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VIRTUAL CATALYTIC REACTOR LABORATORY

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INTRODUCTION

A virtual catalytic reactor laboratory (VCRL) experiment was prepared as a replacement for or complement to a physical laboratory (PL) or as a longer assignment/project for a kinetics/reaction engineering course. This VCRL, which can be used in all modern web browsers for desktop and laptop computers, is available at https://virtual-labs.learncheme.com/catalytic-reactor/. The VCRL aims to imitate a hands-on PL for a gas-phase, catalytic reaction ($A + B \rightarrow 2C$). Students can vary the pressure and molar feed flow rates of the reactants, and the VCRL displays the corresponding effluent composition. Students are expected to use nonlinear regression to obtain kinetic parameters for a Langmuir-Hinshelwood rate expression.

The VCRL interface is an interactive equipment diagram that mimics a laboratory-scale catalytic reactor experiment. Students can left-click on mass flow controllers (MFCs) and a pressure controller to adjust reactor inlet conditions, or right click on various pieces of equipment to display articles describing their function. Documentation describes how to acquire data and how to analyze data using nonlinear regression. The documentation also includes post-lab questions, learning objectives, relevant assumptions, safety considerations, and a video of a physical catalytic reactor. Students are allocated a fixed amount of virtual money, and each experimental run uses some of those funds. Students, as individuals or as part of a group, create a login so they can save their data, which can be downloaded as a spreadsheet. Each student or group has a different set of randomized kinetic parameters. Instructors have a portal where they can view their students' kinetic parameters and the answers their students submit.

COMPARISON OF VIRTUAL AND PHYSICAL LABORATORIES

Some advantages that virtual laboratories (VLs) have over PLs include:

- **Availability at any time and location:**[1] Students can analyze initial results and then plan additional experiments that can be run over multiple days; PLs are location and time-limited.[2]
- **Availability to students worldwide**: VLs provide access to students who may not have access to laboratory facilities and to students who are learning remotely,[3] perhaps due to a pandemic.

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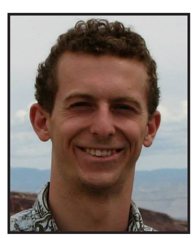

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- **Ability to run experiments that are too time consuming for a PL**: [1,4] Procedures that would each take many minutes in a PL take a few seconds in a VL (furnace reaching a desired temperature, a reactor reaching steady state, a gas chromatograph (GC) analysis). Students can repeat an experiment more easily.[5]
- **Cost-effectiveness**: VLs are less expensive than PLs and easier to maintain.[3]
- **Multiple simultaneous users**: Unlike a PL, many students or groups of students can use a VL at the same time.[3]
- **Ability to update**: The developers can update the VL based on student (and instructor) feedback, allowing for continuous improvement.
- **Ability to make abstract phenomena more visible**: [5] for example, charge flow in an electric circuit, or light rays in an optics experiment.[6]
- **Increased safety**: VLs provide the ability to safely expose students to hazardous techniques that are not available otherwise.[4] Also, different conditions can be tried without the risk of damaging equipment.[3]

Because PLs have constraints (safety, logistic, material), instructors often provide directed procedures that limit students' construction of experimental procedures. Thus, some PLs may not achieve all their learning objectives.[7]

deJong et al.[6] reviewed literature that compared VLs and PLs and concluded that for acquiring conceptual knowledge, VLs can replace PLs; many studies reported no differences in learning outcomes and student performance between VLs and PLs. Altalbe[8] cited a number of studies where student conceptual understanding was as good or better in VLs. Hernandez-de-Menendez et al.[3] also concluded that VLs can replace PLs, but they pointed out advantages and disadvantages of each type of laboratory. They claimed the main disadvantages of VLs are that mentoring is not possible and students cannot touch equipment. However, video conferencing software (ZOOM®, Google Meet™, GoToMeeting®) should allow faculty to mentor students, and other studies suggest tactile information is not needed to develop conceptual knowledge.[6] Instead, manipulation, not physicality, may be important for instruction.[5] Studies that favor PLs are based mostly on student perception.[3] Corter et al.[9] concluded that learning outcomes are roughly equivalent no matter the format. They stated that the majority of comparative studies concluded that VLs are a good substitute for PLs to teach concepts and their applications, and the design of the simulation is responsible for the learning differences reported in different studies. Indeed, the quality of VLs differs significantly between studies. The Physics Education Technology (PhET) project reported that students had a strong preference for VLs over PLs.[10] They found that students could visualize complex phenomena and test their understanding of scientific concepts more easily than with PLs because students were not merely attempting to replicate an expected result.

