Evaluation of an Augmented-Reality-based 3D User Interface to Enhance the 3D-Understanding of Molecular Chemistry

Patrick Maier and Gudrun Klinker
Fachgebiet Augmented Reality (FAR), Technische Universität München, Fakultät für Informatik, Garching bei München, Germany

Keywords: Direct Manipulation, 3D User Interface, Augmented Chemical Reactions, Evaluation, Augmented Reality.

Abstract: The spatial understanding of chemical molecules is crucial for learning chemistry at school. With a good 3D understanding of molecules, chemical processes become obvious compared to a 2D representation in textbooks or just the molecular formula. With the increasing spread of computers, smartphones and tablets, the field of computer aided learning becomes more and more important. Common molecular viewers such as *Jmol* (Jmol, 2012) present chemical simulations as 3D renderings on a regular computer screen in combination with desktop-based user interfaces using a mouse and a keyboard to manipulate 3D molecules. Such interfaces may be cumbersome to use since users have to associate 2D mouse motion and key presses with 3D object motions. In this paper we investigate the hypothesis that the understanding of spatial structures of molecules is enhanced by Augmented-Reality-based 3D user interfaces with which students can directly manipulate the virtual 3D molecules by freely moving and rotating a 3D object in air with their hands. Our results show that a direct manipulation 3D user interface improves the 3D understanding in comparison to the traditional desktop-based user interface with mouse and keyboard.

1 INTRODUCTION

To support students learn chemistry, we have to help them understand the spatial structure of molecules. Knowing the 3D structure of molecules is important to understand the chemical behavior and properties of the molecules. Learning the 3D structure of molecules just by looking at the 2D drawings or formulas of the textbook seams not to be the best method.

Hardware representations that the students can touch have been a well-established method in chemistry education for a long time. Yet, such hardware models are not always available, and it is time consuming to build them for each student and for each molecule. Furthermore, such hardware representations are mostly not flexible or dynamic in their structure.

As computers get more powerful and mobile, interactive 3D representations of the molecules are able to provide a better way for students to inspect and understand the 3D structures. Applications can show complex molecules and animations that the students can inspect. But there is a drawback in the classical 3D presentation programs: the molecules can only be rotated and moved via the mouse and the keyboard. This indirect mapping of mouse movements to the 3D model is not always intuitive. Students have to learn the mapping of 2D mouse movements and keystrokes to 3D object manipulations involving six degrees of freedom. As a result, some of the students' focus may be diverted from the molecules to the user interface, and the structure of the molecules may not be made completely clear.

To combine the benefits of the physical molecule representations with the power of computers, there are direct manipulation 3D user interfaces which use Augmented Reality and tracked real objects to control the position and orientation of the molecules.

In this paper, we report on evaluating the Augmented Reality based 3D user interface of the Application *Augmented Chemical Reactions* (ACR) against the mouse and keyboard based user interface of the Application *Jmol* (Jmol, 2012). The evaluation took place at a secondary school with a class of 14-15 year old students of the 8th grade. In the next section, we take a look at previous work in this field and we describe both types of 3D user interfaces.

Maier P. and Klinker G..
Evaluation of an Augmented-Reality-based 3D User Interface to Enhance the 3D-Understanding of Molecular Chemistry.
DOI: 10.5220/0004349502940302
In *Proceedings of the 5th International Conference on Computer Supported Education* (CSEDU-2013), pages 294-302
ISBN: 978-989-8565-53-2

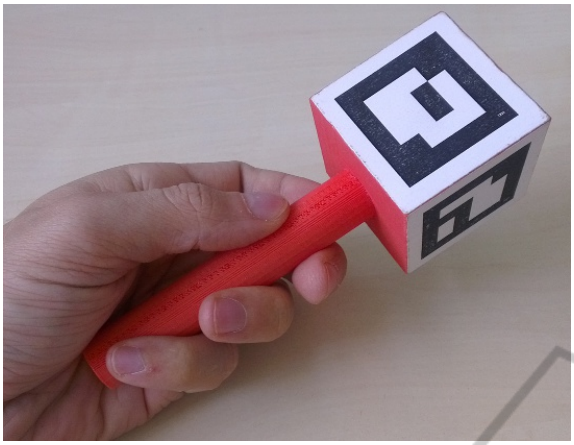


Figure 1: This device is tracked by a computer with a webcam. It is used as a 3D input device for direct manipulation.

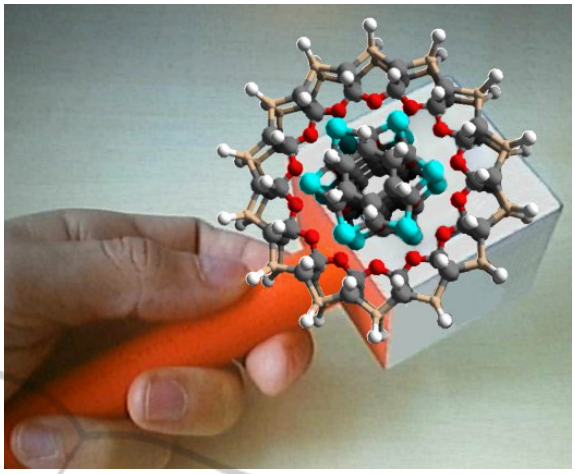


Figure 2: Augmentation of a protein molecule on top of the marker cube.

