

Chemistry Education: A Tangible Interaction Approach

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Abstract: This system paper reports on some of the advantages tangible interaction can bring to chemistry education. The paper describes how we realized a Tangible User Interface (TUI) called Augmented Chemistry (AC), gives details on basic and specialized interactive tools working in this system, and outlines the educational context. Using the basic tools, elements can be chosen from a booklet menu and composed into three-dimensional (3D) molecular models. The system with its tools shows a way to design for seamless integration of the physical and digital realms. Multiple tools can be used concurrently, thereby calling for users' two-handed skills. To teach an aspect of molecular chemistry – the octet rule – we extended the system into an educational workbench drawing on haptic and aural augmentation. The system design required contributions from optics, mathematics, molecular chemistry, software engineering, and 3D programming. Future challenges of this project lie in further system development and educational usability.

Keywords: augmented reality, educational application, chemistry, tangible user interface

Introduction

This system paper shows some of the advantages tangible interaction can bring to chemistry education. Taking an Augmented Reality (AR) approach, an interactive application for handling of three-dimensional (3D) molecular models is presented. We point out the design challenges met and suggest solutions based on haptic and aural augmentation. In particular, we explore the potential and limitations in the use of Tangible User Interfaces (TUIs) for chemistry education. The remainder of this introductory section presents the characteristics of 3D interaction in AR workbenches, shows alternative molecular models, and points out background and related research. The body section of this paper presents the mirror metaphor, interaction form, system setup, basic interactive tools, and specialized interactive tools. This is followed by a section about the instructional content, such as the octet rule, composite models, aural augmentation, and graphical representation. The final section presents a summary of our design practice, including issues of usability and future directions of research.

1.1 3D Interaction in AR Workbenches

While some TUIs offer planar interaction, such as *Tangible Bricks* (Fitzmaurice et al., 1995) and *MetaDesk* (Ullmer and Ishii, 1997), other systems offer 3D interaction, such as *Cubes* (Colella et al., 1998; Goslin, 2001). Wireless tracking of interaction handles may be either optical (Colella et al., 1998; Fitzmaurice et al., 1995; Fjeld et al., 2000; Goslin, 2001) or electromagnetic (Patten et al., 2001). Here, we report on a TUI performing 3D optical tracking of an interaction cube. Such systems can improve 3D interfaces. That is, they mimic more closely the use of “actual” physical artifacts and tools. This interface offers users a more natural use of hand and body movements. Such movements may hence be integrated into the interaction with digital information, thereby supporting a fluent handling of 3D models (Fjeld et al., 2000).

In the *drag-and-drop* operation of the Graphical User Interface (GUI), files are selected and placed into their new folder. In a TUI, which is our interaction form, digital information is represented and manipulated using physical handles. When using a TUI to interact with 3D models, these models can be literally grasped and inspected from all sides, thereby going beyond the *drag-and-drop*

principle. This extension of the classical user interface may be of particular benefit to 3D molecular models, but also to 3D models of furniture, robots, and vehicles.

1.2 Alternative Molecular Models

Schematic and computer-based molecular models used in chemistry are mostly synthetic and highly abstract (Fig. 1). They may represent a physical idea or a mathematical formula.

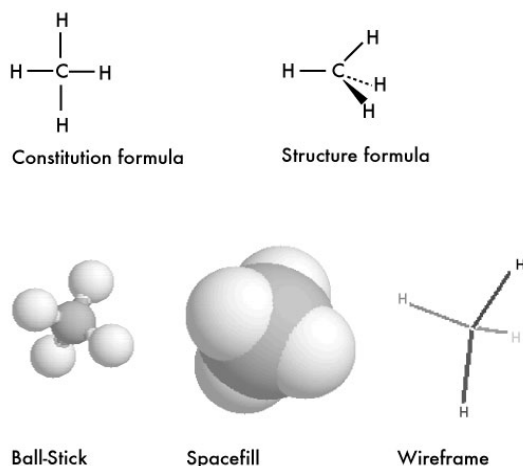


Figure 1: Alternative molecular models.

