Computer Science in the Chemistry Lab: An Interdisciplinary Project Involving Arduino-Based Temperature Sensors*

Brad Bauer[1], Mark Gilder[2], and Judith O'Rourke[2]
[1]Department of Physical and Biological Sciences
[2]Computer Science Department
The College of Saint Rose
Albany, NY 12203
{bauerb,gilderm,orourkej}@strose.edu

Abstract

An interactive activity was developed to connect computer science and chemistry students, allowing both groups to appreciate the applications of computer science to cross-disciplinary fields. Computer science majors are tasked with developing an Arduino system to collect and manage thermal data generated during laboratory experiments. Computer science students must employ a range of techniques .... Once the system is complete, computer science students work alongside chemistry students to implement their program within an introductory chemistry experiment. Aside from the collection, storage, and visualization of laboratory data, chemistry students benefit by gaining experience managing large data sets and an appreciation for computer science and its increasing value in the natural sciences.

1 Introduction

The study of computer science is becoming necessary and fundamental to every academic discipline [**columbia**]. An understanding of computer science concepts and techniques is critical in order to analyze and extract meaningful information from the vast amounts of data generated in fields like biology, healthcare, finance, physical sciences, and mathematics. Due to technological advancements, the ability to store and manage large amounts of data is easily accessible across all major STEM fields.

Comp Sci lead-in to Arduinos as a comp sci teaching tool.

Arduinos are also becoming increasingly common in undergraduate chemistry laboratories. They have recently been utilized to develop low-cost laboratory equipment including (but not limited to) fluorometers [**bullis**], centrifuges [**sadegh**], pH sensors [**qutieshat**], tensile testers [**arrizabalaga**], and calorimeters [**gomes**]. In the current study, arduino systems utilizing thermistors are developed for use in laboratory experiments that require measurements of temperature.

Temperature measurements provide important insight into various chemical and physical processes. By monitoring the variation of temperature of a sample as it is heated or cooled, characteristic transition temperatures such as the freezing/melting point or boiling point can be determined [**atkins**]. When considering mixtures of varying compositions, freezing point decreases proportionally to concentration. Analysis of freezing points over a full range of compositions from pure solvent to pure solute allows for the generation of two-component, solid liquid phase diagrams [**martinez**, **blanchette**]. Thermochemical analysis through calorimetry can also be utilized to determine heats of chemical reaction. When coupled with the method of continuous variations [**jobs**], stoichiometric ratios of chemical reactants or concentration of an unknown reactant can be determined [**vernier**, **vonderbrink**, **tatsuoka**, **mahoney**]. In order to capture key features in the temperature-time profiles, large numbers of data points are often collected. Due to the potentially large data sets generated over reasonably short time periods, prevalence in various introductory through advanced chemistry lab courses, and availability of inexpensive thermal probes, thermal analysis activities are a natural fit for this interdisciplinary project.

2 Application to Undergraduate Chemistry Laboratories

As a proof of concept, the authors applied the thermal analysis Arduino system to an experiment currently used in an undergraduate General Chemistry laboratory course. The objective of this experiment is to determine the optimal (stoichiometric) ratio of two reactants in a chemical reaction using the method of continuous variations [**job**]. Reactants are chosen such that an exothermic (heat-releasing) reaction occurs; the heat released manifests as an increase in the mixture's temperature. Systematically varying the ratio of these reactants and monitoring the associated temperature change (ΔT) allows for the determination of the optimal ratio in the chemical reaction by identifying the proportion that generates the largest ΔT. Two sets of reactants were chosen for this experiment: (1) sodium hypochlorite (NaClO) with potassium iodide (KI) and (2) NaClO with sodium sulfite (Na_2SO_3) [**vonderbrink**]. Other combinations including sodium hydroxide with hydrochloric acid, acetic acid, oxalic acid, sulfuric acid, or phosphoric acid, potassium hydroxide with citric acid, and sodium hypochlorite with sodium thiosulfate have been utilized elsewhere [**mahoney**, **vernier**, **vonderbrink**, **tatsuoka**].

