Center for Connected Learning and Computer-Based Modeling, Northwestern University, Evanston, IL.

[10] Mas, C. J. F., Perez, J. H., & Harris, H. H. (1987). Parallels between adolescents' conception of gases and the history of chemistry. Journal of Chemical Education, 64(7), 616.

[11] Lin, H. S., Cheng, H. J., & Lawrenz, F. (2000). The assessment of students and teachers' understanding of gas laws. Journal of Chemical Education, 77(2), 235.

[12] Levy, S. T., & Wilensky, U. (2009). Students' learning with the Connected Chemistry (CC1) curriculum: navigating the complexities of the particulate world. Journal of Science Education and Technology, 18(3), 243-254.

[13] Wilensky, U. (1999). GasLab—An extensible modeling toolkit for connecting micro-and macro-properties of gases. In Modeling and simulation in science and mathematics education (pp. 151-178). Springer, New York, NY.

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

[15] Stieff, M., & Wilensky, U. (2003). Connected chemistry—incorporating interactive simulations into the chemistry classroom. *Journal of Science Education and Technology*, 12(3), 285-302.

[16] Brady, C., Holbert, N., Soylu, F., Novak, M., & Wilensky, U. (2015). Sandboxes for model-based inquiry. *Journal of Science Education and Technology*, 24(2-3), 265-286.

[17] Horn, M. S., & Wilensky, U. (2012). NetTango: A mash-up of NetLogo and Tern. AERA 2012.

[18] Horn, M. & Wilensky, U. (2011). NetTango [computer software]. Evanston, IL: Center for Connected Learning and Computer-Based Modeling, Northwestern University.

[19] Wilensky, U. (1999b). NetLogo [computer software]. Evanston, IL: Center for Connected Learning and Computer-Based Modeling, Northwestern University.

[20] The Concord Consortium (July 06, 2019). Retrieved from https://codap.concord.org

[21] DiSessa, A. A. (1993). Toward an epistemology of physics. Cognition and instruction, 10(2-3), 105-225.

[22] diSessa, A., & Minstrell, J. (1998). Cultivating Conceptual Change with Benchmark Lessons, Thinking Practices in Mathematics and Science Learning, Greeno, J. and Goldman, S. Eds.

[23] Horn, M. S., Brady, C., Hjorth, A., Wagh, A., & Wilensky, U. (2014). Frog pond: a code-first learning environment on evolution and natural selection. *In Proceedings of the 2014 conference on Interaction design and children* (pp. 357-360). ACM.

[24] Authors (in press). P-prims meet blocks: An introduction to phenomenological programming.

[25] DiSessa, A. (2015). Alternative conceptions and P-prims. Encyclopedia of science education, 34-37.

[26] Koo, T. K., & Li, M. Y. (2016). A guideline of selecting and reporting intraclass correlation coefficients for reliability research. *Journal of chiropractic medicine*, 15(2), 155-163.

[27] Sengupta, P., & Wilensky, U. (2009). Learning electricity with NIELS: Thinking with electrons and thinking in levels. International Journal of Computers for Mathematical Learning, 14(1), 21-50.

8. Appendix A: Figures

Figure 1: The Computational Thinking in Science and Mathematics (CT-STEM) taxonomy

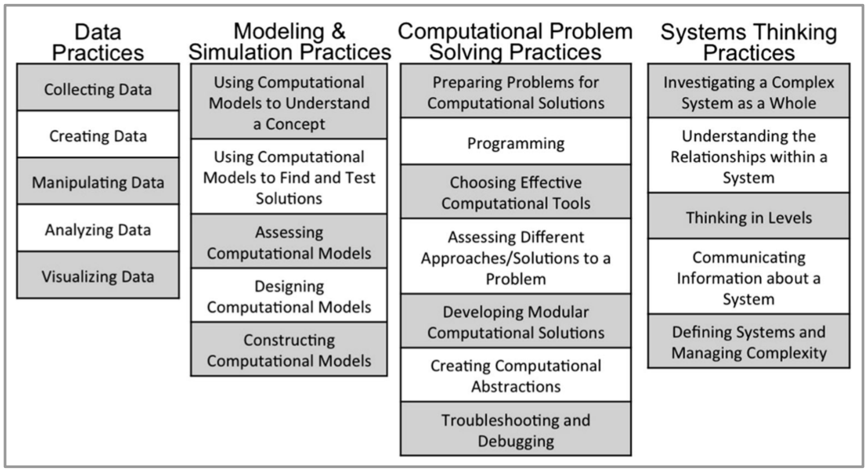


Figure 2: The blocks-based chemistry sandbox toolkit with phenomenological blocks

