Engineering Educators Bringing the World Together
2025 ASEE Annual Conference & Exposition
Palais des congrès de Montréal, Montréal, QC • June 22–25, 2025
Paper ID #46255

Virtual Reality in Chemical Engineering Laboratory Education

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Virtual Reality in Chemical Engineering Laboratory Education

Introduction

Virtual Reality (VR) technology opens the door to tremendous possibilities for engineering educators. Simulation of a fully immersive, virtual environment incorporating visual, auditory, and other sensory elements can enable interactive training experiences that would otherwise be difficult or impractical to deliver in a conventional classroom. Besides chemical engineering applications, educational VR modules have been developed in the fields of construction and civil engineering,[1] architecture,[2] mechanical and electrical engineering,[3] micro/nanoelectronics,[4] robotics,[5] automotive technologies,[6] control systems,[7,8] thermal fluids engineering,[9] renewable energy technologies,[10] and molecular engineering.[11] Assessment of VR-based learning tools in the classroom indicates enhanced student interest levels, improved performance on examinations,[7] and beneficial effects on students' perceptions of the learning experience.[12]

VR technology is gaining momentum in chemical engineering education, as it can provide access to simulated learning environments that would be too expensive, too dangerous, or otherwise impractical to implement on campus. Recent advances in VR software and hardware are creating new possibilities for pedagogical innovations that could transform engineering education by bridging the gap between classroom teaching and hands-on industrial experience.[13,14] Virtual chemical reactors have received some attention due to their inherent risks and costs. Early efforts at the University of Michigan initiated in the 1990s resulted in development of several educational VR models through the Vicher (Virtual Chemical Reactor) project.[15,16] More recently, Schofield described design of an educational module involving a VR polymerization plant.[17] Tehreem and Pfeiffer described a virtual chemical reactor in which a hazardous material (n-butyllithium) is used to carry out a procedure.[18-19] Falconer and Hendren developed a virtual catalytic reactor simulation intended for use as a laboratory experiment or a project in a chemical reaction engineering course.[20] VR simulations are also being developed to train students in design[21], operation[22], or control[23] of chemical plants, to engage high school students with interest in chemical engineering,[24] and for health and safety education.[25-28]

VR has diverse applications in engineering educations, including both in-person and remote education situations. During the recent pandemic, many institutions were forced to switch to remote education on short notice, which posed obvious challenges for effective teaching of (hands-on) laboratory courses. VR technology provides a potentially valuable avenue by which to teach laboratory courses remotely or supplement hands-on courses with experiences on very large-scale equipment. Interactive, immersive simulations of experiments or chemical processes enable students to conduct virtual experiments and collect data at home using a laptop or desktop computer. Virtual laboratory simulations[29,30] or process simulations[31] provide an opportunity to bolster laboratory course content during pandemic times, or more generally to enhance laboratory education at any time.

VR simulations of laboratory experiments addressing unit operations of chemical engineering are a viable avenue to future pandemic preparedness and enhancement of remote education opportunities. During the pandemic period from 2020-2022, our undergraduate chemical engineering program began employing virtual laboratory modules to provide students with an opportunity to collect and analyze laboratory data remotely. Simulations were distributed to students free of cost as an executable "build" file that can be run on laptop or desktop computers with common operating systems, without the need for a VR headset. After the return to in-person education, the VR modules were retained as stand-alone laboratory experiments or hybrid experiments that complement physical data collection in the laboratory.

This paper describes the design and testing of three virtual experiment modules addressing chemical process dynamics and control (CPDC), chemical reactor design and scale-up (CRD), and transport in fluid-particle systems (FPT). All VR simulations were designed in the Unity Real-Time Development Platform 3D game engine, which can generate executable build files that run on the most common operating systems. Each of the modules invokes a different pedagogical approach. Results reveal several advantages of desktop/laptop format vs. fully immersive headset format for VR laboratory experiments. Challenges encountered in developing and distributing the VR modules to students are discussed, along with potential remedies.

Chemical Process Dynamics and Control (CPDC) Module

The CPDC experiment module is a stand-alone VR simulation that does not require any physical laboratory equipment, making it attractive for remote education. This module runs on a desktop/laptop computer, so students do not need to own or purchase headsets for remote use. Students are tasked with designing and tuning a feedback control system for a classic coupled tanks problem in an imaginary biofuels refinery called the RPI Virtual Chemical Plant. Undergraduate students at our institution are required to own laptops capable of running engineering software applications, but no assumptions were made regarding their ownership of graphics cards or machines designed for gaming. Our intention was to make the software accessible to all students enrolled in senior-level laboratory courses without introducing any financial barriers. The 3D simulations emulate a video game format, in which the player is free to walk around the plant, operating buttons to conduct open-ended experiments without any predetermined sequence of actions.

