

Measurement of heat of combustion of stearyl alcohol

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Heat of combustion of stearyl alcohol is measured using bomb calorimeter, the process of which is well simulated using one-dimension model, indicating better way to correct the change of the temperature resulted from the combustion.

Keywords: heat of combustion, bomb calorimeter, simulation

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I. INTRODUCTION

Heat of combustion is a fundamental parameter when giving quantitative analysis on the energy of a substance. It represents the difference of enthalpy of two states: the initial state for the matter, the end state for the stable products after chemical reaction. With this many other data can be deduced or estimated, which provide essential information for researches.

Combustion usually involves forming of gas, which challenges the firmness of the container, while an adiabatic environment is also vital for measuring heat explicitly. A bomb calorimeter is designed to satisfy these requirements, which consists of a small cup to contain the sample, oxygen of high pressure to ensure complete reaction, a stainless steel bomb, water, a stirrer, a thermometer, the dewar or insulating container (to prevent heat flow from the calorimeter to the surroundings) and ignition circuit connected to the bomb. After the sample reacts completely, the heat produced is gradually absorbed by the surrounding water, and the change of temperature is detected, then the Heat of combustion can be derived.

Nonetheless, the calorimeter still cannot eliminate heat exchanges with environment, while stirring also provides extra heat. Thus a correction of temperature is applied, which involves drawing two lines from initial and final temperature curves. Difference exists at different time between these two lines, and the time when the temperature reaches the median is chosen to calculate the corrected change of temperature, thus the loss of heat is compensated, while extra heat introduced by stirring is also reduced from the result.

II. DEVICES AND PROCEDURES

A bomb calorimeter is prepared, containing certain amounts of samples and 1.5 MPa of oxygen compressed in the steel bomb, with precise amount of 3,000 mL of water added to keep the heat capacity of the whole apparatus constant. Copper string is used to ignite the sample. The temperature is measured by Pt-1000 thermometer and recorded by SunyLAB200 Data Recorder. The temperature curve keeps straight for at least 3 minutes before ignition, and for at least 5 minutes before finishing the recording. The water is refreshed after each round. Pure benzoic acid is utilized to measure the exact heat capacity of the apparatus, and the heat of combustion of stearyl alcohol is then measured. The data is analyzed and plotted using *Mathematica*.

III. RESULTS AND ANALYSIS

Correction of the change of temperature is realized by codes:

```
ReynoldsTempCorrect[data_] := Module[{median, center,
  range}, timing
median = (Max[#] + Min[#])/2 &[data];
center =
First@First@
Position[data,
First@Sort[data, Abs[#1 - median] < Abs[#2 - median]
&]];
range =
Normal[LinearModelFit[#, {1, x}, x]] & /@ {Take[data,
100],
Take[data, -100]} /. x -> center;
Abs[Subtract @@ range]
]
```

The data recorded and calculated are shown in Table I. Curves plotted are shown in Fig.1 and Fig.2. The comparison between the result from the experiment and from the reference show that the data is fairly reliable (1.167×10^4 kJ/mol/K *v.s.* $11820. \pm 4$ kJ/mol/K[1]), thanks to the relatively adiabatic environment provided by the bomb calorimeter. Deviations may arise from the incompleteness of the reaction, the insensitivity of the thermometer which affects the process of correction of temperature, and choice of time in the correction process. Deviation from standard room temperature is slightly to

TABLE I. The result of the experiment, where BA stands for benzoic acid, and R for stearyl alcohol.

Data	Test Group				
	R,1	R,2	BA,1	BA,2	BA,3
$m_{\text{sample}}/\text{g}$	0.4235	0.6320	0.7840	0.8406	0.9043
$\Delta m_{\text{Cu}}/\text{g}$	0.0220	0.0202	0.0091	0.0150	0.0164
$\Delta T/^\circ\text{C}$	1.296	1.881	1.452	1.564	1.662
$C_V/(\text{kJ/mol/K})$	N/A		14.30	14.24	14.43
$\bar{C}_V/(\text{kJ/mol/K})$	N/A		14.32		
$Q/(10^4 \text{ kJ/mol})$	-1.182	-1.151	N/A		
$\bar{Q}/(10^4 \text{ kJ/mol})$	-1.167		N/A		

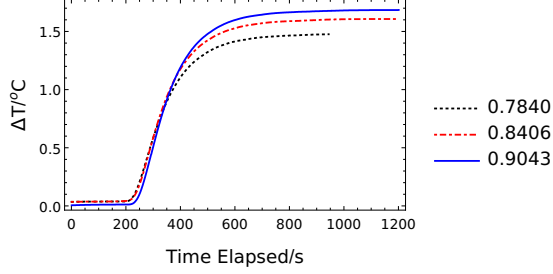


FIG. 1. The $T - t$ curves for combustion of benzoic acid. The legends stand for the mass of the sample.

blame for the error, which affects the heat capacity of the system.