Such models represent concepts, helping us to understand the underlying structures and dynamics of organic and inorganic chemistry. Each kind of model is meant to show a different aspect of chemistry and must be chosen depending on the educational purpose. There is hardly one single kind of model which is best suited to chemistry education. Rather, different kinds must be blended in a way serving educational levels and needs. For reasons of coding, graphics, and educational scope, we employed the *ball-stick* model. However, a specialized tool selecting wireframe viewing mode will be presented later.

1.3 Background and Related Research

A novel educational technology is offered by *learning-objects* (Laleuf, 2001). Learning-objects are reusable components that can be combined in different ways to produce new courseware. Their use promises *reusability*, *component categorization*, and *high levels of interactivity*. Learning objects can be virtual as well as physical models – here we study the integration of both to achieve higher levels of interactivity. In suggesting “visuals to help make abstract chemistry more tangible” (Petrucci et al., 2001), the use of TUIs in education has been put on

the research agenda. This trend has recently been studied and confirmed by Shelton (2002).

One project applying Augmented Reality (AR) technologies for educational purposes is *Construct3D*, a 3D geometric construction tool based on the collaborative *Studierstube* (Kaufmann et al., 2000). 3D model interaction in this tool is reached by combining Head Mounted Displays (HMD) with a Personal Interaction Panel (PIP) – a bimanual 3D interactive tool. Three further realizations suggest alternative ways to make education more tangible by employing highly interactive AR technologies: *Participatory Simulations* (Colella et al., 1998), *Interactive Textbooks* (Koike et al., 2000), and *MagicBook* (Billinghurst et al., 2001). Combination of fiducial markers and chemistry models was studied by Rekimoto (1998).

2 System Description and Use

Next, we show how we based our concept on the mirror metaphor. Constructivist toys, such as Legos, inspired our conception of tangible interaction. The interaction form we offer comes out of the AR Toolkit (Billinghurst et al., 2001; Kato et al., 2000). These components – mirror metaphor, constructivist toys, and AR Toolkit – were all stepping-stones towards our current system. In the context of this system, we report on the design and use of four basic interactive tools: *booklet*, *gripper*, *platform*, and *cube*. We also offer a set of four specialized tools: *browser*, *template*, *template*, and *tag-toggle*. Based on these tools working within our system, we offer an educational workbench serving to teach the octet rule. To enhance the interactive steps in constructing composite molecular models according to the octet rule, we use *aural augmentation*. This section concludes with some descriptions on the 3D graphical models used.

2.1 From the Window to the Mirror Metaphor

When users interact with 3D virtual models, it is advantageous that this interaction is perceived as *direct* (Hutchins et al., 1986). How direct manipulation can be reached in a conventional keyboard-screen-mouse based interface by using metaphors has been examined (Ullmer and Ishii, 1997). Such metaphors even gave inspiration to early TUIs, for instance in the *MetaDesk* (Ullmer and Ishii, 1997).

When working with 3D virtual environments, users are cognitively challenged in understanding and knowing how their actions affect models (Ware

and Rose, 1999). This observation holds true for model positioning, model rotation, and for navigation of the scene (Fjeld et al., 2000). Such insights led to the design of freely movable Web pads and tablets, both drawing on the metaphor of a window with a *virtual camera* sitting on the *backside* of the screen and approximately pointing along the user's line of sight.

Related to the window metaphor, is the alternative mirror metaphor. A *physical camera* records what is taking place *in front* of the screen and projects this onto the screen. This gives users an impression of a mirror. The mirrored image of the physical world is then augmented with the virtual environment. In particular, the interaction handles are augmented with the models of the virtual environment. On the one hand, such an interface may offer a seamless integration to the physical and digital realms. On the other hand – how novel users perceive the *directness* of such interfaces – may be an issue.

The *Virtual Workbench* (Poston and Serra, 1994) (now: *Dextroscope*) also employs a mirror, but in another way. In this system, there is a physical mirror between the screen and the user's hand. Hence, 3D virtual images appear co-located with the user's hand. The focus of *Dextroscope* is on 3D patient-specific medical data manipulation that is enhanced by the use of sound. A related system, called *Reachin*, focuses on the benefit of using haptic feedback (*Reachin*, 1999).