Fig. 1 shows an aerial view of the plant layout and the interactive controls available to students. While the simulation environment mimics a biorefinery with interconnected process equipment, the CPDC experiment takes place on a control platform adjacent to the coupled tanks in question. Only the coupled tanks and the control system have scripts attached to govern their behavior; the remaining process equipment in the plant has limited functionality and serves as a visual backdrop in order to minimize consumption of CPU/GPU resources on the user's machine. Models of tanks and other process equipment were generated in Blender (open-source) computer graphics software and imported into Unity. In general, lower graphics quality and less GPU-intensive processes are favorable features when the software is intended to run on a diverse array of computers owned by students.

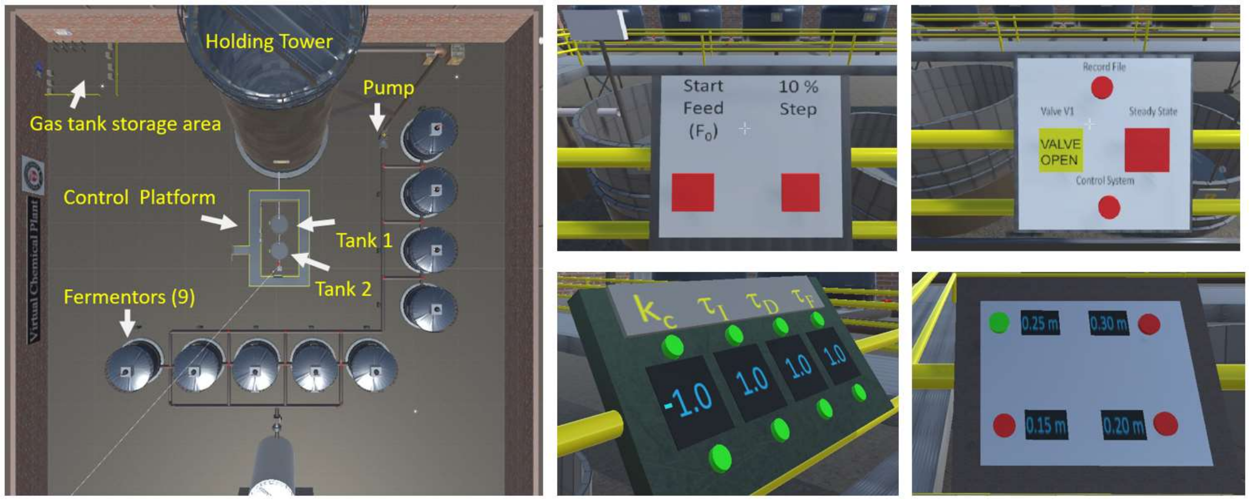

Figure 1. *User interface for the CPDC simulation: plant layout (left) and interactive control panel buttons (right).*

The user is presented with four control panels, which have oversized buttons that resemble a senior laboratory experiment more than an actual plant. Experimentation with virtual controls and indicators revealed that students preferred ease of operation (oversized buttons) over a more realistic user interface, such as virtual workstation computers with small buttons, which can be awkward to click. Without activating the feedback control loop, the user can voluntarily start or stop liquid feed to the first tank, introduce a step increase of 10 % in the feed flow rate, open or close the valve separating the tanks, and export measurements of liquid levels and flow rates vs. time to a text file. A steady state "cheat" button allows the students to fill the tanks to their steady-state levels instantly, which expedites experimentation by skipping the approach to steady state. After activating the control system, the tuning parameter board and setpoint board are used for closed-loop feedback control experiments.

The critical components of the coupled tanks system are shown in Figure 2. State variables are the liquid levels in tank 1 and tank 2 (h_1, h_2). The control objective is to maintain h_1 at a desired setpoint, while h_2 is an uncontrolled output. F_0, the volumetric flow rate of the liquid entering tank 1, is a disturbance input. The valve flow coefficients (C_{v1}, C_{v2}) are parameters when the control system is not activated, but C_{v1} serves as the manipulated input once the feedback loop is closed. Besides h_1 and h_2, additional outputs are the volumetric flow rates F_1 and F_2. With the feedback loop closed, there are two inputs (feed flow rate and control valve coefficient) and two state variables/outputs (liquid levels) of interest, so students are required to consider four process transfer functions in constructing block diagram models of the system.

