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Effects of combined natural and forced convection on thermal explosion in a spherical reactor

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ABSTRACT

The effects of combined natural and forced convection on thermal explosion in a spherical reactor are studied. Upward natural convection arises from internal heating caused by a chemical reaction, whilst downward forced convection is driven by injecting fluid at the top and removing it at the bottom of the reactor. It is shown that explosive behaviour is favoured by a balance between the natural and forced flows. Such a balance establishes a nearly stagnant region close to the centre of the reactor which quickly heats up to explosion. In fact, counter-intuitively, explosion may occur in an otherwise stable reactor by injecting cold fluid or enhancing natural convection. A scaling relation predicting the physico-chemical conditions for which explosion occurs at minimum heat release is developed. The work concludes with a quantitative three-dimensional regime diagram, accounting for the effects of heat transport by conduction, natural convection and forced flow for systems of similar geometry, where the regions of stability and explosion are delimited.

1. Introduction

Explosions arising from the liberation of heat by a chemical reaction in a closed vessel have been studied extensively. Examples include combustion reactions [1,2] and thermal decompositions [3–5]. The classical cases of purely conductive cooling and of a well-mixed fluid with uniform temperature were first considered by Frank-Kamenetskii [6] and Semenov [7], respectively. Many early studies focused on the effects of geometry of the vessel and of a decreasing concentration of reactant on the conditions for onset of explosion in conductive systems [5,8–21]. However, between the limits of pure thermal conduction and perfect mixing lie the interesting effects of natural convection, normally quantified by the magnitude of the Rayleigh number. Merzhanov and Shtessel [13] were the first to propose a diagram of the Frank-Kamenetskii number *Fk* as a function of Rayleigh number *Ra* in which several different hydrodynamic and thermal regimes were identified. Since then many studies have considered the effects of heat transport by both conduction and natural convection on thermal explosion. These include analytical [22], numerical [23–26] and experimental [2–4] investigations of exothermic chemical reactions in closed vessels of various geometries, including infinite parallel plates, vertical and horizontal cylinders with circular cross-sections and spheres [3,23,26,27]. Reactions of zeroth and first order have been preferentially studied. The effects of consumption of reactant in systems with natural convection have been addressed in e.g. [28,29]. In general it has been shown that *Fk* increases with *Ra* and depends on the geometry of the system and on reactant consumption. Liu et al. [29] quantified separately for the first time the stabilising effects of natural convection and of consumption of reactant on the explosive behaviour of a system with a first-order exothermic reaction in a sphere.

The effects of forced convection on thermal explosion have also been studied, particularly in the contexts of continuous stirred-tank reactors (CSTRs) and jet-stirred reactors (JSRs). In theoretical studies on CSTRs complete mixedness is usually assumed (e.g., [30–32]), and thus the contribution of forced convection is restricted to the assumption of uniformity in space in the energy and chemical balances. In practice, mixing is achieved by forced convection driven by an impeller or by re-circulating part of the fluid into the vessel via injection at high flow rate. In JSRs fluid is pumped into the vessel through one or more nozzles at a high Reynolds number. The vessel is commonly operated in the turbulent regime. A review of numerical and experimental work on jet-mixing processes has been given by [33]. Very few studies have been carried out for laminar flows (e.g., [34,35]) and other studies are restricted to inert systems or to combustion processes with very good mixing [36–44].

The combined effects of forced and natural convection (hereafter referred to as mixed convection) have been studied both for inert [45] and reactive [46] fluids in a vertical pipe. In a spherical geometry, Arquis et al. [47] considered the effects of natural convection driven by heating at the walls and forced convection from

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Nomenclature

c_0	concentration of chemical species A
C_p	specific heat evaluated at constant pressure
C_v	specific heat evaluated at constant volume
E	activation energy
Fk	Frank-Kamenetskii number
g	acceleration of gravity
k_0	reaction rate constant evaluated at temperature (T_0)
L	radius of the vessel
L_i	radius of the inlet and outlet pipes of the vessel
n	order of reaction
p	pressure
p_0	initial pressure
Pe_i	Péclet number for the inlet flow based on L_i
Pr	Prandtl number
q	heat of reaction
r	radial coordinate in the inlet pipe
R	universal gas constant
s_A	surface area of the upper and lower hemispheres of the vessel
Ra	Rayleigh number
Re_i	Reynolds number based on L_i
t	time
t_C	time scale for natural convection
t_D	time scale for conduction
t_H	time scale for heating by reaction
t_S	time scale for forced convection
T	temperature
T_0	initial temperature
$u_{ave,i}$	average flow speed in the inlet pipe
u_z	axial velocity in the inlet pipe
u	velocity vector
U	velocity scale
U_{FC}	velocity scale for forced convection in the vessel
U_{NC}	velocity scale for natural convection arising from temperature increase ΔT_H
x	spatial position vector
z	vertical coordinate in the inlet and outlet pipes