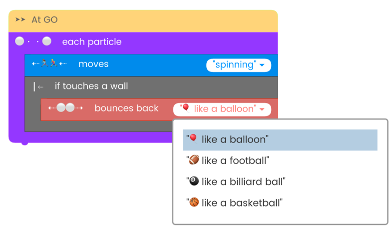
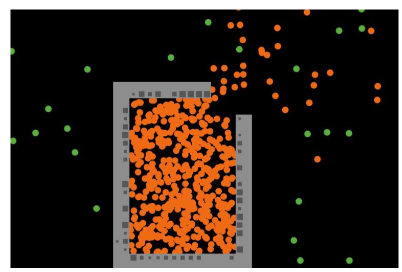
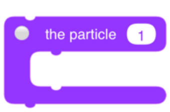
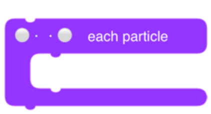
		
(a) static model	(b) coding blocks	(c) running the experiment

Figure 3. The function of the code-blocks of the code-first gas particle sandbox and the assumptions embedded in the phenomenological blocks

Programming Block	**Explanation**
	Procedural block. Code that is attached to this block is executed in a continuous loop when the GO button of the model is clicked.
	Procedural block. The code encapsulated by this block is executed only by the selected particle (e.g., particle 1, particle 10, particle 87).
	Procedural block. The code encapsulated by this block is executed by all particles separately and autonomously.

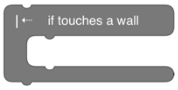
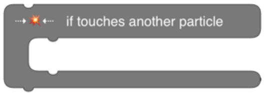
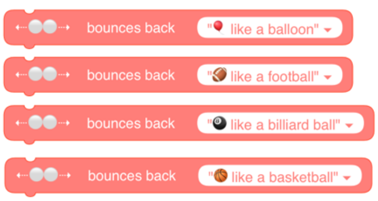
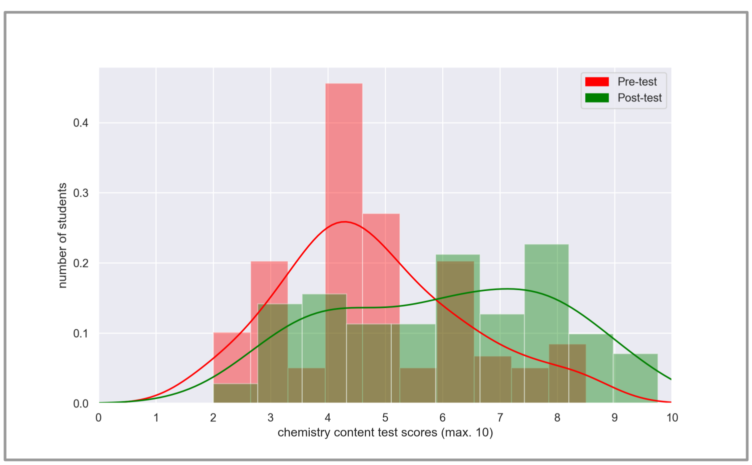
	Procedural block. The code encapsulated by this block is only executed when a particle is touching a container wall.
	Procedural block. The code encapsulated by this block is only executed when a particle is touching another particle.
	Phenomenological block. If a particle is executing this code, it moves 1 unit forward based on the chosen phenomenological statement: <u>Straight</u>: Moves forward 1 unit without changing direction. <u>Spinning</u>: Moves forward 1 unit, changes direction to follow a circular path. <u>Zig-zag</u>: Moves forward 1 unit, changes direction to follow a zig-zag path. <u>Erratic</u>: Moves forward 1 unit, changes direction to follow a path that resembles random walk.
	Phenomenological block. If a particle is executing this code, it changes its momentum and kinetic energy based on the chosen phenomenological statement: <u>Like a balloon</u>: Changes direction as if it is an elastic collision. If collides with another particle, exchanges momentum as if it is an elastic collision. Total kinetic energy is decreased significantly. Recalculates its speed based on its kinetic energy. <u>Like a football</u>: Changes direction randomly. If collides with another particle, exchanges momentum as if it is an elastic collision. Total kinetic energy is decreased slightly. Recalculates its speed based on its kinetic energy. <u>Like a billiard ball</u>: Changes direction as if it is an elastic collision. If collides with another particle, exchanges momentum as if it is an elastic collision. Total kinetic energy is preserved. Recalculates its speed based on its kinetic energy. <u>Like a basketball</u>: Changes direction as if it is an elastic collision. If collides with another particle, exchanges momentum as if it is an elastic collision. Total kinetic energy is decreased slightly.Recalculates its speed based on its kinetic energy.