2.2 Interactive Form

Based on a tangible user interface (TUI), we designed the application Augmented Chemistry (AC). AC is a workbench offering its users the opportunity to use and interact with virtual 3D molecular models in a direct way. The system also offers tools to build composite molecular models. One of our inspirations for this system came from the observation of children playing Legos. In a similar way, users of AC can interact using physical handles to build composite 3D models. Pursuing this analogy, atomic and molecular models – like Legos – inherently offer a wide range of combinations. Several users can use the interactive tools at a time. Thereby, the AC application works for single and for multiple users.

Following the conventional implementation of AR Toolkit, a cube with fiducial marker patterns is connected to an animated 3D model and both are seen in the mirror image. Using a specialized select and rotate tool, single atoms can be picked up, positioned, and composed into complete molecules.

Chemical rules can be formulated and integrated into the application; enabling the construction of basic structures as they appear in nature.

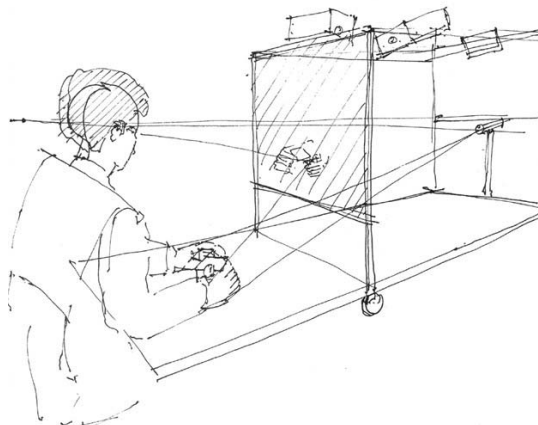


Figure 2: This is an early sketch of the system. In the realization (Fig. 3) we used a camera with a different field of view, hence positioned closer to the user

2.3 System Setup

Augmented Chemistry (AC) is a workbench consisting of a table and a rear-projection screen (Fig. 2). Below the screen is a camera that relays all of the action taking place upon and above the tabletop to the display. This is designed to give the user the feeling of looking into a mirror. This mirror image is then enriched with a virtual environment. Users interact with models in this virtual environment using the booklet, gripper, platform, and cube. Each page in the booklet is used to identify an element of the periodic table. The booklet, the platform, and the gripper each carry a fiducial marker; the cube carries six markers – one per side. A 3D model augments the mirror image of a booklet page, a platform, a cube side, or the gripper. Hence, users can select, position, rotate, compose, and deselect 3D models, thereby affecting the virtual environment.

In the realization of the system (Figs. 3, 13), the screen is based on acrylic glass from Lumin™. It is particularly well suited for rear-projection and also works well under daylight condition. We use a standard projector offering 1000 Ansi Lumens. The screen and the projector sit about 2.5 meters apart. Our camera is a 1/3" CCD color board offering 3 Lux light sensitivity, 450 TV lines, NTSC and S-Video output. We use the S-video output. The computer has a 1.2 GHz Pentium 4, 128 MB RAM, an Nvidia GeForce 3 graphics card, and a Hauppauge WintTV frame grabber. Virtual models are OpenGL, well suited for our Linux operating

system. We chose not to pay particular attention to performance issues such as speed and memory. Due to NTSC camera output rate, frames per second (fps) are around 29. A brief video documentation of the AC system is available (Fjeld et al., 2002).



Figure 3: System realization: User charging the gripper with an element from the booklet (left). The platform (right) holds an unsaturated atom, with in close proximity may trigger a binding with the charged atom.

2.4 Basic Interactive Tools

Bringing together two elements triggers the composition of a molecular model. This operation requires the use of both hands, called bimanual interaction (Balakrishnan and Kurtenbach, 1999). The booklet shows elements by a printed picture and a name. One hand browses the booklet, offering one element per page (Fig. 4). Using the gripper (Fig. 5), users can pick up elements from the booklet. The term gripper stems from robotics and implies a tool with jaws. Instead of employing jaws, our gripper has a button used to bind an atom to the molecular model. First, bringing the gripper into a small perimeter around the element in the booklet charges the gripper with that element. Second, the gripper is positioned next to the platform (Fig. 6). The platform holds a molecule. With the rotation of the cube (Fig. 7), operated by the second hand, users can determine *where* and *how* the element shall connect to the molecule (Fig. 8).



