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Process Safety Assessment of the Entire Nitration Process of Benzotriazole Ketone

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Abstract

To ensure the inherent safety of fine chemical nitration processes, the nitration reaction of benzotriazole ketone was selected as the research object. The thermal decomposition and reaction characteristics of the nitration system were studied using a combination of differential scanning calorimetry (DSC), reaction calorimetry (RC1), and accelerating rate calorimetry (ARC). The results showed that the nitration product released 455.77 kJ/kg of heat upon decomposition, significantly higher than the 306.86 kJ/kg of the original material, indicating increased thermal risk. Through process hazard analysis based on GB/T 42300-2022, key parameters such as the temperature at which the time to maximum rate is 24 h under adiabatic conditions (T_{D24}), maximum temperature of the synthesis reaction (MTSR), and maximum temperature for technical reason (MTT) were determined, and the reaction was classified as hazard level 5, suggesting a high risk of runaway and secondary explosion. Process intensification strategies were then proposed and verified by dynamic calorimetry: the adiabatic temperature increase (ΔT_{ad}) was reduced from 86.70 °C in the semi-batch reactor to 19.95 °C in the optimized continuous process, effectively improving thermal safety. These findings provide a reliable reference for the quantitative risk evaluation and safe design of nitration processes in fine chemical manufacturing.

Keywords: nitration reaction; process safety assessment; thermal behavior; benzotriazole ketone

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1. Introduction

The loss of control of chemical reactions is one of the main causes of safety accidents in fine chemical enterprises. In order to ensure the smooth operation of enterprise production, it is necessary to conduct material thermal decomposition and reaction heat risk research on fine chemical reactions. Based on the research findings, risk levels should be accurately determined, process parameters optimized, and appropriate control measures rigorously implemented. Fine chemical production frequently involves batch or semi-batch operations. These processes are often complex, variable, and have low automation. In some cases, companies are unaware of the inherent safety risks of chemical reactions. There are problems such as lax process control and insufficient professional knowledge, and the production process is prone to accidents such as fires, explosions, poisoning, and personnel injuries. By conducting safety risk assessments for fine chemical reactions, improving safety facilities, and enhancing risk management, we can enhance the intrinsic safety level of enterprises and effectively prevent and curb the occurrence of safety production accidents [1–3].

Nitration reaction is a very important type of chemical reaction in the organic chemical industry. It is widely used in many industries such as pharmaceuticals, spices, pigments, dyes, explosives, and pesticides. Nitration reaction is a fundamental organic chemical unit reaction, which refers to the reaction in which an organic compound introduces one or more nitro groups into its molecular structure under the action of a nitration agent. There are three main sources of thermal hazards in nitration reactions. Firstly, the reaction is highly exothermic, and the product is unstable, which can easily lead to an uncontrolled reaction. Secondly, the decomposition of nitric acid during the reaction usually releases a large amount of heat. Impurities, such as sulfur and organic residues, may catalyze side reactions, further reducing the safety of the nitration reaction system. In addition, insufficient cooling systems and local overheating of reaction equipment during the nitration reaction will also increase the risk of the reaction. The nitration reaction is more dangerous. The exothermic enthalpy of this reaction increases. The reaction heat of most nitration reactions is -145 ± 70 kJ/mol, which is a strong exothermic reaction. If the reaction process has abnormal failures, such as improper operation, it will develop into thermal runaway of the reaction. When the reaction exothermic rate exceeds the cooling threshold of the reactor, it may cause loss of control and eventually lead to serious consequences such as leakage, fire, and explosion. Ray et al. [4] used dynamic scanning calorimetry (DSC) and accelerating rate calorimetry (ARC) to study the thermal decomposition behavior of 1,2,4-triazole-5-one (TO), nitration solution, and dicyandiamide (NTO) under adiabatic conditions. At the same time, the thermal hazard of NTO synthesis at different feed temperatures was evaluated through thermal variables such as adiabatic temperature increase (ΔT_{ad}) and maximum temperature of the synthesis reaction (MTSR), providing key parameters for the safety of NTO during reaction, transportation, and storage. Yao et al. [5,6] optimized the process of nitration of *meta*-xylene to prepare nitrometa xylene using response surface methodology, determined the optimal reaction conditions, and calculated the reaction enthalpy to be 240.9 kJ/mol with a ΔT_{ad} of 98.1 °C.

Although some progress has been made in the safety risk assessment of chemical reactions, there are still some issues that need to be considered. At present, most studies on the thermal decomposition of substances focus on pure components, without considering the effects of solvents, by-products, etc., on their decomposition behavior during the reaction process. Research results cannot accurately reflect the stability of materials in the actual production process. In addition, research on the thermal hazards of hazardous processes mainly focuses on the reaction process, without analyzing auxiliary units such as quenching, extraction, and acid–base neutralization. Research results cannot fully and truly reflect the thermal hazards of fine chemical processes.

This article focuses on the entire process of nitration of benzotriazole ketone, which includes four steps: nitration, quenching, extraction, and alkaline washing. The decomposition risk, reaction risk, and secondary decomposition risk of the reaction products were analyzed by using DSC, reaction calorimetry (RC1), and ARC. The uncontrolled degree of the reaction and the acceptability of the hazards of the reaction process were evaluated. The research results provide a basis for the safety production control of fine chemical enterprises and the supervision of government functional departments.