2 BACKGROUND

Many schemes to support the learning progress of students have been developed. To support the students in understanding the spatial structure of molecules, the most suitable methodologies have to be developed. A number of research efforts have shown that using physical models and therefore using direct manipulation helps students explore and understand the spatial structure of objects (Herman et al., 2006; Arnold et al., 2012; Hoyek et al., 2011). It has also been shown that a direct manipulation interface for rotation via a sensor with 3 degrees of freedom (3 DoF) yields better performance without lacking accuracy, compared to 3D rotation via a mouse (Hinckley et al., 1997). Work at the IBM Almaden Research Center investigated the user performance of different 3D input devices (Zhai, 1998).

2.1 Desktop-based user Interface with Mouse and Keyboard

There are many applications that help users understand the spatial structure and also the resulting dynamics of molecules (Panagiotopoulos et al., 2012; Johnson et al., 2011; Jmol, 2012). Yet, the commonly used user interface to rotate and move virtual objects is still a combination of mouse and keyboard (Chen et al., 1988).

2.2 3D Augmented-Reality-based user Interface

To combine the advantages of the physical direct manipulation with showing complex structures, *Augmented Chemistry* (Fjeld et al., 2007) and *Augmented Chemical Reactions* (Maier et al., 2009b) (Maier et al., 2009a) have been introduced. Both systems use Augmented Reality to deliver a direct manipulation 3D user interface to control the position and orientation of the virtual objects.

Generally speaking, Augmented Reality adds virtual information or objects interactively and in real-time to the real world, generating the impression that the added information is part of the physical world. To this end, the application *Augmented Chemical Reactions* employs a physical cube with a handle that is textured on all sides with black and white patterns (Figure 1). In a typical setup, a student holds the cube by the handle and manipulates it while sitting at a desk in front of a monitor. A webcam records the scene with the cube, and *Augmented Chemical Reactions* uses a marker tracking algorithm similar to the AR-toolkit (Kato and Billinghurst, 1998; Pustka et al., 2011) to detect and recognize the currently visible patterns on the cube. According to the size and deformation of the patterns, the algorithm calculates their position and orientation relative to the webcam – and thus the pose of the cube and handle. With this information, the virtual molecule can be drawn on top of the webcam image, leading to the illusion, that the molecule is attached to the cube (Figure 2). The virtual molecule moves in unison with the physical cube. This is a three-dimensional direct manipulation user interface.

3 EVALUATION

We conducted a user study with 14-15 year old students of a german gymnasium (secondary school) to

determine whether direct manipulation of the position and orientation of virtual molecules leads to a better spatial understanding of virtual molecules than input via a standard mouse and keyboard. We selected a class in the 8th grade – just at the time when they had been taught the basic concept of what a molecule is, but they had not learned yet about the spatial structure of molecules. Therefore they were ideally suited for a study investigating which of the two user interfaces leads to a better 3D understanding of molecules.

None of them already had experience with *Augmented Chemical Reactions* or the *Jmol* application. Most of the students had lots of experience with playing 3D games, but nearly none had already used to use a 3D chemical modeling application or another 3D design application. Only one student stated to have already a good knowledge about the chemical structures of molecules. As his prior results in building the molecules were already correct, he did not have the change to improve. So this results could not be used to get a measurement of the performance of the application and thus was removed (see section 4.1).

3.1 Experimental Setup

In cooperation with a chemistry teacher, we selected ten different molecules to be inspected in this study. Those molecules were (1) Sulfur S_8, (2) Methane CH_4, (3) Ethanol C_2H_5OH, (4) Acetic acid $C_2H_4O_2$, (5) Benzene C_6H_6, (6) Hydrogen sulfide H_2S, (7) Phosphor P_4, (8) Phosphorus trifluoride PF_3, (9) Hexane C_6H_14 and (10) Carbon tetrabromide CBr_4.

We had two computer rooms, one for the *Jmol* and one for the *Augmented Chemical Reactions (ACR)* application. Each student desk was equipped with the respective computer equipment.

Computer Setup for *ACR*. The first computer room was set up to run the *ACR* application with a 3D direct manipulation user interface. Here a monitor, a keyboard, and a marker cube with a handle were placed on each student desk. A webcam on a microphone stand in shoulder height of a sitting person faced towards the student desk and the marker handle. To control the position and the orientation of the virtual molecule, the students had to hold the marker cube into the field of view of the webcam. The video stream, augmented with the currently selected molecule, was shown on the monitor in front of the student, as shown in Figure 3. The students could cycle through the set of molecules by pressing the space-bar on the keyboard.