Figure 4: The distribution of the students' pre-test and post-test scores (n=91)



9. Appendix B: Tables

Table 1: Overview of the Connected Chemistry 2019 CT-embedded chemistry unit

Lesson Title	Length[1]	High-level content objective(s)	CT-Practices
I - Introduction	≈80 mins	Bootstrapping students' naive ideas about the particulate nature of matter and the Kinetic Molecular Theory	Computational Problem Solving Modeling & Simulation Systems Thinking
II - What is pressure?	≈80 mins	Learning how the interactions of gas particles according to the Kinetic Molecular theory at micro-level leads to the emergence of pressure at macro level	Data Modeling & Simulation Systems Thinking
III - Number & pressure	≈40 mins	Understanding the relationship between the number of particles in a container and gas pressure (when other variables are constant). Developing a mathematical model to express this relationship (corresponding to Avagadro's Law)	Data Modeling & Simulation Systems Thinking
IV - Temperature & Pressure	≈40 mins	Understanding the relationship between the gas temperature in a container and gas pressure (when other variables are constant). Developing a mathematical model to express this relationship (corresponding to Charles' Law)	Data Modeling & Simulation Systems Thinking
V - Volume and Pressure	≈40 mins	Understanding the relationship between the container volume and gas pressure (when other variables are constant). Developing a mathematical model to express this relationship (corresponding to Boyle's Law)	Data Modeling & Simulation Systems Thinking
VI - The ideal gas equation	≈40 mins	Combining the three equations from the previous explorations to derive an ideal gas equation	Data Systems Thinking

[1] Recommended length. A class period is assumed as approximately 40 minutes.

Table 2: Demographics of the study participants (self reported)

	N	Male	Female	Non-binary
White	41	27	13	1
African American	34	14	20	-
Latinx	17	9	8	-
Asian	4	3	1	-
Middle Eastern	2	1	1	-
Multiple	23	14	9	-
Total	121	68	52	1

Table 3: Chemistry content test questions

1.What do we mean when we talk about the pressure inside a tire? a) How tightly packed the air molecules are inside the tire b) How much force the air molecules apply to the inside of the tire c) How warm it is inside the tire d) How much space the air molecules take up inside the tire
2. Jeremy kept inflating a balloon until eventually it popped in his face. Why did this happen? a) The temperature of the balloon increased and damaged the balloon b) The balloon was of bad quality and it got ruptured c) There were too much air inside the balloon at room temperature d) It is not possible to pop a balloon just by inflating it
3. Air is often described as being "cold" or "warm". What exactly do we mean when we talk about the temperature of the air? a) How heavy the air is b) How much space the air takes up c) How fast the air molecules are moving d) How much pressure is in the air
4. The gas in an aerosol can is at a pressure of 3.00 atm at 25^{o}C. Directions on the can warn the user not to keep the can in a place where the temperature exceeds 50^{o}C. What would the gas pressure in the can be at 50^{o}C? a) Half b) The same c) Double d) None of the above