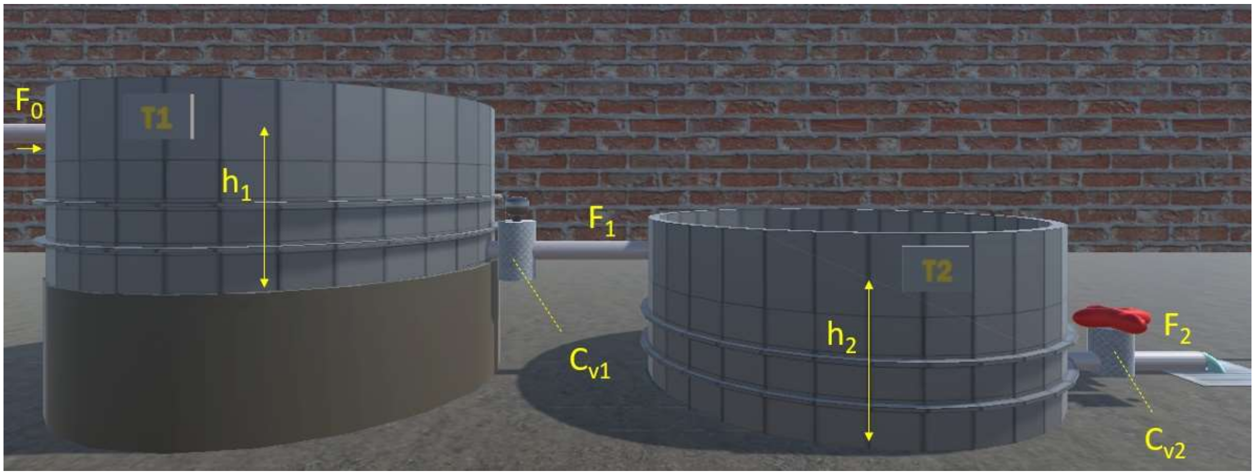

Figure 2. *Coupled tanks with state variables (h_1, h_2 - liquid levels), disturbance input (F_0 - volumetric flow rate) manipulated input (C_{v1} – valve flow coefficient), and outputs (F_1, F_2 - volumetric flow rates) labeled.*

In each simulation frame update, scripts compute the mass balances on the two tanks, handle the input actions of the user, perform control actions on the manipulated input variable in a discrete sense, and govern the recording and exporting of data files. Because the liquid levels in the tanks are derived from frame-by-frame mass balances, rather than from transfer function models, the results obtained from the experiment do not necessarily duplicate the expected outcomes from control theory. For example, approximations made in derivation of transfer functions (e.g., linearization about a steady state) may be challenged by the conditions of the experiment. In addition, a small amount of white noise was added to the measurements of liquid levels and flow rates to simulate experimental measurement noise.

The CPDC experiment proceeds through a series of experimental trials in which students model the response of the system under open-loop or closed-loop conditions. Measurements of liquid levels and flow rate from each experiment trial are exported to a text file, and students are supplied with a MATLAB script that imports and plots the raw data. In post-laboratory analysis, students are expected to solve differential equations and build transfer function models in MATLAB and Simulink to compare the observed response of the system to expectations from control theory. Thus, the VR simulation complements the use of software packages traditionally used to teach process dynamics and control, rather than replacing them.

The first trial involves filling and draining the initially empty tanks under open-loop conditions to find unknown system parameters. Students are asked to measure the values of tank bottom areas, A_1 and A_2, and the flow coefficients of the valves, C_{v1} and C_{v2}, which are not provided, unlike traditional textbook problem. In the second trial, the liquid feed to the tanks is left running until steady-state liquid levels h_{1s} and h_{2s} are determined. In the third trial, the main learning objective is to conduct an input step test[32] to determine gain and time constant values for a process transfer function from experimental data. The fourth trial focuses on closed-loop response for feedback control, using either a PI or PID + filter controllers. After completing each trial, students compare the experimental data to the expected behavior from a Simulink block diagram model that they must construct using process gains and time constants estimated from experimental data. A critical learning objective is for students to construct Simulink block diagram using the correct transfer functions to model the plant and reproduce the experimental trials.