With a well-aligned arrangement of the camera, the user, the hand-held handle and the monitor, the AR illusion via a directly manipulated physical object can be maintained with minimal strain on the hand-eye coordination. A more immersive, perfectly aligned setup can be achieved when the monitor-based arrangement is replaced with a video-see-through or optical-see-through head-mounted display. Yet, such arrangements are costly and thus currently not deployable in classrooms. For this reason, the current test setup was based on webcams and monitors on student desks.

Figure 3: Computer setup for the ACR application, using a webcam a physical cube on a handle and a monitor. The keyboard that is required to cycle through a set of molecules is not shown.

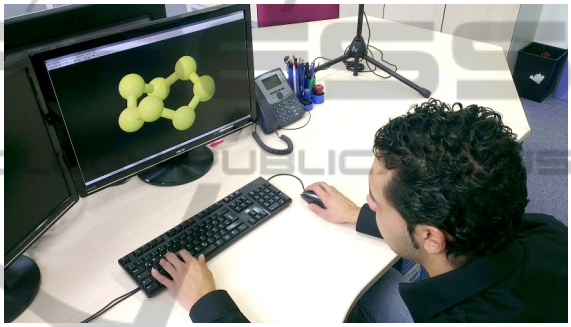
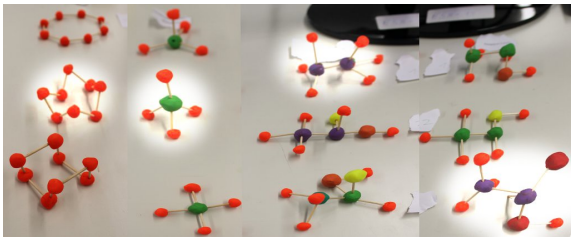
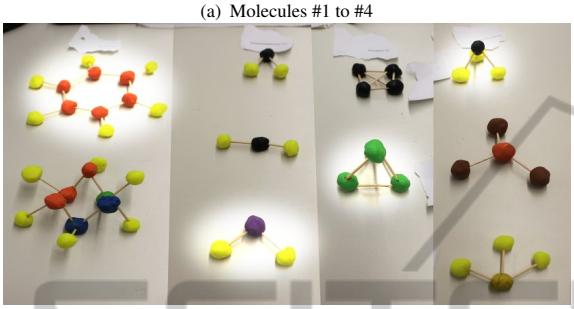


Figure 4: Typical setup to inspect and manipulate molecules on a monitor via keyboard and mouse in the *Jmol* application.

Computer Setup for *Jmol*. The second room was set up to run the *Jmol* application (Jmol, 2012), using a classical mouse and keyboard interface to manipulate virtual 3D molecular structures on the screen. To this end, a monitor, a mouse and a keyboard were placed on each student desk. When started, *Jmol* showed the first of the ten molecules, centered in the middle of the screen. By moving the mouse upwards or downwards, the molecule rotated around its horizontal axis. By moving the mouse leftwards or rightwards, the molecule rotated around its vertical axis. Schemes for translating and zooming molecules do exist in *Jmol*, but they were not required in the current setup. The students could view and explore the molecule from all sides before switching to the next



(a) Molecules #1 to #4



(b) Molecules #5 to #8

Figure 5: This is the set of versions of the first eight molecules. The correct versions are highlighted.

molecule by pressing a button in the application. Figure 4 shows the *Jmol* setup that uses the mouse and the keyboard to manipulate the position and orientation of the molecule.

Further Physical Setups for Further Student Tasks. In addition to the computer setup, the student desks carried papers and pencils and modeling clay with tooth picks. Furthermore, two to three clay models of each molecule were laid out on a table in a separate area in one of the rooms. Only one of these clay models of each molecule was correct. The other two were wrong with different degrees of spatial inappropriateness. Figure 5 shows the set of molecule versions for the first eight molecules. This is described further in task 5 of the next section.

3.2 Evaluation Design

We used a between-subjects design, consisting of two separate groups of students from the eighth grade of a secondary school. The first group, *Group ACR* consisted of 12 students, the second group, *Group Jmol* had 11 students. With the help of their teacher, the students were grouped to form a similar distribution of grades to ensure that both groups had the same knowledge.

The entire evaluation consisted of an introduction phase, five tasks including use of one of the two molecular visualization programs, and a brief subjective interview at the end.

Introduction Phase (5 minutes). At the beginning, all students were in the same room. They received

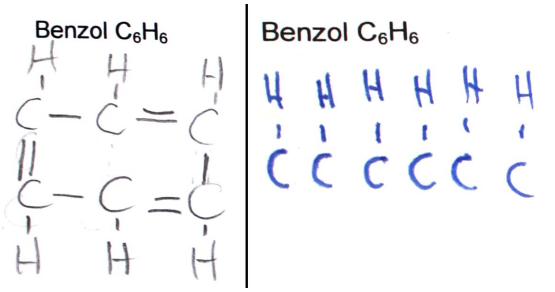


Figure 6: Example of a good and a bad drawing of the chemical formula of molecule #5 as LEWIS structure for Task 1.

an exercise sheet with printed-out molecular formulas of all ten molecules. The paper also contained a short introduction to the topic and explained what the students were asked to do in this evaluation. We additionally explained the topic and the following tasks to the students.