Details of the laboratory procedure can be found in Reference [**vonderbink**], but salient details and modifications are summarized below. 0.50 M NaClO(aq), 0.50 M KI(aq), and 0.50 M Na_2SO_3(aq) solutions were prepared.[1] Nine mixtures with unique ratios of each (1) NaClO solution to KI solution and (2) NaClO solution to Na_2SO_3 solution (by volume) were prepared such that the total volume of each mixture was fixed at 50.0 mL. Components of the mixtures were kept separated until the time of the experiment. For each trial, the component available in the largest volume was added to two nested Styrofoam cups and subjected to moderate magnetic stirring. The thermistor of the Ardunio was inserted into the liquid. Temperature was monitored to ensure thermal equilibrium and a stable initial temperature. The second component was added to the first component in the cups; a button on the Arduino was pushed to record the time of mixing. Temperature of the resulting mixture was monitored for at least two additional minutes.

2.1 Determining the Optimal Ratio of the NaClO and KI Reaction

Profiles of the observed changes in temperature with time for the reactions of NaClO and KI are shown in Figure 1. All temperature changes in Figure 1 are expressed relative to the temperature of solution prior to mixing. This reference temperature for each mixture was determined as the average temperature taken over the fifteen data points prior to mixing. All profiles were shifted horizontally such that the time of mixing corresponds to $t = 0$ s. Each profile is distinguished using the ratio of mL of NaClO(aq) to mL of KI(aq).

From the data sets for each trial, a maximum temperature change (ΔT_{max}) was determined. These ΔT_{max} values were then plotted against the volume of NaClO solution present in the reaction mixture (Figure 2). In addition to the nine measured data points, two additional points corresponding to 0.0 mL NaClO(aq):50.0 mL KI(aq) and 50.0 mL NaClO(aq):0.0 mL KI(aq) were included. Since no reaction occurs at these compositions, ΔT_{max} was taken to

[1] The KI and Na_2SO_3 solutions also contained sodium hydroxide at a 0.2 M concentration. Details are provided in Supporting Information.

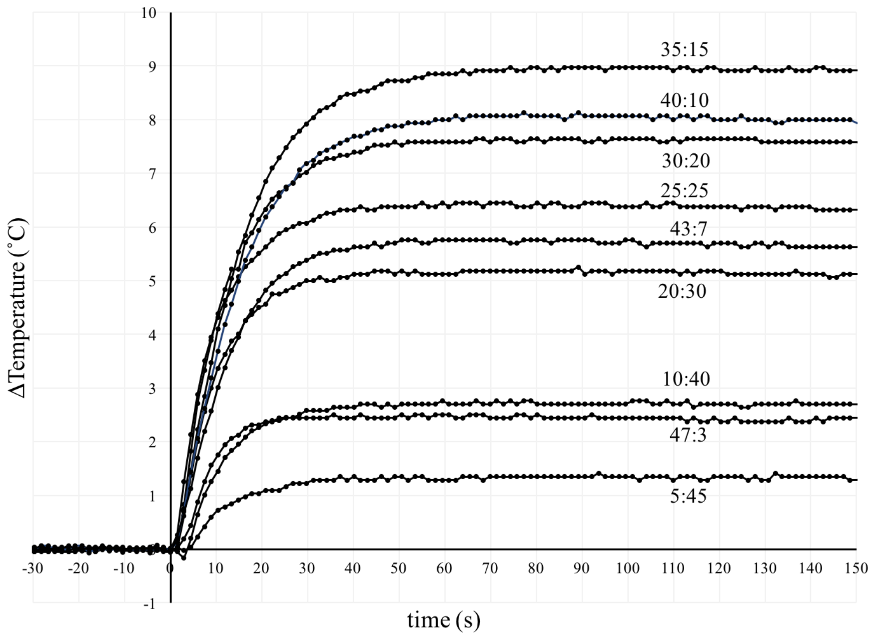

Figure 1: Variation of Temperature with Time for Mixtures of NaClO(aq) and KI(aq)

be 0.0°C for these points. Lines of best fit through points falling on increasing and decreasing ΔT_{max} with volume NaClO(aq) trends were determined.[2]

