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Chemical Papers 2017

Estimation of kinetic parameters from adiabatic calorimetric data by a hybrid Particle Swarm Optimization method

Chemical Engineering Research and Design Volume 122, June 2017, Pages 273–279

Zi-Chao Guo, Li-Ping Chen, Wang-Hua Chen, Department of Safety Engineering, School of Chemical Engineering, Nanjing University of Science and Technology, Nanjing, Jiangsu 210094, China

Abstract

Due to the intense non-linear behavior in the task of estimation of the kinetic parameters from the experimental adiabatic data, a hybrid Particle Swarm Optimization (PSO) is proposed to estimate the kinetic parameters. This method is applied to two real cases: decomposition of DTBP and a nitro-compound under adiabatic conditions. By comparing the experimental and calculated temperature rise rate curve, the accuracy of the fitted parameters is verified. These two cases reasonably prove the validation of this hybrid PSO algorithm in the estimation of kinetic model parameters of adiabatic data.

Link to Purchase Paper: <http://www.sciencedirect.com/science/article/pii/S0263876217302502>

Thermoanalytical investigation of the reactions causing the transuranic waste drum breach that occurred in the Waste Isolation Pilot Plant Thermochimica Acta 650 (2017) 76-87

Randall D. Scheele^{a,*}, Bruce K. McNamara^a, Jon M. Schwantesa, David T. Hobbsb, Michael J. Minettea, Christopher A. Barretta

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Abstract

In February 2014, an energetic gas-producing chemical reaction occurred in remediated plutonium processing waste emplaced in the Waste Isolation Pilot Plant causing the drum's seal to fail and release radioactive material into and outside of the plant. This article provides results of our probative study using simultaneous thermogravimetric and differential thermal analysis and accelerating rate calorimetry to determine the thermal sensitivities of selected simulated characteristic remediated wastes such as hydrogen- and hydrogen, metal-triethanolamine nitrates and nitric acid solidified and stabilized with wheat-based pet litter. These studies found that these nitrate wastes were chemically unstable and susceptible to gas-producing thermal runaway reactions. If undried or partially dried, self-sustaining or accelerating-exothermic reactions were delayed in nitrate- and organic-containing materials to above 100 °C while air-dried nitric acid and pet litter began self-heating exothermic reactions near 30 °C that led to thermal runaway. Caution must be exercised when managing nitrate-containing wastes.

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2016

Evaluation of thermal hazards and thermo-kinetic parameters of N,N'-dinitro-4,4'-azo-Bis(1,2,4 triazolone) (DNZTO)

Thermochimica Acta 623 (2016) 58-64

Jiaping Zhu, Shaohua Jin, Yuehai Yu, Chunyuan Zhang, Lilijie Li, Shusen Chen, Qinghai Shu
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Abstract

Thermogravimetric–differential thermal analysis (TG–DTA) and accelerating rate calorimetry (ARC) were performed to understand thermal characteristics and kinetics of energetic N,N'-dinitro-4,4'-azo-Bis(1,2,4-triazolone) (DNZTO). A single sharp and narrow exothermic decomposition occurred at 143.3, 150.3, 156.4, 157.4, 159.8 and 160.3 °C at different heating rates (0.5, 1, 2, 3, 4, and 5 °C min⁻¹) suggesting that DNZTO composition was vulnerable to thermal hazard. The FTIR–TGA–MS results revealed that the decomposition product was made up of H₂O, NO₂, NO, CO₂, CO, HCN, and N₂O. ARC studies depicted onset temperature at 116.6 °C with temperature step of 5 °C and phi factor of 41.46, and a sharp rise in exothermic reaction at 127.69 °C within the time span of 49.04 min with the maximum heat release rate of 0.47 °C min⁻¹. The exothermic activity resulted in adiabatic pressure rise of the sample up to 300 kPa by the sample pyrolysis into gas. In addition, the kinetic parameters of DNZTO were estimated for the thermal process by TG–DTA and ARC.