Comparative studies have been conducted over a wide range of disciplines. Physics VLs and PLs were found to be equally effective at promoting understanding of concepts and better than instruction without any laboratory.[11] In a biology course, fewer students received D's or F's after using VLs.[4] Finkelstein et al.[12] found that circuits VLs can be more effective than PLs. Students who used a simulation were able to build a real circuit faster than students who used a PL, and VL students performed 12 percentage points better on the exam. In contrast, Alfred et al.[2] reported identical cognitive outcomes for PLs and VLs in a circuits laboratory, but students who used a PL could subsequently construct circuits faster. Holmes and Wieman [13] showed that physics PLs made no difference in performance on final exam questions; they attributed this to the lack of decision making by students in the labs. Learning objectives of PLs can often be met by VLs alone or by using hybrid approaches.[3, 14]

The VCRL incorporates some aspects of the Virtual Bio-Reactor Laboratory,[15] which is a browser-based simulation that can serve as a replacement for a physical bioreactor experiment. This VL assigns different parameters and allocates a fixed amount of virtual money for each student or group. Fogler[16] has prepared a number of reactor simulations that include a quiz where students are expected to input different reactor conditions in order to determine kinetic parameters. These simulations, although not browser-based and not as user-friendly as the VCRL, provide different parameter values for each student, and a large number of simulations are available. Sartorius has a Virtual Bioreactor Training Tool that is freely available to universities and may serve as a VL.[17] Their two bioreactor simulations are realistic, since they model their commercial batch and fed batch reactors and provide the ability to change many parameters.

OVERVIEW OF VIRTUAL CATALYTIC REACTOR LABORATORY

The VCRL models an exothermic, gas-phase, catalytic reaction ($A + B \rightarrow 2C$) in an isothermal, packed bed reactor. Pressure drop is assumed to be small across the reactor, which is modeled as a plug flow reactor. The goal is to determine the values of k, K_A, and K_B and their 95% confidence limits for the Langmuir-Hinshelwood rate expression, shown in Equation (1):

$$r = \frac{kP_AP_B}{(1+K_AP_A+K_BP_B)^2} \qquad (1)$$

where P_A and P_B are the partial pressures of A and B, k is the rate constant, and K_A and K_B are adsorption equilibrium constants. The VCRL home page displays a login, an overview, prerequisites, and the following learning objectives:

- Explain the function of each part of the catalytic reactor system
- Understand how flow rates into a packed-bed reactor (PBR) affect reactants' conversions
- Understand the effect of pressure on the rate of a gas-phase, catalytic reaction
- Efficiently select reaction conditions for PBR measurements
- Explain the reasons that experimental conditions were chosen
- Apply nonlinear regression to determine kinetic parameters and their 95% confidence intervals
- Answer questions about PBR behavior

The instructors' portal contains additional information on the laboratory procedure, examples of typical results, a way to access their students' data (including the kinetic parameters assigned to each student (or group) and the answers their students submit), and an option to run the simulation from a student's perspective. Instructors can request an account by emailing LearnChemE@gmail.com.

The VCRL interface contains documentation (Figure 1) that explains how to get started, how to analyze data, and how to submit kinetic parameters (and confidence intervals) upon completing the lab. Students can log into the VCRL under an instructor's name, as an individual, or as part of a group; they choose a password when they first log in. The simulation stores students' data so experiments can be performed over multiple sessions.

