THERMAL EXPLOSION THEORY
WITH NON-UNIFORM
BOUNDARY CONDITIONS

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A C K N O W L E D G E M E N T S

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ABSTRACT

This thesis investigates the effect of non-uniform boundary conditions on Thermal Explosion Theory. Using Frank-Kamenetskii's postulates of purely conductive heat transfer within the reactant, we seek to determine the critical criteria for the onset of thermal ignition.

Chapter One contains a brief summary of the history and developments of thermal explosion theory. Most of the discussion is dominated by Semenov's and Frank-Kamenetskii's theories.

In Chapter Two, we consider Liouville's nonlinear partial differential equation in an infinite rectangular strip with various surface conditions. This problem arises in the determination of the two-dimensional temperature distribution within a self-heating partially insulated slab, with the remainder of the surface offering no resistance to heat transfer. For symmetrical heating in a dimensionless Cartesian frame of reference Oxyz, with insulating strips at $y = \pm 1$, the critical Frank-Kamenetskii's parameter is found to be

$$\delta_c(\epsilon) = \delta_c(\epsilon)\ (1-\epsilon-0.555\epsilon^{3/2} + \ldots), \quad \epsilon \ll 1$$

where $\delta_c(0) = 0.878$ and ϵ is the ratio of insulation length to the slab thickness. However, for $\epsilon \gg 1$, we are unable to determine an explicit relationship between $\delta_c(\epsilon)$ and ϵ except to note that

$$\delta_c(\epsilon) \sim \frac{\delta_c(0)}{\epsilon^2}, \quad \epsilon \gg 1 .$$

In Chapter Three, we seek to solve the above problem with the boundary condition at $y = \pm 1$ replaced by $\epsilon f(x)$, where $\epsilon \ll 1$ and $f(x)$ is a smooth monotonic function of x with the following asymptotic properties

$$x \to +\infty \quad : \quad f(x) \to 1 ,$$
$$x \to -\infty \quad : \quad f(x) \to 0 .$$

Although the problem is well defined at $x = \pm\infty$, attempts to determine the temperature distribution at criticality and for finite x leads to failure. This paradox is resolved by constraining $f(x)$ to be such that $f'(x) \ll f(x)$. The critical Frank-Kamenetskii's parameter is then found to be

$$\delta_c(\epsilon) = \delta_c(0) \exp(-\epsilon) \qquad 0 < \epsilon \ll 1 \quad .$$

Chapters Four and Five contain details of the numerical schemes for the solution of the problem defined in Chapter Two. Chapter Five has computational results for the schemes discussed and possible suggestions for future implementation of the schemes.

PREFACE

In the following chapters, the figure legends and the tables of results for each chapter are to be found at the end of that particular chapter. However, in Chapters Two and Four, some of the figure legends have been included in the text to make it easier for the reader to follow the text.

CHAPTER ONE: REVIEW OF THERMAL EXPLOSION THEORY

1. INTRODUCTION

The theory of thermal explosion, examines the thermo-kinetic behaviour of chemically reacting systems with respect to the stability of exothermic reactions. An important feature of these systems, is the existence of at least one distinct mode and the possibility of switching from one mode to another under certain conditions. These modes are well defined and distinct from each other. In the steady-state theory, thermal imbalance in heat generation and heat dissipating mechanisms, is considered the predominant factor in understanding the nature and stability of these modes. The kinetics of the reacting system is then relegated to the determination of initial temperatures and the rates of the reacting systems. The kinetics also exhibit the sensitivity of the reacting system to any temperature change. Consequently any temperature rise within the reacting system will be opposed by heat dissipating forces. However, as the ambient temperature is increased, there will exist an ambient temperature such that the heat generating mechanisms will exceed the heat dissipating forces resulting in thermal runaway or ignition. Thus thorough studies of these chemically reacting systems have concentrated on the prediction of this criterion for the onset of spontaneous ignition for self-heating systems.

To facilitate our understanding of this criterion of spontaneous ignition it is necessary to refer to early works on thermal explosion theory. The basis of recent thermal explosion theory rests with earlier works by Semenov [1] and Frank-Kamenetskii [2].

1.1 Semenov's Treatment of Thermal Explosion Theory

In his model, Semenov considered the reacting systems to be in steady-state with uniform temperature T throughout the reactant, different from the uniform temperature T_0 of its surroundings. The reaction rate was considered to be of the Arrhenius form. Hence the rate of reaction is proportional to Exp(-E/RT), where E is the overall activation energy of the reactant. He ascribed the heat losses to convective forces due to Newtonian-Cooling at the interface of the reactant and its surroundings. As a result, the resistance to heat-transfer is directly proportional to the temperature difference $(T-T_0)$, at the boundary. These postulates lead directly to energy equations (1.1.0) and (1.1.1) representing the rate of heat production q and the rate of heat loss ℓ.

$$q = VQA \exp(-E/RT).C_0 \qquad (1.1.0)$$

$$\ell = \chi S(T-T_0) \qquad (1.1.1)$$

where:-

Q is the exothermicity of the reactant

χ is the heat-transfer coefficient at the boundary

C_0 is the concentration of the reactants, assumed constant throughout the reaction.

V and S are the volume and surface area of the reactant vessel.

The graphs of the rates of heat production against temperature of the Arrhenius' rate of reaction exhibit an S-shaped form. However, in Figure 1.1, for example, the graphs of the rate of heat production q_0 and the rate of heat loss ℓ, are shown exhibiting two stationary states P and R, instead of the three states to be expected. This is because in classical thermal explosion theory, the rates of heat release would be insufficient to give rise to the third state. Semenov identified the critical condition as the tangency between the graphs of the heat loss and the rate of heat production, see Figure 1.1. At criticality two conditions have to be met. Firstly an energy balance must exist and secondly the rate of change with temperature of the rate of heat loss should equal the rate of change with temperature of the rate of heat production. Hence at criticality we have,

$$VQAC_0 \ \mathrm{Exp}(-E/RT) = XS(T-T_0) \qquad (1.1.2)$$

$$VQAC_0E \ \mathrm{Exp}(-E/RT) = XS \ RT^2 \qquad (1.1.3)$$

with $T = T_{crit}$.

Dividing equation (1.1.2) by (1.1.3) results in giving the critical temperature and the maximum temperature difference for a stable reacting system. Therefore we get

$$(T_{crit}-T_0) = (RT_{crit}{}^2/E) \qquad (1.1.4)$$

or

$$T_{crit} = \frac{E}{2R} \{1 \pm [1- (4RT_0/E)]^{\frac{1}{2}} \} \qquad (1.1.5)$$

The larger value of T_{crit} in equation (1.1.5) corresponds to the very high rates of heat release. This higher value represents the point of thermal extinction. However, for spontaneous ignition to occur, T_{crit} is given by the lower value of (1.1.5), namely

$$T_{crit} = \frac{E}{2R}\{1-[1-(4RT_0/E)]^{\frac{1}{2}}\} \qquad (1.1.6)$$

Both equations (1.1.5) and (1.1.6) give the range of T_0 for which the system will self-heat and possibly lead to ignition. This will be true for $E \geqslant 4RT_0$ or $0 < T_0 \leqslant (\frac{E}{4R})$. Expansion of equation (1.1.6) as a binomial series results in equation (1.1.7)

$$\frac{E}{RT_0^{\ 2}} (T_{crit}-T_0) = 1 + 2(RT_0/E) + \ldots \qquad (1.1.7)$$

Hence for a reacting system to remain stable, equation (1.1.7) shows that the maximum dimensionless temperature excess is bounded, namely

$$\frac{E}{RT_0^{\ 2}} (T_{crit}-T_0) \leqslant 1 \quad . \qquad (1.1.8)$$

In their 1977 Review paper on thermal explosion theory, Gray and Sherrington [3], rewrote the energy equation and the criticality condition in form of dimensionless variables. They defined the dimensionless excess temperature $\theta = \frac{E}{RT_0^{\ 2}} (T-T_0)$ and a parameter β, such that $\beta = \frac{RT_0}{E}$. On substituting these new variables into the energy balance equation, we get

$$\theta \exp[-\theta/(1+\beta\theta)] = (VQAEC_0/\chi SRT_0^{\ 2}) \exp(-E/RT_0) \qquad (1.1.9)$$

Gray and Sherrington defined $\omega = \omega(\theta)$, such that,

$$\omega(\theta) = \theta \exp[-\theta/(1+\beta\theta)] \qquad (1.1.10)$$

Hence the criticality condition $\frac{dq}{dT} = \frac{d\ell}{dT}$ becomes,

$$(1+\beta\theta)^2 \exp[-\theta/(1+\beta\theta)] = (VQAEC_0/\chi SRT_0{}^2) \exp(-E/RT_0) \qquad (1.1.11)$$

Comparing equations (1.1.10) and (1.1.11) gives the condition for θ at criticality, namely

$$\theta_{crit} = (1+\beta\theta_{crit})^2 \qquad (1.1.12)$$

Consider again equation (1.1.10)

$$\omega(\theta) = \theta \exp[-\theta/(1+\beta\theta)]$$

or $$\log[\frac{\omega(\theta)}{\theta}] = -\frac{\theta}{(1+\beta\theta)}$$

Differentiating with respect to θ, we have

$$\frac{1}{\omega(\theta)} \frac{d\omega}{d\theta} = \{(1+\beta\theta)^2-\theta\}/[\theta(1+\beta\theta)^2]$$

Thus the criticality condition given by equation (1.1.12) corresponds to the stationary value of $\omega(\theta)$. In fact the criticality condition corresponds to the maximum value of $\omega(\theta)$. Expansion of θ_{crit} as a power series in β leads to equations (1.1.13) and (1.1.14)

$$\theta_{crit} = 1+2\beta + 5\beta^2 + \ldots \qquad (1.1.13)$$

$$\omega_{max}(\theta) = e^{-1}(1+ \beta + \frac{3}{2} \beta^2 + \ldots) \qquad (1.1.14)$$

Equations (1.1.13) and (1.1.14) give a mathematical representation of some of Semenov's most important contributions to thermal explosion theory. In the classical theory of thermal explosion (the limit $\beta \to 0$), the reacting system will become unstable and explode if there is an e-fold increase in the rate of heat release above that of T_0. There is also a bound on the dimensionless temperature excess, θ, if the reacting system is to remain stable. Hence in the limit $\beta \to 0$, $\theta \leqslant 1$ and $\omega(\theta) \leqslant e^{-1}$.