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2015

Thermal hazards and kinetic analysis of salicyl hydroxamic acid under isothermal and adiabatic conditions ***Thermochimica Acta 623 (2016) 58-64***

Gui-bin Lu, Cai-xing, Zhang, Wang-hua Chen*, Li-ping Chen, Yi-shan Zhou
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Abstract

Kinetic study and thermal hazards analysis on the thermal decomposition of salicyl hydroxamic acid (SHA) was carried out using differential scanning calorimetry (DSC). The isothermal and dynamic differential scanning calorimetric curves were recorded, respectively. The temperature dependence of the observed induction periods suggests an autocatalytic decomposition mechanism, which was supported by the conversion-reduced time plots. The differential and integral isoconversional methods were used to obtain the kinetic parameters. The decomposition mechanism model of the first peak was $f(\alpha) = \alpha^{1.49}(1 - \alpha)^{1.59}$. Moreover, the isothermal temperature induction period were studied to obtain the activation energy, which was close to that obtained by the iso conversional integral method. The adiabatic accelerating calorimetry (ARC) was also employed to evaluate the thermal hazards. The adiabatic activation parameters were also obtained based on the autocatalytic reaction model

Link to Purchase Paper: <http://www.sciencedirect.com/science/article/pii/S0040603115004384>

Research on the critical temperature of thermal decomposition for large cartridge emulsion explosives
Journal of Loss Prevention in the Process Industries 38 (2015) 199-203

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Abstract

Emulsion explosives are one type of main industrial explosives. The emergence of the large cartridge emulsion explosives has brought new security incidents. The differential scanning calorimeter (DSC) and the accelerating rate calorimeter (ARC) were selected for the preliminary investigation of the thermal stability of emulsion explosives. The results showed that the initial thermal decomposition temperatures were in the range of 232-239°C in nitrogen atmosphere (220e232 °C in oxygen atmosphere) in DSC measurements and 216 °C in ARC measurements. The slow cook-off experiments were carried out to investigate the critical temperature of the thermal decomposition (T_c) of the large cartridge emulsion explosives. The results indicated that the larger the diameter of the emulsion explosives, the smaller the T_c is. For the large cartridge emulsion explosives with diameter of 70 mm, the T_c was 170 °C at the heating rate of 3°C h⁻¹. It is a dangerous temperature for the production of the large cartridge emulsion explosives and it should cause our attention.

Link to Purchase Paper: <http://www.sciencedirect.com/science/article/pii/S0950423015300395>

2014

Thermal risk evaluation on decomposition processes for four organic peroxides
Thermochimica Acta 589 (2014) 11–18

Jiayu Lv, Wanghua Chen, Liping Chen, Yintao Tian, Jiaojiao Yan

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Abstract

Four widely used organic peroxides, namely DTBP, DTAP, BTDH and TBPB, were investigated for hazards caused by their thermal instabilities. Chemically pure materials without diluents were adopted to reveal their thermal decomposition and associated kinetic processes. DSC was employed to carry out experimental thermal study and the Friedman isoconversional method, the Kissinger method, as well as AKTS software were used for kinetic calculations and numerical simulations. Experimental results showed TBPB had the lowest detected “onset temperature”, and unlike DTBP, DTAP and BTDH, all of which showed a two-stage decomposition, TBPB decomposition occurred in a single stage. Heats of reactions measured by ARC were between ca. 37 and 54% of the heats of reaction measured by DSC and reported elsewhere by both, DSC and ARC. The obtained values are compared and discussed. Then, a risk diagram was established to determine the conditionally acceptable conditions of use for the OPs. Furthermore, pressure evaluation results by TSu indicated the generation of non-condensable gas during runaway reactions should be seriously considered.