Fig. 3 illustrates how typical results from the VR experiment complement modeling in MATLAB and Simulink. The experimental data represent the closed-loop response obtained after a change in the liquid level setpoint in tank 1. The closed-loop transfer function $g_{CL}(s)$ for the system is second order, leading to the possibility of oscillating liquid levels after a disturbance or setpoint change. Three sets of tuning parameters were tested with PI control, yielding critically damped ($\zeta=1$), underdamped ($\zeta=0.58$), and overdamped ($\zeta=2$) responses, where ζ is the damping factor for the second order closed-loop transfer function. A key learning objective is for students to conceptually distinguish the closed-loop transfer function $g_{CL}(s)$ from the open-loop process transfer functions, which are first order. Students should also appreciate how tuning parameters (k_c, τ_I, etc.) affect the response after a setpoint change or disturbance.

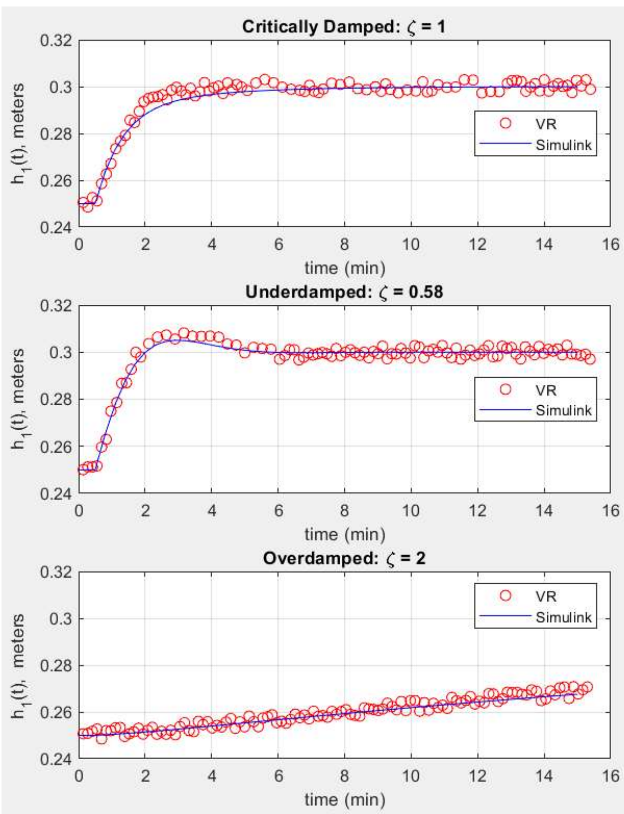

Figure 3. Comparison of a closed-loop feedback control experiment (virtual reality data) and the output of a Simulink block diagram model of the same. Three sets of tuning parameters were implemented with PI control, leading to critically damped, underdamped, and overdamped responses in the liquid level in tank 1 (h_1) after a change in the setpoint.

After exploring given sets of tuning parameters, students are asked to apply IMC-based PID tuning[33] to find a recommended set of tuning parameters. Running a fourth trial with the recommended tuning parameters typically provides a response that is close to the critically damped response. Students are encouraged to explore whether PID + filter control provides any advantage over PI control. Students should understand the actions taken by the P, I, and D terms, and decide whether the D term is even necessary if PI control provides an adequate response.

Chemical Reactor Design (CRD) Module

Whereas the CPDC module serves as a stand-alone VR experiment, the CRD module couples experimentation in the physical laboratory with scale-up and optimization experiments in VR. A hybrid pedagogical approach of this nature mitigates concerns that students lose hands-on experience by performing virtual laboratory experiments. More specifically, the CRD module uses student-generated chemical reaction kinetics data from the physical laboratory to support reactor design, scale-up, and economic analysis in VR. The experiment proceeds through three phases: 1) analysis of batch reactor kinetics data to find reaction rate constants, 2) simulation of a scaled-up, continuous stirred tank reactor (CSTR) in virtual reality, and 3) economic optimization of reactor operating parameters in virtual reality.

The first phase builds upon a historical database of results from a bench-scale chemical reaction experiment in the physical laboratory, from which students quantify reaction order and reaction rate constants. The reaction is a photocatalytic degradation of a toxic organic dye, methylene blue (MB), in the presence of a suitable catalyst (anatase TiO_2 nanoparticles) and an intense light source (solar simulator). Students apply ultraviolet-visible spectroscopy to measure the concentration of MB vs. time in a benchtop batch reactor. During the past several years, a cumulative database of student laboratory team results ("community dataset") has been maintained in order to provide better measurement statistics for reaction kinetics.