Semenov's model of thermal explosion offers several advantages:-

(i) The model itself is a function of the dimensions of the reacting vessel in the form of the ratio of its total volume V to its surface area S.

(ii) Significant results can be obtained by the use of simple mathematics. The mathematical analysis can be applied to both endothermic and exothermic reactions.

(iii) The theory can readily be applied to nonlinear heat transfer (radiation for example) and to reactions with temperature-dependent pre-exponential factors.

(iv) Although Semenov applied his model to reacting systems with high overall activation energies, the case for low activation energy can certainly be discussed.

(v) Its prediction of the maximum dimensionless excess temperature, θ_{crit}, and the e-fold increase in the rate of heat release above that for T_0 for the reacting system to become unstable and explode, have hardly been altered by more sophisticated theories of thermal explosion.

However, the model failed to describe the temperature distribution within the reactant. Its assumption of uniform pre-explosion temperatures does not agree with experimental facts, it is well known that ignition always begins at one point and then the flame spreads through the rest of the reactant. In fact, Semenov's description of uniform pre-explosion temperatures within the reactant can be realised for only two cases:-

(i) Self-heating solid in form of small particles of high thermal conductivity surrounded by a medium of low thermal conductivity.

(ii) Liquid under intense mixing.

1.2 Frank-Kamenetskii's Treatment of Thermal Explosion Theory

Frank-Kamenetskii [2], in his 1939 work, adopted most of Semenov's postulates except the assumption of uniform pre-explosion temperatures within the reactant and the nature of heat dissipating mechanisms. Frank-Kamenetskii attributed the heat resistance to conductive forces within the reactant. In fact, the heat losses were considered to be strictly conductive within the reacting vessel. Furthermore, the reactant was assumed to be surrounded by a medium of infinitely large thermal conductivity. He also postulated that the thermal conductivity of the reactant remained constant throughout the reaction. By invoking the principle of conservation of energy, the temperature of the reactant satisfies the Fourier equation (1.2.1)

$$\lambda\Delta T + QW(T) = 0 \quad \text{in volume}$$
$$T = T_0 \quad \text{at the surface} \qquad (1.2.1)$$

where:

λ is the thermal conductivity of the reactant

Q is the heat of reaction

Δ is the Laplacian operator.

$W(T) = Z_0 \exp(-E/RT)$, is the rate of reaction with Z_0 being the pre-exponential factor.

In his 1939 work, Frank-Kamenetskii studied the stability of reactants within an infinite vessel with plane parallel walls. Equation (1.2.1) was transformed to its dimensionless form by a new choice of variables:-

$$\theta = \frac{E}{RT_0^2}(T - T_0)$$

$$\beta = (RT_0/E)$$

$Z = (r/a)$ where a is half-width of vessel and r is the equivalent length for an infinite vessel.

$$\delta = (E/RT_0^2)(Q/\lambda)\ a^2 Z_0 \exp(-E/RT_0) \qquad (1.2.2)$$

δ is the so-called Frank-Kamenetskii parameter. Hence equation (1.2.1) reduces to

$$\Delta_Z\theta + \delta \exp[\theta/(1+\beta\theta)] = 0 \quad \text{in volume}$$
$$\theta = 0 \quad \text{at surface} \qquad (1.2.3)$$

To simplify mathematical solutions, equation (1.2.3) was solved for the case $\beta = 0$. Thus the one-dimensional energy equation becomes

$$\frac{d^2\theta}{dz^2} + \frac{k}{z}\frac{d\theta}{dz} + \delta e^{\theta} = 0 \quad \text{in volume}$$
$$\theta = 0 \quad \text{at surface} \qquad (1.2.4)$$

where k = 0,1,2 represents the slab, cylinder and the sphere respectively. The criticality condition for thermal ignition was identified as the condition when stable stationary states are impossible to realise for the steady-state zero-order chemically reacting system.

Class A geometries:-

Frank-Kamenetskii further simplified the mathematical solution of equation (1.2.4) by considering symmetrical geometries.

(a) The Slab Solution (k = 0)

$$\frac{d^2\theta}{dz^2} + \delta\exp\theta = 0 , \qquad 0 \leqslant z \leqslant 1 ,$$
$$\theta = 0 , \qquad z = 1 , \qquad (1.2.5)$$
$$\frac{d\theta}{dz} = 0 , \qquad z = 0 .$$

Multiplying (1.2.5) by $\frac{d\theta}{dz}$, we have

$$\left(\frac{d\theta}{dz}\right)\frac{d^2\theta}{dz^2} + \delta e^{\theta}\,\frac{d\theta}{dz} = 0$$

$$\frac{d}{dz}\left\{\frac{1}{2}\left(\frac{d\theta}{dz}\right)^2 + \delta e^{\theta}\right\} = 0$$

Therefore

$$\left(\frac{d\theta}{dz}\right)^2 = \text{constant} - 2\delta\exp\theta \qquad (1.2.6)$$

The maximum temperature rise θ_m will occur, by symmetry, at the centre. Hence equation (1.2.6) becomes

$$\left(\frac{d\theta}{dz}\right) = (2\delta)^{\frac{1}{2}} [\exp\theta_m - \exp\theta]^{\frac{1}{2}}$$

Integrating, we get

$$\int \frac{d\theta}{\exp(\theta/2)\{\exp[(\theta_m-\theta)/2]-1\}^{\frac{1}{2}}} = (2\delta)^{\frac{1}{2}}z + \text{constant} \qquad (1.2.7)$$

We now put; $\cosh\psi = \exp[(\theta_m-\theta)/2]$ into equation (1.2.7). On integrating, we get

$$\psi = \exp(\theta_m/2)\ \{\text{constant} - (\delta/2)^{\frac{1}{2}}z\}$$

and hence

$$\theta = \theta_m - 2\log\cosh\{e^{(\theta_m/2)}[(\delta/2)^{\frac{1}{2}}z+c]\} \qquad (1.2.8)$$

where c is a constant. We now consider the boundary conditions at $z = 0$, and $z = 1$;

at $\qquad z = 0 \qquad \frac{d\theta}{dz} = 0$

therefore $c \equiv 0$. Thus θ becomes

$$\theta = \theta_m - 2\log\cosh z[(\delta\exp\theta_m)/2]^{\frac{1}{2}} \qquad (1.2.9)$$

at $\qquad z = 1, \quad \theta = 0$. Hence

$$\theta_m = 2\log\cosh[(\delta\exp\theta_m)/2]^{\frac{1}{2}} \qquad (1.2.10)$$

Substituting θ_m from (1.2.10) into equation (1.2.9) we obtain

$$\theta = 2 \log \cosh[(\delta \exp\theta_m)/2]^{\frac{1}{2}} - 2 \log \cosh z[(\delta \exp\theta_m)/2]^{\frac{1}{2}} \tag{1.2.11}$$

Putting $\sigma = [(\delta \exp\theta_m)/2]^{\frac{1}{2}}$.

Hence $\delta = 2\sigma^2 \exp(-\theta_m)$ (1.2.12)

Writing θ in terms of σ, we obtain

$$\theta = 2 \log\left(\frac{\cosh \sigma}{\cosh \sigma z}\right) \tag{1.2.13}$$

Note: at $z = 0$, $\theta = \theta_m$. Hence from (1.2.13)

$$\theta_m = 2 \log \cosh \sigma \tag{1.2.14}$$

Substituting θ_m into (1.2.12), δ becomes

$$\delta = 2\sigma^2 \text{sech}^2\sigma \tag{1.2.15}$$

Frank-Kamenetskii identified the critical conditions for the onset of spontaneous ignition by the maximum possible δ in equation (1.2.15). At criticality, this results in the following transcendental equation for the critical parameter $\sigma = \sigma_c$, namely

$$\sigma_c \tanh\sigma_c = 1 \tag{1.2.16}$$

Numerical solution of equations (1.2.16), (1.2.15), and (1.2.14) gives the following critical values for the parameter

$$\begin{aligned} \sigma_c &= 1.2 \\ \delta_{crit} &= 0.878 \\ \theta_{m,crit} &= 1.19 \end{aligned} \tag{1.2.17}$$

(b) The Infinite Cylinder (k=1)

$$\frac{d^2\theta}{dz^2} + \left(\frac{1}{z}\right)\frac{d\theta}{dz} + \delta\exp\theta = 0 \quad , \quad 0 \leqslant z \leqslant 1,$$
$$\theta = 0 \quad , \quad z = 1, \qquad (1.2.18)$$
$$\frac{d\theta}{dz} = 0 \quad , \quad z = 0.$$

The problem is simplified if we follow the approach by Lemke and Reine [4] and Chambré [5]. Thus we put

$$\psi = z\left(\frac{d\theta}{dz}\right) \quad \text{and} \quad \eta = z^2 \exp\theta. \qquad (1.2.19)$$

On substituting ψ and η into (1.2.18), we get

$$\frac{d\psi}{d\eta} = -\delta/(2+\psi) \qquad (1.2.20)$$

On integrating (1.2.20) we obtain

$$\psi^2 + 4\psi + \tau + 2\delta\eta = 0 \qquad (1.2.21)$$

At the centre of the cylinder, that is, at $\eta = 0$, $\psi = 0$ and hence $\tau = 0$. The equation for ψ reduces to

$$\psi^2 + 4\psi + 2\delta\eta = 0 \qquad (1.2.22)$$

Rewriting equation (1.2.22) in terms of θ, we have

$$z^2\left(\frac{d\theta}{dz}\right)^2 + 4z\left(\frac{d\theta}{dz}\right) + 2\delta z^2 \exp\theta = 0 \qquad (1.2.23)$$

By simultaneously solving equations (1.2.23) and (1.2.18), Gray and Lee [6] were able to show that θ is given by

$$\theta = \log[(8G/\delta)/(Gz^2+1)^2] \qquad (1.2.24)$$

and

$$\delta = 8G/(G+1)^2 \qquad (1.2.25)$$

The maximum value of δ occurs when G = 1. On substituting this value of G into (1.2.24) and (1.2.25), we obtain the following critical parameters;

$$\begin{aligned} \delta_{crit} &= 2 \\ \theta_{crit} &= \log[4/(z^2+1)^2] \qquad (1.2.26) \\ \theta_{m,crit} &= \log 4 \\ &= 1.39 \end{aligned}$$

The critical values (1.2.26) are in agreement with the numerical results obtained by Frank-Kamenetskii.

