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Convection characteristics in a closed vessel in the presence of exothermic combustion and ambient temperature oscillations

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ABSTRACT

The influences of ambient temperature oscillations on the convection characteristics generated by an exothermic reaction in a closed vessel have been investigated. The left, right and top walls of the vessel are maintained at a constant temperature while the temperature of the bottom wall is assumed to be oscillating about a constant mean temperature. The governing equations are solved using finite difference method. A demarcation line between the explosion and the oscillatory convection is presented in terms of the Rayleigh and Frank-Kamenetskii numbers. It reveals that when the heat generation is large the convection of heat to the side walls must be higher to circumvent the thermal explosion. When the frequency of oscillation and the amplitude of oscillation of the ambient temperature are increased, the intensity of the stream function and the temperature is found to increase in a certain period of time. After that, the reverse characteristics are seen in the next period of time and these occur periodically. For a certain period of time, a cooler region is recognized near the bottom wall. Results also show that for higher values of the Frank-Kamenetskii number the oscillatory convection tends to chaotic and when it exceeds a certain value there occurs thermal explosion. Moreover, the system encounters a rapid explosion with the increase of Frank-Kamenetskii number and Rayleigh number.

1. Introduction

Thermal explosion in a closed domain occurs due to an imbalance between the heat generation and the heat losses to the surrounding environment. Numerous works are available in the literature of explosive chemical reactions. Semenov [1] and Frank-Kamenetskii [2] accomplished the fundamental works on thermal explosion. Semenov [1] considered a well-mixed reactive fluid within a vessel. The temperature and concentration of the fluid are taken spatially uniform and the heat loss to the exterior is expressed by a heat transfer coefficient. Semenov introduced a dimensionless number and showed that thermal explosion could happen if this number exceeds a critical value of $1/e$. On the other hand, Frank-Kamenetskii [2] observed large temperature gradients in reactive vessels which indicate that heat must be removed from the system to circumvent the thermal explosion. In this case, the conduction of heat could be the controlling mechanism of heat removal from the vessels.

A classical problem of the thermal explosion is free convection that takes place due to exothermic reaction in a liquid or gas mixture contained within a vessel. Most of the past studies have illustrated the thermal explosion with a correlation between the limit of thermal self-ignition and the intensity of natural convection. However, the intensity of convection is measured by the Rayleigh number (Ra). For spherical reaction vessels, Ashmore et al. [3] experimentally showed that the critical Rayleigh number for the onset of convection must be 600. But it is much lower compared to 10^4 which has been determined by the conductive theory of Frank-Kamenetskii [2].

Jones [4] examined the influences of convection in exothermic chemical reaction occurring in the gaseous or liquid phase. A linear stability analysis has been performed for parallel plate geometry and numerically determined the critical Rayleigh numbers for the commencement of convection. He also investigated the effects of convection in gas phase exothermic reaction in a horizontal circular cylinder using numerical integration of the governing equations [5]. It is observed that the Rayleigh number significantly enhances the ignition limit. Moreover, when convection takes place in the vessel, the temperature distribution becomes asymmetrical about the centerline of it.

Shtessel' et al. [6] studied the effects of natural convection and internal heat sources on the thermal explosion. The results were discussed in terms of Frank-Kamenetskii criterion and Ra criterion which characterize, respectively, the thermal and hydrodynamic

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stability. Later, a theoretical study has been performed taking into account the effects of both thermal and concentration convection on the characteristics of thermal self-ignition [7]. Merzhanov and Shtessel [8] illustrated the influences of natural convection on the thermal explosion in a liquid. It is revealed by experimental and numerical results that the explosion could be suppressed by natural convection. Moreover, natural convection is significant when the timescale required for the reactive system to raise its explosion point is larger than the timescale for taking place the natural convection. Belk and Volpert [9] conducted a good work on the thermal explosion considering the effect of natural convection. Results demonstrated that natural convection has considerable influences on the critical conditions of the explosion. It also causes complex oscillations and oscillating thermal explosion. Based on the Semenov's model of the thermal explosion, they proposed a simplified model which can illustrate the main features of a complete problem. Lazarovici et al. [10] studied the interactions of convection and thermal explosion within a square reactor bounded by constant temperature walls. The critical conditions for steady states, oscillations, and thermal explosion are elaborately discussed using numerical simulations.

Liu et al. [11] analyzed the problem of the thermal explosion in the presence of natural convection using a new approach. It illustrates the stable and explosive characteristics of an exothermic chemical reaction in terms of the timescales which are used for heating up the system by the particular exothermic reaction, for cooling by thermal conduction and for natural convection. A theoretical relation is also developed using the aforementioned timescales which distinguish the regions where explosions either do or do not occur. Very recently, Campbell [12] investigated the combined effects of the natural convection and the external heat transfer resistance to the thermal explosion in a spherical vessel. Numerical solutions have been carried out for the variations of Rayleigh and Biot numbers.