2. Experimental Section

2.1. Experimental Principles

The complete nitration process of benzotriazole ketone consists of four sequential steps: nitration, quenching, extraction, and alkaline washing. A schematic diagram of the reaction pathway is presented in Figure 1.

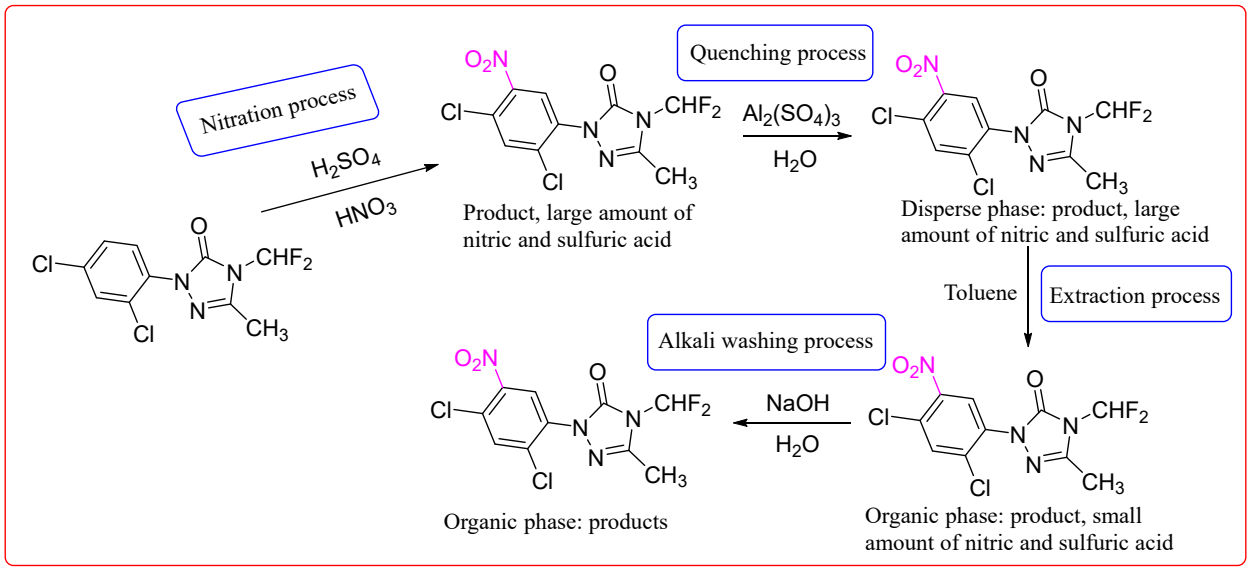


Figure 1. Schematic diagram of the complete process of nitration reaction of benzotriazole ketone.

The complete nitration route for benzotriazole ketone consists of four sequential unit operations—nitration, quenching, extraction, and alkaline washing—executed under rigorously controlled conditions:

(1) Nitration step: The reactor jacket temperature was set to 33 °C. Benzotriazole ketone (186.0 g, 0.63 mol) and fuming sulfuric acid (640.0 g) were charged in a single portion and agitated with an anchor-type impeller at 110 rpm. After the mixture reached thermal equilibrium at 33 °C, concentrated nitric acid (42.0 g, 0.65 mol, 98 wt%) was added dropwise over 30 min while maintaining the bulk temperature at 33 °C. The reaction was then allowed to proceed isothermally until the exotherm ceased (≈6 h). At 33 °C, the post-reaction mixture was sampled to determine the specific heat capacity (Cp) and other thermophysical parameters.

(2) Quenching step: With the reactor at ambient temperature, water (133.0 g) and toluene (140.0 g) were introduced, and the contents were cooled to 5 °C. The stirrer speed was adjusted to 150 rpm before 270.0 g of the nitration mixture was added over 4 h. During the addition process, the temperature rose from 5 °C to 60 °C. After completion, the system was held for 30 min to reach steady state, and Cp, along with other basic parameters of the quenched mixture, were measured.

(3) Extraction step: The quenched liquor (360.0 g) was heated to 63 °C under stirring at 150 rpm. Toluene (140.0 g) was then added in a single charge, followed by a 30 min hold at 63 °C. Once thermal equilibrium was achieved, the mixture was analyzed for Cp and related properties.

(4) Alkaline-washing step: The combined toluene phase (430.0 g) was heated to 63 °C while maintaining agitation at 150 rpm. A single charge of aqueous caustic soda (200.0 g) was introduced, and the biphasic system was held for 30 min. After reaching thermal stability, Cp and other key parameters of the washed organic phase were determined.

This stepwise protocol allowed for a comprehensive evaluation of thermal behavior and heat release characteristics at each stage, providing the data necessary for quantitative safety assessment and subsequent process optimization.

2.2. Reagents

Benzotriazole ketone (AR grade) was obtained from Wuhan Kemike Biomedical Technology Co., Ltd. (Wuhan, China). Oleum, fuming nitric acid, toluene, and sodium hydroxide (all AR grade) were supplied by Nanjing Wangqing Chemical Glassware and Instrument Co., Ltd. (Nanjing, China). All chemicals were used without further treatment.

