International Journal of Heat and Mass Transfer 99 (2016) 452–460

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Modeling and numerical calculation of three-dimensional non-steady state thermal explosion model of cylindrical battery

Zerong Guo *, Jinyuan Hao, Zhiming Du, Quan Xia

State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, Beijing 100081, China

ARTICLE INFO

Article history:
Received 13 November 2015
Received in revised form 31 March 2016
Accepted 31 March 2016
Available online 20 April 2016

Keywords:
Cylindrical battery
Non-uniform heat dissipation
Three-dimensional partial differential equation
Non-steady state
Thermal explosion time to ignition
Safety time

ABSTRACT

In order to study the thermal safety of cylindrical battery deeply, based on the theory of heat transfer, thermal explosion and nonlinear modeling, a three-dimensional non-steady state thermal explosion mathematical model of cylindrical fireworks with non-uniform heat dissipation of the lateral surface was established for the first time (three-dimensional partial differential equation group). Combining seven point difference method and Newton-homotopy algorithm, the numerical calculation method of the three-dimensional non-steady state thermal explosion partial differential equation was established and the numerical calculation program was written base on Matlab. The validity of calculation program has been demonstrated by comparison of numerical solutions and classical solutions. The accuracy of model has been validated by example computation and analysis. The critical parameters describing non-steady state model of cylindrical fireworks when stored individually and stored in combination form were calculated in this paper, including temperature distribution, temperature–time history, thermal explosion time to ignition, etc. The results show that when the ambient temperature is 450 K, the fireworks stored individually do not have thermal explosion, but the fireworks stored in combination form will explode finally and the thermal explosion time to ignition is 19013.53 s. When the ambient temperature is 460 K, thermal explosion will occur in both the fireworks stored individually and stored in combination form, and the thermal explosion time to ignition are 3187.07 s and 3066.60 s respectively. It shows a more exact analytical methods and solutions of thermal safety evaluation of fireworks was established in this paper. Thus, it is need to strengthen the safety monitoring and management of cylindrical battery (combined fireworks) because of the higher thermal hazard.

1. Introduction

The safety accidents of fireworks occur frequently in recent years and major accidents happen occasionally. On February 14, 2008, the warehouse storage of fireworks thermal exploded and 15,000 boxes of fireworks continued burning explosion for 30 h, which generate a lot of energy equivalent to a 1.1 magnitude earthquake. What's more, the rescue measures were unable to carry out and can only wait for the fireworks in the warehouse to burn out because of huge and continuous explosion [1]. The essential reason for the accident is that poor ventilation of warehouse lead to the thermal imbalance of fireworks system. Energetic material product fireworks are vulnerable to external energy in the production, storage, transport and use process. Heat is one of the most common forms of energy and most likely to lead to accidents [2]. The ambient temperature of fireworks may exceed the critical ambient temperature (a certain value) because of thermal stimulation of outside source heat, poor ventilation and so on. And the chemical reaction system of fireworks will lose thermal balance, accumulate heat constantly, temperature rise sharply, and explode eventually. In the non-steady state thermal explosion theory, the time from thermal imbalance to thermal explosion is defined as thermal explosion time to ignition [3]. In practice, the ambient temperature of fireworks should be monitored. It is important to take corresponding emergency measures in time when there is heat imbalance in the system. It not only can control the spread of accident, but prevent the occurrence of secondary accident and reduce the damage of accident effectively. However, the most significant characteristic of emergency is the urgency of time [4]. Emergency measures should be made within thermal explosion time to ignition as soon as possible. Therefore thermal explosion time to ignition can be referred to as thermal explosion safety time from a security perspective.

Since the simulation method base on thermal dynamic was proposed by Misharev, Kossoy and Sheinman [5,6], much research

* Corresponding author. Fax: +86 10 68914153.
E-mail address: zerongguo@gmail.com (Z. Guo).