When a student or group creates an account, the VCRL selects a random temperature and kinetic parameters; each student or group has different parameters. Individual students or groups are allocated virtual money ($10,000), and each experimental run (each time the multi-selector valve sends a sample to the GC) debits their account $250. Instructors can base part of the student grade on the funds remaining in their

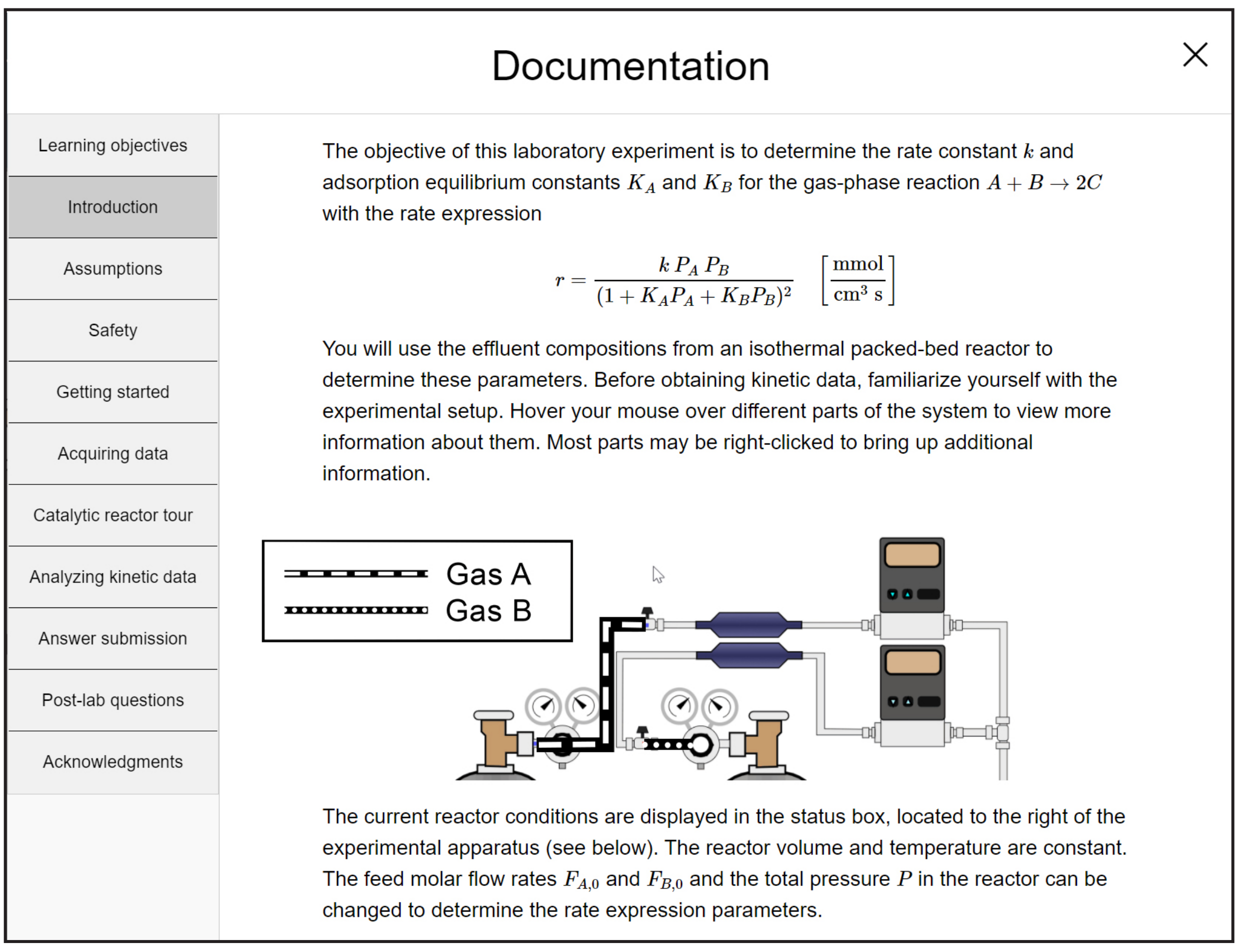

Figure 1. Documentation page that introduces the VCRL and provides resources for using it.