2.3. Experimental Devices

2.3.1. Dynamic Scanning Calorimetry

DSC is a widely used technique for basic thermal analysis. The test was conducted at a heating rate of 10 °C/min under a nitrogen atmosphere at a flow rate of 50 mL/min. The samples were placed in a pressure-resistant, gold-plated crucible (25 μL capacity, 10 MPa max pressure). Prior to testing, calibration was performed using standard indium (In) and zinc (Zn) samples to ensure instrument accuracy [7–9]. The results were analyzed using the STARe software package V16.10 (Mettler Toledo, Greifensee, Switzerland) to determine the key thermal parameters.

The nitration reaction process of benzotriazole ketone is as follows: add benzotriazole ketone to fuming sulfuric acid, stir to dissolve, and add fuming nitric acid dropwise. The product was quenched with water in a maturation kettle, extracted with toluene, and the organic layer was washed with alkali to obtain 1-(2,4-dichloro-5-nitrobenzene)-4-difluoromethyl-4,5-dihydro-3- methyl-1,2,4-triazole-5(1*H*)-one. The tested materials mainly included (1) the benzotriazole ketone solution and (2) the nitration solution of benzotriazole ketone.

2.3.2. Reaction Calorimeter

The RC1 experiments were carried out using an RC1mx atmospheric pressure glass reactor (Mettler Toledo, Greifensee, Switzerland). The reactor was equipped with a glass thermometer probe, a 25 W calibration heater, and a glass anchor-type stirring blade [10–12]. Key measurement parameters included vessel temperature, jacket temperature, reaction heat release power, total sample mass, thermal accumulation, heat conversion rate, and specific heat release rate.

2.3.3. Accelerating Rate Calorimetry

ARC (THT, Milto, Caines, UK) was employed to investigate the thermal decomposition behavior of the reaction products. The instrument features a pressure range of 0–200 bar, a heating rate of 0–200 °C/min, and a temperature resolution of 0.01 °C. Approximately 10 mL of the sample was sealed in a Hastelloy alloy sphere for testing. Experiments were conducted using the heat–wait–search (HWS) mode, with a heating step of 5 °C, a waiting period of 15 min, a search interval of 10 min, and a temperature rise detection threshold of 0.02 °C/min [13–15].

3. Results and Discussion

3.1. Stability of Material

The DSC results of benzotriazole ketone, the benzotriazole ketone solution, and the nitration solution of benzotriazole ketone involved in its nitration reaction are shown in Figure 2 and Table 1. As shown in Figure 2, the benzotriazole ketone sample was found to release heat in the test temperature range (25–350) °C, starting from 264.98 °C to the end of the test (400 °C), with an extrapolated starting exothermic temperature (Tonset) of 353.61 °C and a heat release rate of 421.42 kJ/kg. The sample melted at 118.79 °C. It can be seen that the solution of benzotriazole ketone released heat in two stages within the temperature range of 25.00~400.00 °C. The solution started to decompose at 144.76 °C until reaching

222.46 °C. The calculated onset decomposition temperature (T_{onset}) was 165.28 °C, and the reaction enthalpy (ΔH_1) was 104.38 kJ/kg. The second stage heat release started at 288.24 °C and ended at 345.85 °C, with a ΔH_2 of 202.48 kJ/kg. The above two stages of heat release were both attributed to the decomposition of fuming sulfuric acid. Moreover, a first-stage exothermic signal was detected in the nitration solution of benzotriazole ketone within the temperature range of 25.00~400.00 °C. The solution started to decompose from 295.99 °C until the end of the test, and the heat release was not complete. The calculated T_{onset} was 336.26 °C, and ΔH was 455.77 kJ/kg. This is mainly attributed to the decomposition of fuming sulfuric acid and 1-(2,4-dichloro-5-nitrobenzene)-4-difluoromethyl-4,5-dihydro-3-methyl-1,2,4-triazole-5 (1*H*)-one.

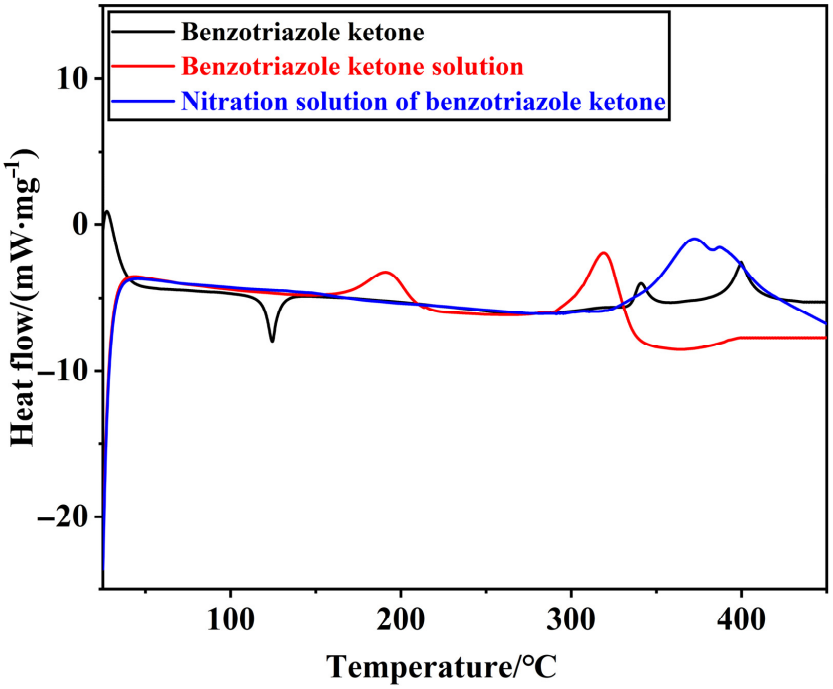


Figure 2. DSC test curve of benzotriazole ketone, benzotriazole ketone solution, and nitration solution of benzotriazole ketone.

