



Thomas James Cresswell

Chemistry Lab Report 3 – Calorimetry

University of Wales Trinity Saint David
Ordnance Munitions and Explosives Professional

BEng
Academic Year: 2024 - 2029

Supervisor: Eva Kazimierska
April 2025

Academic integrity declaration

I declare that:

- the thesis submitted has been written by me alone.
- the thesis submitted has not been previously submitted to this university or any other.
- that all content, including primary and/or secondary data, is true to the best of my knowledge.
- that all quotations and references have been duly acknowledged according to the requirements of academic research.

I understand that to knowingly submit work in violation of the above statement will be considered by examiners as academic misconduct

Table of Contents

1. Introduction	1
1.1. Aim of experiment.....	1
1.2. Hypothesis.....	1
1.3. Experiment variables	1
2. Results.....	2
2.1. Results.....	2
2.1.1. Measuring heat capacity of the calorimeter ($HC_{\text{calorimeter}}$)	2
2.1.2. Measure the specific heat capacity ($C_p \text{ metal}$)	3
2.1.3. Measure the molar heat of reaction (q_{reaction}).....	4
3. Discussion	4
3.1. Significance of results	5
3.2.....	5
3.3. Relevance to OME	6
4. Conclusions.....	6
5. References.....	7
6. Appendices	8
6.1. Annex A – Methodology.....	8
6.2. Annex B – Physical results of experiments.....	10

List of Figures

Figure 1 - Results section 1.....	10
Figure 2 - Results section 2.....	11
Figure 3 - Results section 3.....	12

List of Tables

Table 1 - Results for recorded temperature of the water over time	3
---	---

List of Abbreviations

IM – Insensitive Munitions
OME – Ordnance, Munitions & Explosives

List of Equations

Equation 1 - Heat change equation

$$Q = m \times c_p \times \Delta T$$

Q = Heat energy (J)

c_p = Specific heat capacity (J/g/°C)

m = Mass (g)

ΔT = Change in temperature (°C)

Equation 2 - Heat energy of calorimeter

$$Q_{\text{calorimeter}} = Q_{\text{cold water}} + Q_{\text{hot water}}$$

Q = Heat energy (J)

Equation 3 – Heat capacity of calorimeter

$$HC_{\text{calorimeter}} = \Delta T_{\text{calorimeter}} / Q_{\text{calorimeter}}$$

Q = Heat energy (J)

ΔT = Change in temperature (°C)

HC = Specific heat capacity (J/g/°C)

Equation 4 - Combined equation for Equation 1 and Equation 2

$$m_{\text{metal}} \times c_{p \text{ metal}} \times \Delta T_{\text{metal}} = -(m_{\text{water}} \times c_{p \text{ water}} \times \Delta T_{\text{water}} + HC_{\text{calorimeter}} \times T_{\text{calorimeter}})$$

m = Mass (g)

c_p = Specific heat capacity (J/g/°C)

ΔT = Change in temperature (°C)

HC = Specific heat capacity (J/g/°C)

Equation 5 – Number of reactant moles

$$n_{\text{reactant}} = V_{\text{reactant}} \times C_{\text{reactant}}$$

n = Number of moles (Mol)

V = Volume of solution (L)

C = Concentration of solution (M)

Equation 6 - Heat of reaction for a chemical process

$$Q_{\text{reaction}} = -(m_{\text{water}} \times c_{p \text{ water}} \times \Delta T_{\text{water}} + HC_{\text{calorimeter}} \times \Delta T_{\text{calorimeter}})$$

Q = Heat energy (J)

m = Mass (g)

c_p = Specific heat capacity (J/g/°C)

ΔT = Change in temperature (°C)

HC = Specific heat capacity (J/g/°C)

Equation 7 - Heat energy for a reaction per mole of limiting reactant

$$q_{\text{reaction}} = Q_{\text{reaction}} / n_{\text{reactant}}$$

q = Heat energy per mol of limiting reactant (J)

Q = Total heat energy of reaction (J)

n = Number of moles of limiting reactant (Mol)

1. Introduction

1.1. Aim of experiment

Determine the heat capacity of the calorimeter for calibration. This calibration is used in calculations to determine the heat capacity of the metal as well as determine the heat energy released in the neutralisation reaction between HCl and NaOH.

