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Determination of Heat of Reaction using Calorimetry

Mr. Sagar dure[1], Miss. Sayali Deshmane[2], Miss. Pratiksha Ethape[3],
Miss. Sakshi Dussa[4], Miss. Harshada Gade[5]
Students, Computer Engineering Department [1,2]
Student, Civil Engineering Department [3]
Students, Information & Technology Engineering Department[4,5]
Adsul's Technical Campus, Ahilyanagar, India

Abstract: *The heat of reaction is an important parameter in the safe, successful scale-up of chemical processes. Reaction heat data is used to calculate the potential adiabatic temperature rise of the desired reaction, providing a worst-case scenario for rapid reaction of the entire batch with no heat loss to the surroundings. The data is used in parallel with information regarding the thermal stability of reaction mixtures/components and an intimate knowledge of the process to analyze the risk associated with running it on-scale. If the level of risk is judged to be unacceptable, the analysis can be used to make rational process changes in order to reduce the risk to an acceptable level. The Pfizer global process safety network provides a heat of reaction for all processes run in our kilo laboratories, pilot plant, and manufacturing facilities. In general, there are two methods used to determine reaction heats: (1) experimental measurement using some form of calorimetry, or (2) estimation techniques. Since experimental measurement is not always practical, accurate, or necessary, we set out to show that estimation techniques could be used reliably and efficiently to provide heat of reaction data for a wide range of chemistry. To gain confidence in our ability to accurately predict reaction heats, we carried out a comparative study of measured versus estimated values. The results of this study will be discussed in detail, including rationalization of any significant disparity through further analysis to more fully understand the limitations/advantages of both techniques. To help ensure consistent application of measurement/ estimation across the Pfizer global process safety network, we developed a decision tree to determine whether estimation or measurement should be considered for a particular reaction. In order to maximize the efficiency gain and to ensure accuracy in our estimations, we have created a heat estimation database that allows for (1) rapid archival/retrieval of model compounds, (2) calculation of reaction heat and adiabatic temperature rise, and (3) reporting/documentation of the results.*

Keywords: Calorimeter, Heat of Reaction, Analysis, Thermodynamic

I. INTRODUCTION

Calorimetry studies the exchange of heat, in different processes, through an instrument called calorimeter, which measures the change of energy in a system when operating a process; what It can be physical, chemical or biological. The first calorimeter to measure the heat, was developed in 1783 by Lavoisier and Laplace measured the change in heat of a hot body, to melt a quantity of ice; was waiting until the body warm was at the temperature of the ice, and then it determined the mass of the melted ice. The construction of calorimeters helps to understand the science of energy and its transformations, with a simple experiment you can deduce the change of heat, but implies knowledge of concepts such as; heat capacity, enthalpy, calorific power, thermal power, etc. The calorimeters are designed to determine specific thermodynamic properties; by example, exist calorimeters; from flow, isoperbolic, adiabatic and some indirect as the flash laser method or the photoacoustic calorimeter. To select the right one for determined property is necessary know their main characteristics and factors such as absolute or relative measurement, required accuracy.

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Fig.1 Calorimeter

A. What is calorimeter

The simplest definition of a calorimeter is a device that measures the temperature of the reaction except that the reaction was mechanical, electrical or chemical. It measures the thermal capacity of materials. There are large and varied totals for calorimeter but there are tow types that are the most used is. In constant-pressure calorimetry, the heat lost or obtained for solution is calculated as means of knowing the heat gained or lost for reactivity To measure the temperature of the reaction, the reaction must be isolated so as not to lose heat to the atmosphere and obtain the most accurate results and the calorimeter provides the best isolation of the reaction. The idea of the calorimeter came from joseph black in 1761 where he made the first ice-calometry. In 1780 the ice surrounding his device was than melt by breathing a guinea pig this indicates that gas exchange during breathing is a combustion process The calorimeter measures the temperature of chemical reaction, physiological change and heat capacity. It measures the amount of heat gained or absorbed from the substance during the chemical reaction or physical change.

B. Safety

To take care and safety in the laboratory, wear eye protection at all times. This is because hydrochloric acid and sodium hydroxide acid are highly corrosive when they contact any body (skin, eye, .etc). Concentrated hydrochloric acid it is best to open it only in the fume hood.