Table 1. Summary of DSC testing and extrapolation.

Materials	Mass/mg	Starting Temperature of Heat Release/°C	Peak Temperature/°C
Benzotriazole ketone solution	3.80	I: 144.76 II: 263.96	I: 191.36 II: 319.40
Nitration solution of benzotriazole ketone	3.25	295.99	372.81
Materials	Ending temperature of heat release/°C	Initial decomposition temperature/°C	Heat release/ ($kJ \cdot kg^{-1}$)
Benzotriazole ketone solution	I: 222.46 II: 345.65	I: 165.28 II: 294.41	306.86
Nitration solution of benzotriazole ketone	-	336.26	455.77

Note: "-" indicates that the heat release was ongoing, and the substance was still releasing heat at the ending temperature of the test; "I and II" indicate that the sample underwent multiple stages of heat release with increasing temperature during the testing process. I and II are the ordinal numbers of the samples arranged with increasing temperature.

3.2. Characteristics of Reaction Heat

The exothermic curves of the nitration reaction, quenching process, extraction process, and alkaline-washing process of benzotriazole ketone are shown in Figures 3–6, respectively. The color coding used in the heat release curves is summarized in Table 2. The data are summarized in Table 3. As shown in the exothermic curve in Figure 3, the system exhibited obvious heat release during the process of adding nitric acid and sulfur, and the nitration reaction occurred rapidly at this time. As shown in the exothermic curve in Figure 4, the benzotriazole ketone solution released heat rapidly when it was added to water. It can be seen that the apparent heat release during the quenching process was high, with a ΔT_{ad} of 66.64 °C. As shown in Figures 5 and 6, the heat release during the extraction and alkaline-washing processes was relatively small, with ΔT_{ad}s of 0.22 °C and 5.07 °C, respectively, indicating their high safety. As shown in the exothermic curve in Figure 5, the quenched product was further diluted and released a small amount of heat. As shown in the exothermic curve in Figure 6, when sodium hydroxide solution was added at room temperature, the system temperature decreased, and heat was first absorbed. After reaching the process temperature, a small amount of dilute sulfuric acid reacted with the sodium hydroxide solution and released heat.

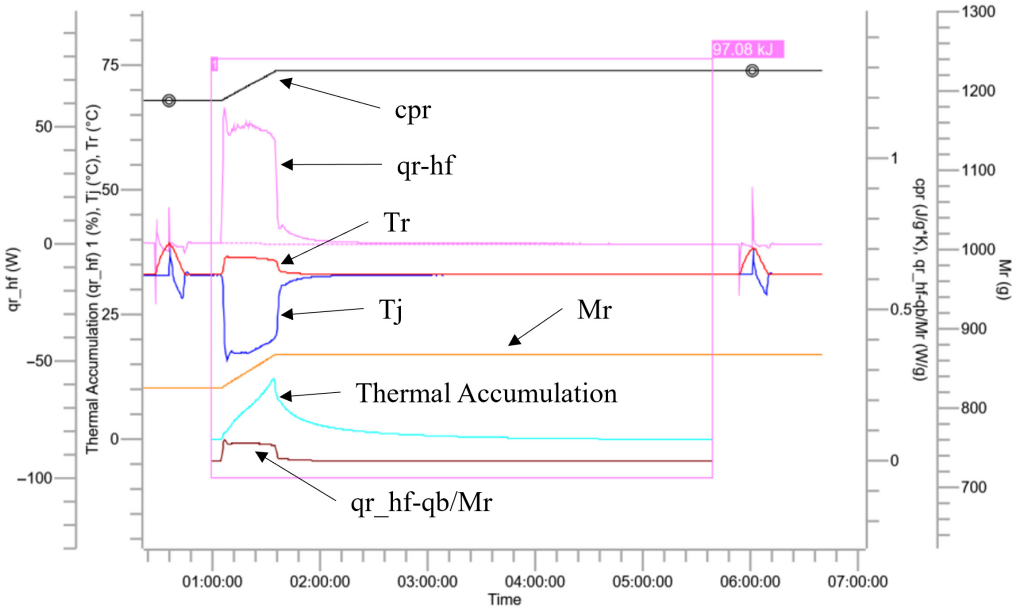


Figure 3. The heat release curve of benzotriazole ketone's nitration reaction.

Table 2. Color explanation of the heat release curves in the whole reaction process.