Simple one-dimension model of such an experiment is fabricated and programmed in *julia*, which fits the curves from the experiment nicely, as revealed in Fig.3. The chamber is set middle of the box of 30 cells, and heat flow is simulated according to the formula

$$\begin{cases} \frac{\Delta q}{\Delta t} \sim D_f \frac{T(x+\Delta x)+T(x-\Delta x)-2T(x)}{2\Delta x} \\ \Delta T(x) \sim \frac{\Delta q/\Delta t}{C_V} \Delta t. \end{cases} \quad (1)$$

It shows that the model is verified, deviation from experimental curve of which is attributed to the absense of stirring process that involves much complicated algorithms to simulate. Fig.4 partly reveals the whole process of the heat flow from the chamber to the very edges of the system. A certain amount of time needs to be spared for the whole system to ‘react’ to the sudden heating

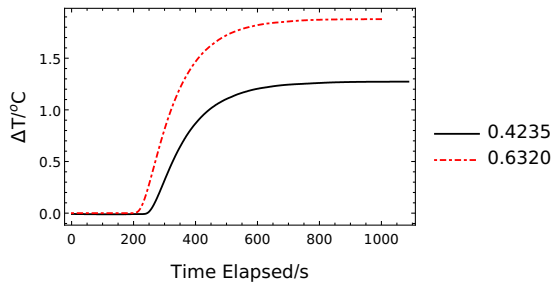


FIG. 2. The $T - t$ curves for combustion of stearyl alcohol. The legends stand for the mass of the sample.

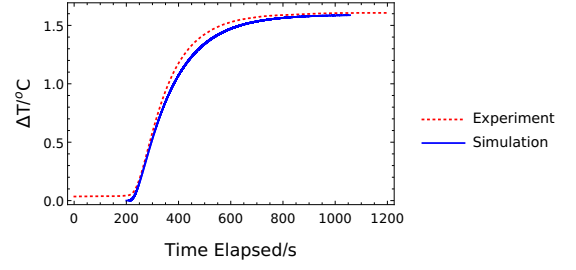


FIG. 3. The curves for experiment *v.s.* simulation

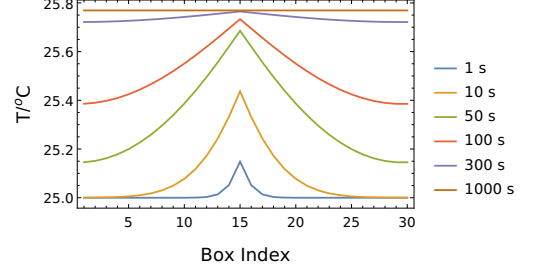


FIG. 4. Temperature curve over the whole box at different time. ‘0 s’ stands for the ‘ignition’.

from the chamber and for the heat to flow over. The relatively slow heat conduction between the chamber and the surrounding water is also simulated, which is also responsible for the delay of the heat flow.

Fig.5 clarifies the change of heating speed over the whole simulation as well as experiment. An initial faster heating and subsequent slow one is identified in the figure, which is very reasonable w.r.t. the gradually reduced gradient of the temperature. This finding also indicates a better point of choice for the correction of temperature. The lines drawn are used to estimate the actual temperature of the initial state and the end state of the reaction, thus the point chosen should be as close as possible to the very beginning of the reaction. The trend of the increasing of temperature shows that the point where the heating speed reaches the highest is much closer, compared with the ‘median’ point.

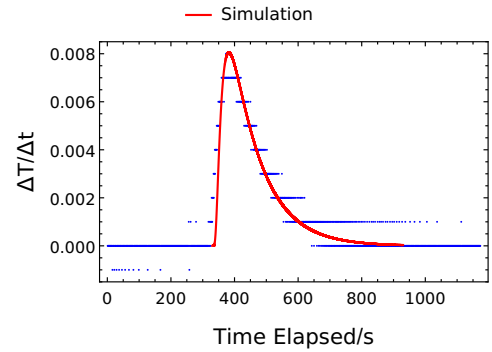


FIG. 5. $\frac{\Delta T}{\Delta t}$ curves for experiment and simulation

IV. CONCLUSION

The heat of combustion of stearyl alcohol is measured, whose result is relatively close to that in references. Sim-

ulations reveal the simplicity of the whole system, as well as indicating that the point where the heating speed reaches the highest better represents the time when the combustion occurs.

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- [1] B Freedman and MO Bagby. Heats of combustion of fatty esters and triglycerides. *Journal of the American Oil Chemists' Society*, 66(11):1601–1605, 1989.