The Application of Virtual Reality to Chemical Engineering and Education

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Introduction

Virtual reality, VR, incorporates high-speed three-dimensional graphics, audio feedback, psychology, and special peripheral devices to produce "realistic" computer generated interactive environments that are (ideally) indistinguishable from reality.[1-3] Although it still requires high-end expensive systems to approach this ideal, the capabilities of personal computers are rapidly increasing to the point where virtual reality is becoming attainable in educational settings.[4-9]. It is also becoming increasingly practical to consider the technology developed for VR as a useful tool for the display and interaction with scientific and engineering data for the solution of practical problems.[10-13]

The educational benefits offered by this technology include the ability to take students into environments otherwise inaccessible, the high memory-retention of "experience" as opposed to passive observation, and the ability to reach out to visually oriented learners and global learners.[14-20] (Hands-on laboratories and plant trips share some of these benefits, but are not available 24 hours a day and are restricted by safety, economic, and logistics limitations.) The benefits offered to scientists and engineers include the high information content of a multi-dimensional, full color, animated, interactive display, as well as the more intuitive interface afforded by VR (as opposed to huge printouts of numbers or traditional two dimensional plots.)

Before we can take full advantage of this new tool, we must first study its strengths, weaknesses, and capabilities, in order to determine how best to apply VR to engineering education, practical engineering, and scientific visualization; We must learn what VR is good for and what it is not good for; We must learn what types of applications are suitable for VR, and what types are better handled through traditional methods; And we must identify which characteristics of a particular problem make it well suited (or not) to VR.

In order to address some of these questions, a series of VR-based educational modules has been developed in the Department of Chemical Engineering at the University of Michigan. Some of these modules are designed to be of immediate practical use in engineering education, and some were developed to explore and test the capabilities of VR as applied to a variety of situations. This paper describes the current status of these modules and some of what has been discovered during their development.

Abstract

Three major educational modules have been produced, as well as a number of smaller modules. The major modules include <u>Vicher I</u>, dealing with industrial methods of handling the decay of catalysts and heterogeneous catalytic mechanisms, <u>Vicher II</u>, dealing with non-isothermal effects in catalytic reactions, and <u>Safety</u>, which allows students to walk through a chemical pilot plant to evaluate the hazards and safety systems present. Of these three, Vicher I is completely finished and available for free download via the world-wide-web.[21] The simulation for Vicher II is complete; However release is being held pending the completion of the associated "help"

documents. Preliminary testing of the safety module has shown that it is not as effective as desired. It is therefore being enhanced to provide more direction and specific tasks for the users.

In addition, a number of minor modules have been developed, in order to test and explore the capabilities of VR as applied to scientific visualization and engineering education. These modules (which are all available on the web site referenced above) deal with the areas of laminar fluid flow visualization, thermodynamic relationships, azeotropic distillation residue curves, crystal structures, and other topics. Some of what was learned during the development of the minor modules was later incorporated into the major modules, and other findings will form the basis for future projects.

The major modules have been tested extensively at the University of Michigan, both during the development process and in their final form (as applicable.) It has been found that VR based educational modules are beneficial to some students in some situations, but not to all students or in all situations. Strengths and weaknesses of VR as an educational tool have been discovered, as well as difficulties and design parameters unique to the development of educational VR. Future projects of the authors are also discussed in this paper.

Results and Discussion

This section briefly describes each of the modules produced for this project, focusing more specifically on the knowledge gained during the development of the modules. Further details regarding the modules themselves can be found in previous papers by the authors.[22-29]

Vicher I

The subject of Vicher I is heterogeneous catalysis. The specific concepts to be delivered to the students are the mechanisms of heterogeneous catalysis and different industrial methods for dealing with different kinds of catalyst decay. It should be noted carefully that Vicher I is NOT intended as a calculational tool for practicing engineers, nor is it intended to teach students how to perform numerical calculations. The important features of Vicher I are that it be able to illustrate the general reaction mechanisms and the reactors, and that it be able to do so efficiently on student-affordable computers.

Figure 1 shows four scenes from Vicher I. The three reactor rooms shown illustrate industrial methods of dealing with slow, medium, and fast rates of catalyst decay, in frames a, b, and c respectively. The time-temperature room heats catalyst up over a time period of days to weeks to compensate for slowly decaying catalyst, until such time as shutdown is required. The moving bed reactor consists of five packed beds (one for reaction and four cleaning stages), and catalyst pellets that move from one bed to another over a time span of hours. The transport reactor (a.k.a. riser reactor or cat cracker) shows catalyst that becomes fouled in a matter of seconds to minutes, and an associated catalyst regeneration unit (both in pilot plant scale.) The catalyst surface shown in Figure 1d is one of three microscopic areas modeled to show the mechanism of catalytic reaction at the molecular level.