Trends	Colors	Units
Temperature inside the reaction vessel (Tr)		°C
Reactor jacket temperature (Tj)		°C
Reaction heat release power (qr_hf)		W
Total mass of materials inside the reaction vessel (Mr)		g
Thermal accumulation		%
Thermal conversion		%
Specific heat release rate (qr_hf-qb/Mr)		W/g
Specific heat capacity of the reaction mixture (cpr)		J/g*k

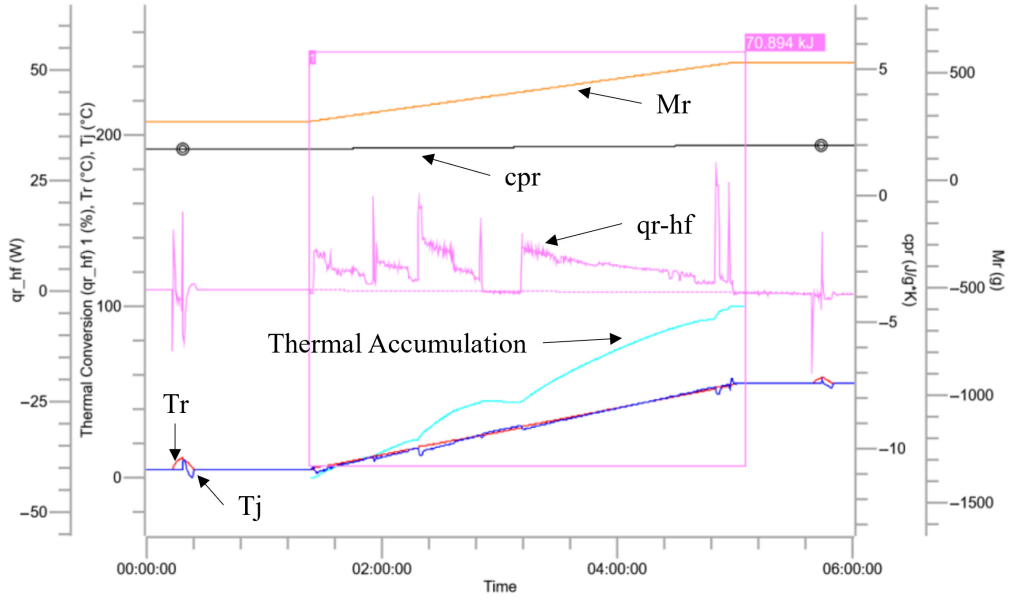


Figure 4. The heat release curve of the quenching reaction.

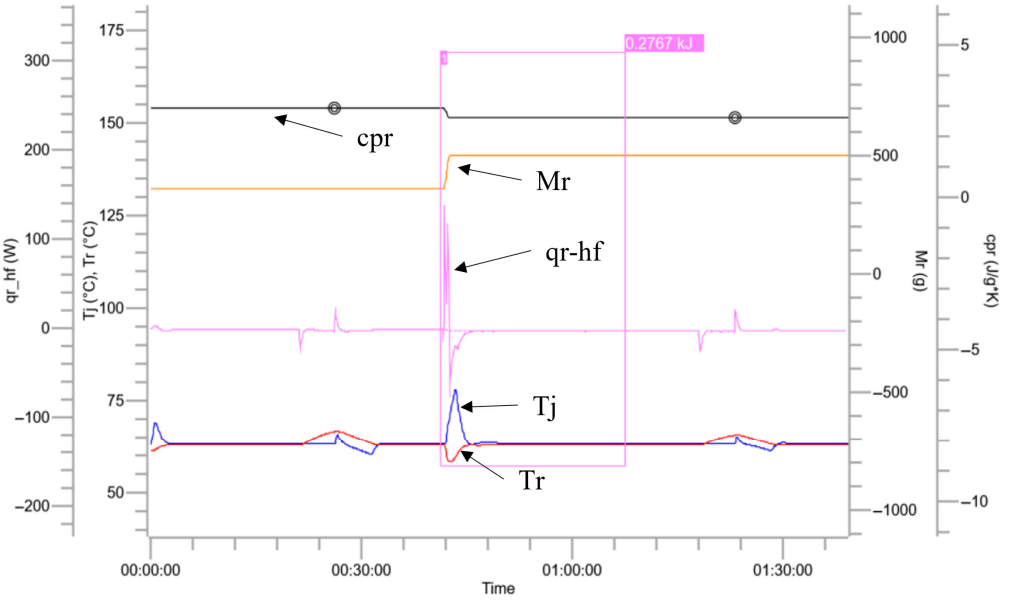


Figure 5. The heat release curve of the extraction process.

As shown in Figure 3, using a semi-batch reactor, the ΔT_{ad} of the nitration reaction of benzotriazole ketone was found to be 86.70 °C. In order to reduce the thermal hazard of the reaction process, an N-type series continuous kettle reactor was adopted in the production process. Using this device, the product could be removed through overflow or a liquid-level control system to ensure a constant volume of reaction materials, volumetric flow rate of feed, and residence time. The N-type series continuous kettle reactor equipment and the process parameters used were as follows:

(1) Process parameters: volumetric flow rate (v_0) = 0.00016 m^3/s, concentration of chlorobenzotriazole ketone at the feed inlet (t = 0) (c_0) = 1298.8 mol/m^3, feed inlet temperature (T) = 25 °C, conversion rate of material at the overflow (X) = 97%, and density of the mixed solution (ρ) = 1800 kg/m^3;

(2) Reactor parameters: volume (V) = 3.99 m^3, heat exchange area (A) = 8.77 m^2, maximum temperature difference with cooling system (ΔT) = 58 K, and comprehensive heat transfer coefficient (U) = 0.0465 kW/(m^2·K).

