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Effect of Computer Simulations at the Particulate and Macroscopic Levels on Students' Understanding of the Particulate Nature of Matter

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ABSTRACT: Computer-based simulations can help students visualize chemical representations and understand chemistry concepts, but simulations at different levels of representation may vary in effectiveness on student learning. This study investigated the influence of computer activities that simulate chemical reactions at different levels of representation in students' conceptual understanding of the particulate nature of matter (PNM). The participants included 170 second semester general chemistry students and were divided into two groups: one interacting with computer simulations at the particulate level and one at the macroscopic level. Students' understanding of the PNM was measured using the Particulate Nature of Matter Assessment. In addition, factor analysis was performed to detect latent concepts in the instrument. Results showed that dynamic simulations at the particulate level helped students understand the PNM in chemistry involving particle motion.

KEYWORDS: *High School/Introductory Chemistry, Chemical Education Research, Computer-Based Learning, Laboratory Computing/Interfacing, Kinetics*

FEATURE: Chemical Education Research

■ INTRODUCTION

Chemistry phenomena are explained in terms of atoms and molecules. It is critical for chemistry students to correctly understand and apply the concepts of the particulate nature of matter (PNM). Nevertheless, the particulate theory of matter is one of the most difficult topics due to the abstract nature of atoms and molecules, which requires students' ability to logically operate on information and symbols beyond personal experience and concrete cases in the real world.[1−12] According to Piagetian theory of cognitive development, students who possess such ability must be in the formal operational stage.[13,14] However, the literature has shown that more than 50% of college freshmen may be in the concrete operational stage, or in the transition state between the concrete and formal operational stages.[9−12] These students often need concrete experiences when conducting mental operations to understand abstract conceptions.[13,14] As a result, they have difficulty learning chemistry at the particulate level, like atoms and molecules that cannot be observed or experienced directly. In particular, many of these students have misconceptions about the structures and behaviors of submicroscopic particles due to the obstacle of building appropriate mental models.[1−8]

To help students comprehend the PNM concepts, chemistry educators have developed various visual representations and integrated them into curricula, trying to build a bridge that connects concrete phenomena and abstract concepts. There are three different levels of chemical representation of matter: macroscopic, symbolic, and submicroscopic or particulate.[15] The macroscopic level comprises real chemicals and observable chemical phenomena. Students learn macroscopic representations from laboratories, demonstrations, and daily experiences. Symbolic representations describe chemical structures and processes with graphs, formulas, equations, etc. Lectures and exams typically focus on this level. The particulate level includes molecules, ions, atoms, and subatomic particles, as well as the movement of particles.[15] Learning at the submicroscopic level often requires the aids of models and imaginations.[16] Computer-based animations and simulations can provide visual representations of particulate structures and processes that may help students build mental models or imaginations. In the past 30 years, numerous research studies have been conducted to evaluate the educational efficacy of computer animations and simulations in chemistry. Researchers and educators have measured student learning outcomes and attitudes by using a variety of methods, such as word problems,[17] open-ended questions,[18,19] interviews,[20] and field observations.[20,21] It has been reported that animations and simulations help students visualize abstract chemistry models,[19,22,23] connect representations of chemical phenomena at all three levels,[22,23] develop advanced conceptual understanding at the particulate level,[21−25] improve performance on exams,[17,18,20,22−24] and form positive attitudes in learning.[2,8,20−24,26−33]

In addition to general measurement such as ordinary exams, researchers employed specifically designed instruments to assess students' conceptual understanding of the PNM. For example, Williamson and Abraham (1995) used the Particulate Nature of Matter Evaluation Test (PNMET) instrument to evaluate the effect of computer animations on college students' mental models and conceptual understanding of the PNM. The results showed that students in the treatment groups scored significantly higher on the PNMET, indicating that the animations helped students form expert-like mental models and improve conceptual understanding of chemistry at the particulate level.[24] Another such instrument is the Particulate