One of the important tools developed for Vicher I was a mechanism for rapidly moving virtual objects in a realistic manner on low-powered computer equipment. The reactors shown in

Figures 1b and 1c have up to 100 moving catalyst pellets that are simultaneously coking and decoking. Inside the catalyst pore (not shown) there are up to 100 molecules diffusing, adsorbing, desorbing, coking, decoking, and undergoing both desired and undesired surface reactions. All of this is made possible via two important simplifications, which the average viewer will never notice: First of all, the moving items are single flat polygons with applied texture maps, much like cardboard cutouts flying through the air. Second, the kinetics are not calculated rigorously at run time; Instead the adsorption, desorption, and chemical reactions are determined using random numbers and pre-determined probabilities. Since the user cannot distinguish between our simplifications and reality, (and considering that the simulation is intended to illustrate a point, not for practical calculations), there is no reason to slow down the simulation with rigorous calculations performed at run-time.



(a) Time-Temperature Reactor Room



(b) Moving Bed Reactor Room



(c) Transport (Riser) Reactor Room



(d) Close-up of Catalyst Surface

Figure 1: Three Reactor Rooms and a View of the Catalyst Surface from Vicher I

Another important tool developed for Vicher I is shown in the graphs of Figure 1a. As each experiment starts, the graphs appear as empty axes. Then, as the reaction proceeds, the graphs gradually appear over time. To the user, it appears much like a strip chart recorder. The data on the graphs are the results from a rigorous solution of a set of simultaneous differential equations. However the equations are all solved off line, and the results stored as (carefully formatted)

finished graphs. The "trick" is that when the graph is first placed on the wall, it is covered with a cover sheet that hides the data. Then, as time progresses, the cover sheet is gradually shrunk in size to reveal the graph a bit at a time. Again, as long as the user cannot tell the difference, there is no reason to slow down the simulation by solving the differential equations on the fly. (It should be noted that low-cost VR display devices have very poor resolution. Users can discern the shape and trends of the graphs, which is what is important, but there is not sufficient resolution to discern precise quantitative values. Many Vicher I data displays, such as the meters in Figure 1c, do not even have a scale shown.)

The time-temperature room (Figure 1a) also incorporates another important learning tool – experience. After the reactor has run for a certain amount of time, it has to be shut down to replace the fouled catalyst with fresh material. At this point in the simulation, the entire screen fills with a shutdown message that the students find very annoying. After a while, the students learn that if they run the reactor at high-temperatures, they get a better product but they have to shut down the reactor more frequently. In this way they learn, *through experience*, about the trade-offs of reactor performance versus increased downtime.

Vicher I incorporates a supplemental help system that can be launched from within the VR simulation or used as a stand-alone resource. The help system was originally based upon the Microsoft Windows "help" standard, but was later switched over to an HTML format when Vicher I was ported to Silicon Graphics computers. This was a very beneficial change, because it not only provides support for a much wider variety of different computer platforms (including some on which the VR simulations do not run), it also allows for the inclusion of many more types of content (gif images, mpeg movies, QTVR panoramas, etc.) as well as links to external web sites. Thanks to photographic images, support for text and equations, and a higher resolution, the help system provides detailed accurate explanations of topics that are by necessity simplified in the VR simulation. Vicher II and Safety have similar help systems incorporated.

Vicher II

The general topic of Vicher II is non-isothermal effects in chemical reaction engineering. Three specific situations are explored in relation to this general theme: Generation of hot-spots in a jacketed non-isothermal packed bed reactor, multiple endothermic reactors in series with interstage heating, and multiple steady states for an exothermic reaction occurring in a jacketed CSTR. Figure 2 shows the three reaction areas of Vicher II, along with the welcome center in which the simulation starts.



There are two important information-representation problems addressed in Vicher II. The most obvious is the representation of temperature, which is a property rather than a physical object. The primary mechanism used in Vicher II to indicate temperature is color, which is unfortunate for those readers seeing this paper in black and white. As in Vicher I, we are not concerned here with exact numerical values for temperature, but rather general trends of "hot" versus "cold". The color scale chosen is fairly intuitive, with bright red indicating very hot conditions, white representing the middle of the scale, and full blue representing very cold conditions, with gradual transitions between these three key values.

In the Multiple Steady States reactor room, color is used to indicate the relative temperature of two key system conditions – the inlet flow temperature and the reactor operating temperature. The reactor feed temperature varies in a relatively narrow range, causing the reactor feed pipe (topmost pipe in Figure 2d) to vary among a few shades of blue. More important is the reactor operating temperature, which changes drastically and suddenly between very cold and very hot, causing the reactor fluid color to change dramatically between strong blue to strong red. Color is also used to indicate temperature in the other Vicher II reactor areas to be discussed.