Potentially confounding factors.

- The students were asked to work by themselves and not to copy from fellow students (cheat), due to the negative consequences to the evaluation. Yet, the potential for such an influence on the evaluation cannot be completely discarded.
- Since this is a between-subject design, learning effects are not crucial. For didactic reasons, we use the same, well-defined sequence through the set of molecules rather than a randomized order. If learning effects occur, they affect both conditions in a similar way and can thus be clearly identified. Yet, the test design consists of a large number of sequentially executed tasks, each involving all eight molecules, and required carry-over experiences between the tasks. Thus, learning can be seen as an omnipresent aspect over time.

Task 1: Drawings of All 10 Molecular Structures (15 minutes). As their first task, the students were asked to draw the LEWIS structure (McNaught and Wilkinson, 1997) for all molecules of the exercise sheet next to the molecular formulas – a topic that had been covered in class during the week before the evaluation. They previously were taught by their teacher how to draw this kind of structures. This should give the students a basic understanding of the connections of the atoms in the molecule. Figure 6 shows an example of a good and a bad drawing.

After this first task the students were split into the two groups and went to their respective computer rooms.

Task 2: Uninformed Modeling of All 10 Spatial Molecular Structures (20 minutes). At their desks, students were asked to build models of the ten molecular formulas with clay and toothpicks, according to

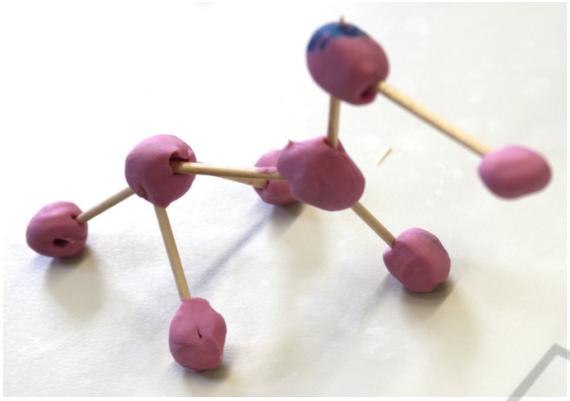


Figure 7: Model of acetic acid $C_2H_4O_2$ (molecule # 4), built by a student for Task 2. Students used modeling clay and toothpicks.

their current guess on what such a 3D structure could look like. They had not yet received any theoretical training on such 3D structures. We requested students to build these models in order to have reference data on the students' understanding of spatial molecular structures prior to using the computer-based chemical visualization applications. The students had 20 minutes to model up to 10 molecules with clay. We accepted that not everyone would complete this task. For the analysis, we therefore only took the finished models into account. Figure 7 shows a model of the fourth molecule, acetic acid ($C_2H_4O_2$), built by a student.

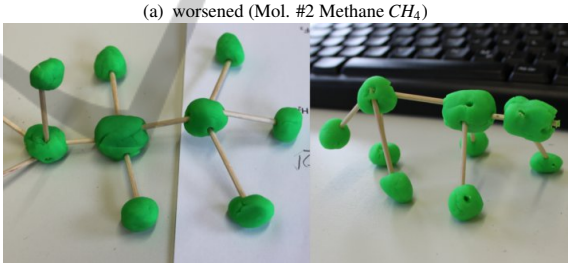
Task 3: Explore 3D Molecular Structures with the Respective Visualization Application (20 minutes). Each group was then asked to use their assigned visualization software to inspect all ten molecules. With *ACR*, the students sat in front of the display with the webcam above their shoulder and the marker cube in their hand. On the screen they saw the captured image plus their controlled virtual molecule rendered on top of the marker cube. The students could cycle through the set of molecules by pressing the space-bar on the keyboard. Figure 8 shows a part of the classroom with students working on the ACR version. With *Jmol*, the students used the mouse and the keyboard to rotate and move the molecules. To switch to the next molecule, they had to click a button in the software.

The students did not receive initial tutoring for either of the two software systems. Rather, they started immediately with the given molecular assignments. None were observed to have difficulties using the user interfaces.

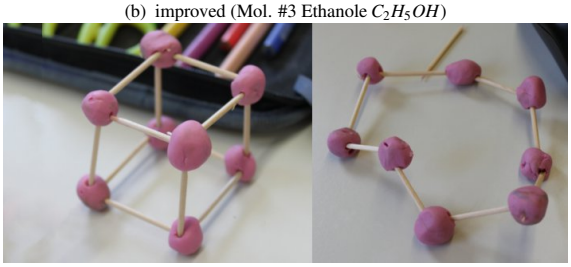
The students had 20 minutes to inspect all ten molecules. After this time, the applications were stopped. In the meantime we took photos of the molecules built for Task 2.

