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Kinetic parameters evaluation for isoprene mixed with aluminum oxide

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Abstract

We analyzed the basic hazard characteristics for isoprene in the manufacturing process by evaluating the runaway reaction, kinetic parameters and safety parameters in this study. Experiments were carried out by calculating the thermal decomposition reactions for isoprene and mixed with aluminum oxide in non-isothermal conditions by differential scanning calorimetry (DSC). Afterwards results indicated that isoprene had a conjugated double bond of unstable structure, and therefore it was prone to produce exothermic reaction during the process of polymerization. Aluminum oxide was applied to mix with isoprene, which could increase the heat release rate. Based on the results, safety information should be provided to government and relevant industries for prevention the accident occur in relevant plants.

Keywords: isoprene, runaway reaction, kinetic parameters, aluminum oxide, differential scanning calorimetry (DSC)

1. Introduction

Isoprene is widely applied as rubber materials for producing the rubber materials (IR), isobutylene-isoprene rubber (IIR), chlorobutyl rubber (CIIR), bromo butyl rubber (BIIR), styrene-isoprene-styrene copolymers (SIS), and epoxy resin [1-4]. In addition, pharmaceutical chemicals are included, such as carrots B, vitamin A, vitamin E, and so on [5-6]. Pesticides also need the isoprene. Many reports have referred to isoprene regarding the applications and toxicity analysis in the world, but thermal hazard analysis for isoprene is rare. The purpose of this study was to determine the thermal hazard characteristics for isoprene during the runaway reactions.

Isoprene has exothermic characteristics in polymerization, which requires inherently safer design during preparation, manufacturing, transportation, storage, and even disposal [7]. Unfortunately, many factories did not have complete material safety analysis or applied insufficient information of material safety data sheets (MSDS), therefore unsafe behavior was happened to induce many potential hazards.

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2. Experimental setup

2.1. sample

Experimental technique of DSC was applied to determine the thermokinetic parameters such as T_0 and the thermal hazardous characteristics of adding aluminum oxide. All these chemicals were stored in a refrigerator at 4℃.

2.2. DSC technique

Dynamic scanning experiments were conducted on TA Q20 system coupled with a measuring test cell that could maintain relatively high pressure about 100 bars [8].

3. Results and discussions

DSC under various scanning rates was applied to determine thermokinetics for evaluating the thermal hazard of isoprene, as illustrated in Fig. 1. It demonstrated a comparison of thermal curves of decomposition of isoprene with two types of heating rates (1 and 4℃min^{-1}) by DSC. The initial reaction of isoprene was endothermic when temperature exceeded 110℃ that caused phase change at the moment. Isoprene had a conjugated double bond of unstable structure. Thus, isoprene was stored at low-temperature environment (0 - 20℃) without sunshine[9]. Exothermic reaction of isoprene had a multi-stage of exothermic in temperature condition of 30 to 500℃. Fig. 2 shows heat production rate vs. time by DSC experiments for isoprene and mixed with aluminum oxide under heating rates 4℃min^{-1}. Temperature control or external thermal hazard should be considered during a purification process in filter tank. In practice, a sound and prudent safe design for isoprene operation was mandatory for avoiding runaway incidents. Furthermore, understanding the thermokinetic characteristics and basic chemical or physical properties of isoprene via calorimetry could provide more information for minimizing industrial disasters.