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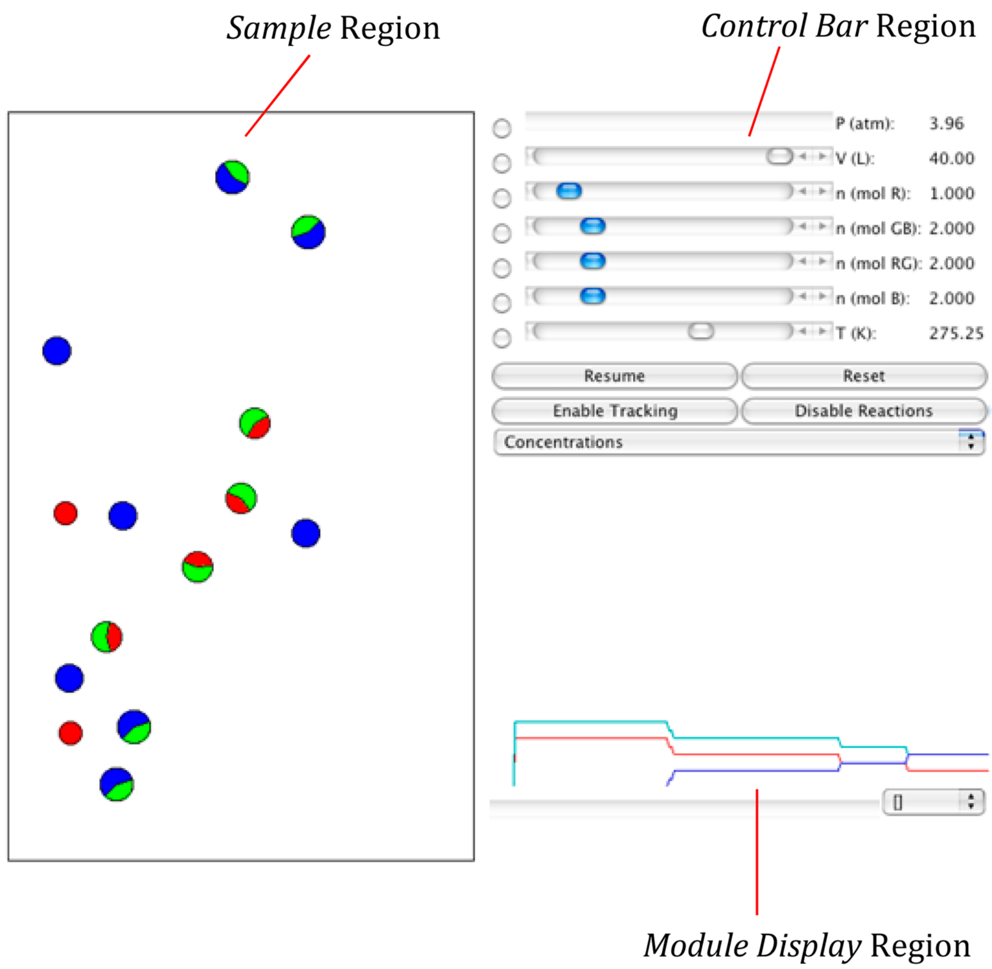

Figure 1. Screenshot of a simulation used in the particulate group: Mechanisms of a Chemical Reaction. The three regions are labeled on the screenshot.

Nature of Matter Assessment (ParNoMA) constructed by Yezierski and Birk.[8] By analyzing the pre- and posttest scores of the ParNoMA, the authors found that students' misconceptions about the PNM were mostly related to phases and phase changes, and animations at the atomic and molecular level aided the students in forming better mental models and changing misconceptions about particle properties and behaviors.

In both studies, the overall scores or the scores for certain predefined categories of the instruments were calculated. For instance, the PNMET consisted of two parts: PNMET 5 contained 11 items that were about properties and behaviors of gases, liquids and solids; and PNMET 7 contained 7 items that covered reaction chemistry.[24] In Yezierski and Birk's study, the ParNoMA was composed of 20 multiple-choice questions including five different topics about particles. The authors compared the overall scores of the pre- and posttests as well as the score gains between the control and treatment groups.[8]