(c) The Sphere (k=2)

Putting k = 2, equation (1.2.4) becomes

$$\frac{d^2\theta}{dz^2} + \left(\frac{2}{z}\right)\frac{d\theta}{dz} + \delta\exp\theta = 0 \qquad (1.2.27)$$

with boundary conditions

$$z = 0 \; : \; \frac{d\theta}{dz} = 0 \, ,$$

$$z = 1 \; : \; \theta(1) = 0.$$

In the survey by Gray and Lee [6], equation (1.2.27) was transformed to model an isothermal gas sphere in gravitational equilibrium. To enable this transformation, new auxiliary variables were chosen such that

$$\psi = \theta_m - \theta \quad \text{and} \quad \eta = z\sqrt{\delta \exp\theta_m} \tag{1.2.28}$$

Using the above substitutions, Gray and Lee then transformed equation (1.2.27) together with the boundary conditions to get

$$\frac{d^2\psi}{d\eta^2} + (2/\eta)\frac{d\psi}{d\eta} - e^{-\psi} = 0$$

with boundary conditions

$$\psi = 0 \quad \text{at} \quad \eta = 0 \quad \text{where} \quad \frac{d\psi}{d\eta} = 0 \tag{1.2.29}$$

and $\psi = \theta_m$ at $\eta_1 = \sqrt{\delta \exp\theta_m}$

Although equation (1.2.29) is no easier to solve by analytical methods than the original equation (1.2.27), nevertheless a numerical solution can be expressed in terms of known tabulated functions developed by Chandrasekhar and Wares [7] and [8]. Thus rewriting the boundary condition at the surface of the sphere, we have

$$\delta = \eta_1^{\,2} \exp(-\psi), \quad \text{since } \theta = 0 \text{ when } \eta = \eta_1 \tag{1.2.30}$$

The maximum value of δ can be obtained from (1.2.30). This critical condition is satisfied by

$$\eta_1 \frac{d\psi}{d\eta_1} = 2 \tag{1.2.31}$$

From the tabulated values in [8], the values of η_1 and ψ satisfying (1.2.31) are

$\eta_1 = 4.07 \quad : \quad \psi = 1.61$

Hence the critical values of δ and θ are

$$\delta_{crit} = 3.32$$
$$\theta_{crit} = 1.60 \qquad (1.2.32)$$

These critical values correspond to those obtained by Frank-Kamenetskii [2].

Summary on Class A geometries:

Figure 1.2 exhibits the bound on δ for thermal stability. Time-dependent linear analysis by Istratov and Librovich [10] for the slab shows that the upper branch of θ_m versus δ curve to be unstable while the lower branch represents a stable state. Istratov and Librovich also showed that the same situation was true for the infinite cylinder with the stable branch corresponding to $\theta_m < 1.387$. Whilst for the sphere the problem was complicated by the lack of analytical solution. However, Steggerda [9] has solved the usual steady-state equation for the sphere by extending the range of tables of Chandrasekhar and Wares [8]. The results of the analysis are indicated by Figure 1.3. In the region of criticality $1.66 \leqslant \delta \leqslant 3.32$, there are more than two centre temperatures, thus more than two temperature distributions for a given δ. Using Istratov and Librovich's notation, the number of temperature profiles becomes infinite as δ tends to 2. Figure 1.4 exhibits the stable temperature profiles at the centre of the vessels for class A geometries. From the work on class A geometries, the temperature profile is roughly parabolic. However, Parks [11], in his numerical work suggests that there is evidence of inflexion points, at least in the case of the sphere. In the work by Enig [12] and confirmed by Gray and Lee [13], they showed that the critical values of δ are determined by critical surface temperature gradients. On examination of class A geometry temperature solutions, they were able to show for the critical case that

$$\left| \left(\frac{d\theta}{dz}\right)_{crit} \right| = 2 \qquad \text{at } z = 1 \tag{1.2.33}$$

A simple physical result follows from (1.2.33). In the stationary state, the total heat transfer from the interior of the reacting vessel is proportional to its surface area and to the temperature gradient at the surface. However, since at criticality, the temperature gradients at the surfaces of class A geometries are equal, we expect the rates of heat generation to be in the ratio of their surface to volume ratios,namely 1:2:3. This result is indeed satisfied by the results obtained for the slab, infinite cylinder and the sphere.

Frank-Kamenetskii postulates of conductive theory for thermal explosion are valid if the following conditions are satisfied;

(i) The temperature difference $(T-T_0)$ at the surface is so low such that radiation plays no part in heat transfer.

(ii) The effect of convective forces is negligible in low densities. However, as the pressure and hence density of the reactant is increased,we expect that there is a limit at which convective forces will have to be taken into account. In effect in regions of Rayleigh numbers of $O(10^2)$ purely conductive heat transfer is still valid.

(iii) If the reactant consistsof large masses of solid explosive and materials such as wood and fibre board.

1.3 Comparison of Semenov and Frank-Kamenetskii Theories for Thermal Explosion

In both theories we assumed, that at the surface of the reacting vessel, the heat transfer was either convective or conductive. However, when there is a resistance to heat transfer, not only due to finite thermal conductivity, we must also take into account both mechanisms for heat dissipation. Thomas [15] considered the case where heat-transfer at the surface is due to Newtonian-Cooling. He replaced the boundary condition at the surface by

$$\frac{d\theta}{dz} + \alpha\, \theta_s = 0 \quad , \qquad \text{at} \quad z = 1 \tag{1.3.0}$$

with $\alpha = \frac{\chi a}{\lambda}$

where:

- χ is the heat-transfer coefficient at the surface
- a width of vessel
- λ thermal conductivity of the reactant.

α is the Biot Number. The significance of the Biot Number is that it compares the internal and external resistances to heat flow. For large values of α, the resistance to heat flow is due to conduction within the reactant with the surface temperature T_s equal to T_0, the ambient temperature. These high values of α are the conditions assumed by Frank-Kamenetskii. Semenov's conditions are satisfied for low values of α in which the heat loss at the surface becomes insignificant resulting in surface temperature T_s being different from T_0. The effect of the Biot Number on the critical parameters for thermal ignition can easily be obtained for class A geometries by imposing condition (1.3.0) on the analysis in above sections. In the review by Gray and Lee [3] the following results were obtained;

(i) The Slab

$$\theta = \theta_m - 2\log \cosh DZ$$

with $$\log\delta = \log 2D^2 - 2\log \cosh D - (2D \tanh D)/\alpha \qquad (1.3.1)$$

and $$\alpha = \frac{D_{crit}.\sinh D_{crit}.\cosh D_{crit} + D_{crit}^2}{(1-D_{crit}.\tanh D_{crit})\cosh^2 D_{crit}}$$

where D_{crit} is the critical value of D for the limiting case on δ.

(ii) Infinite Solid Cylinder

$$\theta = \log[8G/\delta(1+GZ^2)^2]$$

with $$\log\delta = \log[8G/(G+1)^2] - [4G/\alpha(G+1)] \qquad (1.3.2)$$

and $$\alpha = 4G_{crit}/(1-G_{crit}^2)$$

(iii) The Sphere

$$\log\delta = -\psi_s + 2\log\eta_s - (\eta_s/\alpha)\left(\frac{d\psi}{d\eta}\right)_s$$

and
$$\alpha = \left[\eta_s^2 e^{-\psi_s} - \eta_s\left(\frac{d\psi}{d\eta}\right)_s\right] / \left[2-\eta_s\left(\frac{d\psi}{d\eta}\right)_s\right] \qquad (1.3.3)$$

where the subscript s refers to the surface z = 1.

The relationships between θ_m and θ_s, δ_{crit} against α are shown in Figure 1.5 and Figure 1.6, which we have reproduced from [6]. From the figures of δ_{crit} against α, it is apparent that the Frank-Kamenetskii values ($\alpha \to \infty$) are higher than the case for moderate values of α. However, for small values of α, say $\alpha < 0.5$, it is possible to use Semenov's postulates. For small values of α, especially $\alpha = 0$, the critical centre and surface temperatures approach unity, which is in agreement with results of equation (1.1.7).

1.4 Some Steady-State Problems of Asymmetrically-heated Reactants

In above sections all the analytical solutions have been based on symmetrically heated reactants. However, Armittage [14] asserted that if a symmetrical slab is in critical condition so is the asymmetrical slab. In order for us to consider reactants with large temperature differences between the surfaces, it is necessary to alter the specification for θ in terms of ambient temperature at the hotter surface. Thus we re-define a new dimensionless excess temperature $\tilde{\theta}$ such that

$$\tilde{\theta} = \frac{E}{RT_p^{\ 2}} (T-T_p) \qquad (1.4.0)$$

where subscripts p and s refer to the hot and cold surfaces respectively. The definition (1.4.0) implies that temperature will be negative throughout the vessel except at the hot surface where it vanishes. In the heat generation term, we still consider the Frank-Kamenetskii exponentiation to be valid. This assumption will hold good in the region near the hot surface. However, by assuming negligible heat generation at the cold surface compared to the hot region, the Frank-Kamenetskii exponentiation can then be considered valid throughout the whole reactant. We now have α_s and α_p being the Biot Numbers at the cold and hot surfaces respectively. Of the asymmetrically-heated reactants, we only consider slabs which are of interest to us. Thus we consider slabs with the interest of determining the temperature profiles within the reactant and where possible to determine the critical Frank-Kamenetskii parameter δ_c (or δ_{crit}).

1.5 Steady-State Problems in Some Asymmetrically-heated Slabs

The effect of insulating a self-heating slab can be physically understood by considering a slab $0 \leqslant z' \leqslant 2a$ with the hot surface being maintained at temperature T_p. This temperature T_p can be maintained constant by using a heat reservoir. However the other face is then exposed to its surroundings at temperature T_0. Depending on the nature of heat exchange between the slab and the surroundings, we assume a surface temperature T_s at the cold surface.

By varying the Biot Number α_s at the cold surface the effect of insulation can be obtained by letting α_s tend zero.