account. Each time a student logs in, the reactor system in Figure 2 is displayed. Students must start up the equipment. Clicking "start up reactor" does the following:

- Displays a message stating that start up is accelerated in the VL compared to a PL
- Debits their account $125
- Opens the carrier gas valve
- Turns on and calibrates the GC
- Opens the feed gas valves and closes the reactor bypass valve
- Increases the sand heater temperature to the desired value
- Allows the system to reach steady state

All aspects of the startup are much faster than in a PL in order to save time.

RUNNING THE VCRL

Figure 3 shows the VCRL after startup. Tooltips appear when a mouse pointer hovers over a piece of equipment; right-clicking the equipment opens a link that contains more information about the equipment. Not all equipment is drawn to scale; e.g. the sample loop volume is exaggerated so it is easier to see. A typical sample volume in a PL is 1 cm^3. To take a measurement, students adjust the MFCs and pressure controller by left-clicking on them and typing desired values into the input boxes. They then click the multi-selector valve to push the sample to the gas chromatograph (GC) and click the GC to view the effluent composition. Students should plan their experiments since changing either of the molar flow rates (A, B) or the reactor pressure will change effluent molar flow rates. Operating the VCRL is similar in many ways to operating a corresponding PL. In a typical PL, the furnace temperature, the pressure, and the MFC values are set on a computer, the multi-selector valve is computer controlled, and the GC results are analyzed by a computer.

When a MFC flow rate is changed, the VCRL briefly displays the statement "reaching steady state." Red and blue lines represent the feed gases, which mix to form a purple gas that then passes through the preheater coil, the reactor, and the sampling loop before exhausting to the vent. When the multi-selector valve is toggled by left-clicking it, an animation shows the reactor effluent traveling into the GC and the green helium carrier gas flowing through the sample loop (Figure 4). A representative chromatograph is displayed on the computer above the GC. Students must left-click the multi-selector valve again to move it back to the sampling position to collect the next sample. Data can be downloaded as a comma-separated values (CSV) file that can be opened using a spreadsheet.