Figure 4: Booklet offering one element per page – here Na – sodium. Each element is represented by a marker.



Figure 5: Gripper with button (red) and a distinct marker.

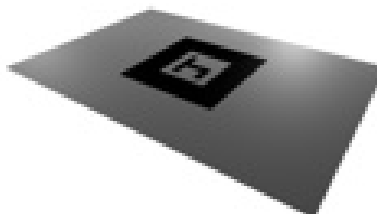


Figure 6: Platform with a distinct marker.



Figure 7: Cube with a distinct marker for each surface.

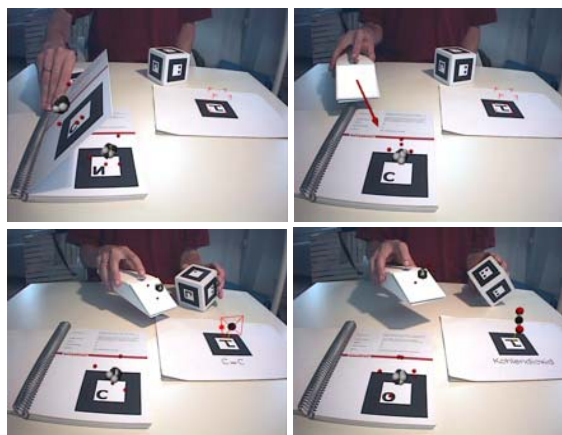


Figure 8: Open booklet with a nitrogen-atom and an animated 3D Bohr-model (core and valence electrons) on top of it (lower left). The platform, or construction space, shows an unfinished molecular model with a wireframe tetrahedron around the selected atom (lower right). A red dot appears where the next bond can be made. Below the molecular model the binding atoms are shown (C-N) before the user confirms by clicking the gripper button.

2.5 Specialized Interactive Tools

During the realization process, we saw a need for several specialized tools. For example, there was a need to provide users with a *browser* to quickly look up all predefined molecules and listen aural information. Further, we saw a need for a *tag-toggle* to switch from viewing atoms as colored to viewing them by their names – thereby switching to a wireframe representation (Fig. 9). These and two further functions were implemented using dedicated symbolic marker cards (Fig. 10). These cards become active when drawn onto the platform and each triggers one of the four tools:

- Browser, enabling users to view all the predefined molecules sequentially by clicking the gripper button.
- Tag-toggle, activating an alternative viewing mode where atoms can be viewed by names.
- Cleaner, emptying the platform, hence enabling users to construct a new molecule.
- Template(s), activating the construction of new molecules predefined ring-structures. For instance, a benzene ring is shown here (Figs. 9-10), consisting of 6 C-atoms.

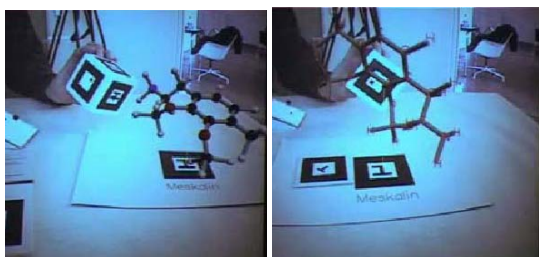


Figure 9: First, a benzene ring was selected using the benzene template. This benzene ring was then expanded into a Mescaline molecule by adding H atoms and can be viewed either as colored spheres (left) or – using the tag-toggle tool – as the names of the atoms (right).

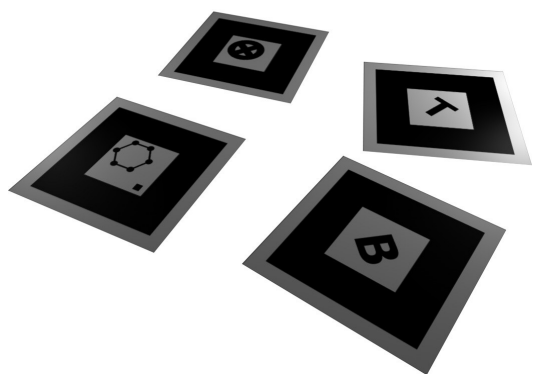


Figure 10: Specialized tools: browser (front), tag-toggle (right), cleaner (behind), and benzene ring template (left).