The second information-representation challenge addressed in Vicher II is to illustrate the *connection* between the mathematics that describe a situation and the physical conditions of the actual equipment. This issue was first addressed in the Non-Isothermal Packed Bed Reactor Room, shown in Figure 2b. In this room, the mathematical representation of the reactor kinetics is materialized as a three-dimensional surface that users can walk around (or on) to view from any desired angle. One of the axes parallel to the floor is the temperature axis, as indicated also by a color shift from blue to red. The other axis parallel to the floor is reaction conversion, which is related to the distance down the length of the reactor. The height of the surface off the floor is inversely related to the reaction rate, and therefore provides a measurement of differential reactor volume. A line on the surface traces current reactor conditions down the length of the reactor, (as pre-calculated from a rigorous solution of simultaneous differential equations.)

The important point to note in all of this, is that the reactor is also color-coded, using the same color scale as the mathematical kinetics surface. Hence a red spot in the reactor has a direct correspondence with the point on the kinetics surface at which the operating line passes through the high-temperature region. Students can change the reactor operating conditions using the (virtual) control panel, and see how the changes affect both the operating line on the kinetics surface and the reactor conditions as indicated by the color coding. In this way, students can directly see the link between the mathematical surface and the physical reactor conditions.

The staged reactor area is also designed to illustrate a link between mathematics and physical equipment, using both color coding and dynamic linked tracers. In this case, there is a tracer that moves through the three-dimensional reaction equipment and a corresponding tracer that moves across the face of a two-dimensional color-coded graph. There is also a moving tie-line that connects the two tracers. Besides the red-white-blue shading on the inset graph, color is also used to relate lines on the graph to specific reactor components. The horizontal lines on the graph, (along which temperature increases but no reaction occurs), are colored green to match the green pipes in the interstage heater (furnace). The diagonal lines, (along which conversion increases while temperature decreases), are each given a different unique shade of yellow-orange to correspond with the colors of the four reactor sections.

Finally, there is a human-factors issue that was first developed in Vicher I and further explored in Vicher II – the Welcome Center. During the development of Vicher I it was discovered that an initial welcome center serves two very important orientation functions. First of all, it provides the user with a comfortable, familiar environment in which to become used to the experience of virtual reality and learn to operate the controls before venturing into more complicated engineering areas. Secondly, it provides a central branching off point from which to explore the other areas of the simulation. Early versions of Vicher I had hallways that users had to navigate to get from one area to another. These hallways were difficult for users and added nothing to the overall simulation, and so they were later replaced with teleports that are much easier to navigate and also much easier to re-configure as needed. The problem that arose in Vicher II is that the Welcome Center is a basically round room which initially had no orientation cues. It is not surprising that teleporting in and out of a bland round room caused many users to quickly become confused and disoriented. Therefore two important changes were made to the Vicher II welcome center, as shown in Figure 2a: One wall was replaced with a large floor-to-ceiling window, and three arrows of different colors were placed on the floor, pointing from the center of the room to each of the three reaction engineering areas. These two changes reduced the symmetry of the room and provided necessary orientation cues sufficiently that users no longer get lost in the Vicher II welcome center.

Safety

The first safety-related module developed focuses on a hazard and operability (HAZOP) analysis of a pilot-plant scale polyether polyol production facility. This module was developed using photographs, measurements, and information provided by a local chemical company and by an expert in the field of chemical plant safety. (Note: The simulation created is not an exact representation of the local company – it is merely based upon information gathered from the local site, as well as from other sources.) The purposes for developing this simulation were to explore the ability of VR to place students into environments that would be otherwise inaccessible due to safety, economic, or logistical limitations, and to evaluate the benefits of an immersive three-dimensional view as opposed to a written description as the basis of a hazard evaluation. Two big differences between the safety module and the Vicher modules are that the safety module has a much greater level of detail and realism (based upon a real facility), but no animations or user interactions (other than the ability to launch the "help" system.)

In order to evaluate the benefit of the VR safety simulation for hazard analysis, an exercise was given to approximately 150 students in the first semester senior design course. The students were divided into three groups, of approximately 70, 70, and 10 students, based upon the last digit of their social security number. All 150 students were given a written description of the process as well as access to the virtual reality simulation, and were asked to write an evaluation (in essay form) of the hazards and safety features present in the pilot plant area. The first group was asked to write their analysis based solely on the written description, and to go through and evaluate the VR module <u>after</u> they had completed their safety analysis. The second group was asked to use <u>both</u> the VR module <u>and</u> the written description when performing their safety analysis. The third group was taken to the local chemical company, where they were allowed to tour the facility that formed the basis for the exercise and to discuss the operation with the operating engineers. The following year the exercise was repeated, with the exception that no students were taken to the chemical plant. The essays of the 300 students were analyzed to determine the astuteness of their analyses, as well as the effort that they put into the assignment.