1.2. Hypothesis

If NaOH and HCl are mixed within a calorimeter of known heat capacity, the energy of the neutralisation reaction can be determined. By measuring the change in temperature (ΔT) and recording the quantity of reactants, you can determine the mixtures heat capacity and therefore the heat released in the reaction. Furthermore, calculating the molar ratios of the reactants through their volume and molar mass will allow for the determination of the energy expected to be released per mole of limiting reactant.

1.3. Experiment variables

Independent variable:

Contents of calorimeter.

Dependant variable:

Change in temperature over time (ΔT).

Control variables:

- Calorimeter assembly
- Ambient temperature: Constant room temperature.
- Thermometer
- Material of stirring rod
- Concentration of HCl
- Volume of HCl
- Concentration of NaOH
- Volume of NaOH

2. Results

2.1. Results

2.1.1. Measuring heat capacity of the calorimeter ($HC_{\text{calorimeter}}$)

$T_{\text{hot}} = 60.0(^{\circ}\text{C})$	$m_{\text{hot water}} = 50(\text{g})$	$\Delta T_{\text{hot water}} = -18.9(^{\circ}\text{C})$
$T_{\text{cold}} = 20.2(^{\circ}\text{C})$	$m_{\text{cold water}} = 50(\text{g})$	$\Delta T_{\text{cold water}} = 20.9(^{\circ}\text{C})$
$T_{\text{max}} = 41.1(^{\circ}\text{C})$		$\Delta T_{\text{calorimeter}} = 20.9(^{\circ}\text{C})$

$$Q_{\text{cold-water}} = 4400(\text{J})$$

$$Q_{\text{hot water}} = 4000(\text{J})$$

$$Q_{\text{calorimeter}} = 420(\text{J})$$

$$HC_{\text{calorimeter}} = 20(\text{J}/(\text{g}^{\circ}\text{C}))$$

Write the calculations for $Q_{\text{HOT-WATER}}$, $Q_{\text{COLD-WATER}}$, $Q_{\text{CALORIMETER}}$, and $HC_{\text{CALORIMETER}}$

$$\begin{aligned} Q_{\text{hot water}} &= m_{\text{hot water}} \times C_p \text{ hot water} \times \Delta T_{\text{hot water}} && \text{(Equation 1)} \\ Q_{\text{hot water}} (\text{J}) &= 50(\text{g}) \times 4.186(\text{J}/(\text{g}^{\circ}\text{C})) \times -18.9(^{\circ}\text{C}) \\ Q_{\text{hot water}} (\text{J}) &= -3956(\text{J}) = -4000(\text{J}) \end{aligned}$$

$$\begin{aligned} Q_{\text{cold water}} &= m_{\text{cold water}} \times C_p \text{ cold water} \times \Delta T_{\text{cold water}} && \text{(Equation 1)} \\ Q_{\text{cold water}} &= 50(\text{g}) \times 4.186(\text{J}/(\text{g}^{\circ}\text{C})) \times 20.9(^{\circ}\text{C}) \\ Q_{\text{cold water}} &= 4374(\text{J}) = 4400(\text{J}) \end{aligned}$$

$$\begin{aligned} Q_{\text{calorimeter}} &= Q_{\text{hot water}} + Q_{\text{cold water}} && \text{(Equation 2)} \\ Q_{\text{calorimeter}} &= -3956(\text{J}) + 4374(\text{J}) \\ Q_{\text{calorimeter}} &= 418(\text{J}) = 420(\text{J}) \end{aligned}$$

$$\begin{aligned} HC_{\text{calorimeter}} &= Q_{\text{calorimeter}} / \Delta T_{\text{calorimeter}} && \text{(Equation 3)} \\ HC_{\text{calorimeter}} &= 418(\text{J}) / 20.9(^{\circ}\text{C}) \\ HC_{\text{calorimeter}} &= 20(\text{J}/(\text{g}^{\circ}\text{C})) \end{aligned}$$