Figure 8: Classroom with students using the ACR for Task 3.

(a) worsened (Mol. #2 Methane CH_4)



(b) improved (Mol. #3 Ethanole C_2H_5OH)



(c) strongly improved (Mol. #1 Sulfur S_8)

Figure 9: Before-after state of a worsening 9(a), normal improvement 9(b) and a large improvement 9(c) (Task 4).

Task 4: Informed Modeling of All 10 Spatial Molecular Structures (10 minutes). With their new knowledge of the spatial structure of the molecules, the students were asked to improve the molecular models they had built in task 2.

To measure how the 3D understanding of the spatial structure of the molecules changed, we compared the initial version of the molecules with the new version. Figure 9 shows typical clay models before and

after using the software.

Task 5: Selection between Several Pre-built Clay Models of each Molecule. To also get an objective measurement of how both 3D user interfaces improved the spatial understanding, we confronted the students with 2-3 pre-built clay models of the first eight molecular structures (see Figure 5). For the first eight molecules, we had built one clay model version that was the correct solution, one that was completely wrong and a third one that was almost correct, but still noticeably different from the correct one. Here, we could evaluate to what extent the students had gained a spatial understanding of molecular structures. Figure 5 shows the alternative clay models for the first eight molecules.

Closing Phase: Informal Interview and Questionnaire. At the end of the evaluation we had a short joint informal interview in front of the whole class. We also handed out a questionnaire to learn a bit about the students' prior knowledge. We asked the students what they liked and what they did not like. The students stated that they liked the idea of learning the molecule structure using a computer application. Especially the group using *ACR* told that they had a lot of fun using the user interface. Where the group with *Jmol* liked the general idea of using an application to show the 3D structure, the *ACR* users were fascinated about the user interface with the marker cube. All stated that they would like to continue using the application in their class to further learn about the geometry of molecules.

4 RESULTS

The evaluation consisted of two parts – the building and the improvement of the clay molecules and the selection of the right version. Table 5 at the end presents the raw absolute scores of all tasks. Empty cells denote that the students did not model the specific molecule or did not select any version in the last task.

The subsequent sections give the results, discuss these scores and suggest interpretations.

4.1 Improvements to Students' Clay Models

To measure how the AR-based and the mouse-based user interfaces of *ACR* and *Jmol* affected the spatial understanding of the virtual molecules, we compared the models built in Task 2 with the models changed in Task 4.

With the help of the chemistry teacher, we scored the molecules (Table 5). Table 1 presents the interpretation of the students' improvements from Task 2 to Task 4 – due to the use of the chemical education applications (*Jmol*, *ACR*). When the second version (Task 4) of the models was worse than the first version (Task 2), we scored this with -1 point. No improvement of the molecule was scored as 0 points, and an improvement was scored as $+1$ point. When the first version was totally wrong and the second was completely correct, we scored $+2$ points. When students already provided a perfectly correct solution in the first version (Task 2) and they did not change anything on the molecule in Task 4, we did not count it – as this does not deliver insight regarding the usefulness of the software system (user interface). The scores are presented in Table 1. A Kruskal-Wallis test shows that there is a significant difference in the medians $\chi^2(3, N = 45) = 32.34, p < 0.0001$ at a significance level of 5%. The results show that the direct manipulation 3D user interface of the *ACR* application helped the students significantly better than the

Table 1: Scores representing students' improvements between uninformed modeling of the molecules in Task 2 and informed modeling in Task 4, i.e., after having visualized the molecules with *Augmented Chemical Reactions (ACR)* or *Jmol* int Task 3.

Group 1 (ACR)								
User \ Mol	1	2	3	4	5	6	7	8
1	-1		1					
2		2	1			2		
3	1		1	0	0			
4	1	1	2	0	0			
5		1	1	0				
6	1	1				0		
7	1	1	1					
8	0	2	1					
9	1	0	0	1	2	0	0	0
10	1	0	0	1		0	2	0
11	2			1			2	
12	0	0	0	0			2	

Group 2 (Jmol)								
User \ Mol	1	2	3	4	5	6	7	8
1	2	2		0		1	0	
2	0	0				0	0	
3	0	0				0	0	
4	1	-1	1					0
5	1	-1	0					
6	2		0	0			0	
7	0				1	1	-1	2
8	1		0	0			1	
9	1		0	0			2	
10	1		0	0			2	
11	1	1	0				1	