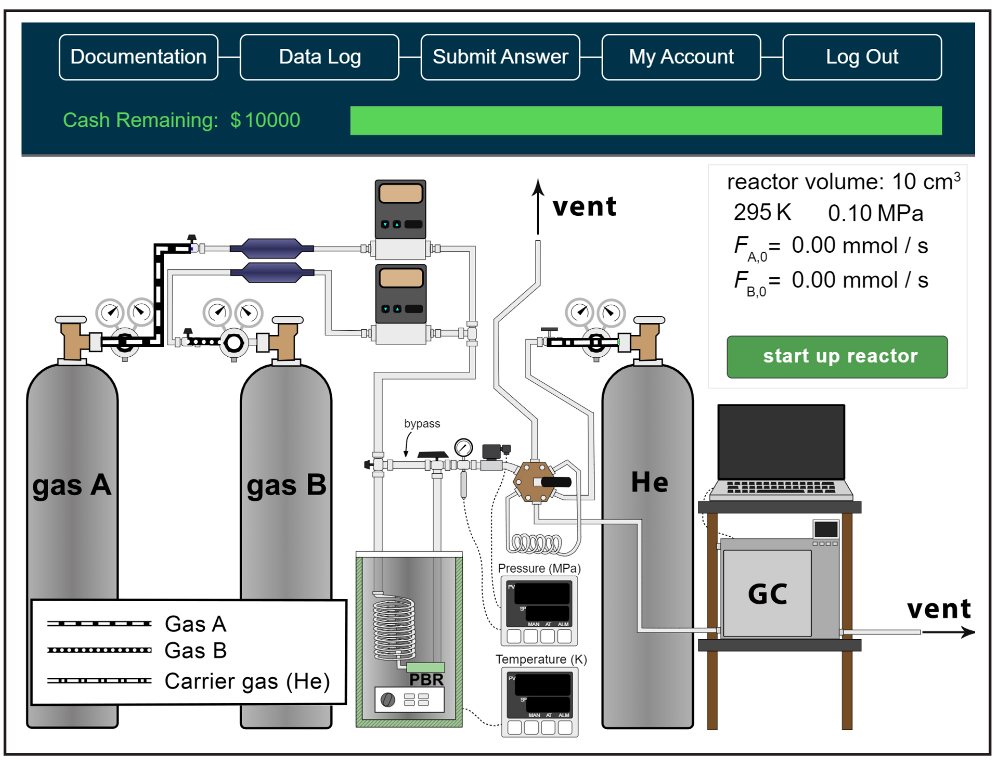

Figure 2. *Main page in VCRL before start up. The valves after the regulators are closed (in the actual VCRL, red, blue, and green colors indicate sections of the lines that contain gas), the sand batch heater is at room temperature, and the GC is turned off.*

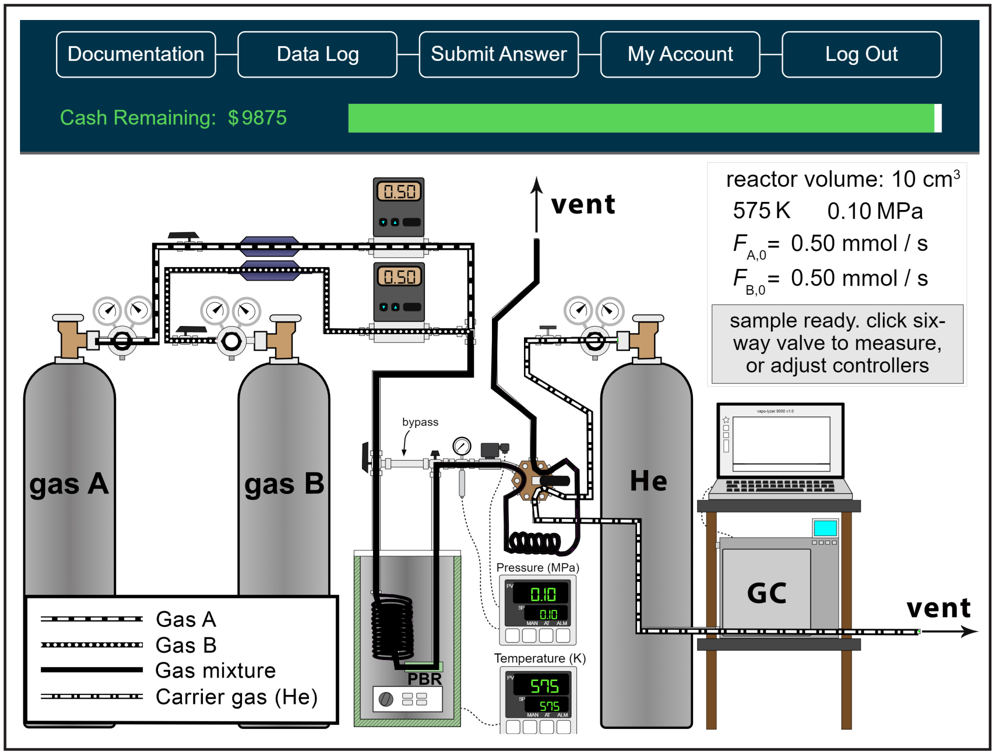

Figure 3. *Main page in VCRL after the system has started up. The gas mixture flowing through the reactor is purple in the actual VCRL, and the reactor effluent flows through the sampling loop. The helium gas line flowing through the GC is green in the actual VCRL.*