Students analyze the community dataset to determine the overall reaction order and find best-fit values of the reaction rate constant at pH values of 7, 10, and 12. Use of a database to perform this analysis equips students with a better appreciation for experimental statistics. Once a suitable kinetic rate law has been determined, students are asked to apply material balance equations for stirred tank reactors to scale up the reaction to run in a 10,000 L CSTR in a hypothetical wastewater treatment facility. The toxic MB must be removed from a wastewater stream totaling 120 m^3 per day. Fig. 4 shows the user interface, through which the user operates a counter-current heat exchanger (not visible) and the 10,000 L CSTR from a control platform.

Figure 4. User interface and control panels for operating the photocatalytic CSTR unit in the chemical reactor design VR module (left). Real-time economics analysis feature (right).

Students are first asked to run the reactor at 298 K to validate that the reaction rate constant is similar to the value from physical laboratory experiments. The students must infer the value of the reaction rate constant from the material balance for a single CSTR at steady state. The reactor is subsequently run at different temperatures, keeping feed flow rate and pH constant, in order to find a value of the activation energy for the reaction (which is coded into the scripts). The learning objective is for students to extract kinetic information from experimental data obtained from both batch and continuous-flow reactors.

In the third phase of the CRD experiment, students use the control panels to characterize the operation of the CSTR at different temperatures, feed flow rates, and pH values. The goal is to solve a constrained optimization problem: treating 120 m^3 per day of wastewater to reduce MB concentration by 100×, while minimizing the daily cost to the company. The given constraints are that the effluent MB concentration must be less than 0.02 mol/m^3, the reactor operating temperature range is between 310 to 350 K, the feed flow rate lies between (0.1 to 1.0) m^3/min, and the pH may be set to 7, 10, or 12. The reactor feed temperature is controlled by manipulating the heat exchanger that conditions the reactor's feed stream (incoming wastewater). Adjusting the (cold side) chilling water temperature or flow rate affects the (hot side) feed temperature, which in turn affects the reactor's operating temperature. Process dynamics are fast enough such that the simulation reaches steady state almost instantly, allowing students to collect data on many operating conditions during a laboratory period.

Students are asked design their own optimization experiments to minimize costs while meeting the given constraints. There is no fixed set of instructions for collecting data on reactor performance or process economics, and there are multiple input variables that can be manipulated. Some guidance is provided in the laboratory manual, where it is suggested that the reactor's operating temperature should be kept constant while other parameters are varied, but students are otherwise free to design their own experiments.

In order to assist students with data collection, a real-time economics analysis feature was introduced (Fig. 4, right). The character in the simulation is equipped with an augmented reality (AR) headset that can be toggled by pressing a console button to view operation costs as they accrue. Economics calculations can be reset after a change is made to the operating conditions in order to erase previous history. The economics AR feature covers a wide array of operating costs, each of which is affected by the user's choice of input variables. Subdividing total operating cost into categories allows students to infer which process variables are driving economics under a given set of conditions.

Fig. 5 shows a representative sample of CRD simulation results. At a reactor temperature of 327 K, students discover that only feed flow rates of 0.2 to 0.7 m^3/min are achievable due to limitations of the heat exchanger. Only some fraction of their trials meets the constraint on the maximum effluent concentration of MB (dashed green line). Among those trials, the lowest operating cost is achieved for pH = 7, despite the fact that the reaction runs faster at pH 10 or 12. After characterizing reactor performance and economics at three or more reactor operating temperatures, students are asked to propose and justify a final set of recommendations for reactor operating conditions (temperature, pH, feed flow rate) in their laboratory report. There is not a unique set of "optimal" conditions, as there are several sets of parameters that provide operating costs approaching the minimum achievable; students must therefore justify their decisions.

