NUMERICAL AND APPROXIMATE SOLUTIONS TO PROBLEMS IN SPONTANEOUS IGNITION

A thesis presented in partial fulfilment of
the requirements for the degree of
Master of Philosophy
in Mathematics at
Massey University

Catherine Margaret Rivers

1994

ABSTRACT

This thesis considers the subject of time-independent spontaneous ignition of materials of arbitrary shape.

Chapter One reviews the major advances up to the work of D.A.Frank-Kamenetskii.

Chapter Two discusses the modern, Gray Wake, formulation of the problem.

In Chapter Three, ignition in the class A shapes is approximated by a numerical finite differences method. The same method is applied to some non-class A geometries.

Solutions to the Gray Wake formulation for ignition in the infinite slab geometry are sought in Chapter Four by approximating the internal energy gradient by the maximum internal energy and by the average internal energy.

Chapter Five considers an industrial application of the spontaneous ignition of moist powder.

CONTENTS

1 INTRODUCTION

1.1 Background

In 1993, at 3:00 am on Good Friday, an explosion occurred in the milk powder factory at Te Rapa, New Zealand (see Figure 1.1). The fire, whose cause is unexplained, resulted in an explosion of milk powder. Extensive damage was caused. The plant, believed to be the largest in the southern hemisphere, was closed for some months at great cost to the parent company.

When materials which contain a heat source are stored in ambient temperatures at or below their internal temperatures, the generated heat builds up to levels where ignition can occur. Powdery masses, like the milk at Te Rapa, can burst into flame, or can explode. The phenomenon is known as spontaneous ignition.

The behaviour and the control of spontaneous ignition is of interest. How hot can materials be assembled? To what temperature should materials be cooled before being stored? Given assembly and storage conditions, what mass of material can be accumulated safely? Can spontaneous ignition be used as a positive factor in manufacturing processes?

Rules of thumb have been developed in many trades, industries and occupations to diminish the risk of spontaneous ignition in the assembly and storage of materials.

Techniques are required to describe the ignition behaviour of materials and to predict safe working limits within which materials can be handled. Modern researchers have endeavoured to disclose the underlying model for spontaneous ignition. This study is a part of that process.

FIGURE 1.1 The aftermath of a dust expolsion.

1.2 Thermodynamic Basis for Ignition

For the elementary reaction $A \Leftrightarrow B$, the activation energy is the energy required to allow the reaction to occur. The greater the activation energy, the fewer are the collisions involving sufficient energy to cause reaction at a given temperature, and the slower is the reaction. As the temperature is increased, more collisions comprise energy equal to or greater than the activation energy, and the reaction rate becomes greater.

For small changes in temperature, the dependence of rate constant on temperature can be represented by the Arrhenius equation,

$$k = A \exp(-E / RT) \tag{1.1}$$

where A is the pre-exponential factor, E is the activation energy, R is the Universal Gas Constant and T is the temperature.

Thermal ignition is an exothermic reaction. Neglecting reactant consumption, the heat balance equation is

$$\nabla \cdot (\kappa \nabla T) + \sigma Q A \exp(-E / RT) = C \frac{\partial T}{\partial t} \tag{1.2}$$

where κ is the thermal conductivity, T the temperature, σ is the density, Q is the exothermicity, C is the heat capacity and t represents time.

The Biot number is the ratio of surface heat transfer to thermal conductivity. If Bi$\rightarrow$0, the temperature becomes uniform throughout the region and there is an abrupt temperature drop at the interface with the surroundings down to the ambient temperature. If Bi$\rightarrow \infty$, the temperature at the boundary becomes equal to the ambient temperature; that is, the boundary condition is

$$T = T_a \tag{1.3}$$

and a temperature gradient exists within the reaction zone. The zero Biot number scenario was developed by Semenov and others; the infinite Biot number by Frank-Kamenetskii and others.

1.3 Frank-Kamenetskii Conditions

In the steady-state equation, $\partial T / \partial t = 0$. For the class A geometries of infinite slab, infinite cylinder and sphere, the steady-state formulation has been investigated by Frank-Kamenetskii as

$$\begin{aligned} \nabla^2\theta + \delta \exp\left(\frac{\theta}{1+\varepsilon\theta}\right) &= 0 \qquad \text{in the region with} \\ \theta &= 0 \qquad \text{on the boundary} \end{aligned} \tag{1.4}$$

with the dimensionless energy parameter,

$$\varepsilon = \frac{RT_a}{E}, \tag{1.5}$$

and the dimensionless Frank-Kamenetskii eigenvalue parameter,

$$\delta = \frac{\sigma Q a_0^2 E A \exp(-E / RT_a)}{\kappa R T_a^2}, \tag{1.6}$$

for which a_0 is some characteristic half-width of the region containing the reaction.

The variable θ represents the dimensionless temperature rise above ambient temperature,

$$\begin{aligned} \theta &= \frac{1}{\varepsilon} \cdot \frac{T - T_a}{T_a} \\ &= \frac{E}{RT_a^2}(T - T_a). \end{aligned} \tag{1.7}$$

The effect on the solution θ of varying δ while keeping ε fixed is shown in Figure 1.3. Of interest is δ_{cr}, the value of δ at which the first bifurcation point occurs on the minimal branch. If $\delta < \delta_{cr}$, the material will warm and will reach a steady temperature distribution; if $\delta > \delta_{cr}$, the material will eventually heat to the point of ignition, that is, thermal runaway may occur; if $\delta = \delta_{cr}$, a metastable state exists.