Most of the studies investigated the characteristics of thermal explosion for processes that occur at a constant or linearly increasing temperature of the surrounding environment. But there are many natural materials such as peat, straw, dry grass etc. where a thermal explosion occurs due to self-heating and autoignition [13,14]. This autoignition process subjected to natural conditions develops owing to relatively high-frequency (diurnal) and low-frequency (seasonal) oscillations of air temperature. In addition to, the thermal explosion can be seen in various configurations of solid materials, namely, piles of food grains, coal, wood chips, biomass or refuse-derived fuels, bagasse and compost, as well as storages containing military munitions, solid propellants, pyrotechnics or similar substances [15]. These arrangements are usually under temperature variations such as day/night variations (in regions close to deserts these are especially significant), seasonal (yearly) variations and weather variations. As a result, thermal equilibrium conditions can break down for the above reactive systems and there might take place thermal explosion resulting in fires. It is worthwhile to note that only a few recent works have presumed oscillating ambient temperature [13–15] for the one-dimensional problem. Among these, Shteinberg and Khudyaev [14] elucidate the justification of such type of boundary conditions. However, no study has taken an attempt for any two-dimensional configurations of thermal explosion with oscillating temperature variations. Thus the objective of the present study is to investigate the influences of oscillating ambient temperature on the thermal explosion in a closed vessel. The system of equations is solved using finite difference method. Results are illustrated to expose how the convection changes its mode depending on the physical parameters such as the frequency of oscillation and the amplitude of oscillation of the ambient temperature, the Frank-Kamenetskii number, and the Rayleigh number.

2. Formulation of the problem

Consider a two-dimensional region $\Re = \{(x, y) : 0 \leqslant x \leqslant L,\ 0 \leqslant y \leqslant L\}$, where x and y are, respectively, the horizontal and vertical Cartesian coordinates. The left, right and top walls arekept at a constant temperature T_0 and the temperature of the bottom wall of the vessel is assumed to be oscillating about a constant mean temperature ΔT. The schematic of the physical configuration is shown in Fig. 1. Following [10–12], it is presumed that the chemical species A contained within the closed vessel undergoes a single step exothermic reaction which can be expressed as

$$A \rightarrow B + \text{heat}, \quad rate = k_0 a e^{-E/(RT)} \tag{1}$$

where k_0 is the pre-exponential factor, E is the activation energy, R is the universal gas constant, T is the temperature of the reactant and a is the concentration of the reactant. According to [10,12], we assume that the supply of reactant is adequate to remain its concentration constant throughout the system.

Now we adopt the Boussinesq approximation so that the density changes can be neglected from all terms except the buoyancy force term. However, it needs to maintain the criterion $\Delta T \ll T_0$, that is, the increase of the system's temperature must be much smaller than its initial temperature. Campbell [12] have pointed out that the Boussinesq approximation is valid for buoyant flows [16], thermal explosion [17–19] and other exothermic reactions [20,21] subject to natural convection.

Based on the above assumptions, the governing equations for mass, momentum and energy in a two-dimensional Cartesian coordinate system are [10–12]:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{2}$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{1}{\rho_0}\frac{\partial (p - p_0)}{\partial x} + \nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) \tag{3}$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -\frac{1}{\rho_0}\frac{\partial (p - p_0)}{\partial y} + \nu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) + \frac{\rho - \rho_0}{\rho_0} g \tag{4}$$

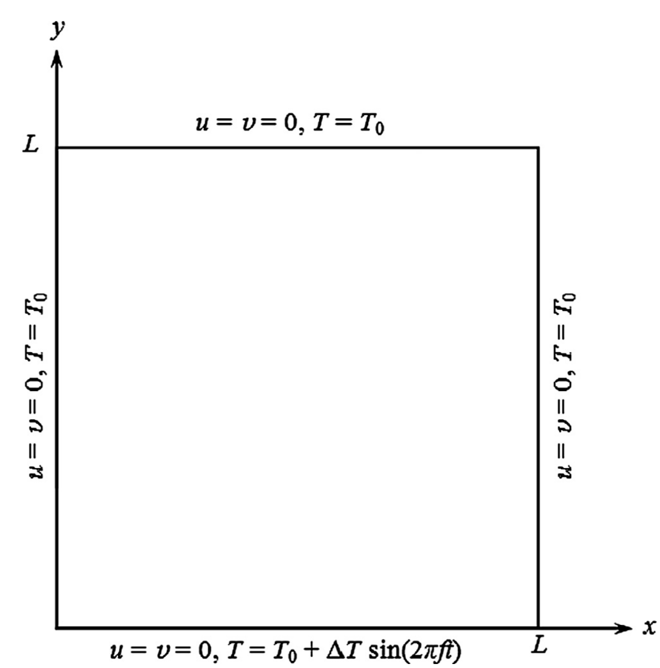

Fig. 1. Schematic of the physical model.