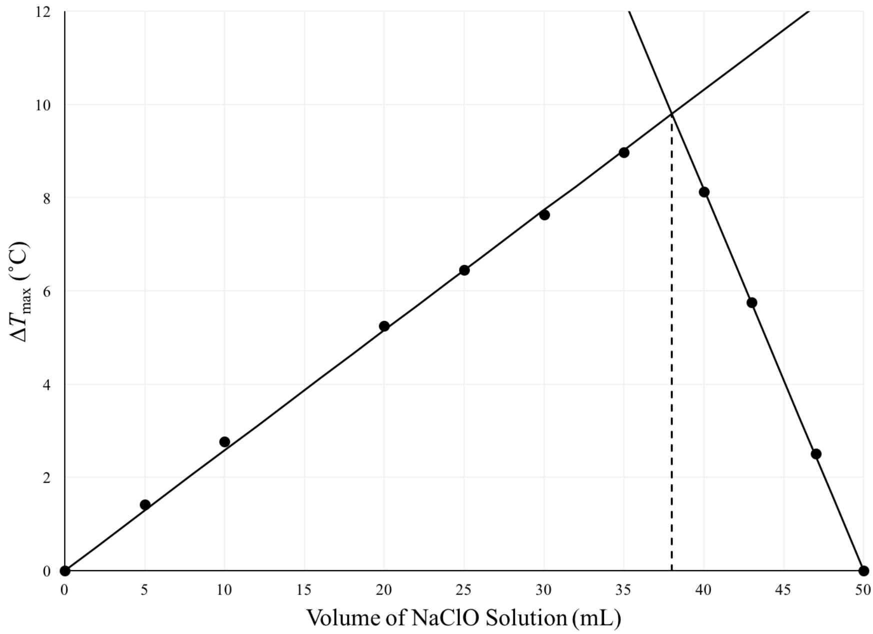

Figure 2: Maximum Temperature Changes Observed for Each Reaction Mixture of NaClO(aq) and KI(aq)

In this experimental method, the heat generated from each reaction (proportional to the ΔT_{max} observed) will increase as components react more completely. The optimal (stoichiometric) proportion of two reactants will yield the largest ΔT_{max}. By extrapolating the two linear trendlines to a point of intersection, we estimate the largest ΔT_{max} to be 9.80°C. This corresponds to an optimal ratio of 38.0 mL NaClO(aq):12.0 mL KI(aq), which is in agreement with the actual 3:1 ratio for this reaction.[3]

[2] The upward trendline was set to include the point (0.0 mL, 0.0°C). The downward trendline was set to include the point (50.0 mL, 0.0°C). The corresponding equations were $\Delta T_{\mathrm{max}} = (0.2578°\mathrm{C/mL})\ V$ ($R^2 = 0.99895$) and $\Delta T_{\mathrm{max}} = (-0.8169°\mathrm{C/mL})\ V + 40.845°\mathrm{C}$ ($R^2 = 0.99983$).

[3] Since solutions are at equal concentrations, the ratio of volumes is equivalent to the ratio of amounts used to establish the stoichiometry of the reaction. The actual stoichiometry of 3:1 is based on the net ionic equation: $3ClO^-(aq) + I^-(aq) \rightarrow 3Cl^-(aq) + IO_3^-(aq)$ [**vonderbrink**].

2.2 Determining the Optimal Ratio of the NaClO and Na_2SO_3 Reaction

The experiment was repeated using sodium hypochlorite (NaClO) with sodium sulfite (Na_2SO_3). Temperature versus time plots for the NaClO and Na_2SO_3 reactions are shown in Figure 3. All temperature changes are expressed relative to the pre-mixing temperature and times are expressed relative to the time of mixing, as discussed previously.