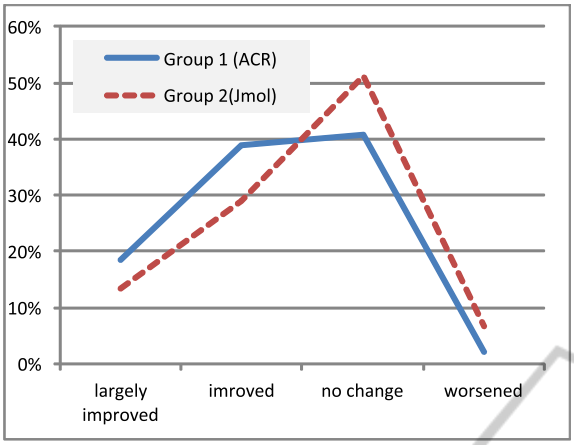


Figure 10: Percentages of the quality of the changes that students made to improve their clay models in Task 4. The height of the graph represents the percentage of the molecules which were *strongly improved*, *improved*, *no change* or *worsened*.

keyboard and mouse 3D User-Interface of *Jmol*.

Table 2 and the corresponding graph in Figure 10 show how many percent of the molecules were *strongly improved*, *improved*, *unchanged* or *worsened* by students using the *Jmol* the *ACR* program, respectively. The numbers enhance the statistical finding that Group 1 (*ACR*) using the direct manipulation 3D user interface had a significantly better improvement than Group 2 (*Jmol*) using mouse and keyboard. Both the percentages for large improvements and for normal improvements are higher for *ACR* than for *Jmol*, whereas the percentages of no change and of worsening changes are smaller. A deeper analysis of the results shows that students of group 1 (*ACR*) who were wrong in Task 2 improved more in task 4 than students of group 2 (*Jmol*). This also shows that *ACR* with the direct manipulation user interface helps more to understand the spacial structures than using an indirect manipulation user interface with mouse and keyboard (*Jmol*).

Table 2: Percentages of the quality the changes that students made to improve their clay models in Task 4.

	ACR	Jmol
Strongly improved	18%	13%
Improved	39%	29%
No change	41%	51%
Worsened	2%	7%

4.2 Students' Ability to Pick the Correct Clay Model out of a given Set of Three per Molecule

Since students' dexterous abilities may vary and the quality of some of the students' clay models may thus have depended on that, we designed Task 5 as a test that was independent of the students' own modeling skills and time limitations. We had prepared three clay model versions of the first eight molecules, with one being correct, one being slightly wrong and one being completely wrong. The students were asked to indicate for each molecule which one they considered to be the correct model. They received 2 points for the correct answer, 1 point for the nearly correct answer, and 0 points when they selected the completely wrong clay model. Although we asked the students not to copy from the others, we cannot guarantee that they did not. Table 3 summarizes the score of table 5, pertaining to Task 5.

Table 3: Scores of students' selections of three clay model versions of each molecule in Task 5.

Group 1 (ACR)								
User \ Mol	1	2	3	4	5	6	7	8
1	2	2	2	2	2	2	2	2
2	2	2	1	1	2	2	2	2
3	1	2	2	0	2	2	2	1
4	1	2	2	2	0	1	2	2
5	1	1	1	1	0	0	2	2
6	1	0	2	2	2	0	2	1
7	2	0	2	2	2	1	2	2
8	2	2	2	2	2	2	2	2
9	2	0	2	1	2	2	2	2
10	1	2	2	1	2	2	2	1
11	2	2	1	2	2	2	2	2
12	2	2	2	2	2	2	2	2

Group 2 (Jmol)								
User \ Mol	1	2	3	4	5	6	7	8
1	2	2	2	1	2	1	2	2
2	2	2	2	1	0	2	2	2
3	2	2	1	2	2	0	2	1
4	2	1	0	2	0	1	2	2
5	2	2	2	2	0	2	2	2
6	1	2	2	2	2	2	2	2
7	2	2	0	1	2	2	2	2
8	2	2	1	1	0	0	2	0
9	2	2	1	1	0	1	2	2
10	2	2	1	1	0	1	2	2
11	2	2	0	1	0	1	2	2

We calculated the average points that students achieved for each molecule. They are shown in Table 4 and in Figure 11. Interestingly, molecule #1 and #2 had a better result with the user interface of *Jmol*. The variance of these results of the group *Jmol* is unusual small in relation to the other molecules. This leads to the assumption that there was some-

Table 5: Scores of all task assignments, T1, T2, T4 and T5.

Group1(ACR)

