



Full Length Article

Modeling of a power compensated adiabatic reaction system for temperature control design and simulation analyses



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ABSTRACT

Principle structure of a power compensation method for sample container in the accelerating rate calorimeter is introduced. Then a simplified model concerning the dynamic heat transfer between the reacting sample and the sample container during the reaction progress is established. A temperature control strategy based the compensation structure are described. Adiabatic reaction experiments were carried out to verify the validity of the simulation model and the effectiveness of the compensation method. At last, the model was used to analyze feasibilities of some typical data processing methods on the reaction kinetics. The modeling and simulation methods used in this research can be applied to study more complex reaction systems and temperature control strategies for obtaining more accurate adiabatic reaction information in the accelerating rate calorimeter.

1. Introduction

Adiabatic calorimetry has become a very popular method for reaction hazard assessments. Measurement results of the accelerating rate calorimeter (ARC) can not only contribute to improve the safety of reactive chemicals' manufacturing, storage and transportation, but also be used for calculating reaction kinetics of unknown substances or mixtures [1–4].

Although in principle, the adiabaticity of the reaction unit (including the sample and the sample container) in the classical ARC is achieved by maintaining equal temperatures between the container outer-surface and the surroundings during the exothermic reaction [5], the ARC still suffers from the “thermal lag” effect due to the fact that a certain part of heat released in the reaction is absorbed by the container. The reaction progress can be notably slowed down for this effect and in turn results in inaccurate reaction kinetics evaluations and hazard assessments [6–8].

The most common method to deal with this effect is the ϕ factor (or thermal inertia) correction [5,9]. However, this method can lead to wrong estimations because it doesn't consider that the kinetics may change during the reaction due to the difference in adiabatic conditions. A more direct and plausible solution is to make the thermal inertia of the sample container close to 1 in the experiment. Dermaut described a method to mimic runaway behaviors at ϕ equals to 1 by multiplying the concentration of the reacting species with exact value of the actual ϕ factor [10]. Chippett proposed a new adiabatic scanning calorimeter which allows the reaction vessel (container) to be

dynamically compensated during tests [11]. Another innovative adiabatic compensation strategy was developed by Frank based on a differential furnace structure [12].

Even the above mentioned compensation methods for the “thermal lag” effect are theoretically feasible, the verification of adiabaticity degree for a newly designed ARC is hard to be carried out in practice. A series of researches on the same reactive chemical DTBP with different types of ARCs resulted in different kinetic evaluations [13–15]. Lack of standard property values for the chemicals makes it time-consuming to evaluate performances of different temperature control methods merely through experimental results. In addition, it cannot be neglected that inaccurate data may be generated from the process of data acquisition and processing, which are also factors influencing the assessments of reaction behaviors.

Modeling and simulation of reactions based on reliable kinetics theories can provide a solution. Wilcock has developed A simulation model for nth-order and autocatalytic reactions to assess data processing methods and to test the effect of changes in physical properties on the kinetics [16]. Arcady Kossoy has studied the temperature distribution in the sample cell (including the sample and the container) and its influences on hazard evaluation parameters based on numerical simulations using a kinetic based model [17–19], in turn a new temperature control method for the ARC has been proposed [20].

This paper presents the modeling and simulation of a power compensated reaction system and sequential analyses of some data processing methods based on the simulation results. First, the principle structure of power compensation for sample container used in this

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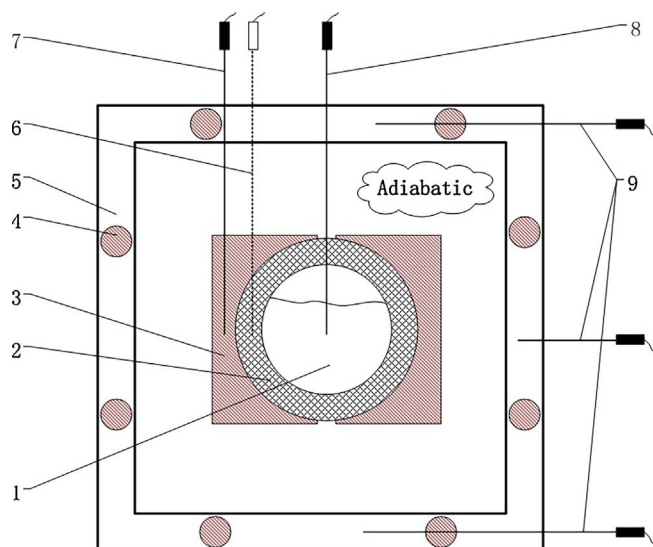


Fig. 1. An ARC with power compensation for the sample container.

research is introduced. Then a dynamic reaction model of n th-order is developed considering the real time heat transfer between the sample and the container. From the perspective of energy equations, the temperature control strategy for compensation is discussed. The improved control effect is shown by simulated thermal behaviors and calculated kinetics of DTBP and verified by experiments. At last, inaccurate kinetics caused by some typical data processing methods for the ARC are demonstrated using the simulation results.