Another way to investigate students' responses is to statistically identify groups of questions in an instrument and then analyze the characteristics of each of the groups. The number of groups can be determined by performing exploratory factor analysis (EFA). EFA is generally used to reduce data dimensionality by classifying common variables of the items into descriptive groups that represent the internal data structure. It has the potential to uncover latent features in responses, and hence may provide information that cannot be measured directly from overall scores or the scores of individual questions. Chemistry education researchers have conducted factor analysis to analyze survey data, e.g., determine the structure of survey items with a certain number of factors, such as attitude, belief, motivation, and interest.[34−39] However, factor analysis has rarely been used to explore student conceptual understanding in chemistry. In the two recent examples where students' understanding of concepts related to the PNM was investigated, the authors utilized factor analysis to verify the existence of the factors in the instruments.[40,41]

■ PURPOSE OF THE STUDY

The aim of the present study was to investigate the effect of particulate-level simulations and macroscopic-level simulations on students' conceptual understanding of the PNM, which was evaluated using an existing instrument. The authors sought factors in student responses, trying to explore the commonalities among the items in each factor and the correlations between different factors. Accordingly, in addition to the overall scores of the instrument, the researchers compared the scores between the two experimental groups (simulations at two different levels of representation) for each factor. The research questions were as follows:

1. How do computer simulations at the particulate and macroscopic levels affect students' conceptual understanding of the PNM?

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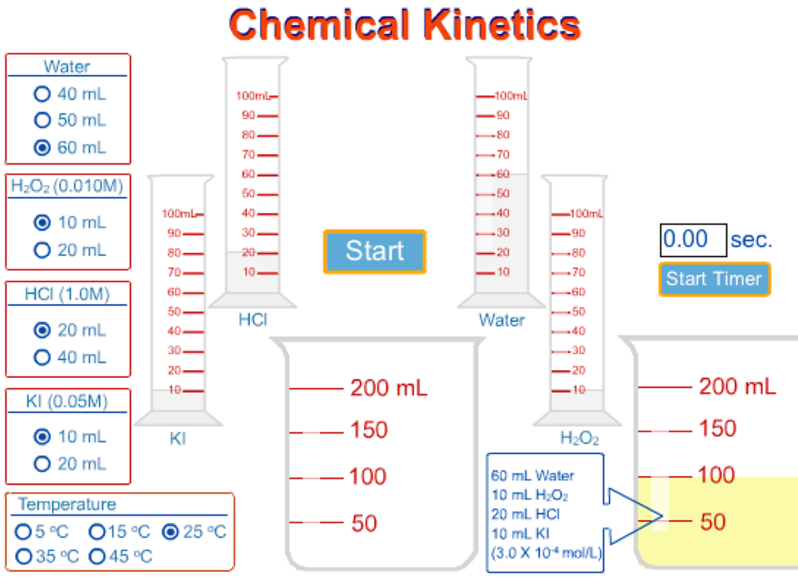

Figure 2. Screenshot of a simulation used in the macroscopic group: Concentration/Temperature Effects.

2. Do meaningful and apparent factors exist in student responses to the questions in the instrument? Are there differences in student performance between the two experimental groups for one or more factors?
3. What characteristics can be extracted from the factors, focusing especially on characteristics that cannot be (easily) observed from overall responses to the questions or even predefined groups of questions in the instrument?

■ METHODS

Participants

The participants were students in the second semester general chemistry course at a large Midwestern comprehensive university in the spring 2008 semester. 511 students were enrolled in the course at the beginning of the semester. All the students were required to enroll in one of the 24 laboratory/recitation sections in addition to the lectures. Each section met for a 3 h chemistry laboratory and an 80 min recitation each week. Every section had a maximum of 24 students and was taught by an experienced graduate teaching assistant (TA). Students were freely and randomly enrolled in the laboratory/recitation section. Nine sections were randomly selected as the particulate group and 11 sections as the macroscopic group. There were 182 students in the particulate group and 190 students in the macroscopic group who initially volunteered to participate in the research study. Because the participants could leave the experiment at any time, we only included those who took both pre- and posttests when analyzing the data (56 in the particulate group and 114 in the macroscopic group). The study was approved by the Institutional Review Board (IRB), and all the participants signed the consent form prior to the experiment.