Greek symbols

β	coefficient of thermal expansion
ΔT_H	characteristic temperature increase at equilibrium of heat generation by chemical reaction and loss by thermal conduction
ΔT_S	scale for temperature increase to explosion
γ	ratio of specific heat capacities
κ	thermal conductivity
ν	viscosity
Π	dimensionless pressure
ρ	density
τ	dimensionless time
θ	dimensionless temperature increase
υ	dimensionless velocity vector
ξ	dimensionless position vector
η	dimensionless inverse activation energy

injection and removal of fluid at two directly opposite sides of the vessel along its equator. He used the parameter $Ra/(Re_i^2 Pr)$ to indicate the relative importance of natural and forced convection, and estimate the temperature distribution of the bulk fluid. However, to the authors' knowledge, no studies have been carried out on the effect of mixed convection on thermal explosions.

The present work investigates the effects of combined natural and forced convection on thermal explosion in a spherical geometry. Here, forced convection is caused by a stream of reactant slowly injected at the top and simultaneously withdrawn at the bottom of the vessel, along its vertical axis. Natural convection arises as the fluid heats up owing to an n-th order chemical reaction; the consumption of reactant is neglected so that there is no effect of the order of the reaction, other than determining the rate of heat release. Such a system benefits from simplicity and yet allows us to examine a wealth of interesting phenomena arising from the opposed flows due to natural and forced convection. This new configuration is also very interesting from an energetic perspective, where the potential energy of the heavy fluid entering at the top is used to enhance mixing inside the reactor. The results are compared with those obtained previously for a closed spherical vessel [48].

2. Theoretical analysis

2.1. Governing equations and non-dimensionalisation

Consider a fluid, initially at temperature T_0, undergoing an n-th order exothermic reaction $A \rightarrow B$ in a spherical vessel of radius L. The concentration of A in the reactor is spatially uniform at c_0. A stream of pure reactant at concentration c_0 and temperature T_0 is injected at the top of the vessel and the mixture in the vessel is withdrawn at the bottom, along its vertical axis, at a constant flow rate. Figure 1 shows the axisymmetric configuration. The vessel wall is maintained at T_0. The consumption of reactants is neglected.

Non-dimensionlising temperature T, velocity $\boldsymbol{u}$, pressure p, spatial position $\boldsymbol{x}$ and time t as

$$\Theta = \frac{T - T_0}{\Delta T_s} \upsilon = \frac{\mathbf{u}}{U}, \quad \Pi = \frac{p - p_0}{\rho_0 U^2}, \quad \xi = \frac{\mathbf{x}}{L}, \tau = \frac{Ut}{L}, \qquad \text{(1a-e)}$$

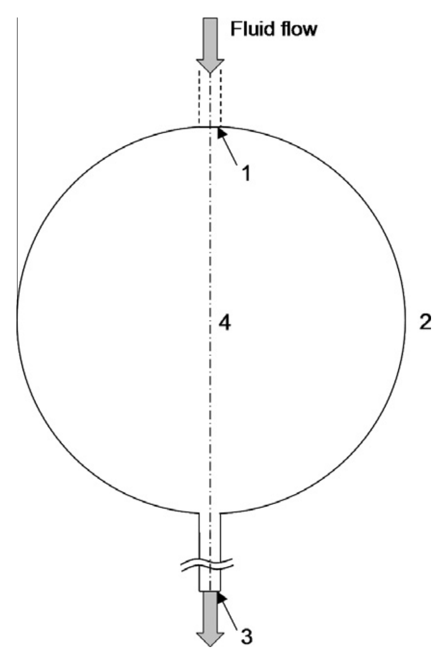

Fig. 1. Configuration of an open-sphere system. Boundaries 1 and 3 indicate the inlet and outlet, respectively. Boundary 2 is the vessel wall, and boundary 4 is the axis of symmetry.