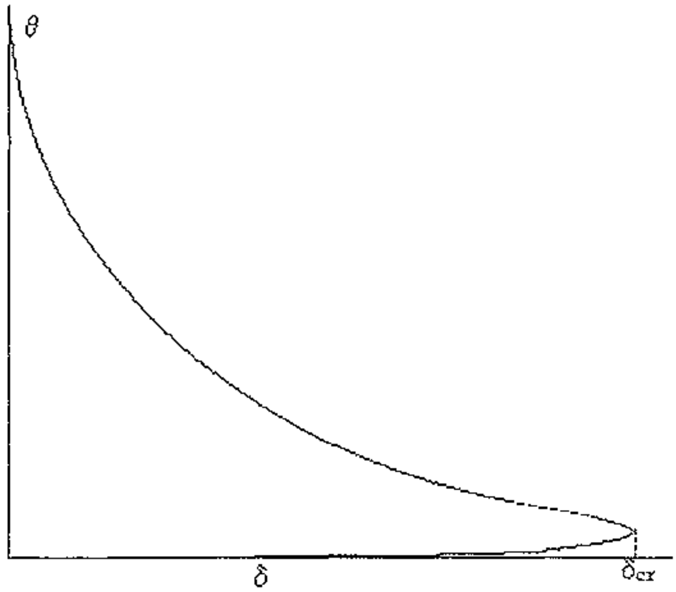

FIGURE 1.2 Bifurcation diagram.

When $\varepsilon << 1$, the instantaneous heat balance equation can be written as

$$\frac{d^2\theta}{d\rho^2}+\frac{j}{\rho}\frac{d\theta}{d\rho}+\delta\exp(\theta)=0$$
$$\theta|_{\rho=1}=0 \tag{1.8}$$
$$\left.\frac{d\theta}{d\rho}\right|_{\rho=0}=0$$

where the dimensionless shape factor, j, has value 0 for slab, 1 for cylinder and 2 for sphere. The variable ρ is a function of distance, r, from the centre of the body;

$$\rho=\frac{r}{a_0}. \tag{1.9}$$

In general, the boundary condition is

$$\frac{ha_0}{\kappa}\theta_s=\begin{cases}\mp\frac{d\theta}{d\rho} & \text{when } j=0, \text{i.e. when } \rho=\pm1\\ -\frac{d\theta}{d\rho} & \text{when } j=1,2, \text{i.e. when } \rho=1,2\end{cases} \tag{1.10}$$
$$=Bi\,\theta_s$$

where h is the surface heat transfer coefficient and θ_s is the dimensionless temperature excess at the surface.

By symmetry,

$$\frac{d\theta}{d\rho} = 0 \qquad \text{when } \rho=0. \tag{1.11}$$

Equation (1.4) cannot be solved explicitly when ε is non-zero. Solution of (1.8) yields the values in Table 1.1.

Shape	δ_{cr}	
infinite slab	0.88	(analytical)
infinite cylinder	2.00	(analytical)
sphere	3.32	(no exact solution)

TABLE 1.1

The variation of δ_{cr} with Bi is shown in Figure 1.3. Under Semenov conditions (Bi→0), Bi and δ_{cr} are related by

$$\delta_{cr} = (j+1)\frac{Bi}{e} \tag{1.12}$$

shown in Figure 1.3 by the dashed line. When Bi is small, δ_{cr} is proportional to Bi. As Bi becomes larger, δ_{cr} tends asymptotically to a maximum value, the Frank-Kamenetskii limit.

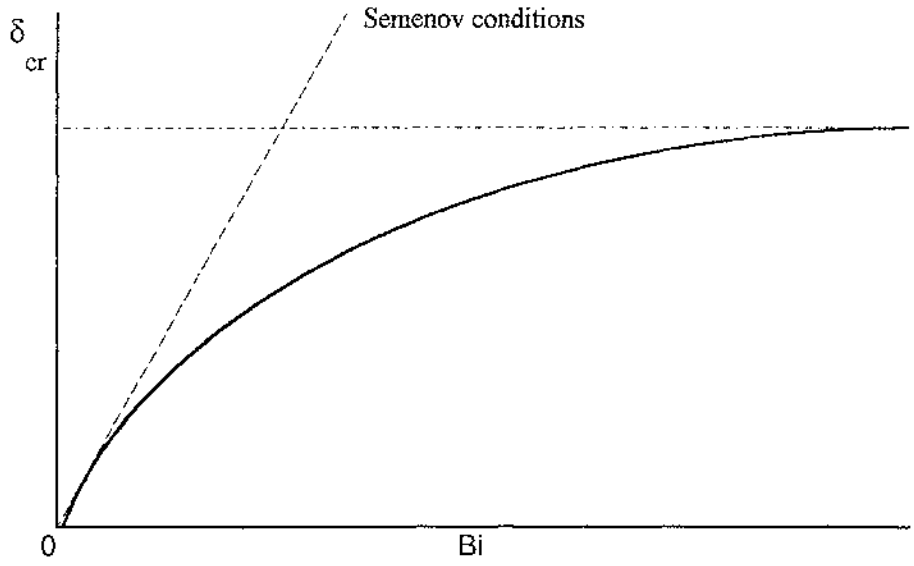

FIGURE 1.3 Variation of δ_{cr} with Biot number, Bi.