Tangible User Interface for Chemistry Education: Visualization, Portability, and Database

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Abstract

Augmented Chemistry (AC) is an application that utilizes a tangible user interface (TUI) for organic chemistry education. Based on the outcome of an extensive evaluation, we are in the process of extending the AC system[5]. Firstly, for enhanced interaction, keyboard-free system configuration, and internal/ external database (DB) access, a graphic user interface (GUI) has been incorporated into the TUI. Three-dimensional (3D) rendering has also been improved using shadows and related effects, thereby enhancing depth perception. Secondly, AC has been ported to different operating systems and is now compatible with Linux-, Windows-, and Mac OS X based platforms. This enables the use of a wider range of hardware: USB and Firewire (IEEE1394) cameras are now supported. Finally, system capacity to import and visualize molecules from an extensive XML-based DB has been realized. This gives users the ability to download and interact with any molecule up to a certain complexity.

Keywords

Augmented Reality, Tangible User Interface, Education, Organic Chemistry, Octet Rule, GUI, TUI

CCS

Input devices; Three-dimensional displays; Display algorithms; Viewing algorithms; Virtual device interfaces; Curve, surface, solid, and object representations; Color, shading, shadowing, and texture; Virtual reality

1. Introduction

Augmented Chemistry (AC) was developed at HyperWerk FHBB[6] [Voegtli, 2002; Fjeld and Voegtli, 2002]. It was extended with additional functionality and evaluated in a joint project which involved ETH[7], HyperWerk FHBB, and the aprentas[8] school of chemistry [Fjeld et al., 2004]. As part of the project, an empirical evaluation of AC was conducted by Bötschi [Bötschi, 2005], who studied how AC compares to the traditional ball-and-stick method of learning organic chemistry. Subjective preferences of the two alternative systems was one of the many variables measured (Fig. 1). On the basis of the first version and Bötschi's findings, we have further extended the AC system addressing three objectives:

- improved visualization
- extended portability
- ability to import from public chemistry DBs

All three objectives called for further implementation in the AC system. Aiming for improved comfort of use, ease of use, and ease of learning the system [Bötschi, 2005] (Fig. 1), we established a set of goals and informal requirements. Following these, visualization has been significantly improved utilizing shadows and luster to facilitate user comprehension of complex 3D models and information. (See the included video documentation[5]). Secondly, to increase the potential software and hardware compatibility, portability was extended. The new import functionality from public chemistry DBs offers users an expanded library of molecules for viewing and manipulation. Finally, for enhanced interaction, keyboard-free system configuration, and internal/external DB access, a GUI was incorporated into the TUI.

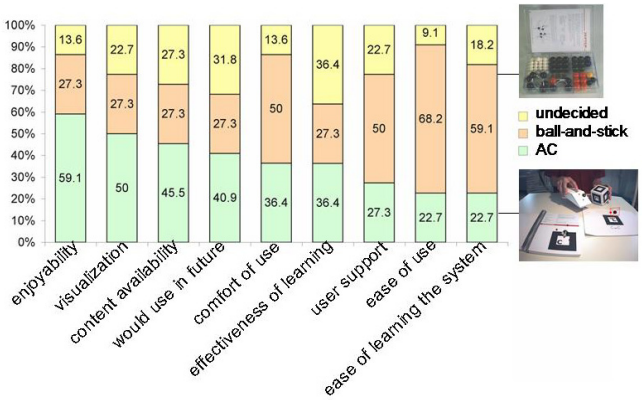

Figure 1: Test subjects' mean preferences for AC (bottom), ball-and-stick (middle), or undecided (top). AC ranked higher in enjoyability, visualization, content availability, future use, and effectiveness of learning. AC ranked lower in comfort of use, user support, ease of use, and ease of learning the system [Bötschi, 2005].

2. Tangible user interface (TUI)

AC uses a TUI enabling its user to compose and directly interact with 3D molecular models. The system was designed to assist in teaching abstract organic chemistry concepts such as molecular forms, the octet rule, and bonding. Following the conventional implementation of the AR Toolkit [Kato et al., 2000], physical tools carry one or more fiducial markers, connecting each tool to an animated 3D model so that both the tool and the model can be seen in a composite image.