(a) Slab with insulation at the cold surface ($\alpha_p=\infty$; $\alpha_s=0$)

Curve 2 in Figure 1.7 represents the asymmetrical slab with perfect conduction ($\alpha_s=\infty$) at the cold surface. However, as α values are reduced, the temperature profiles take the form of curves 3 to 6. The significant feature of these curves is that maximum temperature within the slab shifts from the 'hot surface' to the 'cold face' with T_{s2} representing the maximum temperature for the onset of thermal ignition. This temperature T_{s2} represents the symmetrically-heated case with $0 \leqslant z \leqslant 2$. Hence the corresponding limiting δ_{crit} can be determined in the same approach as in the earlier section on class A geometries. In fact, for the limiting case we have

$$\tilde{\theta}_{max} = 2\log\cosh(2\delta\exp\tilde{\theta}_{max})^{\frac{1}{2}}$$

and $$\delta_{crit,\alpha_s=0} = 0.22 \qquad (1.5.0)$$

The result (1.5.0) can also be derived from physical arguments, since when $\alpha_s = 0$, the slab corresponds exactly to one half of symmetrically heated slab subject to the Frank-Kamenetskii surface condition. Curve 1 is for the trivial case for an inert material in which case the temperature profile is linear.

(b) Slab with hot face on a perfect conductor and with restricted heat loss at the cold face ($\alpha_p=0$; α_s finite)

The slab is once again assumed to have temperature T_p

maintained at the hot face by a heat reservoir with Newtonian-Cooling at the cold face. By defining $z = z'/a$, we have at the cold surface

$$\frac{d\tilde{\theta}}{dz} + \alpha_s(\tilde{\theta}_s - \tilde{\theta}_0) = 0 \qquad \text{at } z = 2 \tag{1.5.1}$$

with $\tilde{\theta}_s = \frac{E}{RT_p^2}(T_s - T_p)$ and $\tilde{\theta}_0 = \frac{E}{RT_p^2}(T_0 - T_p)$

Note for $\alpha_s = 0$, this correponds to the symmetrically heated slab with the limiting case (1.5.0). In general the slab solution is given by

$$\tilde{\theta} = \log A - 2\log\cosh[z(\tfrac{A}{2})^{\frac{1}{2}} + c] \tag{1.5.2}$$

We expect from (a) that for a finite α_s the maximum temperature will occur within the slab. We let the maximum temperature $\tilde{\theta}_{max}$ correspond to the point $z = z_{max}$. Therefore our problem becomes

$$\frac{d^2\tilde{\theta}}{dz^2} + \delta\exp\tilde{\theta} = 0, \qquad 0 \leqslant z \leqslant 2.$$

with boundary conditions;

(i) $\tilde{\theta} = 0, \quad z = 0$

(ii) $\frac{d\tilde{\theta}}{dz} = 0, \quad \tilde{\theta} = \tilde{\theta}_{max} \quad \text{at } z = z_{max}$ (1.5.3)

(ii) $\frac{d\tilde{\theta}}{dz} + \alpha_s(\tilde{\theta}_s - \tilde{\theta}_0) = 0 \quad \text{at } z = 2$

Imposing boundary condition (i) into (1.5.2), we get

$$A = \cosh^2\left(\frac{A\delta}{2}\right)^{\frac{1}{2}}$$

But at the point $z = z_{max}$,

$$\frac{d\tilde{\theta}}{dz} = -2\left(\frac{A\delta}{2}\right)^{\frac{1}{2}} \tanh\left[z_{max}\left(\frac{A\delta}{2}\right)^{\frac{1}{2}} + c\right]$$

$$\equiv 0$$

Therefore

$$c = -z_{max}\left(\frac{A\delta}{2}\right)^{\frac{1}{2}}$$

Hence $\tilde{\theta}$ solution is

$$\tilde{\theta} = \log A - 2\log\cosh\left[\left(\frac{A\delta}{2}\right)^{\frac{1}{2}}(z-z_{max})\right] \qquad (1.5.4)$$

Note once again at $z = z_{max}$, $\tilde{\theta} = \tilde{\theta}_{max}$. Thus

$$A = \exp\tilde{\theta}_{max}$$

Finally (1.5.4) becomes

$$\tilde{\theta} = \tilde{\theta}_{max} - 2\log\cosh\left[(\delta\exp\tilde{\theta}_{max}/2)^{\frac{1}{2}}(z-z_{max})\right]$$

$$\text{with} \quad \tilde{\theta}_{max} = 2\log\cosh(\delta\exp\tilde{\theta}_{max}/2)^{\frac{1}{2}} z_{max} \qquad (1.5.5)$$

<u>Considering the boundary condition at $z = 2$</u>

$$-\frac{d\tilde{\theta}}{dz} = \alpha_s(\tilde{\theta}_s - \tilde{\theta}_0)$$

Differentiating $\tilde{\theta}$ with respect to z in (1.5.5) and then imposing the boundary condition we obtain

$$\alpha_s(\tilde{\theta}_s-\tilde{\theta}_0) = P\ \tanh P(1-\frac{z_{max}}{2})$$

$$\equiv P\Phi \qquad (1.5.6)$$

where $$P = (2\delta\exp\tilde{\theta}_{max})^{\frac{1}{2}} \qquad (1.5.7)$$

Hence

$$\delta = \frac{P^2}{2} e^{-\tilde{\theta}_{max}}$$

$$= \frac{P^2}{2} \operatorname{sech}^2 \frac{P}{2} z_{max}$$

$$= \frac{P}{2} (1-\tanh^2 \frac{P}{2} z_{max}) \qquad (1.5.8)$$

But

$$\tilde{\theta}_s = \tilde{\theta}_{max} - 2\log \cosh P(1-\frac{z_{max}}{2})$$

$$= 2\log[\cosh \frac{P}{2} z_{max}/\cosh P(1-\frac{z_{max}}{2})]$$

Therefore

$$e^{(\tilde{\theta}_s/2)} = \frac{\cosh \frac{P}{2} z_{max}}{\cosh P(1-\frac{z_{max}}{2})}$$

We note

$$\cosh P(1-\frac{z_{max}}{2}) = \cosh P \cosh \frac{P}{2} z_{max} - \sinh P \sinh \frac{P}{2} z_{max}$$

Thus

$$e^{(\tilde{\theta}_s/2)} = \frac{1}{(\cosh P - \sinh P \tanh \frac{P}{2} z_{max})}$$

OR

$$\tanh^2 \frac{P}{2} z_{max} = \frac{[\cosh P - e^{-(\tilde{\theta}_s/2)}]}{\sinh^2 P}$$

Hence on substituting $\tanh^2 \frac{P}{2} z_{max}$ into (1.5.8), we get

$$\delta = \frac{P^2}{2\sinh^2 P}[\sinh^2 P - \cosh^2 P + 2\cosh P\, e^{-(\tilde{\theta}_s/2)} - e^{-\tilde{\theta}_s}]$$

$$= \frac{P^2}{2\sinh^2 P}[2\cosh P\, e^{-(\tilde{\theta}_s/2)} - e^{-\tilde{\theta}_s} - 1]$$

$$= \frac{P^2}{2\sinh^2 P}[2\cosh P - (e^{(\tilde{\theta}_s/2)} + e^{-(\tilde{\theta}_s/2)})]\, e^{-(\tilde{\theta}_s/2)}$$

Therefore

$$\delta = (P^2/\sinh^2 P)[\cosh P - \cosh(\tilde{\theta}_s/2)]\ \exp(-\tilde{\theta}_s/2) \qquad (1.5.9)$$

A summary of the above analysis is contained in [6]. However, attempts to determine the limiting case when $\frac{d\delta}{dP} = 0$ for all values of α_s and $\tilde{\theta}_0$ is not possible. Thomas and Bowes [16] were able to determine the limiting case for a wide range of practical interest by assuming large values of parameter P. Infact they chose $\Phi = 1$ which is the implicit condition $P \to \infty$ in (1.5.6). Hence the maximum δ is obtained when

$$2(1-P\coth P)(\cosh P - \cosh N) + (P/2\alpha_s)e^{-N} + [1-(\coth P/2\alpha_s)]\, P\sinh P = 0 \qquad (1.5.10)$$

where

$$N = (P/2\alpha_s) + (\frac{\tilde{\theta}_0}{2})$$

Note: From equation (1.5.6) we have

$$\tilde{\theta}_s = \tilde{\theta}_0 + \frac{P}{\alpha_s}\ \Phi$$

Hence $N = (\tilde{\theta}_s/2)$ corresponds to the case when $\Phi \equiv 1$.

The determination of P that satisfies (1.5.10) is essentially numerical. Thomas and Bowes were able to determine P and z_{max} for a wide range of $\tilde{\theta}_0$ and in the process did determine $\Phi \sim 1$. They also showed that both z_{max} and θ_{max} were small for $\alpha_s > 0.5$. However as α_s tends to zero, z_{max} was noticed to move towards the 'cold face'. For $\alpha_s < 0.5$, the temperature was approximately uniform, the Semenov condition. To determine the limiting case for $\alpha_s < 0.5$, Thomas and Bowes assumed the heat generation term to be constant and equal to $\delta \exp \tilde{\theta}_{max}$. Thus for $\alpha_s \ll 1$, the critical Frank-Kamenetskii parameter becomes

$$\delta_{crit} = \delta_{crit,\alpha_s=0} \cdot (1+2\alpha_s|\tilde{\theta}_0|) \qquad (1.5.11)$$

with $\delta_{crit,\alpha_s=0} = (\frac{1}{2e}) = 0.182$, which is a good approximation to (1.5.0).