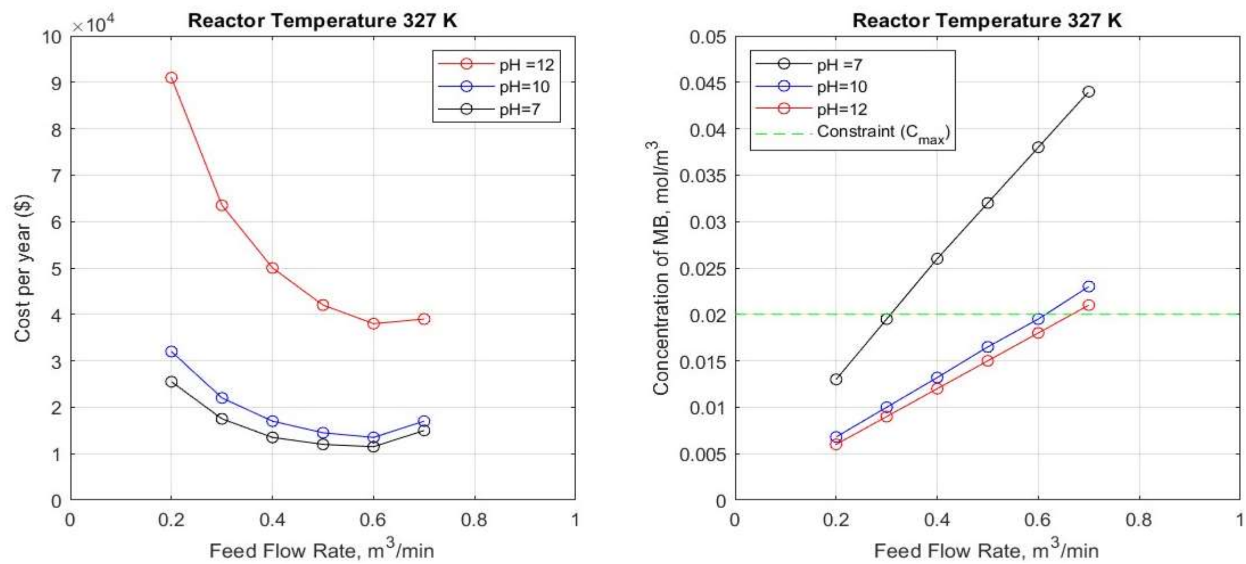

Figure 5. Results from the CRD simulation characterizing CSTR performance and economics.

Fluid-Particle Transport (FPT) Module

This module simulates transport of particles in fluidic systems, supporting a design-build-test paradigm within our senior laboratory course. Like the CRD module, the FPT module combines VR simulations with experimentation in the physical laboratory. The FPT simulations provide predictive capability, enabling students to design a separator device *in silico*, optimize its performance in a particle separation scenario, and subsequently fabricate/test a replica in the laboratory. The VR simulation works in tandem with MATLAB scripts and COMSOL Multiphysics® simulations of fluid flow to predict transport of particles in a liquid stream flowing through two-dimensional, maze-like architectures at low Reynolds number. The mazes could serve as prototypes for passive microfluidic separators, or they may be taken as models of flow in porous media (e.g., the channels in filtration membranes).

Students are asked to separate a mixture of large, spherical particles (color coded red) and small, spherical particles (color coded green) by passing them through a maze-like structure of their design. Students may opt to design a maze that captures the larger particles (filtration maze) or one that splits a mixed particle feed stream into red-rich and green-rich effluent streams (splitter maze). Fig. 6 shows simulations of both types of mazes. Neutrally buoyant particles are generated at the top edge of the maze, and the fluid flow carries particles downward in each case. The user controls the number and size of each type of particle generated. When particles exit the lower edge of the maze, they are regenerated above the maze and recycle through the system. Thus, the simulations embrace some aspects of a multistage separation process.

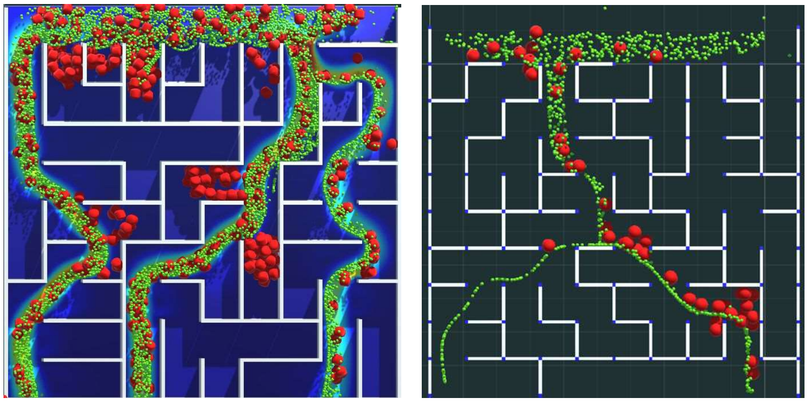

Figure 6. Simulation of fluid-particle separations in maze-like structures. Left: a maze designed to filter out larger particles. Right: a maze designed to split particles into streams with different compositions. Fluid flows downward in both cases.