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[6] HyperWerk FHBB: http://www.hyperwerk.ch/
[7] Eidgenössische Technische Hochschule Zürich: http://www.ethz.ch/
[8] aprentas: http://www.aprentas.com/

The system consists of the booklet, the gripper[9], the cube, the platform, a camera, and software. The booklet contains one element per page, each with its name and relevant information (Fig. 2). By using the gripper, users can pick up elements from the booklet and add them to the molecule in construction on the platform (Figs. 3, 4).

Figure 2: The booklet, the gripper, the cube, and the function cards (clockwise from top left).

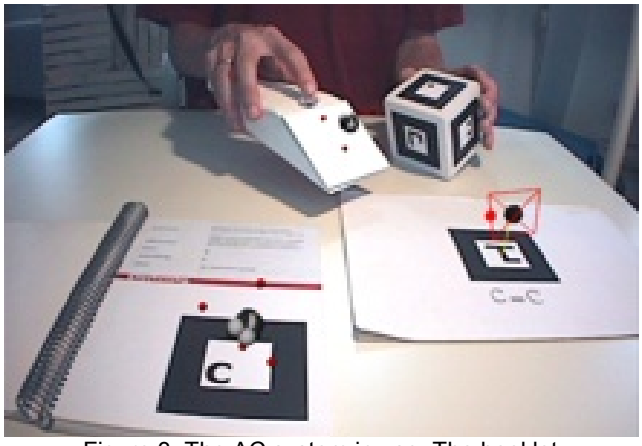

Figure 3: The AC system in use: The booklet, the gripper, the cube and the platform (left to right).

By rotating the cube, the user rotates the molecule, which determines how and where the new element shall bond. The function cards represent specialized functions which are activated when drawn onto the platform. These include the browser, the tag-toggle, the cleaner, the benzene-template, and the dipole [Fjeld and Voegtli, 2002; Fjeld et al., 2004]. While optical tracking systems enabling smaller markers and function cards do exist and would free up tabletop real estate[10], their source is not yet open. At the same time, we did not consider utilizing more cards for system configuration and internal/external DB access because of limited hardware real estate. Consequently, the limited physical space triggered the idea of integrating a GUI into the TUI. The idea of combining TUI with GUI has been explored in other projects [Ishii et al., 2002].

[9] The gripper first consisted of a wireless mouse rebuilt into a cage with a marker. Now, the marker is simply fastened to a conventional wireless mouse.

[10] ARTag, http://www.cv.iit.nrc.ca/research/ar/artag/, is not available under a open/free license.

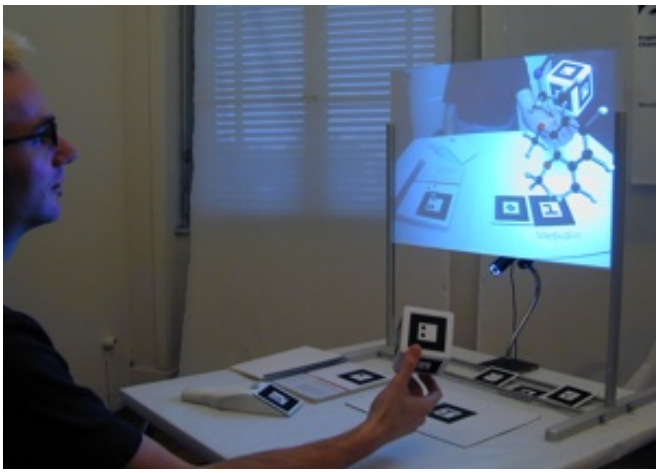

Figure 4: The AC system running on a standard workstation with a frame grabbing camera. USB and FireWire cameras are equally supported.

3. GUI and TUI, dual mode, 3D rendering

Here, we present realizations where particular attention is paid to integration of a GUI into the existing TUI. Firstly, we will explain the benefits of a GUI to support system configuration and, internal/external DB access. Secondly, we will show how dual mode presentation of the learning content was realized. Finally, we will present the 3D display and rendering issues and then the consequential improvements.