2. Power compensation structure

Principle structure of the power compensation method for sample container presented herein is shown in Fig. 1. The adiabatic condition for the reaction unit (including 1, 2 and 3) is achieved by traditional ARC's furnace structure which comprises a guard 5, several guard heaters 4 and associated thermocouples 9 mounted at corresponding positions. For power compensation, a container heater 3 is coupled to the outside surface of the sample container 2. The compensation heater 3 is made of material with high thermal conductivity and low heat capacity to guarantee adequate uniformity of temperature in the body of container heater 3 and on its interface with the container 2. The container thermocouple 7 inserted into the heater 3 and the sample thermocouple 8 inserted into the sample 1 are used to measure outer surface temperature of the container and temperature of the sample respectively. An alternative thermocouple 6 can be mounted in the wall of the container for sensing the container temperature, providing more information during tests.

1-sample 2-container 3-container heater 4-guard heater 5-guard 6-container thermocouple (alternative) 7-Heater thermocouple 8-sample thermocouple 9-guard thermocouples

A controller (not shown in the figure) will record temperature data from all the thermocouples during reaction tests and conduct real time calculation of power required for each heater in the system. Guard heaters are provided with powers to maintain the guard temperature at the same temperature of the outer surface of the container. The container heater is controlled to supply sufficient compensating power for heating the container, preventing heat absorption by the container from the reacting sample.

3. Dynamic modeling and analysis

The rate of a reaction is related to the real time sample temperature. As a result heat transfer between the sample and the container changes the sample's temperature rate and then definitely influences the

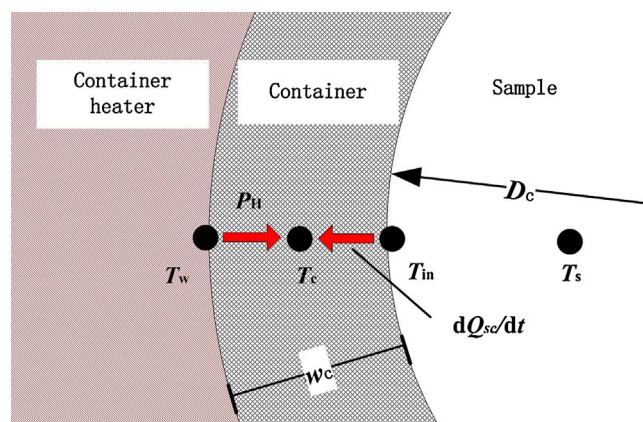


Fig. 2. Heat transfer principle of the lumped parameter model.

reaction progress. The model takes into account not only the classical reaction theories but also more importantly, the real time heat transfer between the sample and the container. Considering the model complexity and calculation efficiency, a lumped parameter model concerning temperature gradients between finite mass points rather than a distributed parameter model was chosen to simulate the thermal behaviors of the reaction system.

3.1. Hypotheses

Heat transfer principle of the simplified reaction unit model is shown in Fig. 2, and assumptions used in the model are made as followings:

- (1) Temperature control of the guard is ideal so that there is no heat transfer between the reaction unit (including the sample, the container and the container heater) and the surroundings.
- (2) Heat transfer in the reaction unit is simplified as thermal conductions between three mass points along the radius direction of the container's wall, representing the sample, the container heater and the container body (geometrically located at the middle surface of the container wall), whose temperatures indicated by T_s , T_w and T_c respectively, as shown in Fig. 2.
- (3) The sample is considered to be at a uniform temperature T_s and have complete contact with the container's inner wall at the boundary, thus T_s equals to temperature of the container's inner wall T_{in} all the time. Considering the temperature gradient within the sample in practice, boundary condition of the third kind is applied at the boundary with an equivalent overall thermal conductivity. Temperature of the container heater's body is also assumed to be uniform and has complete contact with the container's outside surface. Boundary condition of the third kind is applied between the heater and the container with an equivalent thermal conductivity.

Main equations used in the modeling of the reaction unit are described as followings.

3.2. n th-order reaction equation

According to related theories [5], for a n th-order reaction with a single reactant, when the sample temperature T_s is above the initial decomposition temperature and the reactant concentration $c_m > 0$, the reaction rate can be expressed by:

$$r = -\frac{dc_m}{dt} = kc_m^n \quad (1)$$

where c_m [mol L⁻¹] is the molar concentration of the reactant in the

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