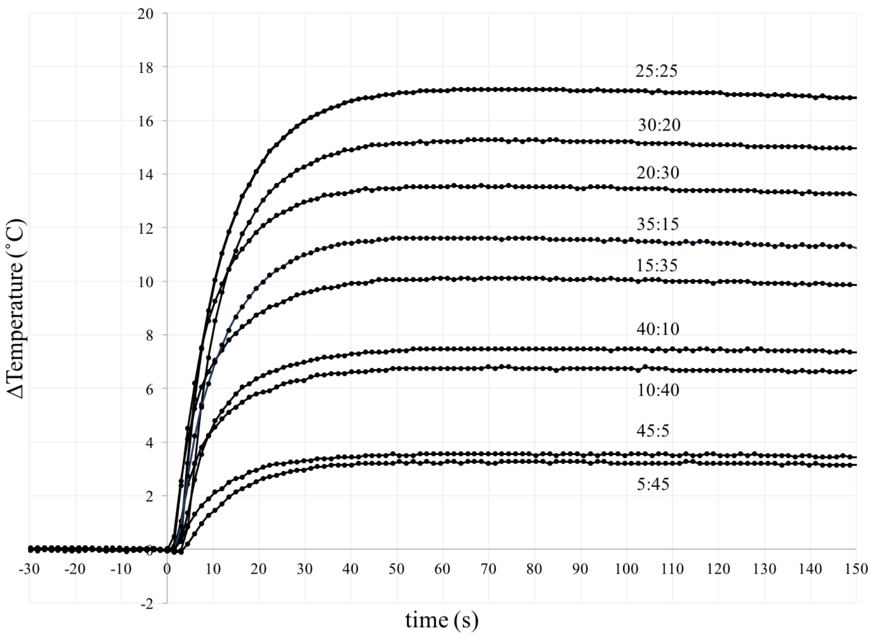

Figure 3: Variation of Temperature with Time for Mixtures of NaClO(aq) and Na_2SO_3(aq)

The maximum ΔT for each mixture was recorded and plotted against the volume of NaClO(aq) in the mixture; these results are shown in Figure 4. Points corresponding to 0.0 mL NaClO(aq):50.0 mL Na_2SO_3(aq) and 50.0 mL NaClO(aq):0.0 mL Na_2SO_3(aq) (each with $\Delta T_{\text{max}} = 0.0°C$) were included. Lines of best fit were generated through each the upward and downward trends.[4] The intersection of these lines occurs at 26.4 mL NaClO(aq)

[4]The point corresponding to 25.0 mL NaClO(aq):25.0 mL Na_2SO_3(aq) was included in the upward trend. As before, the lines were forced through the end points. The resulting

and $\Delta T_{\max} = 18.0°\mathrm{C}$. This corresponds to a predicted optimal ratio of 26.4 mL NaClO(aq) to 23.6 mL Na_2SO_3 (simplified to 1.12:1), which is in agreement with the predicted stoichiometry of 1:1.[5]

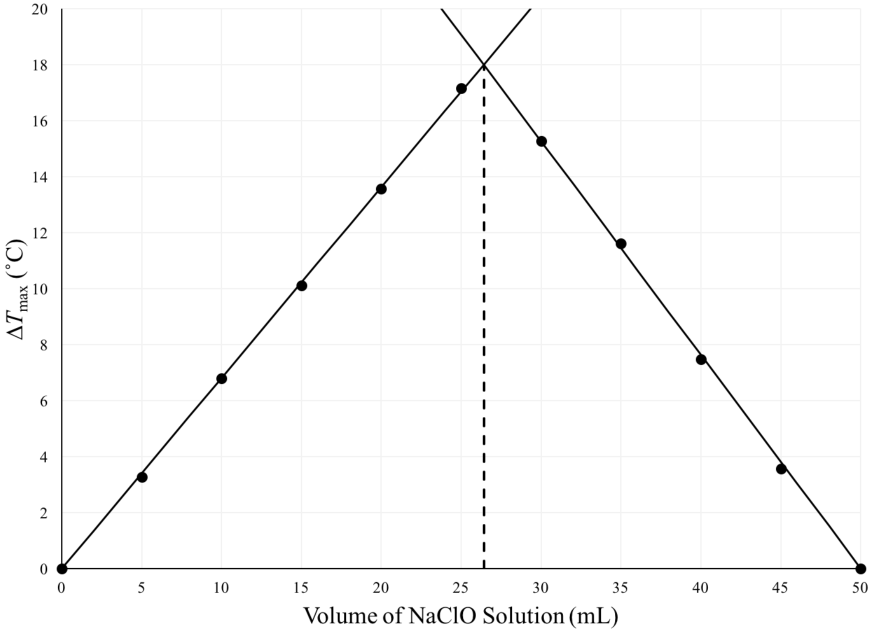

Figure 4: Maximum Temperature Changes Observed for Each Reaction Mixture of NaClO(aq) and Na_2SO_3(aq)

2.3 Improving the Accuracy of Results

The method employed above allows students to quickly and easily determine the stoichiometric ratio in a chemical reaction with minimal calculations. The determined ratios of 3.17:1 (NaClO:KI) and 1.12:1 NaClO:Na_2SO_3 were of sufficient accuracy to conclude the correct ratios of 3:1 and 1:1 when rounded to the nearest whole number. The accuracy of these ratios can be improved using some post-lab corrections. One notable correction involves the adjustment

equations of the lines of best fit are: $\Delta T_{\max} = (0.6813°\mathrm{C/mL})\ V$ ($R^2 = 0.99977$) and $\Delta T_{\max} = (-0.7629°\mathrm{C/mL})\ V + 38.145°\mathrm{C}$ ($R^2 = 0.99923$).