3.1. GUI and TUI: design issues

User studies showed that a problem in using the AC system – as compared to a traditional ball-and-stick method – was that controlling system settings often obstructed the learning process [Bötschi, 2005]. Many configuration settings are more suited to a GUI such as molecule size, element labeling, and system parameters. Such settings were initially mapped onto keyboard function keys. However, many users had difficulty using function keys while keeping complex chemical models in mind. The importation of molecules from external DBs also made it necessary to visualize large DB lists of molecules. So, to simplify interaction with system configuration settings and the new DB functionality, a purely mouse-controlled GUI was integrated into the primary TUI. Consequently, the GUI allows for a much more user-friendly system. Plus, keyboard-free operation allows for more efficient use of tabletop real estate.

In order to assure portability, the GUI was realized using OpenGL. To avoid a one-to-one reclaim of screen real estate, we designed a GUI with a permanent button in the corner that activates a pop-up menu with each alternative activating a graphic overlay dialogue box (Figs. 5-10).

Since OpenGL was already being utilized in AC for video image display and molecule rendering, it was the only application programming interface (API) feasible for GUI drawing. OpenGL has an adequate capability for high-quality GUI drawing because of its fast hardware acceleration. It is significantly faster than X or Win32 GDI when running on 3D-capable hardware. Alpha-blended texture mapping makes it possible to draw not only well designed 3D objects, but also smooth 2D windows and buttons.

And a normal painting program is all that is required to customize the appearance in detail.

Alpha-blending also made it possible to easily implement the GUI's unique fading feature. When users click on the AC background video image, the entire GUI fades, allowing for a better view (Fig. 8). Then, when clicking anywhere on the translucent GUI, it regains full visibility. This effect would have been practically impossible with most traditional windowing APIs.

Since there was no suitable, light-weight GUI toolkit using OpenGL available under the GPL license, we implemented a toolkit designed in-house. We foresee to base future GUI development on the current achievements (Figs. 5-9).

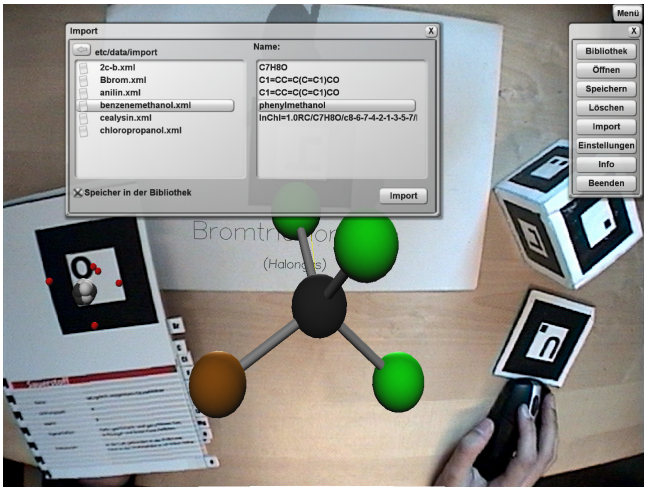

Figure 5: The GUI's import function from an external DB.

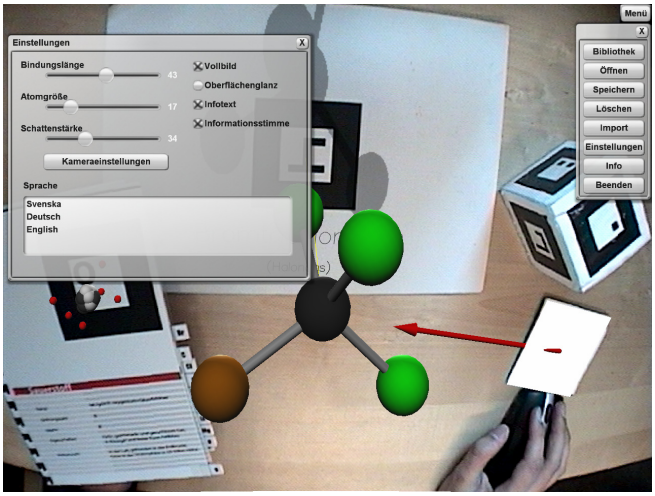

Figure 6: The GUI's configuration menu.