2.1.2. Measure the specific heat capacity (C_p metal)

Type of metal = Aluminium

$$T_{\text{hot}} = 91.4(^{\circ}\text{C}) \quad m_{\text{metal}} = 18.6(\text{g}) \quad \Delta T_{\text{metal}} = -59.8(^{\circ}\text{C})$$

$$T_{\text{cold}} = 21.5(^{\circ}\text{C}) \quad m_{\text{water}} = 30(\text{g}) \quad \Delta T_{\text{water}} = 10.1(^{\circ}\text{C})$$

$$T_{\text{max}} = 31.6(^{\circ}\text{C}) \quad \Delta T_{\text{calorimeter}} = 10.1(^{\circ}\text{C}) \quad C_p \text{ metal} = 1.3(\text{J}/(\text{g}^{\circ}\text{C}))$$

time (s)	$T_{\text{WATER}} (^{\circ}\text{C})$	time (s)	$T_{\text{WATER}} (^{\circ}\text{C})$	time (s)	$T_{\text{WATER}} (^{\circ}\text{C})$
0	31.0	120	27.7	240	26.8
10	30.4	130	27.6	250	26.8
20	29.9	140	27.5	260	26.8
30	29.5	150	27.5	270	26.7
40	29.3	160	27.5	280	26.6
50	28.9	170	27.3	290	26.6
60	28.6	180	27.3	300	26.6
70	28.5	190	27.2	310	26.6
80	28.3	200	27.1	320	26.6
90	28.1	210	27.0	330	26.6
100	28.0	220	26.9	340	26.6
110	27.8	230	26.9	350	26.6

Table 1 - Results for recorded temperature of the water over time

Write the calculations for C_p metal:

$$m_{\text{metal}} \times C_p \text{ metal} \times \Delta T_{\text{metal}} = -(m_{\text{water}} \times C_p \text{ water} \times \Delta T_{\text{water}} + H C_{\text{calorimeter}} \times T_{\text{calorimeter}}) \quad (\text{Equation 4})$$

$$C_p = - (m_{\text{water}} \times C_p \text{ water} \times \Delta T_{\text{water}} + H C_{\text{calorimeter}} \times T_{\text{calorimeter}}) / (m_{\text{metal}} \times \Delta T_{\text{metal}})$$

$$C_p = - (30(\text{g}) \times 4.186(\text{J}/(\text{g}^{\circ}\text{C})) \times (10.1(^{\circ}\text{C})) + (20 (\text{J}/(\text{g}^{\circ}\text{C})) \times 10.1(^{\circ}\text{C})) / (18.6(\text{g})) \times (-59.8(^{\circ}\text{C}))$$

$$C_p = 1.321(\text{J}/(\text{g}^{\circ}\text{C})) = 1.3(\text{J}/(\text{g}^{\circ}\text{C}))$$

2.1.3. Measure the molar heat of reaction (q_{reaction})

$$T_{\text{start}} = 19.4(^{\circ}\text{C})$$

$$T_{\text{end}} = 26.7(^{\circ}\text{C})$$

$$\Delta T = 7.3(^{\circ}\text{C})$$

$$V_{\text{HCl}} = 50(\text{mL})$$

$$C_{\text{HCl}} = 1.0(\text{M})$$

$$n_{\text{HCl}} = 0.050(\text{mol})$$

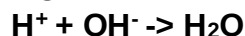
$$V_{\text{NaOH}} = 52(\text{mL})$$

$$C_{\text{NaOH}} = 1.0(\text{M})$$

$$n_{\text{NaOH}} = 0.052(\text{mol})$$

Write the formula of the limiting reactant:

HCl



$$Q_{\text{reaction}} = - 3300(\text{J})$$

$$q_{\text{reaction}} = - 65(\text{KJ/mol})$$

Write the calculations for Q_{reaction} and q_{reaction} .