■ SIMULATIONS

All the simulation activities were chosen from a book that the students used in their recitation sections, named *General chemistry: During class inventions and computer lab activities (Volume II)*.[42] Each unit in the book is composed of several inquiry activities for students to learn the key concepts in the unit. These activities include two types of computer-based experiments that simulate general chemistry laboratories: Molecular Laboratory Experiments (MoLEs)[32,42] and Laboratory Simulations.[42,43]

A typical interface of a MoLE simulation consists of three regions: the Sample Region, the Control Bar Region, and the Module Display Region. Figure 1 is an example of a MoLE simulation interface. The Sample Region is a two-dimensional container with simulated particles that can move, collide, and react. Students can change parameters such as temperature and pressure in the Control Bar Region to control the simulation. The Module Display Region displays the simulation results in graphs or tables. The actions of the three regions are linked so that changes in one region are reflected in the other two.

A Laboratory Simulation window integrated the Macroscopic Region and the Symbolic Region. In the window, students can read measures from the equipment or glassware, change variables in the experiments, and view chemical phenomena such as color change. Figure 2 shows the interface of a Laboratory Simulation.

The complete collections of both MoLEs and Laboratory Simulations were designed to explore concepts at the particulate, macroscopic, and symbolic levels. However, the MoLE activities in this study were selected purposely to have more particulate features, while the Laboratory Simulation activities selected in this study focused on the macroscopic level.

Two sets of simulations that the particulate group interacted with were from MoLEs,[32,42] including Mechanisms of a Chemical Reaction about chemical kinetics, and Shifting Reaction A and Shifting Reaction B, which linked concepts of chemical equilibrium in the gas phase. There was no simulation of chemical equilibrium in Laboratory Simulations that met the requirement of this study (e.g., only had macroscopic features). Thus, the two sets of simulations that the macroscopic group interacted with were two kinetics experiments called Concentration/Temperature Effects, and Decomposition of H_2O_2 and Acid/Base pH from Laboratory Simulations.[42,43]

Designed as guided-inquiry learning activities, each simulation in the book is accompanied by associated questions.[42] The questions were developed in a similar structure with three

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main steps: guiding students to collect data, analyze and interpret data, and draw conclusions. For example, the major steps in the Mechanisms of a Chemical Reaction (particulate simulation, Figure 1) and Concentration/Temperature Effects (macroscopic simulation, Figure 2) are described in the following:

Step 1. Data Collection: Students record the initial concentrations and volumes of the reactant solutions (macroscopic simulation) or the volume of the container and the numbers of particles (particulate simulation), as well as the initial temperature. Next, students are guided to design trials to change the above parameters and then to record the results (e.g., amount of reaction time) in each trial.

Step 2. Data Analysis and Interpretation: Students are required to explore the relationship between the change in reaction rate and concentration/temperature change as well as to draw a graph to show and explain either the relationship (macroscopic simulation) or what is happening to each kind of particle during the reaction (particulate simulation).

Step 3. Conclusion: Students are asked to generalize how concentration and temperature changes influence the rate of a chemical reaction (macroscopic simulation) or to propose the mechanism of the reaction by drawing the particles before, during, and after the reaction (particulate simulation).

The experimental treatments took place during the second and third weeks of the semester. That is, students in both particulate and macroscopic groups conducted the computer-based laboratory simulations and answered the associated questions in their recitation sessions during these 2 weeks, one in each week. The amount of time to complete each simulation activity was approximately 60 min. The TAs collected students' reports at the end of each recitation.

INSTRUMENTS

Particulate Nature of Matter Assessment

The ParNoMA is an instrument that assesses students' conceptual understanding in the PNM.[8] The instrument consists of 20 multiple-choice questions about water molecules. As listed in Table 1, the design of the ParNoMA questions was based on five concepts: (a) size of particles, (b) weight of particles, (c) compositions of particles, (d) phases and phase changes, and (e) energy of particles. The second version of the ParNoMA was employed as both pre- and posttests in this study. Because the ParNoMA was not directly related to the concepts (kinetics or equilibrium) in the experiment, it was utilized as a general measure of understanding of the PNM in this research.