Link to Purchase Paper: <http://www.sciencedirect.com/science/article/pii/S0040603114002184>

Water induced thermal decomposition of pyrotechnic mixtures: Thermo kinetics and explosion pathway
Journal of Loss Prevention in the Process Industries 30 (2014)

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Abstract

Pyrotechnic mixtures are susceptible to explosive decompositions. The aim of this paper is to generate thermal decomposition data for flowerpot tip, which is a mixture used in the tip of flowerpot fireworks for easy ignition. Several accidents were reported by using this mixture. The mixture is prepared by mixing barium nitrate, potassium nitrate, aluminum (666) and dextrin in a slurry manner with water. In the manufacturing process 40% water wt/wt is added to the mixture. The thermal characteristics of pure sample and water added sample were studied. Differential Scanning Calorimeter is used for screening tests and Accelerating Rate Calorimeter is used for detailed studies in adiabatic and isothermal mode. The self heat rate data obtained showed onset temperature for pure sample at 170.62 °C and the sample with water showed a much earlier onset at 95.71 °C in adiabatic mode. Also it gets decomposes even at 40 °C and starts exothermic characteristics with a substantial rise in system pressure of 32 bar in isothermal mode. The heats of exothermic decomposition and Arrhenius kinetics were computed.

Link to Purchase Paper: <http://www.sciencedirect.com/science/article/pii/S0950423014000436>

2013

Effects of incompatible substances on the thermal stability of dimethyl sulfoxide
Thermochimica Acta 559 (2013) 76– 81

Xiao-Wu Yang, Xiang-Yang Zhang, Zi-Chao Guo, Wen-Shuai Bai, Lin Hao, Hong-Yuan Wei

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Abstract

Thermal decomposition of pure dimethyl sulfoxide (DMSO) and DMSO in the presence of different incompatible substances including N,N-dimethyl formylamine, NaOH, KBr and FeCl₃ were investigated using accelerating rate calorimeter. Hazard indicators such as onset temperature Tonset, adiabatic temperature rise ΔT_{ad} , maximum pressure Pmax at Tfinal, residual pressure Presidual at 50 °C, maximum rate of pressure-rise (dP/dt)max and self-heating rate (dT/dt)max have been determined directly. Activation energy Ea of decomposition reaction and time to maximum rate TMRad of pure and impure DMSO have been studied from the measured self-heating rate data by assuming a zero-order reaction. Moreover, the decomposition mechanisms of pure and impure DMSO have also been discussed.

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Evaluation of thermal hazards and thermo-kinetic parameters of a matchhead composition by DSC & ARC
Thermochimica Acta 557 (2013) 13– 19

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Abstract

From the process safety point of view, irrespective of the kind of stimulus (friction, impact, heat), the final event is “thermal” in nature. Differential Scanning Calorimetry (DSC) and Accelerating Rate Calorimetry (ARC) were performed to understand thermal characteristics and kinetics of a matchhead composition. A single sharp and narrow exothermic transition occurred at 200, 210, 215 and 220 °C at different heating rates (5, 10, 15 and 20 °C min⁻¹) suggesting that the matchhead composition was vulnerable to thermal hazard. ARC studies depicted onset temperature at 115.5 °C and a sharp rise in exothermic reaction at 127.64 °C within the time span of 14 s with the maximum heat release rate of 598.4 °C min⁻¹. The exothermic activity resulted in rapid pressure rise (50.45 bar) confirming the vulnerability of this mixture to undergo catastrophic explosion. Kinetic parameters were estimated for the thermal process observed in DSC and ARC. Such data were validated.

Link to Purchase Paper: <http://www.sciencedirect.com/science/article/pii/S0040603113000646>

Thermal stability evaluation of β -artemether by DSC and ARC

Thermochimica Acta 569 (2013) 134– 138

Haisu Gao, Liping Chen*, Wanghua Chen, Shilong Bao

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Abstract

The thermal stability of β -artemether under dynamic, isothermal and adiabatic conditions were investigated by differential scanning calorimeter (DSC) and accelerating rate calorimeter (ARC), respectively. The dynamic DSC measurements at various heating rates (1, 2, 4 and 8 °C min⁻¹) displayed that β -artemether experienced polymorph transformation in the melting process. According to the isothermal DSC results at different temperatures 86, 88, 90 and 92 °C, β -artemether decomposed after the completion of the melting and the polymorph transformation, and the thermal decomposition of β -artemether is hazardous for its characteristic of autocatalytic decomposition. The kinetics analysis dynamically and isothermally described by Friedman method indicated the thermal decomposition of β -artemether did not comply with a single mechanism. The ARC results showed that the pressure increased with the increase of temperature, and indicated obvious linear relationship. Based on the ARC data, the value of SADT of β -artemether in 50 kg package was obtained.