(c) <u>Slab with the hot face insulated and the cold surface in contact with a perfect conductor</u> $(\alpha_p=0, \alpha_s=\infty)$

This problem has been studied by Semenov [17] and Zeldovich [18] for a slab with large temperature differences. Their assumption of zero temperature gradient at the hot face and a linear temperature profile at the cold face is a good model to problem (a), which is a special case of (b). In (b) Thomas and Bowes found $\tilde{\theta}_{max}$ to be independent of α, and $\tilde{\theta}$ satisfies the above assumptions. Gray and Lee [3] were able to show that the Semenov - Zeldovich treatment leads to the limiting case

$$\delta_{crit} = \tilde{\theta}_0^{\,2}/8 \qquad (1.5.12)$$

By assuming $\tilde{\theta}_s \gg 1$ Thomas and Bowes [16] replaced T_0 by T_s and hence replaced $\tilde{\theta}_0$ by $\tilde{\theta}_s$ in (1.5.12). Thomas and Bowes extended the analysis of Semenov-Zeldovich to include the cases where $\alpha_s \neq \infty$ and accordingly modified the limiting case for δ. Hence they were able to determine $\tilde{\theta}_s$ and δ_{crit}, namely

$$\tilde{\theta}_s \cong [2\alpha_s/(1+2\alpha_s)]\tilde{\theta}_0$$

and
$$\delta_{crit} \cong \tfrac{1}{2}[\alpha_s(1+2\alpha_s)]^2\tilde{\theta}_0^{\,2} \qquad (1.5.13)$$

with the proviso that

$$[2\alpha_s/(1+2\alpha_s)]|\tilde{\theta}_0| \gg 1$$

Zeldovich also studied the problem (b) with $\alpha_p = 0$ and α_s finite and was able to determine δ_{crit} such that

$$\delta_{crit} \cong \frac{1}{2}[\alpha_s/(1+2\alpha_s)]^2(1.4-|\tilde{\theta}_0|)^2 \qquad (1.5.14)$$

Equation (1.5.14) gives a value of δ_{crit} greater than (1.5.13) by a factor $[(1.4-|\tilde{\theta}_0|)^2/\tilde{\theta}_0^{\,2}]$. However, when $|\tilde{\theta}_0|$ becomes large both approaches of (1.5.13) and (1.5.14) give the same value of δ_{crit}. This result corresponds to the case when α_s becomes large.

1.6 Multi-dimensional Self-heating Bodies

The discussions in the earlier sections have concentrated on the solution of problems with one spatial variable. However, techniques and methods have also been developed to cater for thermal ignition for generally shaped bodies. J.T. Stuart [19] developed a general analytical solution of the Liouville problem by using complex analysis methods. In fact his 1967 paper suggested typical solutions of Liouville's problem for given fluid conditions. Of importance is the solution he suggested for spatially periodic problems, this was used by Adler [20] to determine the critical parameters for the slab with a periodic surface temperature.

(a) Procedure for determining solution of Liouville's problem using complex analysis methods

Consider the Liouville's problem

$$\frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial y^2} + \delta\exp\theta = 0 \qquad (1.6.0)$$

We define complex variables z and $\bar{z}$ by putting

$$z = x + iy \quad \text{and} \quad \bar{z} = x - iy$$

and treat them as new independent variables. Hence

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial z} + \frac{\partial}{\partial \bar{z}} \quad \text{and} \quad \frac{\partial}{\partial y} = i\left(\frac{\partial}{\partial z} - \frac{\partial}{\partial \bar{z}} \right)$$

Thus equation (1.6.0) becomes

$$\frac{\partial^2\theta}{\partial z\partial \bar{z}} = -\frac{\delta}{4}\, e^{\theta} \qquad (1.6.1)$$

Differentiating (1.6.1) with respect to z, we obtain

$$\begin{aligned}\frac{\partial^3\theta}{\partial z^2\partial \bar{z}} &= -\frac{\delta}{4}\, e^{\theta}\, \frac{\partial\theta}{\partial z} \\ &= \frac{\partial\theta}{\partial z} \cdot \frac{\partial^2\theta}{\partial z\partial \bar{z}}\end{aligned}$$

Therefore

$$\frac{\partial^3\theta}{\partial z^2\partial\bar{z}} - \frac{\partial\theta}{\partial z}\ \frac{\partial^2\theta}{\partial z\partial\bar{z}} = 0$$

$$\frac{\partial}{\partial\bar{z}}\left\{ \frac{\partial^2\theta}{\partial z^2} - \frac{1}{2}\left(\frac{\partial\theta}{\partial z}\right)^2\right\} = 0$$

Integrating the equation with respect to $\bar{z}$, we get

$$\frac{\partial^2\theta}{\partial z^2} - \frac{1}{2}\left(\frac{\partial\theta}{\partial z}\right)^2 = -2G(z) \qquad (1.6.2)$$

where $G(z)$ is as yet an unspecified analytic function of z. We now define a solution $f(z,\bar{z})$ for equation (1.6.2) by putting

$$f(z,\bar{z}) = e^{-\theta/2}$$

On substituting $f(z,\bar{z})$ into (1.6.2), we have a condition on $f(z,\bar{z})$, namely

$$f_{zz}(z,\bar{z}) - G(z)\ f(z,\bar{z}) = 0 \qquad (1.6.3)$$

On repeating the same procedure with $\bar{z}$ instead of z, we obtain

$$f_{\bar{z}\bar{z}}(z,\bar{z}) - H(\bar{z})f(z,\bar{z}) = 0 \qquad (1.6.4)$$

$H(\bar{z})$ is an arbitrary analytic function of $\bar{z}$. In general the solution of equation (1.6.3) is

$$f(z,\bar{z}) = \alpha_1(z)\beta_1(\bar{z}) + \alpha_2(z)\beta_2(\bar{z})$$

where α_1,α_2 are linearly independent solutions. However, $f(z,\bar{z})$ must be real, therefore

$$\beta_1(\bar{z}) = \bar{\alpha}_1(\bar{z})$$

and $$\beta_2(\bar{z}) = \bar{\alpha}_2(\bar{z}).$$

Hence θ becomes

$$\theta = -2\log[\alpha_1(z)\,\bar{\alpha}_1(\bar{z}) + \alpha_2(z)\bar{\alpha}_2(\bar{z})] \qquad (1.6.5)$$

By imposing Wronskian constraint on (1.6.3) we get

$$\alpha_1(z)\,\frac{d\alpha_2}{dz} - \alpha_2(z)\,\frac{d\alpha_1}{dz} = \lambda \quad , \quad \text{say.}$$

On substituting into (1.6.1) it can be shown that

$$|\lambda^2| = \frac{\delta}{8} \qquad (1.6.6)$$

In his 1975 paper Adler [20] solved the symmetrically heated slab (1.6.0) with conditions;

$$\text{(i)} \quad y = 1 \quad : \quad \theta(x,1) \cong \varepsilon\cos\omega x$$

where the wavelength $= \frac{2\pi}{\omega}$, with ω being the wave number.

$$\text{(ii)} \quad y = 0 \quad : \quad \frac{\partial\theta}{\partial y} = 0$$

Adler chose a periodic solution in x such that

$$G(z) = -\frac{\omega^2}{4}, \quad \alpha_1(z) = A^{\frac{1}{2}}\cos(\frac{\omega z}{2}) \quad \text{and} \quad \alpha_2(z) = B^{\frac{1}{2}}\sin(\frac{\omega z}{2})$$

He was able to express the Frank-Kamenetskii parameter as a function of the wave number and the amplitude, namely

$$\delta = 2\omega^2\left[\frac{\cosh^2(\frac{\varepsilon}{2})}{\cosh^2\omega} - \sinh^2(\frac{\varepsilon}{2})\right] \qquad (1.6.7a)$$

OR

$$\sinh^2\left(\frac{\varepsilon}{2}\right) = \frac{\operatorname{sech}^2\omega-(\delta/2\omega^2)}{\tanh^2\omega} \qquad (1.6.7b)$$

$$\geqslant 0$$

Adler [20] also determined the dependence of temperature profile $\theta(x,y)$ on ω and ε, namely

$$\theta(x,y) = -2\log\left[\cosh\left(\frac{\varepsilon}{2}\right)\frac{\cosh \omega y}{\cosh \omega} - \sinh\left(\frac{\varepsilon}{2}\right)\cos \omega x\right] \qquad (1.6.8)$$

We have reproduced the curves of δ versus ω for various values of ε, see Figure 1.8. Adler observed that the maximum δ decreased for an increase in ε. Hence his conclusion that the oscillatory motion decreased the critical δ and that this amount of decrease is dependent on the amplitude of the oscillation.

(b) Many other attempts have been made to determine the critical conditions for multi-dimensional bodies, for example, the Frank-Kamenetskii [2] practical approach on finite cylinders. An important feature of these solutions is the dominance of the harmonic mean-square lengths in the relevant formulae of the critical parameters. One of the most practical aids is the concept of an equivalent sphere . In essence this method replaces an arbitrary body by an equivalent sphere of appropriate radius such that the equivalent sphere will reach the same critical conditions as the arbitrary body under the same surface temperature. Since the limiting case for the spheres is known and is expressed in terms of its radius, the problem reduces to determining the equivalent radius of the sphere and hence the critical parameters of the arbitrary body. Gray and Lee [6] have used this concept with reasonable success for the cube and the regular cylinder. They calculated δ_{crit} (cube) = 2.65 and δ_{crit} (regular cylinder) = 2.89. These values compare favourably with the 'exact' values quoted by Gray and Sherrington [3], namely δ_{crit} (cube) = 2.52 and δ_{crit} (regular cylinder) = 2.77.

In [3] Gray and Sherrington describe three further approaches which can be used to generalize the steady-state problem. These methods are summarised below:-

(i) Collocation Methods

This method involves defining a suitable polynomial for the temperature profile within the reactant, and satisfying the boundary conditions. The degree of accuracy and complexity of the chosen polynomial will be determined by the number of internal points, since the coefficients of the polynomial must be chosen such that the polynomial satisfies exactly the energy equation at these internal arbitrary number of points. The profile chosen may 'blur' the bifurcation (or turning point, see Figure 1.2) point which occurs at $\delta = \delta_{crit}$, thus it is necessary to 'impose' the critical condition. Gray and Sherrington define this 'criticality' as the condition underwhich a small change in temperature at some point well removed from 'centre' results in large changes in central excess temperature. This definition is consistent with results from experiments discussed in [3]. This method has been used successfully for class A geometries and other bodies, see Table 1.

In practice this method results in solving numerically a pair of transcendental equations which completely specify the critical values of δ and the central excess temperature. Note the method avoids the integration of the energy equation though the work itself is tedious. Another advantage of the scheme is that no approximation of the heat generation term is necessary, namely the term $\delta\exp[\theta/(1+\beta\theta)]$, need not be altered. Thus the method can also be used to determine the effect of β on the Frank-Kamenetskii parameter. However, the polynomial exhibits some non-symmetrical terms where there should be symmetry. A major weakness of this scheme is that it offers no scope for a transient study due to its lack of a theoretical basis.

