

The Oxidation of Iron: Experiment, Simulation, and Analysis in Introductory Chemistry

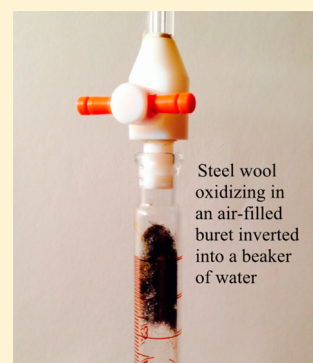
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S Supporting Information

ABSTRACT: In this exercise, an actual chemical reaction, oxidation of iron in air, is studied along with a related analogue simulation of that reaction. The rusting of steel wool is carried out as a class effort. The parallel simulation is performed by students working in small groups. The analogue for the reacting gas is a countable set of discrete marble “atoms.” The iron is represented by a strip of tape. This combined exercise is designed to be done at the beginning of the school year. No prior chemical knowledge is required for gathering, plotting, and comparing the raw data sets. Data obtained show comparable trends for decreasing rate of reactant consumption with real time and simulated time. The simulation offers a reference point for discussion of aspects of the real system. Analysis of the raw data is presented that can be carried out later in the year, if desired, by more advanced students, as a kinetics example. When worked up, the simulation data yield linear first-order plots and the results from the real system generally do as well.

KEYWORDS: First-Year Undergraduate/General, Demonstrations, Laboratory Instruction, Hands-On Learning/Manipulatives, Analogies/Transfer, Inquiry-Based/Discovery Learning, Kinetics, Rate Law, High School/Introductory Chemistry



Steel wool oxidizing in an air-filled buret inverted into a beaker of water

OVERVIEW

Oxidation of iron and other metals represents a cost of hundreds of billions of dollars, about 4% of GDP, for the United States annually.¹ H. Alyea,² in a basic look at the important and familiar case of iron rusting, inverted a test tube, containing only a plug of dampened steel wool, into a beaker of water and monitored the rise in water level as the steel corroded. Here, a buret replaces the test tube. In conjunction with the actual reaction, run as a class experiment, an analogue simulation, using marbles for air and a strip of tape for steel wool, is carried out by students working in small groups. Two plots are prepared from the raw data obtained: consumption of oxygen with time and consumption of marble “atoms” over simulated time.

Analogue simulations are used often in science education. Examples discussed in this journal involve using marbles in the study of thermal energy transmission³ and in a simulation of Rutherford’s atomic scattering experiment.⁴ Harsch,⁵ in a general study of the use of marbles in kinetics simulations, associates time units, as this paper does, with marble movements according to a given model’s scheme. In the example here, each placement of marbles on the “reactive” surface represents a time interval. Pedagogically, he notes that, for maintaining interest, simulation “games” are better performed by students in small groups, as is done here, than by individuals working alone.

Recently, Pergiovanni⁶ presented a simulation–experiment combination, analogous in organization to the current work, where molecular adsorption was studied as an experiment and

also by using an analogical model employing LEGO blocks as molecules.

EXPERIMENTAL DETAILS

Fine steel wool was purchased at a hardware store. While grade 0000 was used for the data in this article, 00 also works well. A plug of the material with a mass of about half a gram was moistened with DI water and patted to near dryness. The volume of air used was approximately 50 mL. Others^{7–9} have mixed acetic acid with the wetting water to accelerate the reaction. The wool was placed in the buret at the stopcock end. The buret was then inverted into a large beaker containing 600 mL of deionized water and clamped in place. The water level in the buret was initially adjusted onto the graduated scale using the stopcock and the information was recorded. This setup produces a system stable for a week or so. No corrections were made in the raw data collected for pressure and temperature variations, as the experiment assumes the beginning students have no knowledge of the gas laws. For the simulation, marbles of various colors were found at local stores. The reaction container is a shoebox, into which the marbles were poured. Figure 1 is a photograph taken during the running of the simulation.

HAZARDS

The steel wool can be safely handled without danger of cuts. Gloves may be worn as bits of the metal do come loose. Goggles should be worn as well and caution taken to keep



Figure 1. Marbles in simulated reaction poured from a bag and settled into a shoebox. White marbles represent oxygen. Orange marbles represent the portion of air not involved in the reaction. The strip of tape running down the center represents the steel wool. Here, a group would select the six white marbles that sit on the tape as having reacted. They would be set aside and the remainder of the marbles put back into the bag, shaken, and then poured again into the box. Each pour represents a simulated day.

hands away from eyes. Managing the glassware, particularly the buret, deserves normal laboratory care. Caution should be taken to minimize the likelihood of large numbers of marbles spilling in the lab.

■ OXIDATION OF IRON IN AIR: THE REAL SYSTEM

The beaker–buret setup was left in the lab and referred to for a new volume data point periodically as the reaction proceeded. One setup can be used for several classes. Figure 2 shows data from two contemporaneous runs followed for 8 days. The decrease in the rate of gas consumption over time is clear.