User	Mol.1				Mol.2				Mol.3				Mol.4				Mol.5				Mol.6				Mol.7				Mol.8			
	T1	T2	T4	T5	T1	T2	T4	T5	T1	T2	T4	T5	T1	T2	T4	T5	T1	T2	T4	T5	T1	T2	T4	T5	T1	T2	T4	T5	T1	T2	T4	T5
1	1	2	0	2	2			2	2	1	2	2	0			2	0			2	1			2				2	0			2
2	2	3	3	2	2	1	3	2	2	1	2	1	0			1	2			2	1	0	3	2	1			2	2			2
3	1	0	2	1	2	3	3	2	2	1	2	2	0	1	1	0	1	0	0	2	1	3	3	2	1			2	3			1
4	2	0	2	1	2	2	3	2	0	1	3	2	0	2	2	2	2	1	1	0	1			1	0			2	2			2
5	2			1	2	1	2	1	0	0	1	1	0	0	0	1	1			0	1			0	0			2	2			2
6	1	0	2	1	2	0	1	0	1			2				2				2	1	0	0	0	0			2				1
7	2	0	2	2	2	1	2	0	0	1	2	2	0			2	1			2	1			1	1			2	2			2
8	1	2	2	2	2	1	3	2	0	1	2	2	0			2	0			2	1			2	1			2	2			2
9	1	1	2	2	2	1	1	0	0	1	1	2	0	0	1	1		0	3	2	1	0	0	2	1	0	0	2	2	0	0	2
10	1	0	2	1	2	0	0	2	2	1	1	2	1	0	1	1	2	3	3	2	1	0	0	2	1	0	3	2	2	1	1	1
11	1	0	3	2	2	3	3	2	2			1	2	2	3	2	1			2	2	3	3	2	1	0	3	2	2			2
12	1	0	0	2	2	0	0	2	2	0	0	2	2	0	0	2	1			2	1			2	1	0	3	2	2			2

Group2(Jmol)

User	Mol.1				Mol.2				Mol.3				Mol.4				Mol.5				Mol.6				Mol.7				Mol.8			
	T1	T2	T4	T5	T1	T2	T4	T5	T1	T2	T4	T5	T1	T2	T4	T5	T1	T2	T4	T5	T1	T2	T4	T5	T1	T2	T4	T5	T1	T2	T4	T5
1	1	1	3	2	2	1	3	2	2			2	0	0	0	1	0			2	1	0	1	1	1	0	0	2	2	3	3	2
2	1	1	1	2	2	1	1	2	2			2	0			1				0	1	0	0	2	1	1	1	2	2			2
3	1	1	1	2	2	1	1	2	2			1	0			2	0			2	1	0	0	0	1	1	1	2	2			1
4	2	0	2	2	2	3	1	1	0	1	2	0	0			2				0	1	3	3	1	0			2	2	1	1	2
5	0	0	2	2	2	2	0	2	0	1	1	2	0			2	0			0	1	3	3	2	0			2	2			2
6	1	0	3	1	2	3	3	2	2	2	2	2	2	2	2	2	2			2	1	3	3	2	1	2	2	2	2			2
7	2	0	0	2	2	3	3	2	2			0	2			1	0	2	3	2	1	1	2	2	1	1	0	2	2	1	3	2
8	1	0	2	2	2	3	3	2	2	1	1	1	2	1	1	1	2			0	1			0	1	1	2	2	2			0
9	1	0	2	2	2	3	3	2	2	1	1	1	2	1	1	1	2			0	1	3	3	1	1	0	3	2	2			2
10	1	0	2	2	2	3	3	2	2	1	1	1	2	1	1	1	2			0	1	3	3	1	1	0	3	2	2			2
11	1	0	2	2	2	2	3	2	2	2	2	0	1			1	2			0	1	3	3	1	1	1	2	2	2	1	1	2

Table 4: Average number of points students achieved for each molecule in Task 5.

	ACR	Jmol
1	1.58	1.91
2	1.42	1.91
3	1.75	1.09
4	1.50	1.36
5	1.67	0.73
6	1.50	1.18
7	2.00	2.00
8	1.75	1.73

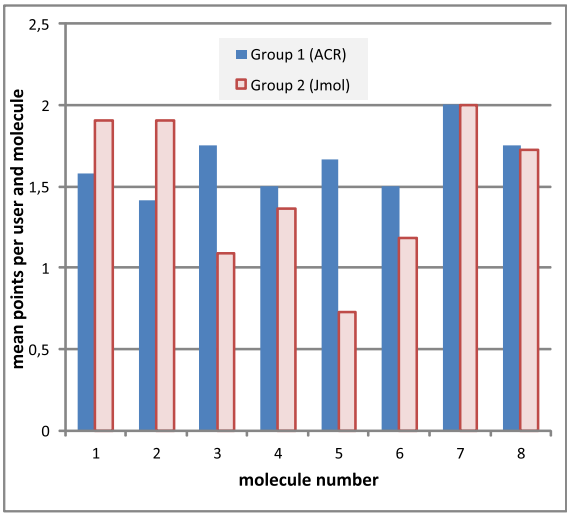


Figure 11: This diagram shows the mean points users had for each molecule with Task 5 (Selecting the right version of the molecules).

thing unintended going on (copying from others). Molecule #1 with its crown-like structure can be seen in Figure 11. Molecule #2 has a simple tetrahedron structure with the carbon atom in the middle. For molecules #3, #4, #5, and #6, group *ACR* was better than group *Jmol*, while molecules #7 and #8 faired approximately even in both groups. The large difference in the results of Molecule #5 could be explained in the following way: Students using the *Jmol* application could not remember the flat structure of the molecule anymore, so they probably took the more complex looking structure, whereas the students with the *ACR* could have remembered the flat structure. Molecule #7 and #8 were so easy that nearly everyone has picked the right version.