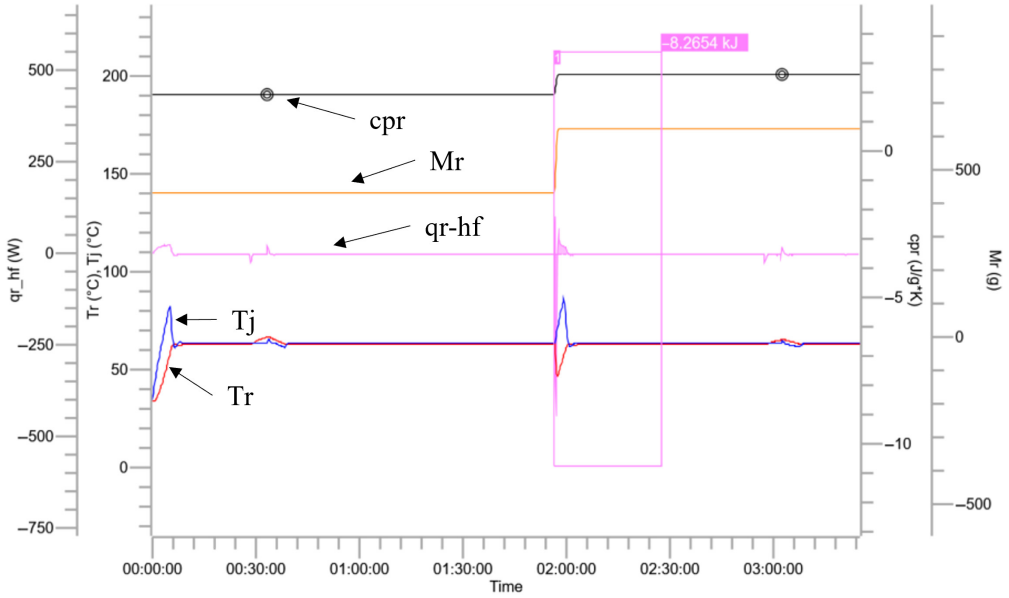


Figure 6. The heat release curve of the alkaline-washing process.

Table 3. The tests and analyzed data of RC1.

Reactions		Apparent Heat Release/kJ	Specific Heat Release/ (kJ·kg^{-1})	Specific Heat Capacity After Reaction/(kJ·kg^{-1}·K^{-1})	
The whole process of nitration of benzotriazole ketone	nitration process	97.08	111.84	1.29	
	quenching reaction	70.89	131.28	1.97	
	extraction process	0.28	0.56	2.59	
	alkaline-washing process	8.27	13.13	2.59	
Reactions		ΔT_{ad}/K	T_P/°C	MTSR/°C	MTT/°C
The whole process of nitration of benzotriazole ketone	nitration process	86.70/11.95#	33.00	119.7/44.95#	320.00
	quenching reaction	66.64	63.00	66.06	100.00
	extraction process	0.22	63.00	63.22	100.00
	alkali washing process	5.07	63.00	68.07	100.00

#: Data corresponding to n-type series continuous kettle reactor. T_p refers to temperature for the process. MTT refers to the maximum temperature for technical reasons.

The calculation of reaction heat for a series continuous stirred tank reactor is shown in Equation (1).

$$Q_{rx} = v_0 c_0 X(-\Delta H_r) \quad (1)$$

The heat exchange calculation of the series continuous stirred tank reactor is shown in Equation (2).

$$Q_{ex} = UA\Delta T \quad (2)$$

At this point, the heat generation exceeds the heat exchange capacity and cannot be removed through the jacket. The temperature difference that must be compensated for through heating and cooling effects is shown in Equation (3).

$$\Delta T_1 = \frac{Q_{rx} - Q_{ex}}{v_0 \rho C_P} \quad (3)$$

The calculated ΔT_{ad} of this reaction process was 19.95 °C, which is 77% lower than the ΔT_{ad} of 86.70 °C in the kettle reactor, indicating that it is safer to use a series continuous kettle reactor than a semi-batch kettle reactor.

3.3. The Secondary Decomposition Behavior of Matter

As shown in Figure 7a, three exothermic signals were detected within the temperature range of 30.00~350.00 °C. The first stage started at 111.00 °C and ended at 125.00 °C, with slow heat release. The temperature increased by 14.00 °C, with a heat release of 92.25 kJ/kg, and the initial temperature increase rate was 2.80×10^{-2} °C/min. The second stage started at 140.90 °C and lasted for a short period of time, ending at 141.90 °C, with a heat release of 6.59 kJ/kg. The instrument entered a search mode again, with the third stage starting from 160.80 °C and ending at 349.10 °C, releasing 1238.90 kJ/kg of heat. Comparing its temperature increase rate, it was found that at this stage, the temperature increase rate reached a maximum value of 0.74 °C/min, the maximum pressure increase rate was 1.19 bar/min, and the temperature corresponding to the maximum temperature increase rate was 240.90 °C. A nitro group, an energetic functional group, was added to benzotriazole ketone. ARC results show that its thermal stability was poor. Therefore, the temperature had to be strictly controlled during the highly exothermic nitration reaction to avoid thermal decomposition. Adiabatic kinetic calculations were conducted at this stage.