http://dx.doi.org/10.1016/j.ijheatmasstransfer.2016.03.128
0017-9310/

Nomenclature

Parameter	The meaning of parameter
χ	heat transfer coefficient (W m^{-2} K^{-1})
χ_r	cylinder radial heat transfer coefficient (W m^{-2} K^{-1})
χ_z	cylinder axial heat transfer coefficient (W m^{-2} K^{-1})
λ	thermal conductivity coefficient of propellant (W m^{-1} K^{-1})
λ_a	thermal conductivity coefficient of air (W m^{-1} K^{-1})
T	system temperature (K)
T_a	ambient temperature (K)
E	activation energy (J mol^{-1})
Q	reaction heat (J kg^{-1})
A	pre-exponential factor (s^{-1})
R	universal gas constant (J mol^{-1} K^{-1})
τ	dimensionless time
τ_{ign}	thermal explosion time to ignition (s)
σ	reactant density (kg m^{-3})
c_v	specific heat (J kg^{-1} K^{-1})
c	reactant concentration (kg m^{-3})
θ	the dimensionless temperature rise
Bi_r	Biot number of the lateral surface
Bi_{z1}	Biot number of the upper surface
Bi_{z2}	Biot number of the lower surface
ρ_1	dimensionless coordinate variable in the r direction
ρ_2	dimensionless coordinate variable in the z direction
ρ_3	dimensionless coordinate variable in the z direction
R_c	thermal contact resistance (m^2 K/W)
R_r	thermal resistance of the lateral surface (m^2 K/W)
R_{z1}	thermal resistance of the upper surface (m^2 K/W)
R_{z2}	thermal resistance of the lower surface (m^2 K/W)
R_a	thermal resistance of the air layer (m^2 K/W)
δ	Frank-Kamenetskii number
ε	the dimensionless activation energy
H	length diameter ratio
n	reaction order

of thermal explosion about the self-accelerating decomposition temperature had been made [7–9]. Nowadays thermal explosion theory keeps improving, especially in the thermal safety problems of fireworks. Zhou [10] solved the one-dimensional thermal safety criticality problems of spherical fireworks base on thermal explosion theory. Ji [11] expanded the one-dimensional thermal explosion theory to the two-dimensional. Seen from the recent year's literature, most of the studies focused on the steady state theory. Researchers studied little on the non-steady state theory and the research of three-dimensional or multidimensional non-steady state thermal explosion of fireworks and crackers is still blank. However, it is urgent to establish a scientific non-steady state thermal explosion model of fireworks and study to obtain a scientific and reliable thermal explosion time to ignition. The model and the calculation program of fireworks should be improved gradually to reflect the objective facts as far as possible. In the study of non-steady state thermal explosion theory, the research results and current situation of the domestic and foreign thermal explosion theory were summarized by Professor Feng [3] in his monograph *Thermal Explosion Theory*, including the one-dimensional non-steady state thermal explosion theory within boundary conditions of Semenov, Frank-Kamenetskii and Thomas. In 1990s, the influence of the reaction on thermal explosion is systematically studied by Ahmad Shouman [12–15] with analytical and numerical methods. The effect of variable heat transfer coefficient on criticality of Semenov system is studied by El-Sayed Saad [16]. At the beginning of 21st Century, two-dimensional non-steady state thermal explosion model is proposed in *Limited Space Explosion and Ignition in Theory and Experiment* [17] published by Wang et al. In 2012, two-dimensional non-steady state thermal explosion model of fireworks with complex shell structures was established by Ji [11]. The thermal safety problem of fireworks is such a problem coupling of heat field, space field and time field in view of the non-steady state thermal explosion theory that increases the difficulty of research to a certain extent. Meanwhile, fireworks are stored in a complex environment or in combination (battery) for the most part in the production, storage, transport and use process. Thus, the non-steady state thermal explosion theory of single cylinder fireworks is no longer applicable in these cases. A accurate non-steady state thermal explosion model and calculation method of battery is imperative.

Above all, it is necessary to study the thermal explosion time to ignition (thermal explosion safety time) to evaluate the thermal safety of battery. Based on heat transfer theory, this paper applied thermal explosion theory, nonlinear modeling and numerical simulation to solve the heat spontaneous combustion and thermal explosion problem of fireworks and obtained the critical parameters of non-steady state. Then it can be used to evaluate the thermal safety of fireworks. A three-dimensional non-steady state thermal explosion mathematical model of cylindrical fireworks with non-uniform heat dissipation of the lateral surface, numerical calculation method and Matlab calculation program (This program can be used for both two-dimensional and three-dimensional thermal explosion calculation of cylindrical system.) were established for the first time. And the thermal safety of cylindrical battery was analyzed.

2. Three-dimensional non-steady state thermal explosion model of cylindrical battery

A common cylindrical battery is treated as the research object, which made up of several single cylinders as shown in Fig. 1.

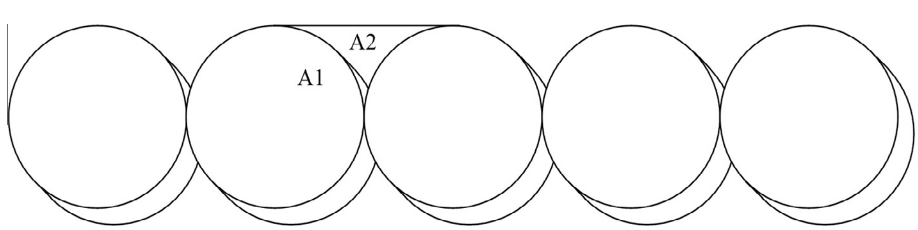

Fig. 1. Diagrammatic sketch of cylindrical battery.