Table 1. Category of Concepts in ParNoMA

Concept	Name	Question	Number of Questions
a	Size	3, 14	2
b	Weight	6, 19	2
c	Composition	4, 7, 8, 9, 11, 15	6
d	Phase change	1, 2, 10, 13, 16, 17, 20	7
e	Energy	5, 12, 18	3

The pretest was held 1 week before the treatment, while the posttest was carried out 6 weeks after the treatment. The interval between the treatment and the posttest was relatively long so that students would not be able to recall the questions they answered in the pretest. The effects of the treatment were measured by comparing students' performance on both tests.

DATA ANALYSIS

Most statistical analyses were carried out using Statistical Analysis Software (SAS). Independent t-tests were used to compare the mean scores statistically between the particulate and the macroscopic groups. These scores include (a) the pretest and the gain scores of the ParNoMA and (b) the gain scores of each factor in the ParNoMA. Paired t-tests were used to compare the mean scores between the pre- and posttests for the two groups of participants. Factor analysis was performed to determine the factors in the ParNoMA. Only students who took both pre- and posttests were included in the analyses of student responses. The software R (version 2.15.3)[44] was used to measure Cronbach's α, Pearson's correlation, and the effect sizes.

RESULTS

Reliability of the Instrument

The reliability of the ParNoMa was measured by calculating Cronbach's α using the R function cronbach in the package psy. Cronbach's α evaluates the internal consistency of the instrument items. The values were $\alpha = 0.856$ for the pretest and $\alpha = 0.889$ for the posttest, which indicates "good" consistency[45] for both pre- and posttest data sets. In addition, the reproducibility of students' responses on both tests was measured by calculating Pearson's correlation r using the R function cor.test. The correlation for the overall data set was $r = 0.605$ ($p < 0.001$); the r values were 0.683 ($p < 0.001$) for the particulate group and 0.597 ($p < 0.001$) for the macroscopic group. The relatively high positive correlations between the pretest and the posttest indicated a reasonably good reproducibility of students' responses in the instrument.[45]

t-Tests

There was no significant difference between the particulate and macroscopic groups on the pretest ($t = 0.909$, $p = 0.365$, Cohen's $d = 0.148$). Paired t-tests showed no significant difference between the pre- and posttests for the particulate or macroscopic group ($p > 0.05$). However, a significant difference in the gain scores between the two groups was found ($t = 2.272$, $p = 0.0246$). The particulate group gained more after the treatment than the macroscopic group did, with an effect size (Cohen's $d = 0.371$) in the moderate range.[46] The average scores and the gain scores are listed in Table 2.

Factor Analysis

Students' responses to each question on the pretest and the posttest were combined to form a 340 × 20 matrix. To evaluate the suitability of factor analysis, Bartlett's Test of Sphericity and

Table 2. ParNoMA Scores

	Pretest		Posttest		Gain	
Group	Mean	SD	Mean	SD	Mean	SD
Macroscopic (n = 114)	14.25	4.45	13.68	5.36	−0.57	4.48
Particulate (n = 56)	13.59	4.38	14.41	3.94	0.82	3.34

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Kaiser–Meyer–Olkin (KMO) Measure of Sampling Adequacy were performed. The Bartlett's test checks how the items in an instrument are correlated. It showed a statistical significance of the correlation matrix (χ^2 = 2380.012, df = 170, p = 0.000). The KMO index determines whether the items can be factorized efficiently.[47] The overall KMO index was 0.85, and the value of each question was greater than 0.50. Thus, factor analysis was appropriate[47] for the ParNoMA data.

The EFA[48] of the 20 questions suggested three factors according to eigenvalues greater than 1 and the shape of the scree plot. The factor extraction method was "prinit" (iterated principal factor analysis), and the rotation method was "varimax". Each factor consists of four to nine questions, as shown in Table 3. The criterion 0.32 was used as the cutoff of the factor loadings.[49] That is, a question was categorized to a factor if the factor loading was greater than 0.32. For example, the first question had a loading 0.37 in factor 2 and therefore it was grouped to factor 2. There was only one item crossloading (question 6), that is, the item had loadings greater than 0.32 on two factors. In this case, we assigned the question to the group that had the higher factor loading. According to the content of each question in the ParNoMA, three concepts associated with each set of questions were derived. The three concepts are sizes of particles, compositions of molecules, and particle motion and energies (Table 3). Table 4 summarizes the groups of questions and the name of each factor.