[5] The actual stoichiometry of 1:1 is based on the net ionic equation: $ClO^-(aq) + SO_3^{2-}(aq) \rightarrow Cl^-(aq) + SO_4^{2-}(aq)$ [**vonderbrink**].

of the initial temperature. Initial temperature was determined using only the component in the mixture with the largest volume; this assumes that both reactants are at this initial temperature. If the components are at different initial temperatures, a weighted average can be utilized [**vonderbrink**] to determine a more representative initial temperature as:

$$T_{i,\text{avg}} = \left(\frac{V_\text{A}}{V}\right) T_{i,\text{A}} + \left(\frac{V_\text{B}}{V}\right) T_{i,\text{B}}$$

where V_A and V_B represent the volumes of components A and B in the mixture, V represents the total volume of the mixture, and $T_{i,\text{A}}$ and $T_{i,\text{B}}$ represent the initial temperatures of components A and B.[6] This temperature correction was applied to the $NaClO/Na_2SO_3$ reactions; results are shown in Figure 5.[7]

The corrected data yield a more accurate ratio of 25.6 mL NaClO(aq) to 24.4 mL $Na_2SO_3(aq)$, which simplifies to 1.05:1. The observed variations are also more symmetric about the intersection composition, as is expected for a 1:1 ratio.

The method used assumes equal concentrations of the reactants. Slight differences in concentrations may lead to deviations from the true ratios. Concentrations can be incorporated using the expression

$$\text{Ratio} = \frac{n_\text{A}}{n_\text{B}} = \frac{M_\text{A} V_\text{A}}{M_\text{B} V_\text{B}}$$

where M represents the molar concentration of component A or B, V represents the volume of A or B at the optimal ratio, and n indicates the amount of the component A or B at the optimal ratio. This can be an important correction if the NaClO(aq) solution was prepared from an older bleach solution, as some decomposition is possible. An accurate concentration of NaClO(aq) can be determined through titration analysis [**vonderbrink**].

2.4 Reference List

The `\printbibliography` command prints a list of references for you. Please use `sample.bib` as an example to create your bibliography entries.

[6] In order to apply this correction, an additional measurement of the initial temperature of the minor component must be obtained using a separate thermometer.

[7] When conducting the experiment using these reactants, initial temperatures varied by as much as 2°C. Initial temperature variations for the NaClO/KI reactions were less significant at approximately 0.5°C.

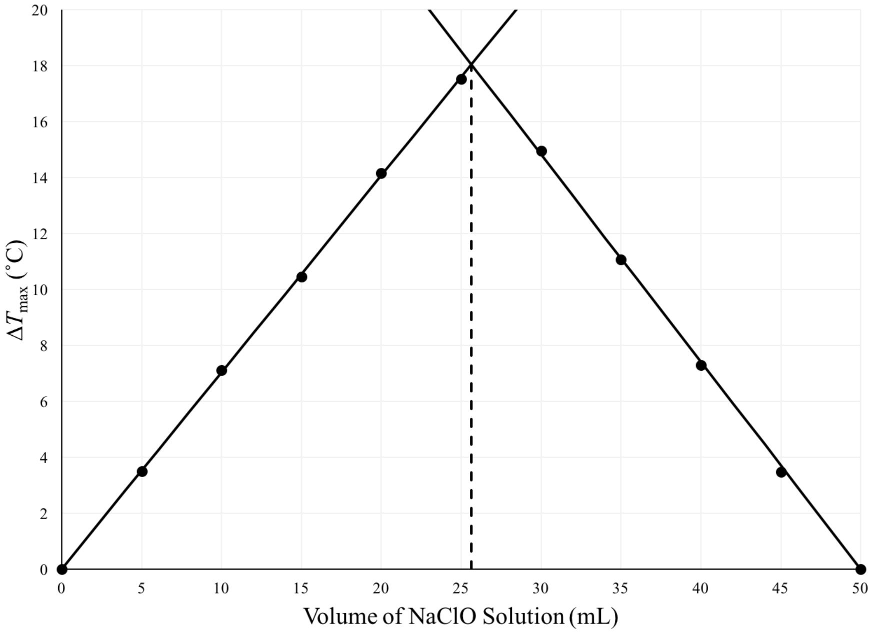

Figure 5: Maximum Temperature Changes for Mixtures of NaClO(aq) and Na_2SO_3(aq) with Initial Temperature Correction