The iterative design and testing process is summarized in Fig. 7. An initial design for a maze can be generated randomly using one of several available algorithms,[34] or it can be drawn up manually. Using custom MATLAB scripts, the maze structure is converted to two file formats: a *.DXF graphics file that can be imported into COMSOL, and a "maze directions" text file that can be read by the Unity3D package. The velocity profile for fluid flow in the empty maze is found using COMSOL Multiphysics®. Fluid velocity profiles are fitted to fourth-order polynomial expressions by curve-fitting in MATLAB, generating coefficient matrices that are imported into Unity to guide particle motion through the mazes. Simulations of fluid-particle flows through the mazes are generated in VR by applying forces to the particles that are consistent with the velocity profiles. A MATLAB utility program allows students to rapidly iterate on their initial design after observing the simulation results. Once a student team is satisfied with the design of their separator, the design is converted to a stereolithography (*.STL) file using NX software. Finally, a three-dimensional replica of the maze is 3D printed in poly(lactic acid) for testing in the physical laboratory.

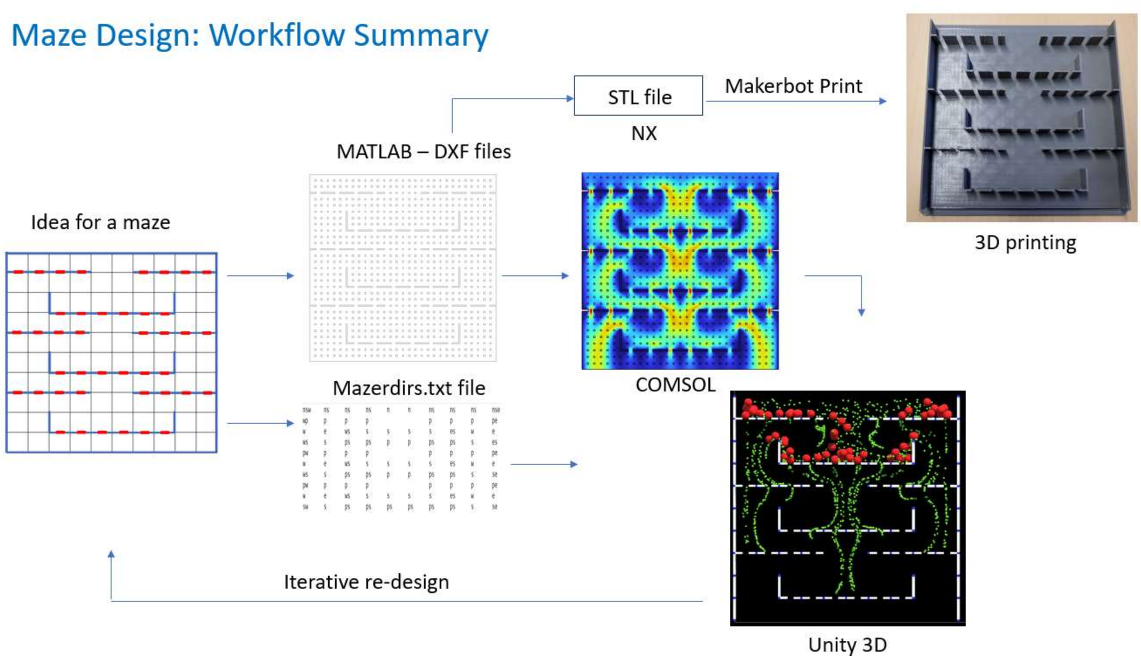

Figure 7. Workflow for iterative design, simulation, and 3D printing of a student maze design.

A laboratory apparatus for physical testing of the mazes was recently constructed, which allows 3D printed mazes to be inserted and removed from a slotted fluid flow channel. To maintain low Reynolds number flow ($Re \approx 0.1$), we chose silicone oil (dynamic viscosity 1.0 Pa·s) as the fluid. Gravity-driven flow is achieved by feeding silicone oil to the top of the apparatus via peristaltic pump. A flow restrictor at the exit of the apparatus controls the fluid flow rate and enables a steady-state liquid level to be maintained at a level above the maze. The particles, which should be neutrally buoyant, are high-density polyethylene (HDPE), which has nearly the same mass density as the fluid. HDPE particles were selected from commercially available flow visualization particles or injection-molded spheres. One unexpected complication encountered is that the densities of the fluid and the particles must be closely matched; slight differences in density produce noticeable buoyancy effects.

The first round of student maze tests with the flow apparatus was conducted in early 2025. Generally speaking, the physical experiments did not validate the results obtained from predictive simulations, although several of the student groups did observe size-based separations in their experiments. In their final project reports, students were asked to comment on the differences between simulations and experiment, and to explain observations based on potential contributing factors such as buoyancy forces and inertial forces that can impact particle separation mechanisms.