(ii) General Series

This method was developed to offer a unified solution of class A geometries making use of the harmonic mean-square lengths in the formulae. The equation to be solved is

$$\frac{d^2\theta}{dz^2} + \left(\frac{K}{z}\right)\frac{d\theta}{dz} + \delta e^{\theta} = 0$$

with boundary conditions;

$$\theta = 0 \quad \text{at} \quad z = 1 \tag{1.6.9}$$

$$\frac{d\theta}{dz} = 0 \quad \text{at} \quad z = 0$$

A parametric solution of (1.6.9) was expressed as

$$\theta = \theta_0 - 2\log\sum_{j=0}^{\infty} b_j (yz^2)^j$$

On imposing the condition at $z = 1$, it can be shown that

$$\sum_{j=0}^{\infty} b_j (yz^2)^j = \exp(\frac{\theta_0}{2})$$

For the recurrence relation of b_j see [3]. Gray and Sherrington sought to determine the solution for an arbitrary body by considering $\theta = \theta(\theta_0, z, K)$. For the limiting case they obtained

$$\delta_{crit} = \frac{2(K+1)(K+3)}{(K+7)}$$

$$\left(\theta_{max}\right)_{crit} = 2\log(\frac{K+7}{4}) \qquad (1.6.10)$$

where K is the shape factor, with K = 0,1,2 representing the slab, infinite cylinder and the sphere respectively.

Gray and Sherrington were also able to show that θ depended feebly on the shape factor K and wrote

$$\theta \cong \theta_0(1-z^2)[1- \frac{K+1}{2(K+3)} z\, \theta_0^{\,2} + \ldots] \qquad (1.6.11)$$

The justification of this method can be seen from Table 1, in that its solutions broadly agree with the results independently obtained by other schemes. However, its advantage is that the temperature attains its maximum value at the centre and that the total heat balance equation is satisfied. It also offers a unified solution for class A geometries, even though the bodies differ widely in shape.

(iii) Variational Methods

This method was developed to cope with the transient behaviour of a reacting system. However, Sherrington [21] and Wake

[22] have shown how powerful this method is even for the stationary state problems. Both authors have solved the class A geometries, cube and other geometries (see Table 1). The method involves choosing a physically realistic temperature polynomial satisfying exactly the boundary conditions. Thus the temperature polynomial must exhibit parabolic or convex temperature profiles with the maximum temperature occurring at the centre of the reactant. The coefficients of the polynomial are then considered to be functions of time only and hence independent of spatial coordinates. The power of the variational method is that any errors in approximating the temperature are reduced by the following procedures:-

(a) Two vector fields H and G are defined representing the heat flow and heat generation fields respectively. G is defined as an integral in time. Thus we have

$$\text{div } H = -\rho\mu\theta \tag{1.6.12}$$

$$G = \int_0^t Q.K_0(T)dt \tag{1.6.13}$$

where

ρ = density of the reactant

μ = specific heat

K_0 = kinetic rate

(b) Fourier law and heat conduction gives

$$\text{grad}\theta + \frac{1}{\lambda}.H = 0 \tag{1.6.14}$$

A variational in θ can be obtained from combination of equations (1.6.14) and (1.6.13). Hence, we get

$$\int_V \rho\mu\theta \, \delta\theta \, dv + \int_V \frac{1}{\lambda} \dot{H} \, \delta H \, dv' = - \int_V \frac{1}{\lambda} \dot{G} \, \delta H \, dv \qquad (1.6.15)$$

Equation (1.6.15) can be made more tractable to analysis by defining the temperature profile. Gray and Sherrington [3] chose

$$\theta = (1-z^2)(q_0+q_1z^2+q_2z^4 + \ldots) \qquad (1.6.16)$$

By substituting (1.6.16) into (1.6.15) we obtain n equations;

$$\int_V \rho\mu\theta \frac{\partial\theta}{\partial q_i} dv + \int_V \frac{1}{\lambda} \dot{H} \frac{\partial \dot{H}}{\partial q_i} dv = - \int_V \frac{1}{\lambda} \dot{G} \frac{\partial H}{\partial q_i} dv \qquad (1.6.17)$$

$$i = 1(n)$$

The n equations are equivalent to the Lagrangian equations of classical mechanics. However, for the steady-state problem equation (1.6.17) becomes

$$\int_V \rho\mu\theta \frac{\partial\theta}{\partial q_i} dv = - \int_V \frac{1}{\lambda} \dot{G} \frac{\partial H}{\partial q_i} dv \qquad (1.6.18)$$

Equations (1.6.18) now represent n algebraic equations. For nonlinear heat generation, equations (1.6.17) are not always amenable to analysis. However, the Frank-Kamenetskii conditions of criticality can be obtained when the solutions of the n-equations cease to be bounded. Sherrington [21] considered the solution for class A geometries, the cube and other geometries (see Table 1, variational (1)), using a quadratic heat generation rate. Sherrington obtained the results by using a temperature polynomial as described above. He further assumed that $\theta = 0$ at surface. Wake [22], on the other hand, generalised the surface condition by imposing the condition

$$\frac{\partial \theta}{\partial z} + \alpha\theta = 0, \quad \text{at the surface}$$

Unlike Sherrington, Wake chose trigonometric terms to represent the temperature profile within the reacting mass. By assuming the heat losses to be purely due to heat conduction within the reactant, Wake further investigated the effect of the Biot Numbers on the critical Frank-Kamenetskii parameter. He defined this criticality as the condition when solution of the time-dependent variational equations is just possible. His results are shown in Table 1; variational (2) corresponds to the Frank-Kamenetskii condition, $\alpha = \infty$.

1.7 The Effect of β Values on the Ignition Phenomena

In the above sections, we have limited our discussions to the case $\beta = 0$ in the heat generation term. However, it is of interest to investigate the effect of non-zero β values on the possibilities of existence of the conditions for thermal ignition. It is known that the curve in Figure 1.2 represents the simplest bifurcation of a self-heating medium, in which no temperature solutions exists for $\delta > \delta_{crit}$. However, for $\beta \neq 0$ and $\delta > \delta_{crit}(\beta=0)$, there exists a stable state, given by the upper part of curve in Figure 1.9, for which the temperature is sufficiently high to lead to ignition. This stable state is called the supercritical state. Fradkin and Wake [23], have investigated the disappearance of the critical phenomena for thermal explosion, when $\beta = \beta_{tr}$. In fact they have shown that criticality always exist for thermal ignition for small values of β, namely $0 < \beta \leqslant \beta_{tr}$, in which $\delta_{crit}(\beta)$ monotonically approaches $\delta_{crit}(\beta=0)$ from above as $\beta \to 0$. Several authors have sought to determine β_{tr} for various rates of heat generation and geometries. Fradkin and Wake suggested a variational model for determining β_{tr} by assuming a local critical δ. However, their scheme results in considerable difficulties even for simple geometries. Bazley and Wake [24] have successfully computed β_{tr}, using an approximate reaction rate form, $\beta_{tr} = 0.2138$ for the infinite slab and $\beta_{tr} = 0.1732$ for the infinite circular cylinder. On the other hand, Boddington and Gray [25] have conducted an extensive study of the transition region for the slab using Arrhenius and 'bimolecular law' rates of heat generation, namely $\delta\exp[\theta/(1+\beta\theta)]$ and $\{\delta(1+\beta\theta)^{\frac{1}{2}}\exp[\theta/(1+\beta\theta)]\}$ respectively. They also determine the shape of the critical locus, the bifurcation set, a curve in three dimensional space (δ,β,θ_m) for the two rate laws for both Frank-Kamenetskii and Semenov extremes. Curves in Figure 1.10 represents some of their results. Table 2 contains some of the data with a comparison of the transition and critical parameters for both Frank-Kamenetskii and Semenov conditions for the infinite slab. The main conclusions of Boddington and Gray's investigation are:-

(i) The size of the excess central temperatures $\theta_m(\beta_{tr})$ is nearly four times the classical value with temperatures (T_m-T_0) being of the order 400K greater than T_0. T_m and T_0 are temperatures at the centre and surface of the vessel respectively.

(ii) For any particular rate law, the Semenov extreme sets an upper bound on β_{tr} for the Frank-Kamenetskii extreme and all the intermediate Biot Numbers.

(iii) The suddenness with which the criticality is lost with the ignition phenomena persisting to within 0.025 of β_{tr}.

Kordylewski [26] has also investigated numerically the β effect on the disappearance of the criticality for thermal explosion using the reduced Frank-Kamenetskii rate of heat generation. Figure 1.11 exhibits the loci of the δ curves for extinction and ignition dependence on β, with the stable solutions possible within the confines of δ_1^* and δ_2^* curves.

1.8 Conclusions

The effect to which the postulates and approximations of thermal explosion theory provide an adequate description of the gas phase reactions has been the subject of interest to many authors. However, due to lack of satisfactory precision instruments most of the experimental data are erroneous. Gray et al [27] have conducted an extensive study on the decomposition of diethyl peroxide in the gas phase. By limiting the heat losses due to convection and radiation, any heat losses could then be attributed to the conductive heat transfer. In spite of the deviation in practice of the reacting systems from the various assumptions of the steady-state conductive theory, their results are in excellent agreement with the predictions of the thermal explosion theory. The experimental results may be summarized as follows:-

(i) Ignition is always preceded by self-heating with the largest temperatures occurring at the centre of the reactant. At the vessel walls the temperature is $O(T_0)$, where T_0 is the temperature of reactant's surroundings.

(ii) A critical temperature increment exists above which ignition is inevitable. The size of this increment is a multiple of RT_0^2/E.

(iii) The dimensionless critical temperature gradient at the wall is given by

$$\left| \left(\frac{d\theta}{dz} \right)_{crit} \right| = 2 \quad .$$

(iv) The temperature differs significantly from a parabola close to criticality, being less steep at the walls and more curved at the centre.

The assumption of the Arrhenius rate of reaction in the postulates of thermal explosion theory implies a monotonic increase in the reaction rate with an increase in temperature. However, this case is true for chemically simple reactions. The interaction of chemical kinetics sometimes exhibit reaction rates which fall over certain temperatures ranges leading to many interesting and complex phenomena. One of these is the substantial self-heating that may be tolerated in a reaction without ignition. This is the case for the oxidation of hydrazine with the reaction being overwhelmingly thermal in origin.