3 Instructional Content

As for the instructional content, we take a more detailed look at the octet rule and composite models. We also explain how we employ aural augmentation as part of the educational concept. Finally, we comment on the representation mode chosen, which corresponds to the molecular model of Bohr.

3.1 Octet Rule

A major didactical aim of Augmented Chemistry (AC) is to teach the *octet rule*. This rule comes from the realization that since atoms aim to have noble gas structure and all noble gases have eight electrons in their valence shell, atoms should have eight electrons around them. They achieve this state through bindings with other atoms. The atoms that commonly follow the octet rule are: C – Carbon, N – Nitrogen, O – Oxygen, and the halogens F, Cl, Br, and I. Each of these atoms will eventually have eight electrons around it in a molecular configuration. For the atoms in the second period, the rule is always fulfilled. The octet rule can only be partly applied to elements of the third and higher periods.

Period	1	2	3	4
Valence 1	H (hydrogen)			
Valence 2	Li (lithium), F (fluorine)	O (oxygen)	N (nitrogen)	C (carbon)
Valence 3	Na (sodium), Cl (chlorine)			
Valence 4	K (potassium), Br (bromine)			

Figure 11: Some elements from the first few periods and their valence.

In AC, we focus on the atoms given in the second, third, and some of the fourth period (Fig. 11). Each of these atoms has four pairs of electrons in their valence shell. The valence of an atom indicates how many of these four pairs are free. For each free electron pair, an atom can connect to another atom. Since the two electrons in a binding search for a maximum of distance, each of the atoms can be seen as a tetrahedron (Fig. 12). Atoms with valence two or higher (e.g. O, N and C), can connect with two or three free pairs of electrons. These are called double- and triple-binding. When the distance between the two electrons in binding is small, the binding is strong.

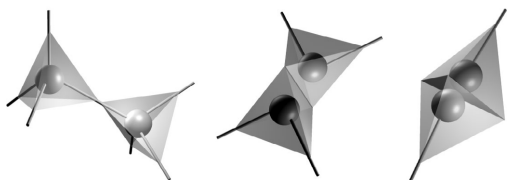


Figure 12: Different bindings between two atoms, here single-, double- and triple-bindings (left to right).

In typical use of AC (Figs. 10-12), an atom is added to an existing molecule. The atom is selected from the booklet using the gripper. A cube holds the molecule. The atom can connect to the molecule in three different ways: by single-, double- and triple-binding (Fig. 12). When the atom approaches the molecule, virtual auxiliary lines representing a tetrahedron are shown at the molecule on the display. These lines appear at the atom inside the molecule with the shortest distance to the approaching atom, enabling the user to choose *place* (which atom inside the molecule) and *kind* (single, double or triple) of the next binding. The two connect as soon as the user clicks the button on the gripper (Figure 4). Additionally, the name of the involved elements and the corresponding bond appears right below the molecule model on the workbench. The size of the tetrahedron is large enough to cover the underlying atom/sphere. Depending on the rotation of the molecule, a corner (single-binding), an edge (double-binding), or the whole side (triple-binding) appears as highlighted with a red dot. In the case of double- and triple-bindings, the atoms always connect in the middle of the corners. The ratio of distance between the corners to the binding atoms determines the kind of binding (Fig. 11). In the case of an atom approaching a molecule with the closest atom of valence three, there are seven distinct ways for a new atom to connect to the molecule: with one of the three corners, with one of the three edges, or with the whole side. In this case, the user may rotate the molecular model until the preferred binding is indicated. To activate the selected binding, the button of the gripper is pushed.

3.2 Composite Models and Aural Augmentation

Using the atoms and bindings described so far, numerous molecules can be constructed. In the current realization of Augmented Chemistry (AC), we focused on some of these molecules only – typically stemming from household products, environmental agents, poisons, and explosives. Investigating the use of these molecules, we set out to offer an audio feedback cue suited to each

constructed molecule. Such feedback can be considered as *aural augmentation* of the molecular models.

During the constructions of a molecule, different states trigger visual and audio events:

- When a molecule reaches a saturated level (state), i.e. no more bindings can take place, an acoustic signal is triggered (event). This tells the user that she can move on to construct the next molecule.
- When a molecule belongs to the predefined list (state) the user is offered additional spoken information about the molecule (e.g. „water covers 75% of the surface of the earth ...”) (event) (Fig. 12). Additionally, there is a separately designed sound used to identify one of the above-mentioned categories (household, environment, poisons, explosives).