As shown in Figure 7b, a heat release signal was detected within the temperature range of 60.0~245.0 °C, starting from 161.63 °C and ending at 238.09 °C, with a heat release of 484.06 kJ/kg, an ΔT_{ad} of 76.46 °C, a maximum pressure increase rate of 0.02 MPa/min, and a maximum temperature rate of 195.09 °C. As shown in Figure 7c, a heat release signal was detected within 60.0~300.0 °C, starting at 155.80 °C and ending at 201.90 °C, with a heat release of 311.03 kJ/kg, an ΔT_{ad} of 46.10 °C, a maximum pressure increase rate of 0.10 bar/min, and a maximum temperature rate of 182.90 °C. During the thermal decomposition process of the mixture after the reaction, T_{D24} was 120.45 °C. As shown in Figure 7d, no obvious exothermic signal was detected within the temperature range of 60.0~315.0 °C for the sample, and the T_{D24} of the solution after the reaction was calculated to be 250.0 °C.

The relationship between the time to maximum rate under adiabatic conditions (TMR_{ad}) and the temperature for the secondary decomposition of nitration, quenching, and extraction products of benzotriazole ketone is shown in Figure 8. As shown in Figure 8a, during the thermal decomposition process of the reacted mixture, the temperature at which the time to maximum rate was 24 h under adiabatic conditions (T_{D24}) was 86.20 °C and the temperature at which the time to maximum rate was 8 h under adiabatic conditions (T_{D8}) was 98.40 °C. As shown in Figure 8b, the T_{D24} during the thermal decomposition process of the mixture after the reaction was 101.90 °C. As shown in Figure 8c, during the thermal decomposition process of the mixture after the reaction, T_{D24} was 85.10 °C and T_{D8} was 94.20 °C.

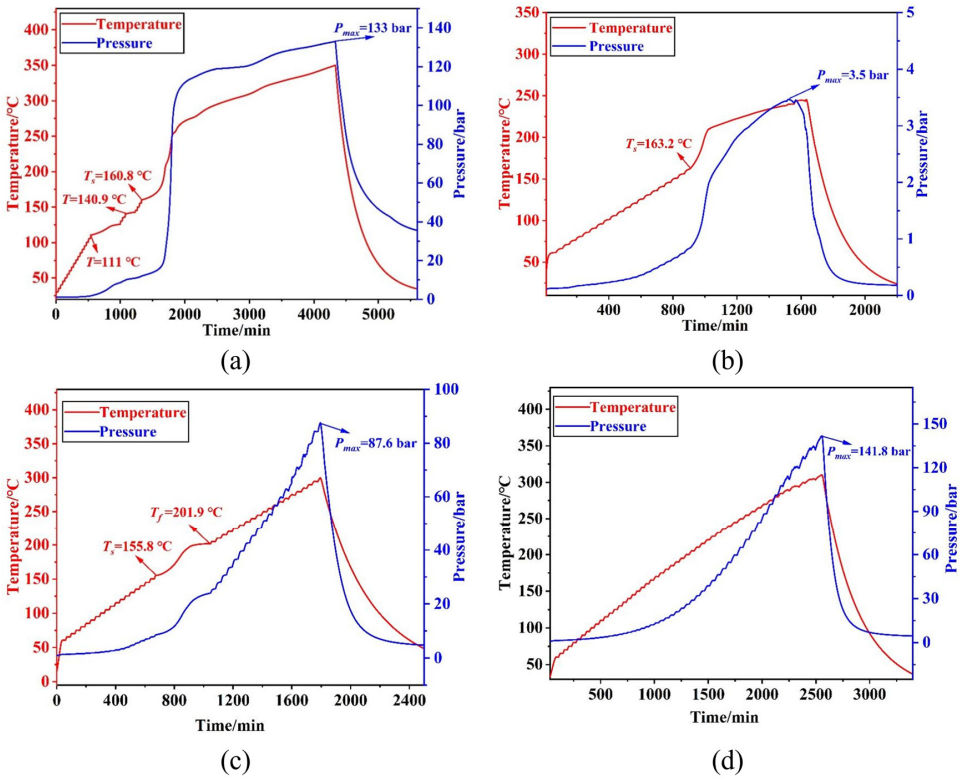


Figure 7. Time–temperature–pressure variation curves of the secondary decomposition of benzotriazole ketone's (**a**) nitration, (**b**) quenching, (**c**) extraction, and (**d**) alkaline-washing products.