Table 3. Factor Loadings of ParNoMA Questions and the Corresponding Concept Categories

Question	Factor 1	Factor 2	Factor 3	Concept	Name
3	0.57[a]	0.31	0.13	1	Size
6	0.66[a]	0.39	0.20		
14	0.77[a]	0.22	0.14		
19	0.6[a]	0.27	0.20		
4	0.31	0.47[a]	0.17	2	Composition
5	0.30	0.62[a]	0.19		
7	0.18	0.76[a]	0.03		
8	0.16	0.75[a]	0.08		
9	0.16	0.58[a]	0.19		
11	0.16	0.61[a]	0.24		
15	0.19	0.70[a]	0.12		
1	0.10	0.06	0.37[a]	3	Motion-energy
2	0.13	0.08	0.37[a]		
10	0.12	0.06	0.32[a]		
12	−0.07	0.22	0.51[a]		
13	0.18	0.11	0.58[a]		
16	0.11	−0.04	0.54[a]		
17	0.10	0.09	0.63[a]		
18	−0.15	0.17	0.45[a]		
20	0.17	0.19	0.47[a]		

[a]These values indicate factor loadings greater than 0.32, and the corresponding question is categorized to that factor. If a question has two factor loadings greater than 0.32, the higher factor loading is used.

When the pretest and the gain scores were compared between the particulate and macroscopic groups, there were no significant differences in the compositions factor or the size factor ($p > 0.05$). For the motion and energy factor, there was no significant difference in the pretest ($p > 0.05$). However, a significant difference of the gain scores was found (t = 3.060, p = 0.003). The particulate group gained more than the macroscopic group did, and the effect size (Cohen's d = 0.499) was medium. The average scores of the motion and energy factor are shown in Table 5.

Table 4. Summary of Factors of ParNoMA Items from Factor Analysis

Factor	Concept Name	Question	Number of Questions
1	Size	3, 6, 14, 19	4
2	Composition	4, 5, 7, 8, 9, 11, 15	7
3	Motion-energy	1, 2, 10, 12, 13, 16, 17, 18, 20	9

Table 5. Average Scores of Motion-Energy Factor in ParNoMA

	Pretest		Posttest		Gain	
Group	Mean	SD	Mean	SD	Mean	SD
Macroscopic (n = 114)	7.96	1.12	7.41	2.34	−0.55	2.10
Particulate (n = 56)	7.68	1.65	8.00	1.16	0.32	1.55

■ DISCUSSION

The operation of the factor analysis of the ParNoMA resulted in three factors, which were named as (1) sizes of particles, (2) compositions of molecules, and (3) particle motion and energies based on the commonality of the concepts in the questions within each factor. Recall that five concepts were implemented in the ParNoMA when Yezierski and Birk designed this instrument: (a) size of particles, (b) weight of particles, (c) composition of particles, (d) phases and phase change, and (e) energy of particles.[8] It can be seen that both size and weight (concepts a and b) are physical properties of substances, and contain the same questions as in factor 1 (sizes of particles) from the factor analysis. Moreover, concept c is equivalent to factor 2 (both are "compositions"). Additionally, phases and energy (concepts d and e) can be considered as phenomena involving motion of particles, and the questions in these two concepts are identical to those in factor 3 from the factor analysis. In other words, the groups that the factor analysis classified were conceptually consistent with what Yezierski and Birk designed.[8] Thus, this study validated the conceptual categories of the ParNoMA[15] to a new population of students. Furthermore, it can be seen that the sizes and compositions factors were about static phenomena of atoms and molecules, while the motion and energy factor was associated with the dynamic features of particles. Therefore, the EFA reduced the 20 questions in the ParNoMA to only three meaningful subscales of concepts through which the latent construct of the instrument (static and dynamic attributes of the questions) could be easily disclosed. Compared to using the five predefined concepts, the usage of factor analysis demonstrated a clearer and more concise way to further explore the effect of the experiment and to interpret the features of the differences found in the results.