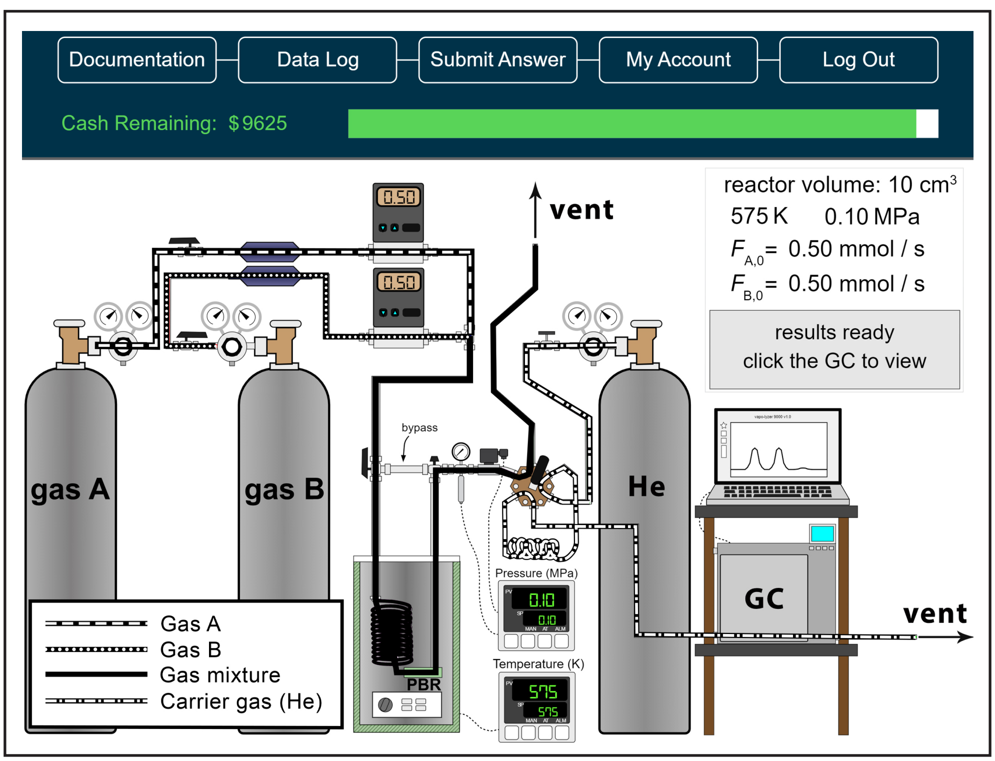

Figure 4. *Main page in VCRL after injecting gas in the sample loop into the GC.*

Students can work in groups, with each student logged onto the VCRL at the same time; they each can run experiments independently, and within a few seconds, their data will show up on the data log for the other students to see. Alternatively, one student can log in and share his/her screen with group members using conferencing software. They can then jointly plan experiments. This is similar to many PLs where one student makes changes in the equipment and others record data, make suggestions, and discuss the results.

DATA ANALYSIS

Three screencasts in the Documentation explain Langmuir-Hinshelwood kinetics, nonlinear regression, and the approach used to analyze data from a PBR. Four more screencasts demonstrate the use of nonlinear regression in Microsoft Excel® spreadsheets to analyze kinetic data. The Excel spreadsheets are available at http://www.learncheme.com/student-resources/excel-files. The spreadsheets solve the differential-equation mass balances numerically and apply nonlinear regression to the parameters used in the mass balances. Spreadsheets were used to demonstrate nonlinear regression because spreadsheets are widely available, but other software (Mathematica®, MATLAB®, Python®) can also be used.

SUMMARY

A virtual catalytic reactor laboratory (VCRL) that runs in most browsers was created and made available online. Each student or group of students is assigned a different set of kinetic parameters that they must determine by running the reactor at different pressures and with different flow rates of reactants. The VCRL has extensive documentation and screencasts that explain catalytic mechanisms and how to carry out nonlinear regression. The VCRL was made available near the beginning of the Fall 2020 semester, and currently 21 instructors at other universities have accounts. During the fall semester, seven of those instructors had a total of 196 students who created accounts and collected data.

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