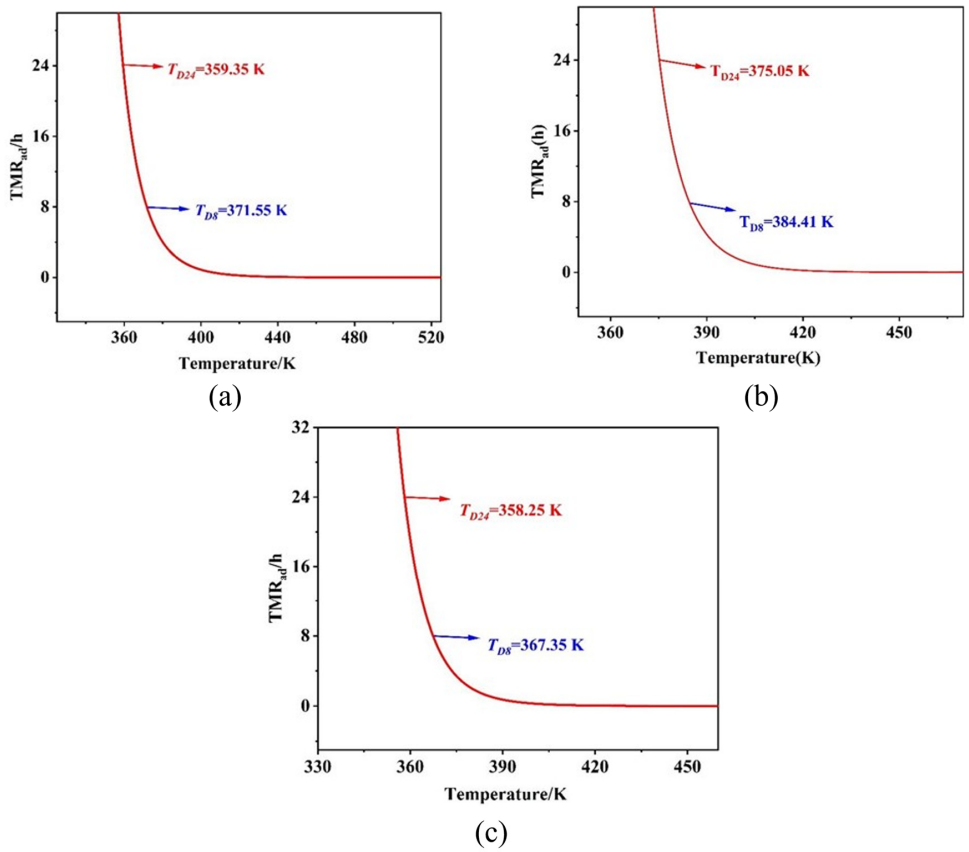


Figure 8. TMR_{ad} curves of the secondary decomposition of (**a**) nitration, (**b**) quenching, and (**c**) extraction products.

3.4. Process Hazard Assessment

A process hazard assessment was conducted based on T_p, MTT, MTSR, and T_{D24}, with evaluation criteria shown in Table 4.

Table 4. Risk assessment criteria for reaction processes [16].

Level	Temperature	Consequences and Explanation
1	$T_p \leq$ MTSR < MTT < T_{D24}	Low risk. When MTSR is less than MTT and T_{D24}, there will be no secondary decomposition of reaction products or material flushing. However, the reactants should avoid prolonged heating to prevent them from reaching MTT.
2	$T_p \leq$ MTSR < T_{D24} < MTT	There is a potential for decomposition of the reactants. MTT is higher than T_{D24}. Once the reaction is out of control for a long time, it may cause secondary decomposition of the reaction products. Continuing to release heat will reach MTT and cause material flushing, etc.
3	$T_p \leq$ MTT $\leq$ MTSR < T_{D24}	Possible material flushing may occur. MTSR is greater than MTT, which can easily cause material flushing and even sudden pressure increase. At this time, MTSR is less than T_{D24}, and the possibility of secondary decomposition of reaction products is not high. The exothermic rate during the MTT reaction affects safety. It is recommended to increase emergency pressure relief and emergency cooling to avoid material flushing.
4	$T_p \leq$ MTT < T_{D24} < MTSR	There is a high possibility of secondary decomposition of materials and reaction products, which may lead to explosions. The temperature may exceed MTT, causing material flushing and secondary decomposition of reaction products, which seriously affects process safety in terms of heat release rate. Emergency pressure relief and emergency cooling have a certain protective effect, but cannot avoid secondary decomposition.
5	T_p < T_{D24} < MTSR < MTT T_p < T_{D24} < MTT < MTSR	There is a high possibility of explosion. MTSR greater than T_{D24} is prone to secondary decomposition of reaction products, which can continue to release heat and exceed MTT temperature, increasing the risk. Relying solely on emergency cooling, emergency pressure relief, etc., cannot meet safety requirements. Therefore, the process should be optimized, area isolation should be increased, and the entire process should be automated.

When using a semi-batch reactor, it can be seen from Table 3 that the nitration process of benzotriazole ketone yielded a T_P of 33 °C, an MTSR of 119.7 °C, an MTT of 320 °C, and T_{D24} of 86.20 °C. The order of the four parameters was T_p < T_{D24} < MTSR < MTT, and the risk of the reaction process was level 5.

4. Conclusions

In this study, DSC, RC1, and ARC were employed to investigate the thermal behavior of the nitration of benzotriazole ketone with mixed acid. The results are as follows:

(1) The decomposition heat release rates of the benzotriazole ketone solution and nitration solution were 306.86 kJ/kg and 455.77 kJ/kg, respectively.

(2) The nitration reaction was a strongly exothermic reaction and underwent a semi-batch kettle reaction. The ΔT_{ad} of benzotriazole ketone nitration was 86.70 °C. The series kettle continuous reaction was safer than the semi-batch kettle reaction.
(3) The secondary decomposition reaction order of the digestion product of benzotriazole ketone under adiabatic conditions in the entire nitration process of benzotriazole ketone was 1.0, E_a was 111.66 kJ/mol, A was 1.1097×10^{10}, and T_{D24} was 86.20 °C. Under adiabatic conditions, during quenching, T_{D24} was 101.90 °C, whereas during the extraction process, T_{D24} was 120.45 °C, and during alkaline washing, T_{D24} was greater than 250 °C.

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Conflicts of Interest: Author Qianjin Xiao was employed by the Jiangsu TaiJieZhiBang Testing Technology Co., Ltd. The remaining authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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