Previous studies have shown that students exposed to simulations and animations performed significantly better in assessments and demonstrated better conceptual understanding than students who only viewed computerized static representations.[24,26,50] This is because dynamic chemical processes are usually more complex than static phenomena and simulated visualizations can help students develop appropriate mental models to comprehend the concepts and processes.[51,52] In this study, a significant difference was found in the overall gain

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scores of the ParNoMA between the two groups of participants. Further analysis revealed that the difference was in the motion (of particles) and energy factor, that is, the gains in the particulate group were significantly higher than that in the macroscopic group. Because this factor was associated with the dynamic nature of particles, the results not only supported the findings in the literature that computer simulations improved students' conceptual understanding at the particulate level,[21−25] but more specifically indicated that dynamic simulations at the particulate level helped students understand the PNM involving dynamic chemical phenomena.

The overall mean scores of the pretest and the posttest of the ParNoMA for the entire participants in this study were 13.92 and 14.05, respectively. These scores are close to 15.2 in Yezierski and Birk's pilot study[8] when the participants were also in a second semester general chemistry course. In another experiment reported by them,[8] the participants were a mixture of students from middle school, high school, and college general chemistry and the authors did not differentiate the scores of students at different academic levels. The overall mean scores were 10.31 on the pretest and 12.85 on the posttest. Compared to the significant increase in their study,[8] the overall gain scores in our research were statistically insignificant. The reason might be that college students had relatively better understanding of the PNM than high school and middle school students, especially after college students took first semester general chemistry. Thus, it could be difficult to improve their overall ParNoMA scores in weeks intervened by a few simulations.

■ LIMITATIONS

The limitation of this study was the recruitment of the participants. In the course, four of the 24 sections were taught by four TAs, one for each section. The rest of the 20 sections were taught by ten TAs, i.e., each of the ten TAs taught two sections. We selected these 20 sections and intended to assign one section from each TA to the particulate group and the other taught by the same TA to the macroscopic group. However, with the exception of one TA, the other nine TAs considered that this assignment would double their teaching burden because they had to teach two different types of activities and grade two types of reports. As a result, we randomly assigned five of these TAs to the macroscopic group and four to the particulate group, with ten and eight sections, respectively. For the TA who agreed to follow the initial assignment, the two sections were randomly assigned to different experimental groups. In the end, students in 11 sections were assigned to the macroscopic group, and students in nine sections were in the particulate group. In addition, the students participated in this study voluntarily and could leave the experiment at any time. Thus, although the numbers of participants taking the pretest were roughly the same in the two groups (182 in the particulate group and 190 in the macroscopic group), participants in the particulate group who took both pre- and posttests were approximately half of those in the macroscopic group (56 vs 114). The recruitment method and the loss of the participants in the particulate group from the pretest to the posttest might affect data validity. However, because the lab/recitation sections were randomly assigned to different experimental groups, and there was no significant difference in the pretest, it could be assumed that the two groups of students should not differ in their abilities to understand the PNM before the treatment.

■ IMPLICATIONS

Factor analysis has been widely used to study survey data in chemistry education research. This work demonstrates that it can also be a useful tool to explore students' conceptual understanding. Researchers in chemistry education can employ exploratory factor analysis to reduce the dimensions of an instrument. Through the process, groups of items in the instrument may be formed with a latent construct. Interpreting students' responses in these groups of items can be more informative than analyzing the overall score of the instrument, as well as be more efficient than examining each question in the instrument individually.

The present study confirms that the ParNoMa produces valid and reliable data from the sample of college students. Researchers and educators can utilize this instrument to measure students' general understanding of the PNM even though it is about phases/phase changes of matter. Furthermore, some questions in the ParNoMa were associated with dynamic characteristics of atoms and molecules, while others were associated with static characteristics. Thus, chemistry educators can use the instrument to investigate students' understanding of the PNM in both dynamic and static aspects.

A significant difference in the gain scores was found between the participants in the particulate-level simulation group and the macroscopic-level simulation group. Further analysis revealed that the difference was associated with students' understanding of the PNM involving dynamic chemical phenomena. In other words, if the questions in the instrument were related to neither the particulate level of matter nor the dynamic nature of particles, the differences between the two groups might not be detected. Therefore, the findings in this study suggest that it is critical for researchers to utilize an appropriate instrument that consists of relevant subscale conceptions to assess students' understanding of certain topics.

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The authors declare no competing financial interest.

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