The GUI's graphical overlay is utilized for the import function (Fig. 5), system configuration (Fig. 6), and as a browser for the internal molecule DB (Fig. 7). All the molecules loaded into the system, whether predefined or imported from external DBs, are indexed by their chemical name (Fig. 5). This allows users to quickly browse through the molecules and select one by clicking its name. The browser then displays the selected molecule as a simplified 3D representation (Fig. 7).

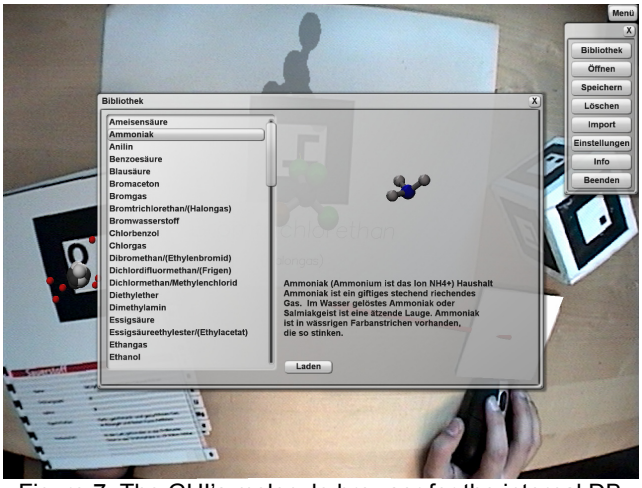

Figure 7: The GUI's molecule browser for the internal DB.

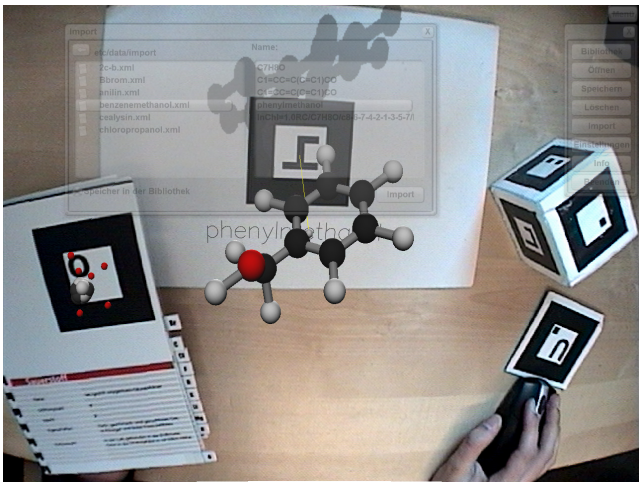
Figure 8: The focus shift from the GUI to the TUI.

3.2. Dual mode: textual and aural information

Evaluations demonstrated that there was a need to improve the presentation of the educational texts. Students have different learning styles, some preferring aural methods and some visual [Bötschi, 2005]. The first versions of AC did not take this into account. In these versions, when a predefined molecule was loaded or a constructed molecule was recognized, audio information was output. One problem with this was the inability to rewind or replay the audio information. To enhance user control of the information flow we are developing a dual mode system which would include a graphical overlay with the information in textual form. This display of educational text has been partly realized (Fig. 9). The realization of a user option between textual display, audio output, and both is foreseen.

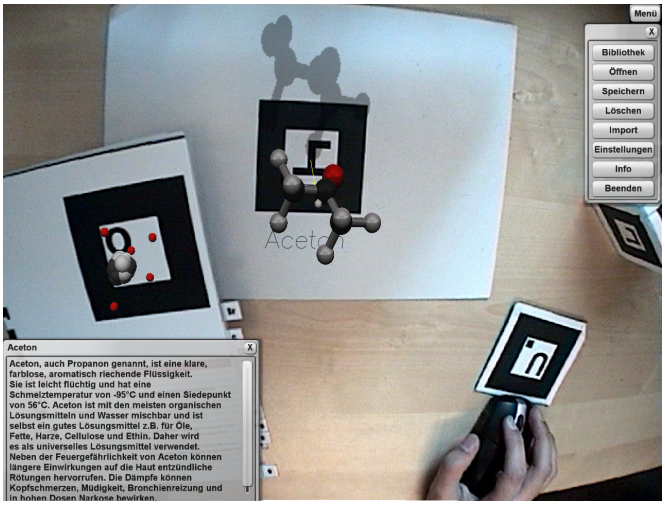

Figure 9: Educational text is displayed.