On average across all molecules, students of group *ACR* achieved 13.17 points, compared to 11.91 of group *Jmol*.

5 DISCUSSION AND CONCLUSIONS

Although the time for using the software was not very long, there is already a significant difference in the improvement of the spatial understanding of the 3D molecules. We think that by using a direct manipulation 3D user interface, students can literally grasp the spatial structure. Whereas with mouse and keyboard, there is a mapping of the movements (2D horizontal movement of the mouse on the table results in a rotation of the virtual molecule on the screen). With this mapping, it seems to be not so easy to concentrate on the spatial structure of the virtual molecules. People are used to direct manipulation from their childhood.

Consequently this user interface is more natural and supports the learning of the spatial structures.

All students also mentioned that they had fun using the application and would like to use it more often in class. Fun is also one of the most important enablers in learning.

Our evaluation showed that this assumption seems to be valid. Further investigations with a longer period of the study could investigate this finding in more detail.

ACKNOWLEDGEMENTS

We would like to thank the Josef-Hofmiller-Gymnasium for their kind support. Special thanks go to Nina Hefter and Andreas Dippon who helped a lot in this study.

REFERENCES

Arnold, O., Fujima, J., Jantke, K. P., and Tanaka, Y. (2012). Exploring and understanding the abstract by direct manipulation of the concrete. In *CSEDU (2)*, pages 100–107.

Chen, M., Mountford, S., and Sellen, A. (1988). A study in interactive 3-d rotation using 2-d control devices. In *ACM SIGGRAPH Computer Graphics*, volume 22, pages 121–129. ACM.

Fjeld, M., Fredriksson, J., Ejdestig, M., Duca, F., Bötschi, K., Voegtli, B., and Juchli, P. (2007). Tangible user interface for chemistry education: comparative evaluation and re-design. In *Proceedings of the SIGCHI conference on Human factors in computing systems*, pages 805–808. ACM.

Herman, T., Morris, J., Colton, S., Batiza, A., Patrick, M., Franzen, M., and Goodsell, D. (2006). Tactile teaching: Exploring protein structure/function using physical models*. *Biochemistry and Molecular Biology Education*, 34(4):247–254.

Hinckley, K., Tullio, J., Pausch, R., Proffitt, D., and Kassell, N. (1997). Usability analysis of 3d rotation techniques. In *Proceedings of the 10th annual ACM symposium on User interface software and technology*, pages 1–10. ACM.

Hoyek, N. E., Collet, C., Guillot, A., Thiriet, P., and Sylvestre, E. (2011). Experimental research validation for the use of 3d in teaching human anatomy. In Verbraeck, A., Helfert, M., Cordeiro, J., and Shishkov, B., editors, *CSEDU (2)*, pages 225–227. SciTePress.

Jmol (2012). Jmol: an open-source Java viewer for chemical structures in 3D. http://www.jmol.org/.

Johnson, E. M., Khoo, E., Cowie, B., de Lange, W., and Torrens, R. (2011). Ict/ elearning for developing visual spatial thinking in university science teaching. In *CSEDU (2)'11*, pages 73–78.

Kato, H. and Billinghurst, M. (1998). Marker tracking and hmd calibration for a video-based augmented reality conferencing system. In *2nd IEEE and ACM International Workshop on Augmented Reality (IWAR 99)*, pages 85–94.

Maier, P., Tönnis, M., and Klinker, G. (2009a). Augmented Reality for teaching spatial relations. In *CD-ROM Proceedings from the Conference of the International Journal of Arts and Sciences*. ISSN: 1943-6114.

Maier, P., Tönnis, M., and Klinker, G. (2009b). Dynamics in Tangible Chemical Reactions. In *Proceedings from the International Conference on Chemical Engineering (ICCE 2009)*. ISSN: 2070-3724.

McNaught, A. and Wilkinson, A. (1997). *Compendium of chemical terminology*, volume 1669, chapter Lewis formula (electron dot or Lewis structure), page 1135. Blackwell Science Oxford, UK.

Panagiotopoulos, C. G., Manolis, G. D., and Athanatopoulou, A. (2012). Edusoft package for structural engineering - web-based educational material using java for structural dynamics. In Helfert, M., Martins, M. J., and Cordeiro, J., editors, *CSEDU (2)*, pages 299–303. SciTePress.

Pustka, D., Huber, M., Waechter, C., Echtler, F., Keitler, P., Newman, J., Schmalstieg, D., and Klinker, G. (2011). Automatic configuration of pervasive sensor networks for augmented reality. *IEEE Pervasive Computing*, 10(3):68–79.

Zhai, S. (1998). User performance in relation to 3d input device design. *ACM Siggraph Computer Graphics*, 32(4):50–54.