$$n_{\text{HCl}} = V_{\text{HCl}} \times C_{\text{HCl}}$$

(Equation 5)

$$n_{\text{HCl}} = (50 \times 10^{-3})(\text{L}) \times 1.0(\text{M}) = 0.050(\text{mol})$$

$$n_{\text{NaOH}} = (52 \times 10^{-3})(\text{L}) \times 1.0(\text{M}) = 0.052(\text{mol})$$

Lower number of moles means HCl is the limiting reactant.

$$Q_{\text{reaction}} = - (m_{\text{water}} \times C_{p \text{ water}} \times \Delta T_{\text{water}} + HC_{\text{calorimeter}} \times \Delta T_{\text{calorimeter}})$$

(Equation 4)

$$Q_{\text{reaction}} = - (102(\text{mL}) \times 4.186(\text{J}/(\text{g}^{\circ}\text{C})) \times 7.3(^{\circ}\text{C}) + 20(\text{J}/(\text{g}^{\circ}\text{C})) \times 7.3(^{\circ}\text{C}))$$

$$Q_{\text{reaction}} = - 3263(\text{J}) = - 3300(\text{J})$$

$$q_{\text{reaction}} = Q_{\text{reaction}} / n_{\text{reactant}}$$

(Equation 7)

$$q_{\text{reaction}} = - 3263 (\text{J}) / 0.050(\text{mol})$$

$$q_{\text{reaction}} = - 65260(\text{J}) = - 65(\text{KJ/mol})$$

3. Discussion

3.1. Significance of results

3.1.1. Section 1 – Determining heat capacity of calorimeter

By determining the heat capacity of the calorimeter, it is possible to use the result in further calculations to determine the heat of the neutralisation reaction from within the same calorimeter. The heat capacity is the amount of energy, measured in Joules (J), required to raise the temperature of 1g of solution by 1°C.

In this experiment, water of known heat capacity was used as a calibration for the calorimeter. The exchange of energy from the water was calculated using Equation 1 and the measured parameters. The energy required to heat the water is greater than the energy required for it to reach equilibrium due to the retention of heat by the calorimeter (Equation 2). Finally, the heat capacity is determined through Equation 3 and gave a result of 20(J/(g°C)). This was expected as the Styrofoam is a stronger insulator than water so would require more energy to raise its temperature.

3.1.2. Section 2 – Determining the heat capacity of the aluminium

The heat capacity of the aluminium was determined using the previous calibration of the calorimeter. As the calorimeter's heat capacity is known, the value is used in Equation 4 along with recorded parameters during the experiment. The result of the calculations that followed showed that the aluminium test piece requires 1.3 (J/(g°C)).

The rate at which the energy transfer is carried out was not determined due to the measurements being taken from maximum temperature and not the initial introduction of the test piece.

3.1.3. Section 3 – Determining the heat energy released per mole of reactant

The neutralisation reaction between the HCl and NaOH was carried out with different quantities of reactant. Due to both solutions having a concentration of 1M, the limiting reactant in this reaction was the HCl. The number of moles for each reactant in the solution was calculated to confirm this using Equation 5.

The total energy of the reaction was then calculated using Equation 4 where a conversion can then be applied to determine the energy per mole of the limiting reactant.

3.2. Relevance to OME

3.2.1. Bomb calorimetry – determination of enthalpy of combustion

This experiments relevance to OME is through a process called bomb calorimetry. This is where the heat energy (enthalpy of combustion) is calculated. The enthalpy of combustion is the amount of energy released in heat by the complete combustion of the substance within the calorimeter in Joules.

An example on the use of this method is through a set of experiments by W. Kicinski and W.A. Trzcinski. This experiment tested the enthalpy of combustion for multiple non-ideal explosive compounds and was able to determine the released energy. In figure 6 of the reference, a diagram is provided of a bomb calorimeter. [1]

Bomb calorimetry can also be used for determining the thermal stability of an explosive compound. This feeds directly into the development of Insensitive Munitions (IM) where they require a resistance to external stimuli, in this case heat. [2]

4. Conclusions

Overall, the heat capacity of the calorimeter and the aluminium metal was able to be determined through the expected methods. The heat of reaction for the neutralisation reaction, along with the energy released per mole of limiting reagent, were also able to be determined. The rate of heat transfer could not be determined for the aluminium due to the temperature being recorded from maximum and not when the metal was initially submerged.