Although thermal explosion theory has led to an excellent prediction of chemical ignition of simple chemical systems in open stirred systems, its prediction of the critical dimensionless temperature excess offers a bound on closed systems. It has also led to a better understanding of hydrocarbon oxidation, in that a unified theory of both thermal and kinetic theories does play a part in determining chemical reactions of more complex systems (see Reference [3]).

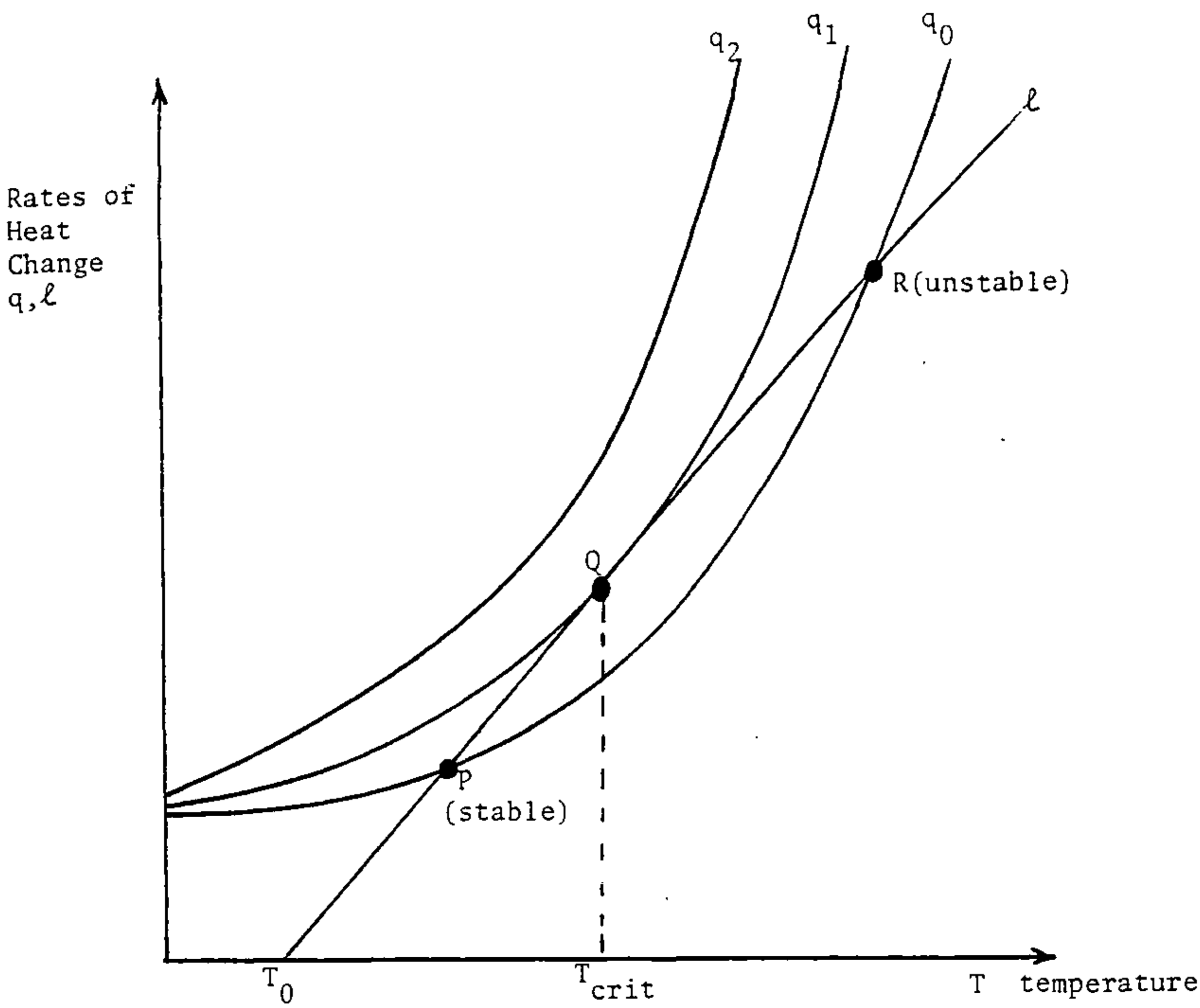


Figure 1.1: Semenov's diagram of heat release rates q_0, q_1, q_2 and heat loss ℓ. P and R of q_0 and ℓ represent stable and unstable modes. However, the intersection Q represents the highest attainable temperature T_{crit} for the reacting mass to remain stable. T_{crit} is given by the tangency of q_0 and ℓ. Hence Q represents the critical condition for the onset of thermal ignition.

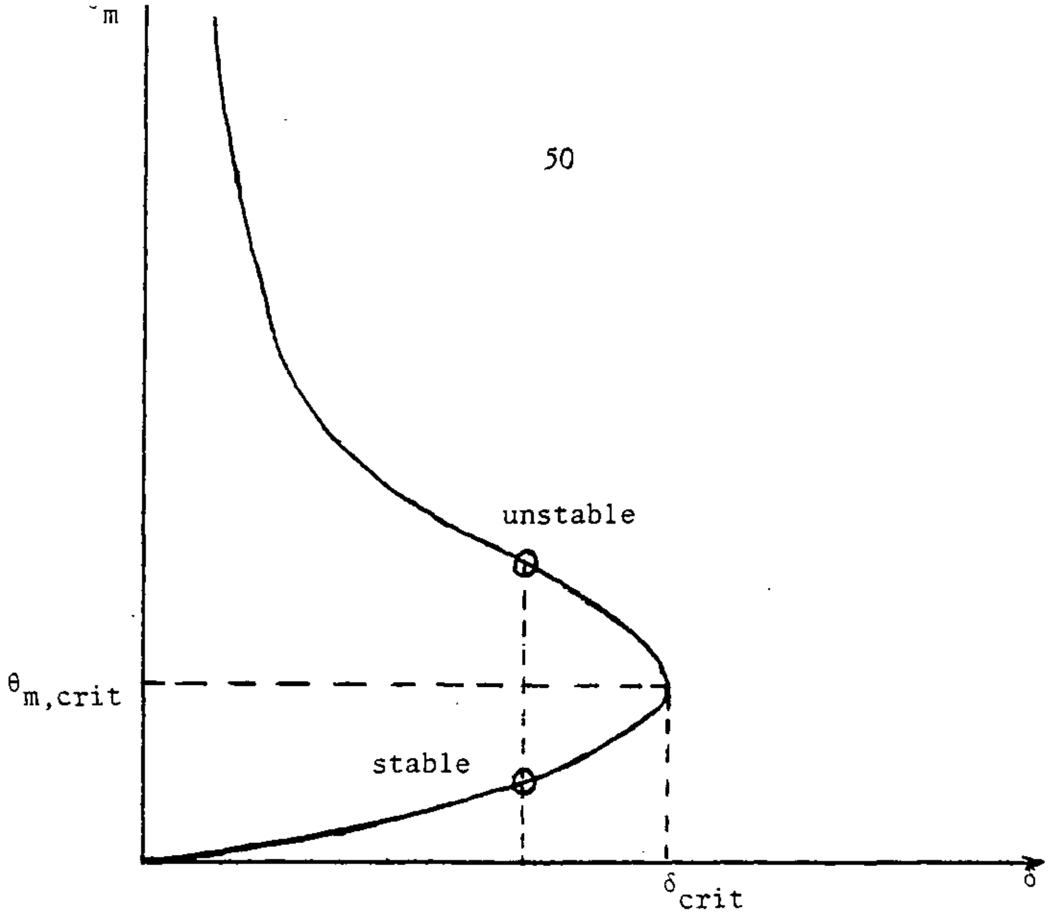


Figure 1.2: Schematic diagram of the temperature of the centre of slab versus the Frank-Kamenetskii parameter, exhibiting stable temperature for $\theta < \theta_{crit}$ with δ_{crit} being the limiting case.

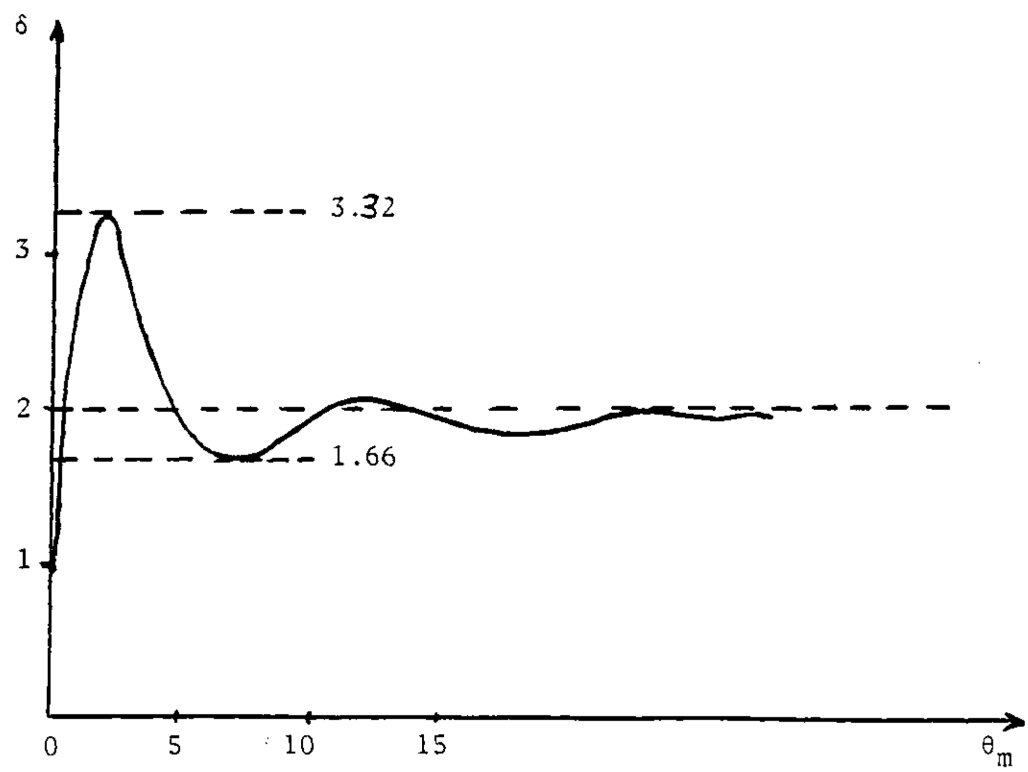


Figure 1.3: δ as a function of θ_m from a sphere as data published by Steggard [9].