In pursuing the issue of composite models, we have met perceptual and technical challenges. One challenge stems from so-called *isomerism*, describing molecules of *same sum formula* but of different constitution (i.e. bindings / connections). Stereoisomers are molecules of the same constitution but different geometries (diastereomers) or topographies (enantiomers). AC cannot distinguish stereoisomers. With the educational scope of our application, it is of crucial importance to keep track of a user's actions and to identify the resulting molecule to provide her with appropriate information. We do not know of any general way to compare such complex structures. However, we have found a feasible solution to identify *constitutional isomers*.

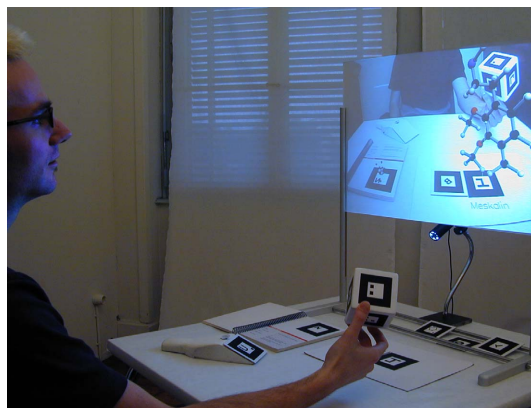


Figure 13: Viewing a predefined (saturated) molecule in the browser mode while using the cube to rotate the model.

3.3 Graphical Representation

To represent molecular models graphically, Augmented Chemistry (AC) employs a well-known principle, namely the *ball-stick* model. In the booklet, working as an interactive menu, the valence electrons of an atom can be seen. Visualizing the number of electrons in the valence shell shows the valence. On the one hand, the visual representation of atoms is different from that of the molecules. On the other hand, atoms are not only shown as colored balls. Rather, they are visualized with a clearly visible nucleus and the outermost valence shell. This representation of atoms is in accordance with the model of Bohr. Wireframe representation can be achieved using the tag-toggle (Figs. 8-9).

4 Discussion and Outlook

We have shown some of the advantages tangible interaction can bring to chemistry education. This was done through the realization of a Tangible User Interface (TUI) where 3D molecular models can be easily handled and composed using basic and specialized interactive tools. The design and implementation of this system required contributions from optics, mathematics, molecular chemistry, software engineering, and 3D programming, making it a truly interdisciplinary project.

The source code of Augmented Chemistry (AR) will be made – as far as possible – platform independent. The code will then be published in the Internet, together with further documentation.

Later on, we are planning to extend the functionality of AR. In particular, we aim for a more exact molecular-mechanical model (MM).

The mirror image presented to the user sometimes caused a perceptual problem. Some users reported that they needed a time to become acquainted with mirrored image of both the interaction and the virtual environment.

We have not paid particular attention to the use of the dominant and non-dominant hand. Normally, a tool will be held by the dominant hand (mostly right), whereas a work-piece will be held by the non-dominant hand (mostly left). In our case, the gripper may be viewed as the *tool* and the cube the *work-piece*. For our future research an issue to consider will be to investigate the design of the system for effective two-handed interaction.

Aural augmentation has proved to be an important factor. It may serve as an ambient media (Wisneski et al., 1998) (typically a background sound) or give foreground, task-related information (typically spoken information). The use of sound

may also improve the usability of Tangible User Interfaces (TUIs), e.g. by explaining the steps of use and interaction. In an educational workbench, such as ours, we believe haptic and aural augmentation is particularly suited to avoid the overuse of one perceptual channel. However, we also see the potential peril of overusing sound, since some users may perceive it as intrusive.

We have mentioned the importance of distinguishing *same sum formula*, this representing a perceptual and a technical challenge. Hence, we will evaluate alternative methods to compare such complex structures.

Finally, we aim to evaluate the *educational usability* of the AC workbench. This may be performed as field-studies in high-school chemistry courses. We wish to compare AC with traditional means of chemistry education. This will require well-defined use cases and scenarios corresponding to existing textbooks and educational methods.

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