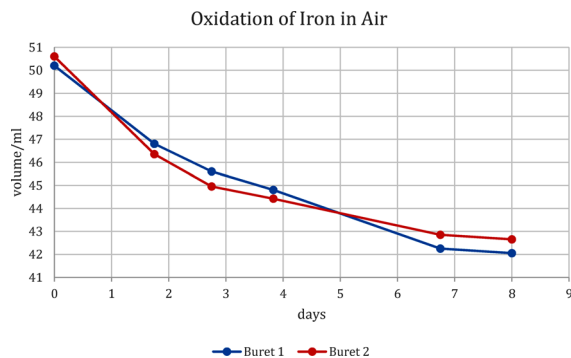


Figure 2. Volume over time of confined quantities of air in two burets as samples of steel wool oxidize. The setups ran concurrently. The volume of oxygen in each sample is between 10 and 11 mL. The decrease in volume indicates consumption of oxygen. Days five and six were a weekend. Points are connected by line segments.

■ OXIDATION OF IRON IN AIR: THE SIMULATION

Each small group was given 100 “air” marbles, 20 of which were white, representing reactive oxygen and the other 80, which were orange, stood for the unreactive portion of the air, mostly nitrogen. The rounding to air being 1/5 oxygen was done to help manage the distribution of 400 marbles. Each group’s marbles were placed in a bag and shaken. They were then poured into an open box that was tilted slightly to let the

marbles settle into a single layer at one end. The tray had a strip of tape running down its middle, sticky-side down, that represented a strand of steel wool. White oxygen marbles settling on the tape strip, were considered to have reacted. Figure 1 shows the setup after one pour out of marbles into the box. Six white marbles are counted as having reacted. That number of white marbles was then removed from the sample. All other remaining marbles were placed back into the bag. The bag was shaken and the process repeated, with each round taken as one “day” of rusting. Data collection was cut off after five “days” when only a few oxygen marbles remained. Plots were made of the number of white marbles remaining versus “days.” Group results were combined into class plots. Results for four classes, a total of 400 marbles in each case, are presented in Figure 3. Analogous to the real system data in

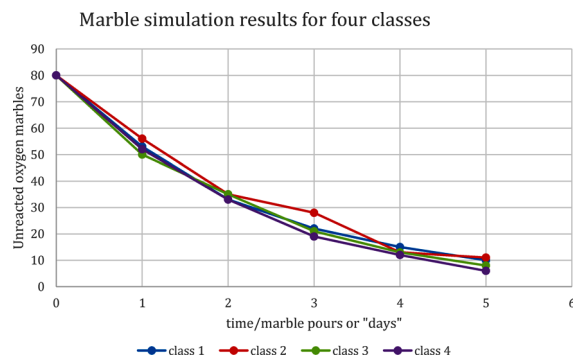


Figure 3. Results of marble simulation for four classes. $N = 400$ marbles for each plot. Points are connected by line segments.

Figure 2, the rate of marble reaction decreases monotonically with “time”. Additional data for individual small groups, with $N = 100$ marbles, is presented, for comparison, in the Supporting Information.

For beginning students, the exercise entailed only the gathering of data to generate and discuss the similar profiles of the real and simulated oxidations. As an option, the data can be revisited later in the year, by advanced students, for the analysis given below, once kinetics has been covered in detail.

■ OPTIONAL ADVANCED WORK

This experiment and simulation have been used at Friends Seminary with two groups of students. For the average introductory set of sophomores, only the work described thus far was carried out. Another group, mostly seniors, the Advanced Chemistry students, nearly all of whom were also in AP Calculus, was able to successfully navigate the analysis given below. When this work is done later in the year, students will be familiar with kinetics concepts.

Studies of this reaction by Gordon and Chancey,⁹ Birk, et al.⁷ and Wilson¹⁰ indicate that the oxidation proceeds as a first-order process in oxygen at pH of 7 or less. To check on agreement with these authors for the system and its simulation, parallel concentration units were developed for oxygen gas and “oxygen” marbles. Graphs of log of concentration versus time and simulated time were then generated.

In the simulation, the marble atoms are countable, and the fraction of reactive marbles remaining in the sample is the concentration unit, calculated as shown in eq 1. In this formula, the cumulative total of oxygen marbles removed is labeled “O marbles reacted.”

fraction O marbles

$$= \frac{\text{initial O marbles} - \text{O marbles reacted}}{\text{initial total marbles} - \text{O marbles reacted}} \quad (1)$$

A parallel equation can be written for the fraction of O₂ molecules, eq 2,

fraction O₂ molecules

$$= \frac{\text{initial O}_2 \text{ molecules} - \text{O}_2 \text{ molecules reacted}}{\text{initial total air molecules} - \text{O}_2 \text{ molecules reacted}} \quad (2)$$