5. What do we mean when we talk about the volume of an object? a) The number of molecules inside the object b) The speed of the molecules of the object c) How much space the object takes up d) How warm the object is
6. A gas has a pressure of 1.26 atm and occupies a container with a volume of 8.2 L. If the container and gas are compressed to a volume of 4.1 L, what will its pressure be, assuming constant temperature? a) Half b) The same c) Double d) None of the above
7. Why did reducing the volume of the gas in Question 6 have this effect on its pressure? a) The molecules are striking the container the same number of times as before, but with more energy. b) The molecules are striking the container with the same energy, but there are more molecules now. c) The molecules take up the same amount of space as before. d) The molecules are each striking the container with the same energy as before, but more frequently now.
8. A dented ping-pong ball can be repaired by placing it in a pot of hot water and stirring constantly until the dent pops out by some force. Why does this happen? a) The air molecules inside the ball speed up from the heat and try to take up more space, and as a result pop out the dent. b) The heat from the water makes the walls of the ping-pong ball soft, allowing the dent to pop out from the unchanged pressure inside the ball. c) More air molecules are moved into the ball, creating more pressure inside to push out the dent. d) Other - none of these explain why the dent is removed
9. Most car tires need a pressure of around 32 psi to work effectively, so drivers check the pressure of their tires regularly to see if they need to be filled. In the winter the pressure will read lower when the tires are cold from sitting all night and higher again after the tires have been driven for a few minutes. Why does this happen? … … …

Table 4: The grading rubric for the question 9

Relevant gas laws concepts	**Mentioned in the answer?**
There are particles inside the tire.	☑
The particles are always moving around.	☑
Particles constantly hit the walls of the tire.	☑
Pressure is the result of the particles' impacts with the walls of the tire	☑
Temperature decrease during cold nights cools down the tire.	☑
The particles lose energy from the impacts with colder tires.	☑
Losing energy slows the particles down.	☑
Slower particles means fewer impacts with the walls of the tire.	☑
Driving creates friction between the tire and the road, thus heats up the tire.	☑
The particles gain energy from the impacts with warmer tires.	☑
The particles speed up from increased energy.	☑
Faster particles means more and stronger impacts with walls of the tire.	☑
* *Total student score (between 0 to 2) is calculated by dividing the number of mentioned concepts by 6.*	

Table 5: Examples from the student's pre-and post responses to an open-ended gas laws question

Question 9: *Most car tires need a pressure of around 32 psi to work effectively, so drivers check the pressure of their tires regularly to see if they need to be filled. In the winter the pressure will read lower when the tires are cold from sitting all night and higher again after the tires have been driven for a few minutes. Why does this happen?*

Pre-test response	Score	Post-test response	Score
When the temperature is higher, pressure increases, so once the wheels start moving and warm up, the pressure returns to a safe level.	0.08	When the air temperature is cold, the walls of the tire have a small amount of energy. Therefore, the particles inside the tires, when hitting the sides, will lose energy and slow down. The slower the particles are, the less pressure there is, so after sitting all night in the cold, the particles will have lost energy and the pressure will have dropped. Once the car starts and the tires have been driving for a few minutes, the walls of the tire are warmer, speeding up the particles inside, and ultimately raising the pressure.	1.75
Because the friction on the tires affects the heat of the tire, affecting the pressure.	0.17	Because the colder the temperature, the slower the air molecules will move. Creating less pressure. But when the tires are being driven, that creates friction, which in turn creates heat. Which speeds up the air molecules inside the tire, making them strike the walls of the tire more, which creates more pressure.	1.33
Because the cold air interferes with the pressure	0	Because there is less heat there is like kinetic energy so when the air molecules bounce of the tires they wont get transfered heat to make them go faster. There will be less pressure because there is less heat.	1.25
Cold temperature make the particles come together so they occupy less space	0.17	The temperature of the tire is going to change when is just sitting there it will freeze meaning the walls (tires) will be cold and we study that when they are cold particles tend to hit the wall less times. When you start driving it the friction will make the tires warm and the particles will start to move around faster meaning the pressure will increase.	1.17