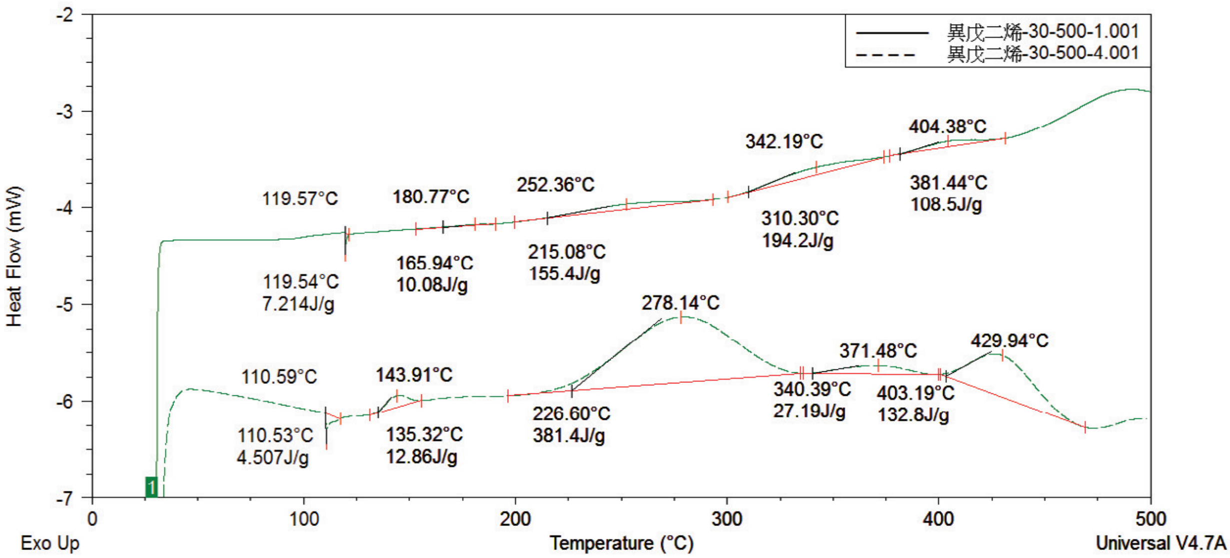

Fig. 1. Heat flow vs. temperature for thermal decomposition of isoprene under 1 and 4℃min^{-1} by DSC.

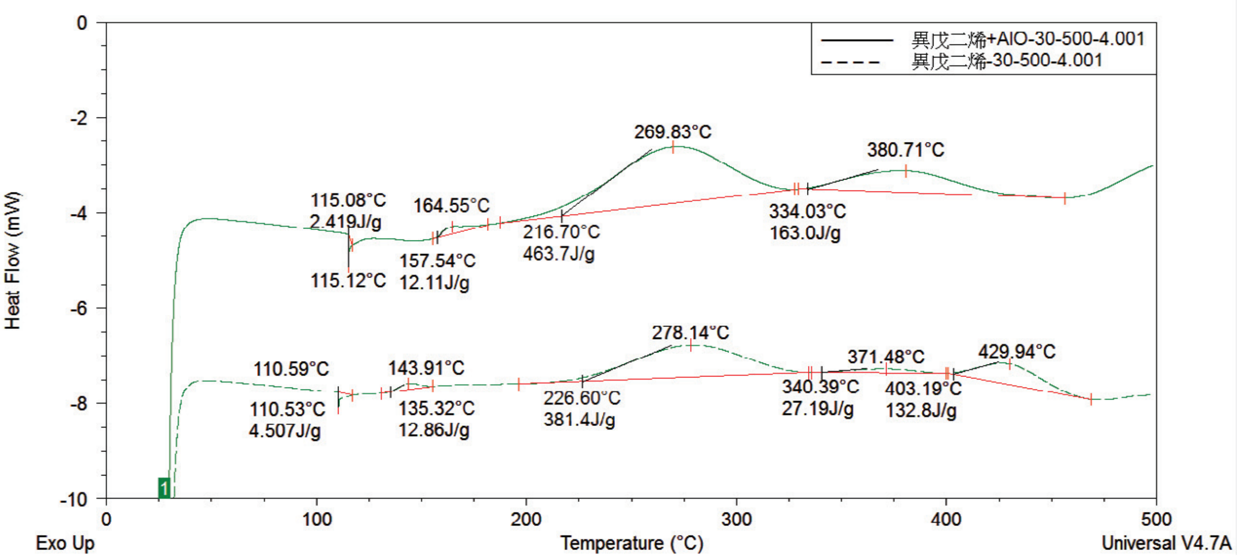

Fig. 2. Heat flow vs. temperature for thermal decomposition of isoprene and mixed with aluminum oxide under 4℃min-1 by DSC.

Table 1. Heat of decomposition, endothermic onset temperature, and exothermic onset temperature of isoprene and mixed with aluminum oxide by DSC tests

Sample	1	2	3
Heating rates (℃/min)	1	4	4
Isoprene mass (mg)	0.9	1.6	2.4
aluminum oxide mass (mg)	-	-	1.1
Total heat release (J/g)	461.0	549.7	636.4

4. Conclusions

A thermokinetic analysis can effectively reduce the occurrence of disasters, if engineers to improve production process by the results of analysis. Experimental results by DSC provided evidence to show that the isoprene had complex reaction. Isoprene is a highly volatile transparent liquid. Isoprene products must be storage under temperature control without sunshine, due to it had an decomposition reaction at 110℃. In practice, results of this study are necessary for safe conditions of application, storage, and transportation in terms of isoprene.

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