Potential directions for future research of this reaction could be to test the heat energy from different types of explosives in comparison to how much of the composition consists of nitrogen bonds. This would allow for the exploration of how strongly the nitrogen bonds affect the energy released during combustion of these compositions.

5. References

- [1] W. Kicinski and W. Trzcinski, "CALORIMETRY STUDIES OF EXPLOSION HEAT OF NON-IDEAL," *Journal of Thermal Analysis and Calorimetry*, vol. 96, no. 2, pp. 623-630, 2009.
- [2] M. I. Pakadaki, W. Zhu, S. Horsch, M. Karuse and C. V. Mashuga, "Calorimetric Studies on the Thermal Stability of 2-Nitrotoluene Explosives with Incompatible Substances," *Industrial & Engineering Chemistry Research*, vol. 58, no. 29, pp. 13366-13375, 2019.

6. Appendices

6.1. Annex A – Methodology

6.1.1. Procedure to measure $HC_{\text{calorimeter}}$:

1. Add 50.0 mL of water to the Styrofoam coffee cups, and close with a lid. Add the thermometer and stirring rod to set up your calorimeter.
2. Take 50.0 mL of water in a separate beaker and heat to about 80°C. Close the gas and wait till the temperature reaches 60°C. When the "hot water" is ready, record its temperature as T_{hot} .
3. Measure the temperature of the water in the calorimeter and record it as T_{cold} .
4. Add the hot water to the water in the calorimeter, and mix thoroughly, while watching the thermometer. Record the maximum equilibrium temperature of the mixture, record it as T_{max} .
5. Calculate the heat capacity of the calorimeter, $HC_{\text{calorimeter}}$, using Equations 1-3.

6.1.2. Procedure to measure c_p metal:

1. Obtain a piece of the metal sample. Weigh the metal and record its mass as m_{metal} .
2. Set up a water bath, heat the water until boiling, and then carefully put your metal into it. Keep boiling for another 5 minutes, to allow the metal to reach the same temperature as the water. Try to avoid heating the metal directly! To reduce the effect of direct heating, close the gas after 5 min and wait 2 minutes for the temperature of boiling water and piece of metal to equilibrate.
3. While this is being done, measure 30.0 mL of water and add it to the calorimeter. Measure the temperature of the water in the calorimeter, as done previously, and record it as T_{cold} .
4. Once the metal has reached "thermal equilibrium" with the boiling water, measure and record the temperature of the hot water as T_{hot} and quickly add the metal to the water in the calorimeter using the tongs.

5. Stir the water and record the temperature every 10 seconds, filling in the datasheet provided at the end of this script with the entries (time, T_{water}). The temperature will increase at the start. Continue until the temperature of the water has reached a maximum and then cooled down by about 2°C . Record the maximum temperature reached by the water as T_{max} .
6. Calculate c_p metal the specific heat of the metal using Equation 4 and the value of heat capacity of the calorimeter found previously. Assume that calorimeter and water are in thermal equilibrium, $c_p \text{ water} = 4.186 \text{ J/(g}^{\circ}\text{C)}$, and always give the units of the results of your calculations.

6.1.3. Procedure to measure q_{reaction} :

1. Place 52.0 mL of 1.0 M NaOH into the calorimeter and pour 50.0 mL of 1.0 M HCl into a beaker.
2. Place the two side-by-side until they attain the same temperature. Record this value as T_{start} .
3. Add the HCl quickly to the calorimeter and record the temperature when it reaches a maximum as T_{end} .
4. Calculate Q_{reaction} , the heat of reaction, using Equation 6 and the heat capacity of the calorimeter found previously. Again, assume that calorimeter and water are in thermal equilibrium, $c_p \text{ water} = 4.186 \text{ J/(g}^{\circ}\text{C)}$, and always give the units of the results of the calculations.
5. Calculate q_{reaction} , the molar heat of reaction, as the heat of reaction per mole of the limiting reactant using Equation 7.