The O₂ molecules are not countable, but since Avogadro's Law holds for the gas, the number of molecules is proportional to its volume. It follows also, that the number of moles is proportional to the gas volume. Any proportionality constant would cancel for each term, leading to the volume fraction of O₂ being equivalent to the mole fraction of O₂ in the sample. The volume of air consumed is taken as the volume of O₂ reacted. This yields eq 3,

$$\text{mol fraction O}_2 = \frac{\text{initial volume O}_2 - \text{volume O}_2 \text{ reacted}}{\text{initial volume air} - \text{volume O}_2 \text{ reacted}} \quad (3)$$

The unitless concentrations of eq 1, fraction of O marbles, and eq 3, mole fraction O₂, are used for the analysis. The initial volume of oxygen was taken as 21% of the air volume. As indicated earlier, in the simulation, the "air" was taken as simply 1/5 oxygen, or 20 reactive marbles per 100. Logarithmic plots were made of the two sets of data in Figure 2 and the four sets of simulation data in Figure 3.

Figure 4 presents logarithmic plots of [mole fraction(O₂)] vs time derived from the two data sets in Figure 2 individually and

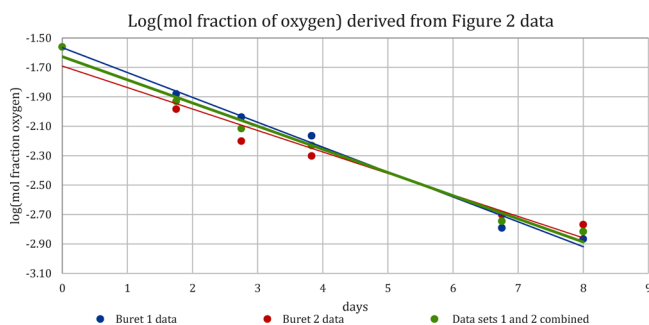


Figure 4. Thin lines are for values derived from data in Figure 2. $r^2 = 0.99$ for the buret 1 data and $r^2 = 0.96$ for the buret 2 data. For the combined data, the two sets were collected concurrently, and a thicker line is shown. For this line, $r^2 = 0.99$.

in combination. The individual data sets give correlation coefficients, r^2 values, of 0.96 and 0.99. When they are combined, they were collected at the same time in side-by-side burets, an r^2 value of 0.99 is obtained. The combined plot yields a half-life of just over 4 days. Other runs at Friends yielded half-lives varying from three to 8 days. Additional runs are presented in the Supporting Information that also show significant variation in half-life. Also, in the appended information is a discussion of why the rate of this complex multiphase reaction might be likely to vary from sample to sample and run-to-run.

Figure 5 presents logarithmic plots of [fraction of oxygen marbles] vs simulated time, using eq 1 applied to the data sets for classes 1–4, presented in Figure 3. They give correlation

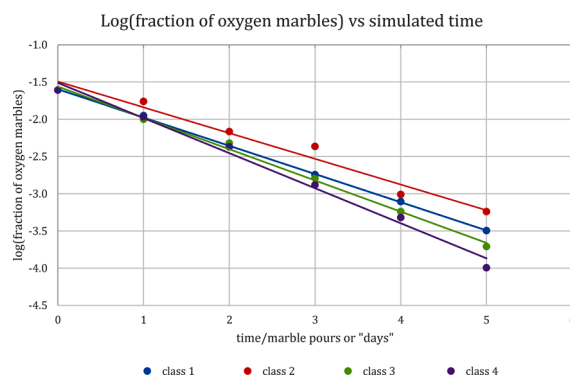


Figure 5. Log plot of the data sets in Figure 3, employing eq 1 concentration units. r^2 values are 1.00 for class 1, 0.97 for class 2, 0.99 for class 3, and 0.99 for class 4. $N = 400$ for each plot.

coefficients, r^2 values, of 1.00, 0.97, 0.99, and 0.99, respectively. The marble simulation involves an arrangement that approximates first-order kinetics in that the number of white marbles "reacting" will be proportional to the fraction of white marbles present. While pouring is imperfect, as Figure 1 shows, and the marble level in the box drops a bit with each new pour, with enough groups of students working, the shape of the simulation plot does follow the pattern of the actual oxidation.

FINAL COMMENTS

The goal of this combined reaction–simulation exercise is to present, a week or two into the school year, an example showing the explanatory utility of picturing a dynamic reaction system as a set of discrete atoms. The simulated oxygen consumption data, obtained by students from a countable number of marble atoms, is shown to relate graphically to the observed trend in the real iron–oxygen system. In the author's view, this is a valuable correspondence. Analysis of the data is presented that has been successfully carried out by Advanced Chemistry students, later in the year, when kinetics has been covered. In this analysis, the close parallel between eq 1, for marbles, and eq 2, for molecules, captures the thinking underlying the development of this combined exercise.

ASSOCIATED CONTENT

Supporting Information

In the accompanying file are a student handout for the lab and some instructor notes. Also, data on a number of additional experimental runs are presented, including one for the oxidation in pure oxygen. Finally, a detailed discussion is given of some important factors affecting results obtained for this complex multiphase reaction system. This material is available via the Internet at <http://pubs.acs.org>.

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Notes

The authors declare no competing financial interest.

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