Findings

Implementation of VR modules in educational settings requires that the technology is accessible to all students and therefore, does not depend upon students owning specialized hardware or operating systems. VR experiments can be distributed to students as an executable file in a desktop/laptop screen format that does not require any additional hardware. In a remote education situation, these distributable VR experiments can replace experiments in the physical laboratory. Our VR modules were initially developed in desktop/laptop format, either for distribution during the pandemic (CPDC and CRD) or due to license restrictions on some components of the software suite that complicate distribution to students (FPT). We are presently developing a fully immersive version of the CRD module for use on a single workstation with a headset for in-person education.

A significant challenge encountered is the inability to foresee the CPU and GPU capabilities of every student's computer. Despite efforts to design the software to consume minimal resources, our first pilot test of the software with a group of 52 students revealed that approximately 10 % of the students' laptop computers struggled to run the executable files due to CPU or GPU limitations. This issue was addressed by forming teams of up to four students who were able to run virtual experiments together on a single computer, either in-person or through web-based video conferencing.

Another challenge was the variability in the GPU or CPU speeds of the user's machines. The VR simulations run in a discrete, frame-by-frame sense. Faster computers (e.g., gaming machines) therefore can produce faster process dynamics by achieving a higher frame rate, potentially altering the results of experiments. This issue was addressed by capping the frame rate at 60 frames per second. Provided all students' machines can achieve this frame rate, similar process dynamics are obtained on different computers, facilitating collaboration.

The reactor design module was later refactored to work in fully immersive format with headsets, which were purchased by the school and kept in the undergraduate laboratory for in-person use. With a headset, students gain three-dimensional perception of conducting the experiment in a virtual environment. However, headsets with hand-controllers pose significant challenges that must be addressed during software development. Scripts may need to be written to map the available input buttons on hand controllers to specific actions in VR. Depending on the compatibility between the game engine and the headset in question, coding to achieve optimal function of the hardware can be challenging and may require an experienced programmer. Once the application is fully functional, it is unlikely the same scripts will work with other headset models without substantial modifications. The simplest approach is therefore to ask students to conduct the experiment using compatible VR packages and headsets furnished by the school.

Another challenge posed by the use of immersive headsets is that the collection of data from the simulation may be slow or cumbersome. For example, students using a computer mouse to run the CRD simulation in desktop format were able to complete tasks substantially faster than they could with a headset and hand controllers. In desktop format, students were able to rapidly record data from the economics AR feature by taking photos or screenshots. When numerical data are transmitted through a headset instead, it becomes necessary to code a new feature that allows the results to be exported to a text file. In addition, it should be noted that some VR headset users suffer from nausea or motion sickness,[35] a risk that can be exacerbated if the experiment takes a long time to complete. These issues can be mitigated by asking students to complete just part of the experiment with the VR headset in order to gain experience, while finishing the remaining trials in desktop format.

Assessment of student learning outcomes from VR laboratory experiments was conducted via laboratory reports after in-person education resumed following the pandemic. Student teams were asked to perform one VR experiment and two or three physical experiments in the same semester. Laboratory reports concerning VR experiments were of similar or better quality than reports received from the same students after conducting physical laboratory experiments, an improvement that was attributed to students' ability to run (or re-run) additional experimental trials at home to continue learning after laboratory hours ended. However, we observed that students were less thorough about analyzing sources of experimental uncertainty or estimating error bars when the data were sourced from a computer simulation. When surveyed about their self-assessment of learning through VR experiments vs. physical experiments, students overwhelmingly recommended that one VR experiment should be made available in the laboratory course, but that it should be optional, rather than required.

Conclusions

Three VR modules have been developed for laboratory education to address the subjects of process control, chemical reactor design and scale-up, and transport in fluid-particle systems.

Three different pedagogical approaches were explored: stand-alone VR experiments (CPDC), VR simulations that build upon physical experimentation (CRD), and predictive VR simulations that enable a design-build-test paradigm (FPT). A crucial outcome was that students were able to conduct experiments remotely during the pandemic when the physical laboratory was inaccessible. The VR modules continue to be an important component of our in-person laboratory courses. For in-person education, hybrid approaches involving synergistic VR simulations and physical experiments enhance laboratory course outcomes, rather than sacrificing hands-on experience, providing an efficient means to link laboratory experimentation with design and scale-up concepts.

Acknowledgements

We gratefully acknowledge the Teaching and Learning Collaboratory at RPI (https://undergrad.rpi.edu/teaching-and-learning-collaboratory) for supporting the Virtual Chemical Plant project under a 2019 seed grant. We would like to thank Dr. Corey Woodcock for assisting with the 3D printing process and William Marshall and Alex Guo for preparing the initial maze generation scripts in MATLAB.

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