6.2. Annex B – Results of experiments

DATA SHEET TO RECORD OBSERVATIONS, CALCULATIONS and RESULTS

STUDENT'S NAME: THEODOSIOS

PARTNERS' NAMES: JAMES BOUTON, JOSEPH H. HARRIS

REPORT IS DUE MAY 02, 2025 (DD May 09, 2025) submitted via Moodle

$C_p \text{ H}_2\text{O, water} = 4.184 \text{ J/g}^\circ\text{C}$

1. Measure the value of the heat capacity of the calorimeter ($HC_{\text{calorimeter}}$)

Use these entries to record your experimental data, results, and calculations.

$T_{\text{hot}} = 60.0^\circ\text{C}$ $m_{\text{hot water}} = 50 \text{ g}$ $\Delta T_{\text{hot water}} = -19.9$

$T_{\text{cold}} = 20.2^\circ\text{C}$ $m_{\text{cold water}} = 50 \text{ g}$ $\Delta T_{\text{cold water}} = 20.9$

$T_{\text{max}} = 41.41^\circ\text{C}$ $\Delta T_{\text{calorimeter}} = 20.9$

$Q_{\text{cold water}} =$ $Q_{\text{hot water}} =$ $Q_{\text{calorimeter}} =$

$HC_{\text{calorimeter}} =$

Write the calculations for $Q_{\text{HOT-WATER}}$, $Q_{\text{COLD-WATER}}$, $Q_{\text{CALORIMETER}}$, and $HC_{\text{CALORIMETER}}$:

Page 6

Figure 1 - Results section 1

2. Measure the specific heat capacity of a metal ($c_{p, \text{metal}}$)

Use these entries to record your experimental data, results, and calculations.

Type of metal = ALUMINIUM $T_{\text{hot}} =$ 91.4 $m_{\text{metal}} =$ 18.6 $\Delta T_{\text{metal}} =$ -59.8 °C $T_{\text{cold}} =$ 21.5 $m_{\text{water}} =$ 80.2g $\Delta T_{\text{water}} =$ +10.1 °C $T_{\text{max}} =$ 31.6 $\Delta T_{\text{calorimeter}} =$ +10.1 °C $c_{p, \text{metal}} =$ _____

time (s)	$T_{\text{WATER}} (^{\circ}\text{C})$	time (s)	$T_{\text{WATER}} (^{\circ}\text{C})$	time (s)	$T_{\text{WATER}} (^{\circ}\text{C})$
10	21.6	130	27.7	250	24.8
20	20.4	140	27.6	260	24.8
50	20.4	150	27.5	270	24.7
40	21.5	160	27.5	180	26.7
58	29.3	170	27.3	220	26.6
60	28.9	180	27.3	300	26.6
70	28.6	190	27.2	310	26.6
80	28.5	200	27.1	320	26.6
90	28.3	210	27.0	330	26.6
100	28.1	220	26.9	340	26.6
110	28	230	26.9	250	26.6
120	27.5	240	26.9	360	26.6

Write the calculations for c_{metal} :**Figure 2 - Results section 2**

3. Measure the molar heat of reaction of HCl with NaOH (q_{reaction})

Use these entries to record your experimental data, results, and calculations.

 $T_{\text{start}} = 19.4^{\circ}\text{C}$ $T_{\text{end}} = 26.7^{\circ}\text{C}$ $V_{\text{HCl}} = 50$ $C_{\text{HCl}} = 0.1$ $n_{\text{HCl}} =$ $V_{\text{NaOH}} = 50$ $C_{\text{NaOH}} = 0.1$ $n_{\text{NaOH}} =$ Write the formula of the limiting reactant: HCl $Q_{\text{reaction}} =$ $q_{\text{reaction}} =$ Write the calculations for Q_{reaction} and q_{reaction} .**Figure 3 - Results section 3**