II. THEORETICAL BACKGROUND

Thermodynamic processes (mix of cold and hot water, mix of two liquids, chemical reaction, ...) can be characterized from the variations of energy produced as a result of the completion of the process. Bearing in mind that in the In most cases the processes take place under constant pressure, the energy function most suitable for the experimental measure will be the enthalpy (H). In this sense, the enthalpy variation of a process measures the amount of heat exchanged between the system and the environment at constant pressure

$\Delta H = Qp$

Now, experience shows that the exchange of heat manifests itself with a modification of the temperature in the system. This modification is a function of the nature of the materials that form it. This fact introduces the convenience of define a magnitude that allows to qualify each substance in terms of capacity to exchange heat at constant pressure. In this sense, Capacity is defined Calorific Molar of a substance such as the amount of heat to be supplied to one mole of substance to increase its temperature by one degree. If the process has place at constant pressure, the molar heat capacity at constant pressure, C p, can be express mathematically as:

$Cp = dH/dT$

If the unit of mass is the gram, the heat capacity is called heat specific. In general, the heat capacity, Cp, is a function of temperature, which is why it is necessary to know the function Cp = f(T) in order to solve the equation (1). Assuming that Cp = constant (valid approximation for temperature increases small), the solution to the above equation

allows us to conclude that

$\Delta H = Cp * \Delta T$

Based on equations (1) and (2), calorimetry can be defined as the set of techniques and methods that allow the determination of Cp of a substance or H of a process from the measurement of temperature changes experienced by the system as a result of heat exchange.

A. Thermal Balance

The thermometer that usually gives us its value in degrees Celsius (C). Heat is a form of energy, it is difficult to conceive. The heat the fireplace warms the living room, hot tap water flows into the sink and warms especially your cold hands. In these examples, there are two systems involved, one having a higher temperature than the other and therefore hotter than the other and each of these systems undergoes a transformation, because its temperature varies, so there is a heat exchange between the two systems, one of them yielded heat and the other received heat. If two systems put in front do not exchange heat, we say that they are in equilibrium, that is, they are at the same temperature. If they exchange heat, they are not in equilibrium: their temperature is different, the one that gives heat to the other is the one the temperature is the largest. The device used to identify temperatures is called a thermometer. The first ones devices intended to indicate a temperature were invented at the end of the XVI century, by Galileo in particular: it was an open tube filled with water. The influence of pressure atmospheric distorted the results. It is in 1654 that the Grand Duke of Tuscany, Ferdinand II, invented the sealed tube: the thermometer with dilatation of liquid.

1. Thermometers for dilatation of liquids. These are the most common. A variation of temperature causes dilation of the liquid but also of the glass envelope. In practice, these thermometers cover an area ranging from -180 C to +650 C depending on the chosen liquid (mercury, alcohol, toluene, pentane). They give good results but this requires some corrections.
2. Thermometers dilating solids. They can be used up to 1000 C and their accuracy is a few degrees. There are also bimetallic thermometers used in the temperature regulation from 30C to 300C.
3. Electric thermometers. They use a physical phenomenon. The resistance of a metallic filament increases with temperature. The most used metal is platinum (-250C at 1000C). For temperatures not exceeding 300C, nickel may be used. CTNs (Negative Temperature Coefficient) Coefficient) are thermistors whose resistance decreases uniformly with the temperature. CTP (Positive Temperature Coefficient, PTC, Positive Temperature Coefficient) are thermistors whose resistance increases strongly with temperature in a limited temperature range (typically between 0C and 100C), but decreases in outside this area
4. The thermocouple. This is a second type of electric thermometer. It consists of two different metal wires welded together at their ends. If these two welds are not not at the same temperature, it appears in the circuit a fem that we measure with a voltmeter. Practically, one of the welds is immersed in melting ice and the other is placed where you want to measure the temperature. Next to the temperature range where we find ourselves, we choose the metals. The most common pair is platinum / platinum rhodium to 10% (from 0 C to 1700 C).

B. Heat of Reaction

It The changes in temperature caused by a reaction, combined with the values of the specific heat and the mass of the reacting system, makes it possible to determine the heat of reaction. Heat energy can be measured by observing how the temperature of a known mass of water (or other substance) changes when heat is added or removed. This is basically how most heats of reaction are determined. The reaction is carried out in some insulated container, where the heat absorbed or evolved by the reaction causes the temperature of the contents to change. This temperature change is measured and the amount of heat that caused the change is calculated by multiplying the temperature change by the heat capacity of the system. The apparatus used to measure the temperature change for a reaction system is called a calorimeter (that is, a calorie meter). The science of using such a device and the data obtained with it is called calorimeters. The design of a calorimeter is not standard and different calorimeter are used for the amount of precision required. One very simple design used in many general chemistry labs is the Styrofoam ”coffee cup” calorimeter, which usually consists of two nested Styrofoam cups. When a reaction occurs at constant pressure inside a Styrofoam coffee-cup calorimeter, the enthalpy change involves heat, and little heat is lost to the lab (or gained from it). If the reaction evolves heat, for example, very nearly all of it stays inside the calorimeter, the amount of heat absorbed or evolved by the reaction is calculated. When a chemical reaction occurs in the coffee cup calorimeter, the heat of the reaction is absorbed by the water. The change in the water temperature is used to calculate the amount of heat that has been absorbed(used to make products, so water temperature decreases) or evolved (lost to the water, so its temperature increases) in the reaction. Heat flow is calculated using the relation:

$$q = (\text{specif icheat}) * m * \Delta T.$$

Where q is heat flow, m is mass in grams, and ΔT is the change in temperature. The specific heat is the amount of heat required to raise the temperature of 1 gram of substance 1 degree Celsius. The specific heat of water is 4.18 J/(g. C). For example, consider a chemical reaction which occurs in 200 grams of water with an initial temperature of 25.0 C. The reaction is allowed to proceed in the coffee cup calorimeter. As a result of the reaction the temperature of the water changes to 31.0 C. The heat flow is calculated:

$$\text{qwater} = 4.18\text{J/(g.C)} * 200\text{g} * (31.0\text{C}-25.0\text{C}) \quad \text{q water}=+5.0 \text{ x } 103\text{j}$$

III. CALORIMETERS

The calorimeter is a device intended to measure heat exchanges (heat energy, from Latin calor meaning heat). This exchange can occur between several bodies, it can involve changes of state or chemical reactions. The calorimeter constitutes a thermodynamic system, there is no exchange of matter and energy (work or heat) with the external environment. The determination of the thermal changes that accompany the processes Thermodynamic tests are carried out with devices recognized by the name of Calorimeters. Schematically a calorimeter consists of the following elements:

1. Container in which the process takes place. This container is integrated in an insulation system through which it is tried to avoid heat losses by radiation or convection.
2. Device for measuring temperature changes (thermometer of contrasted mercury, thermocouple, resistance thermometer, ...).
3. Device for controlled heating of the system (electrical resistance connected to a power supply with stabilized voltage).
4. Device for mixing components and stirring to ensure the Uniformity of the temperature in the mixture.

Fig.2 Calorimeter

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In the figure it is collected in a schematic the structure of a calorimeter being to the vessel or calorimetric vessel and the outer shirt for the isolation. Operation of this type of calorimeters can be of two ways:

- The outer vessel is kept at a constant temperature.
- The temperature of the outer vessel is maintained at all times as close as possible possible to the calorimetric vessel. In this case, the device is recognized as adiabatic calorimeter. The use of any of the two types of calorimeters requires the adoption of experimental precautions if you want to get results reasonably precise. The main points that need to be controlled are: agitation, losses for evaporation, minimizing the possible heat losses by radiation and convection. In this sense, adiabatic calorimeters in which the temperature of the outer vessel is maintained with differences less than 0.1C to that of the glass Calorimeter by electronically controlled heating devices that allow to minimize the losses by radiation and convection.

Fig. 3:

Readings before the process and after it has took place and the temperature modification regime is again reached to the agitation and the losses by radiation and convection. The graph shows the variation of the system temperature over time in a calorimeter in which an exthermic process has taken place. 1. This section corresponds to the stage of thermal steady state between the system and the environment. Since the slope is positive, it can be assumed that during this stage the system takes heat from the environment which implies that the outside temperature is higher than the system. In a well-designed calorimeter, the slope of this section of the curve should be as small as possible (0.01 C/min). 2. The section corresponding to the stage of completion of the process that, According to the temperature change observed, it should be noted that it is a process exothermic. The shape of the curve and the time it takes to reach the new state thermal stationary, (section 3), is a function of the speed with which the process, the efficiency of the homogenization of the temperature in the system and the speed response of the temperature measuring device. In the construction of a calorimeter, its operation must be optimized minimizing the duration of the stage of change between the steady state process (I) and the post-process (III)

IV. CONCLUSION

In conclusion, We should study well the sample and know the specific heat of it to avoid the error . • In the first experiment requires interaction to a high current because of the presence of the composite in the case of stability and after we have installed the amount of voltage and give the compound a certain current we find that after a period of time, this compound needs a minimum amount of current to complete the interaction and this indicates the high resistance contained in the compound so it needs a high current at the beginning of the experiment. As for the temperature of the composite will increase and almost regularly and gradually because of the lack of resistance to the composite heating over time because of the fragmentation of the composite to its components. • In the second experiment and when the current is constant.

Increasing the voltage due to the high temperature and when the arrival of the voltage to the greatest amount at this point begins the composite in breaking the chemical bonds and a decrease in the resistance of the composite and the need for the greatest Volte after that decrease in volte, then increase the voltage to break other bond of the composite and continue this process to reach to steady state .

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