Link to Purchase Paper: <http://www.sciencedirect.com/science/article/pii/S0040603113003869>

Accelerating rate calorimeter studies of water-induced thermal hazards of fireworks tip mixture

Journal of Thermal Analysis and Calorimetry June 2013, Volume 112, Issue 3, pp 1335-1341

Thermochemical Laboratory, Department of Chemical

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Abstract

The objective of this article is to generate thermal decomposition data on fireworks tip mixture, a mixture used to coat the tip of fireworks, for easy ignition. This mixture has reportedly involved in triggering many accidents in fireworks industry. Different quantities of water were added to the mixture and its thermal characteristics were studied. Differential scanning calorimeter was used for screening tests and accelerating rate calorimeter was used for detailed studies in adiabatic and isothermal modes. The self-heat rate data obtained showed onset temperature for different quantity of water, at a range of 80–170 °C. The mixture with 40 % water wt/wt had onset at 80 °C in adiabatic mode. The same mixture on isoaging at 40 °C exhibited exothermic characteristics with a substantial rise in system pressure (57 bar). The heats of exothermic decomposition and Arrhenius kinetics were also computed.

Link to Purchase Paper: <http://link.springer.com/article/10.1007%2Fs10973-012-2716-5>

Thermal behavior pattern of tributyl phosphate under adiabatic conditions

Journal of Thermal Analysis and Calorimetry January 2013, Volume 111, Issue 1, pp 849-856

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Abstract

Violent decomposition of Tributyl Phosphate (TBP), a widely employed extractant in the Plutonium Uranium Extraction process of nuclear fueling reprocessing plants in the presence of Nitric acid at temperatures in excess of 130 °C is a matter of concern in serious accidents including in the Savannah River (USA) and Tomsk (Russia). The thermal behavior of TBP under adiabatic conditions employing the world's benchmark adiabatic calorimeter, the Accelerating Rate Calorimeter is examined. TBP shows multiple self heating exothermic activities with the onset of primary exotherm at 250 °C. The exothermic activity is accompanied by considerable pressure rise. The thermal decomposition of TBP is found to follow first order Arrhenius kinetic model. TBP loses about 70% of its chemical moieties as volatile matter during the exothermic decomposition. Spectroscopic methods are used to elucidate the degradation pathway.

Link to Purchase Paper: <http://link.springer.com/article/10.1007%2Fs10973-012-2197-6>

Thermal hazard analysis of cyclohexanone peroxide and its solutions
Thermochimica Acta 568 (2013) 175– 184

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Abstract

Cyclohexanone peroxide (CYHPO) is widely used in the chemical industry, but unfortunately, as an organic peroxide, it has been involved in many serious fires and explosions in daily manufacturing, storage, and transportation. We present an advanced methodology of application of thermal analysis for thermal hazard investigation of complex chemical reactions. The applied method is based on a differential isoconversional approach and involves the combination of non-isothermal differential scanning calorimetry (DSC) and adiabatic measurements by accelerating rate calorimeter (ARC) for kinetic analysis and prediction. The kinetic parameters and heat balance were analyzed and used for a simulation of the adiabatic behavior: time to maximum rate under adiabatic conditions (TMRad) and self-accelerating decomposition temperature (SADT). Applications of finite element analysis (FEA) for heat balance and accurate kinetic description allowed us to determine the effect of scale, geometry, heat transfer, thermal conductivity, and ambient temperature on the heat accumulation process. The presented explosion simulations of the thermal behavior of 100 kg storage tank at different temperatures, related to the possible storage scenarios, may help in the elucidation of a real accident which occurred in Beijing during CYHPO storage.