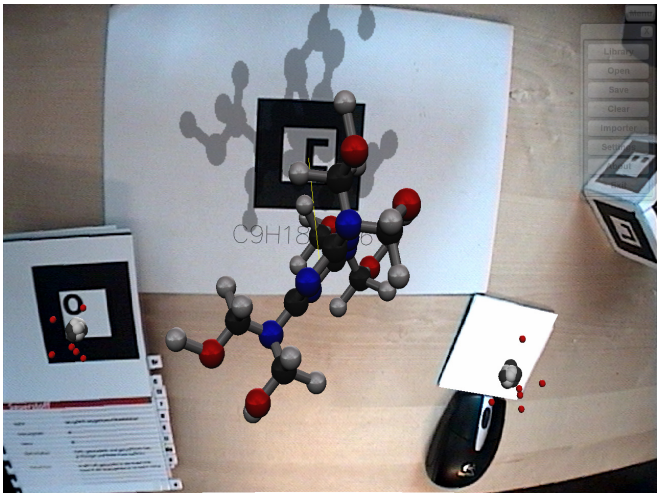
Figure 10: Molecule shadow and luster rendering; the use of shadows may potentially be expanded for projecting information on multiple planes.

3.3 Improved 3D visualization and rendering

Molecule visualization is being iteratively improved and evaluated. The user study [Bötschi, 2005] showed that manipulating the structure of the molecules using the TUI was relatively difficult. Small mistakes, e.g. misplacement and accidental removal of atoms, disrupted the learning process. To increase the ease of learning and operating the system, we believe that the interface needs to feel more natural and more like the conventional ball-and-stick method, but with the benefits of a TUI. To enhance the appearance of the computer-generated molecules, shadow rendering was added to the graphics engine. The projection of shadows and information on different planes (Fig. 10), lends a sense of order and structure to the complex information. Shadows play an important role in visualizing 3D models by improving the user's depth perception [Shon and McMains, 2004]. This allows users to manipulate the molecules with greater precision, enhancing the TUI experience. However, when viewing more complex molecules, the shadows have little or no added value [van Liere, 2005]. Addressing this issue, the system allows users to change the shadow darkness and turn it on or off easily.

4. Portability

The AC system's portability has been extended, so it is now compatible with a wider range of software and hardware platforms, including laptops. Furthermore, new options and an easy-to-install CD-ROM enable user-friendly installation. Newly enabled for multilingual configuration, the AC system is now accessible to a potentially larger user community.

4.1. Operating systems and cameras

Originally, AC was developed for Linux and only supported video cameras connected through a frame grabber. We have recently ported it for use on Windows and Mac OS X and switched to a newer version of ARToolKit. This allows for operation with a much wider range of hardware, including standard, low-cost USB and Firewire (IEEE1394) cameras. The increased compatibility maximizes the number of potential users and simplifies the use of AC.

4.2 Multilingual configuration

The AC system's first version presented language information exclusively in German. In order to make it accessible to more users, we have prepared it for translation into multiple languages. This required that molecule names, structure information, and educational text/audio be stored in the internal DB, enabling display in multiple languages. So far, the GUI has been translated into English and Swedish. Meanwhile, most of the educational information remains to be translated from German.

5. Ability to import from an external molecule DB

By enabling users to construct and examine organic molecules in 3D, a greater understanding of organic chemistry is expected. However, interviews with subject-matter experts revealed that there was a need to not only visualize and interact with user-defined molecules, but also with predefined molecules.