It came as no surprise that the students who went to the chemical plant performed the best on the exercise. While it cannot be determined whether this is due to a better view and understanding of the facility, the benefit of discussing the plant with operating personnel, increased enthusiasm inspired by the plant visit, or some other cause, there has never been any question that "real reality" is better than virtual reality when the choice is available. However it should be noted that out of a class of 150 students, only 10% (15 students) could be given the option to tour the plant, due to logistical constraints at the host facility, and of those 15, only 10 could actually go, due to class conflicts. One could easily argue that the group that went to the chemical plant was biased, in favor of students who had enough interest in the assignment to rearrange their schedules.

Between the other groups, there was no statistically significant difference in the results. In fact, there was a very slight (statistically insignificant) lower average score among the students who used the VR module to perform their safety evaluations. While we cannot be certain of the reason for these findings, we do have several ideas. First of all, there is not enough specific direction in the VR simulation. It stands to reason that if a group of students were place in a *real* chemical plant, without a tour guide of any kind, and given no more instructions than to just "explore the area and analyze the hazards present", that they would not learn very much from the experience. Secondly, a lot of the information necessary to conduct a thorough safety evaluation is not evident from a visual inspection. For example, a safety expert analyzing a plant would want to know about maintenance records and training policies. Third, we believe that some of the students who went through the VR simulation before conducting their analysis spent so much time in the simulation that they were unwilling to spend as much time on the written portion of the exercise as those who did not use the VR simulation for their analysis. Finally, the simulation is not a perfect representation of reality, and some students had difficulty discerning between weaknesses in the simulation versus weaknesses in the safety of the plant.

Nevertheless, the students who used VR did make some very astute observations that were not apparent from the written description. In general these observations had to do with spatial relationships, such as the proximity of housing to the chemical plant and the accessibility of exit doors and fire fighting equipment to the pilot plant area. We therefore conclude that there is some benefit to be gained from an immersive three-dimensional view of the facility, but that the VR simulation needs to have more specific user direction and more detailed information provided before it becomes a useful teaching tool. (It should be noted that practicing engineers, who have a better understanding of plant operations and safety analysis, have used VR successfully for analysis of chemical plants prior to construction.[30])

In order to improve the effectiveness of the safety simulation, some major enhancements are underway. A series of specific safety scenarios are being assembled, to be dispersed throughout the pilot plant environment. Students will have to find each of the scenarios, (marked with a three-dimensional question-mark icon), that will be fully described using full-screen photographic images, auditory narration, and possibly movies. The students can repeat the scenario descriptions as many times as desired. The students will then be asked to evaluate whether the scenario represents a dangerous hazard, a reason for caution, or an example of a good safety system in action, as indicated by red, yellow, and green lights respectively. (The lights will be arranged in traffic-light order to accommodate color-blind students.) When the student has made their choice, they will be given further feedback, and the opportunity to make another choice (if the correct choice has not yet been determined.) There will also be a point system implemented in order to provide further incentive for careful analyses.

Minor Modules

In addition to the major modules described above, a number of minor modules were also developed, to test and explore the capabilities of virtual reality for scientific visualization and educational applications. Two modules were developed for the examination of crystal structures (face centered cubic and body centered cubic) to explore the benefits of interactive stereoscopic display for the comprehension of three-dimensional spatial phenomena. A fluid-flow visualization was developed to explore the use of color and shape for conveying information,

and to examine the benefits of *experiencing* fluid flow phenomena from a viewpoint within the flow field. An azeotropic residue curve representation was produced for a four-component system, to test the capabilities of VR technologies to visualize higher dimensional problems. Two different applications were developed for the visualization of thermodynamic information – One explores the use of a single icon to represent four different thermodynamic quantities (pressure, volume, temperature, and entropy), and the other utilizes that icon and some interactive function surfaces to visualize the *relationships* between important thermodynamic variables (Maxwell's relationships.) The evaluations of these minor modules are not yet completed.

Conclusions

This paper has discussed a series of VR-based educational modules developed at the University of Michigan, focusing primarily on the pedagogical issues that have been addressed during their development. In addition to educational applications, the authors have also explored the potential for VR as a general information-delivery tool, for eventual use in scientific visualization and practical engineering applications. Regarding the educational benefits of VR, we feel that VR can benefit some students in some situations, when it is properly implemented. However that implementation is not straightforward, and VR should not be considered as a replacement for real experiences when the latter is available. VR should be used as a supplement to real experiences, and/or in situations where the real experience is inaccessible. The authors intend to continue the development of VR as a useful tool in engineering, science, and education, initially in the areas of higher-dimensional scientific visualization and the development of virtual accident scenarios for the reduction of laboratory accidents.

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