Link to Purchase Paper: <http://www.sciencedirect.com/science/article/pii/S0040603113003559>

2012

Study on thermal properties and kinetics of benzoyl peroxide by ARC and C80 methods
Journal of Thermal Analysis and Calorimetry March 2012, Volume 107, Issue 3, pp 943-948

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Abstract

Benzoyl peroxide (BPO) has been widely used in the industrial and food field, it is sensitive to shock, heat and friction, and causes thermal explosion incidents easily. Therefore, it is important to understand its thermal behaviors and kinetics for loss prevention and safety management. Two kinds of experimental methods (C80 calorimetry and accelerating rate calorimetry) were used to study the hazardous characteristics of BPO, and idea kinetic parameters, such as the pre-exponential factor and the activation energy were obtained. These results contribute to improve the safety in the reaction, transportation, and storage processes and help to the stability criterion of decomposition reaction of BPO

Link to Purchase Paper: <http://link.springer.com/article/10.1007/s10973-011-1536-3>

Thermal hazard research of smokeless fireworks
Journal of Thermal Analysis and Calorimetry September 2012, Volume 109, Issue 3, pp 1151-1156

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Abstract

The problem of dealing with expired military propellant is paid wide attention throughout the world. Currently, destruction is adopted as the main disposal route; however, the process is cumbersome, dangerous, costly, and even more non-environment-friendly. As a result, it is absolutely necessary to find out an appropriate recycling method. Nowadays a feasible method, by

which the expired military powders are used to make smokeless fireworks, has already been proposed. However, the security of expired military propellant is still making all those concerned anxious on account of the stabilizer's volatilization during long-term storage. In this article, waste single base propellant (named powder 128, one of expired military propellants) and waste single base propellant/potassium perchlorate mixed powder are analyzed by differential scanning calorimeter (DSC) and accelerating rate calorimeter (ARC). The mixtures of these two are considered as the ideal raw materials of smokeless fireworks. DSC results show onset temperature, peak temperature, and normalized heat release of thermal decomposition under the condition of linear heating. Based on DSC data, activation energy and pre-exponential factor of the test samples are calculated according to Kissinger method, Ozawa method, and Friedman method. Furthermore, TD24 is derived by means of AKTS-Thermokinetics software using DSC data. ARC results reveal onset temperature, adiabatic temperature rise, self-heat rate, time to maximum rate and pressure-temperature profile. TD24, which can be applied for the evaluation of thermal and pressure hazards, can be obtained in two ways from the data measured by ARC. One is calculated directly from the experiment, and the other indirectly from the fit-calculations. Based on these results, the thermal hazards of these two mixtures were analyzed preliminarily

Link to Purchase Paper: <http://link.springer.com/article/10.1007/s10973-012-2367-6>

Adiabatic thermokinetics and process safety of pyrotechnic mixtures

Journal of Thermal Analysis and Calorimetry September 2012, Volume 109, Issue 3, pp 1387-1395

Sridhar Vethathiri Pakkirisamy, Surianarayanan Mahadevan, Sivapirakasam Suthandathan Paramashivan, Asit Baran Mandal
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Abstract

Pyrotechnic mixtures are susceptible to explosive decompositions. The aim of this paper is to generate thermal decomposition data under adiabatic conditions for fireworks mixtures containing potassium nitrate, barium nitrate, sulfur, and aluminum which are manufactured on a commercial scale. Differential scanning calorimeter is used for screening tests and accelerating rate calorimeter is used for other studies. The self heat rate data obtained showed onset temperature in the range of 275–295 °C for the fireworks atom bomb, Chinese cracker and palm leaf cracker. Of the three mixtures studied, atom bomb mixture had an early onset at 275 °C. The mixtures in general showed vigor exothermic decompositions. Palm leaf mixture exhibits multiple exotherm and reached a final temperature of 414 °C. The thermal decomposition contributes to substantial rise in system pressure. The heats of exothermic decomposition and Arrhenius kinetics were computed. The kinetic data are validated by comparing the predicted self heat rates with the experimental data

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