5.1. Advantages of an external DB

A new system feature is the ability to visualize any pre-defined, existing molecule[11]. While manual assembly of a molecule, atom by atom, is an effective way of learning structural details, it can be wearisome for larger molecules. That is to say, the pedagogical benefits of the TUI may be lost when user attention is drawn more to interaction than learning. We wanted to avoid such undesirable effects and create a more versatile TUI, so access to an external DB of predefined molecules was viewed as advantageous. While the first version of the AC system used its own proprietary format for storing molecule definitions and information, we have newly enabled the system for standard molecule file formats.

However, the import of molecules into the AC system from an external DB is limited to simpler molecules that conform to the octet rule and have a tetrahedron-based structure. In order to construct and visualize more complex organic and inorganic molecules, the current static composition model in AC would have to be replaced by a dynamic model based on molecular mechanics.

[11] There are still limitations in molecule complexity. For example, only one benzene ring can be represented in a molecule.

5.2. Database format

A variety of molecule DBs are available, including Beilstein[12], ISIS[13], and PubChem[14], all of which are used by professionals for many purposes. These DBs differ in many ways, but most importantly in file format. After extensive research into molecule file formats and interviewing subject-matter experts, we chose an XML based format because it is a standard that is easily convertible to non-standard formats. PubChem is just one XML enabled DB containing a vast amount of molecule information, created by the National Center for Biotechnology Information[14]. And by having access to PubChem, users can easily choose to import a molecule of interest, visualize it in 3D, and interact with it through AC.

5.3. Conversion from external to internal data structure

While most standard data formats like PubChem include predefined, spatial offset coordinates for the positioning of the atoms in a molecular model, the AC internal data structure does not. Therefore, AC does not consider molecular structure separately from the positioning of single atoms. Rather, the placement of atoms in a molecule is determined by their composition following a tetrahedral pattern [Fjeld and Voegtli, 2002].

When importing a PubChem molecule into AC, the data is converted into the internal data structure. Currently, the AC system can only process molecular model data that complies with its internal data structure. For example, only molecules with up to one benzene ring can be imported.

6. Discussion and outlook

Based on the AC system's first version and the outcome of its comparative evaluation [Bötschi, 2005], we have implemented a new set of functions and features into the system, as described in this paper. First, we have integrated a GUI into the TUI and improved 3D visualization and rendering. Then, we have extended portability to Windows and Mac OS X, enabling the use of different camera types. Finally, we have made AC compatible with an external XML database. Currently, we are in the process of translating information into languages other than German, supporting the dual mode of aural and textual learning content, and capitalizing on multiple-plane shadow rendering.

To evaluate our work we conducted a small, qualitative user study in which six secondary school students tested the system before and after our implementations. They constructed a set of molecules and then gave their subjective opinions about the system's ease of use, ease of learning the system, and if they would be likely to use it in the future when learning organic chemistry. Most of their opinions of the earlier version coincided with those found in the major user study [Bötschi, 2005]. Their opinions of the later version indicated that we had successfully improved both the system's ease of use and ease of learning the system. Their general opinion was that the additional functionality and added features had increased the probability of their using a similar system in an actual learning situation. We foresee a more extensive usability evaluation of the GUI/TUI integration and the GUI functionality in the future.

A possible improvement for AC would be the implementation of an alternative viewing mode for externally created molecular models from PubChem that do not comply with the internal data structure. Structural comparisons as internally carried out when building new models would not be used in this alternative viewing mode. Hence, a conversion of the PubChem data to the AC internal data structure could be bypassed. We will consider this in the future.

In a related project, researchers at The Scripps Research Institute have added markers to passive, ready-made ball-and-stick structures [Gillet, 2005]. Like in Fjeld et al. [Fjeld et al., 2004], they have visualized electrostatic fields and a local field vector. Going beyond the results of Gillet et al., we foresee the exploration of intelligent, physical balls and sticks. The imagined use would require spatial tracking of individual balls and sticks which would communicate the constructed molecule composition, position, and rotation. Hence, a one-to-one 3D virtual augmentation should become possible, enriching the physical ball-and-stick model with color-coding, atomic information (electrostatic fields, valence number, atom name), and other relevant information.

[12] MIMAS; http://www.mimas.ac.uk/crossfire/
[13] MDL; http://www.mdl.com/
[14] PubChem; http://pubchem.ncbi.nlm.nih.gov/

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