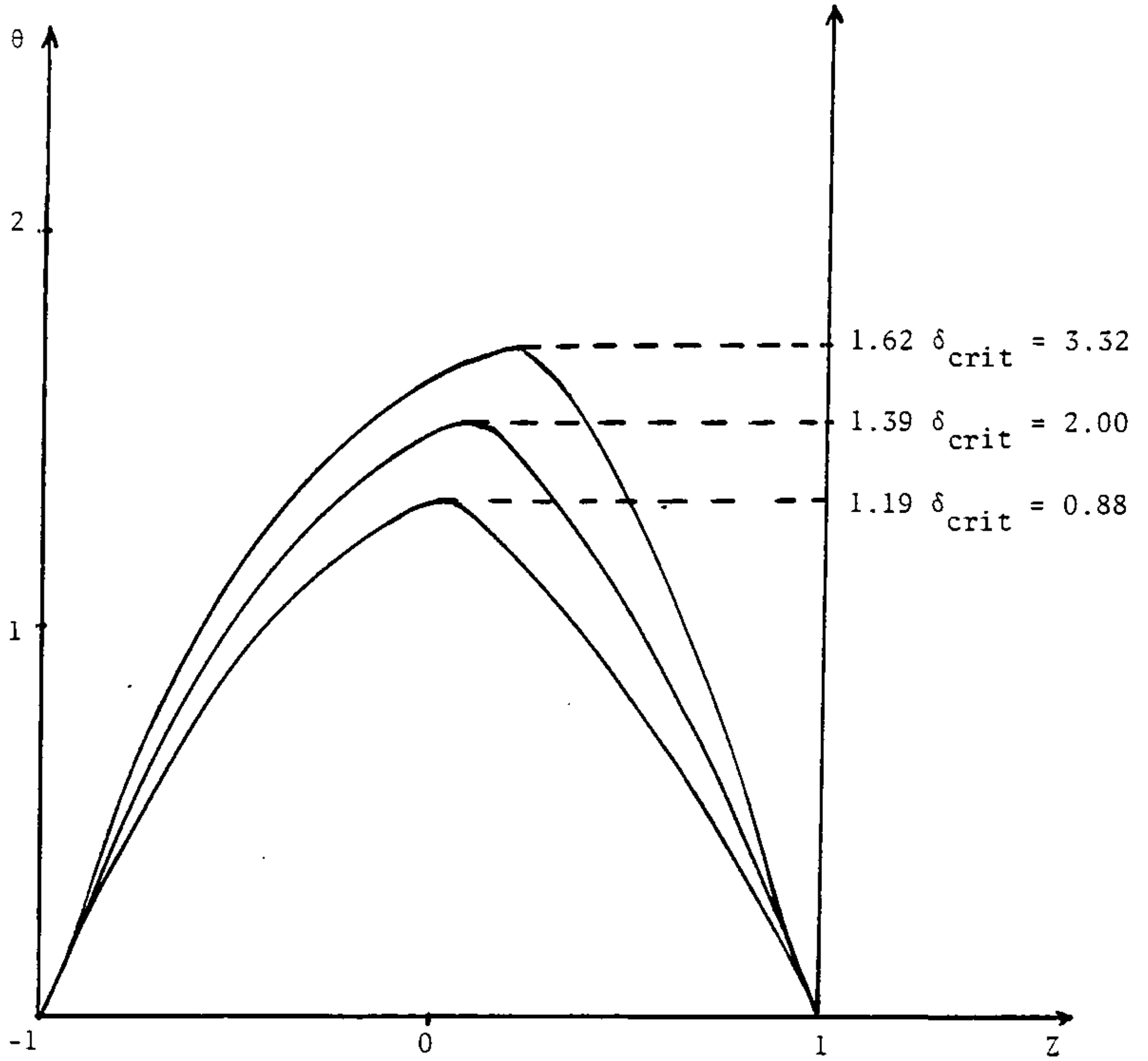


Figure 1.4: Temperature profiles for the class A geometries across the reactant's vessel.

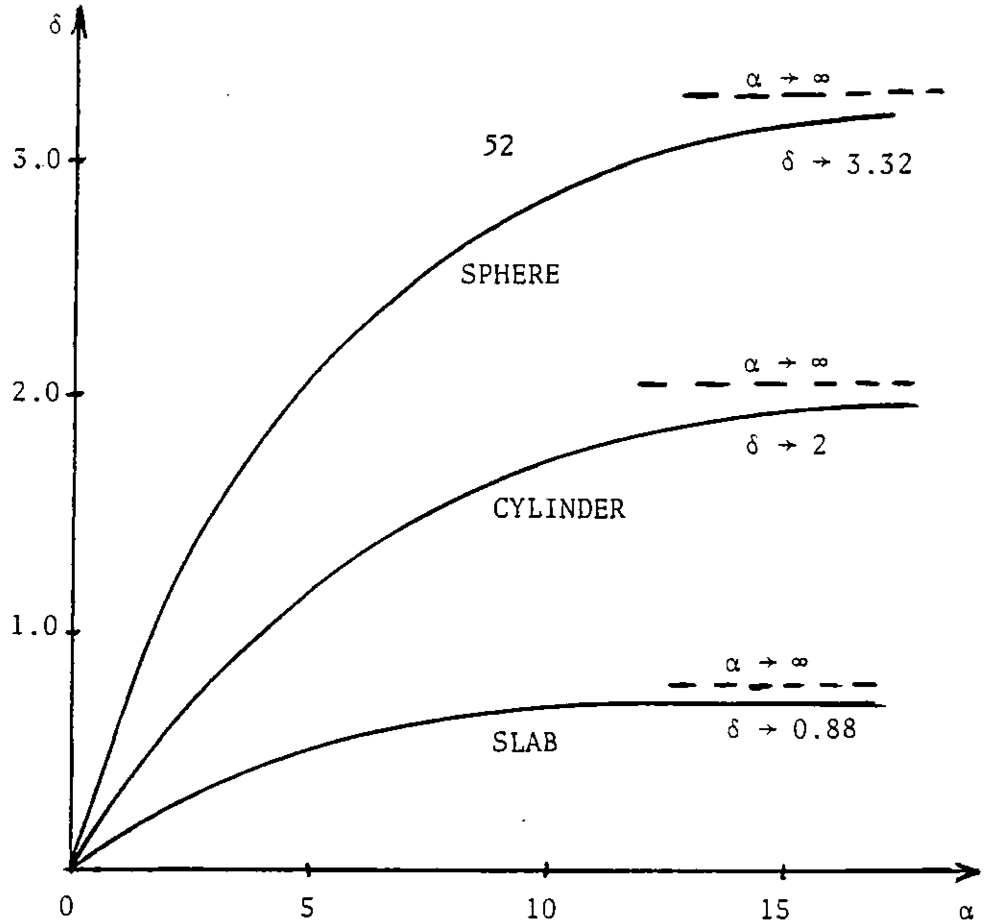


Figure 1.5: The critical values of δ against α for class A geometries.

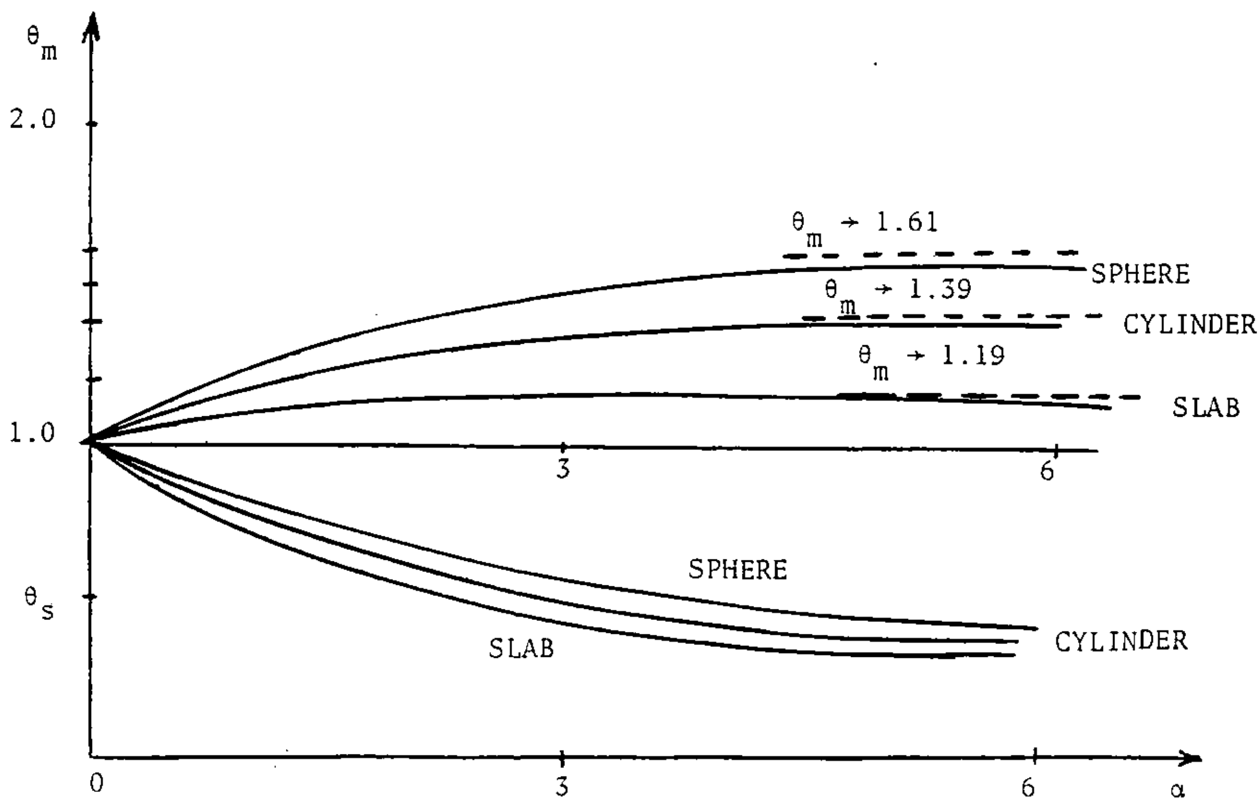


Figure 1.6: θ_m and θ_s are the centre and surface temperatures respectively for the infinite slab, infinite cylinder and the sphere at criticality.

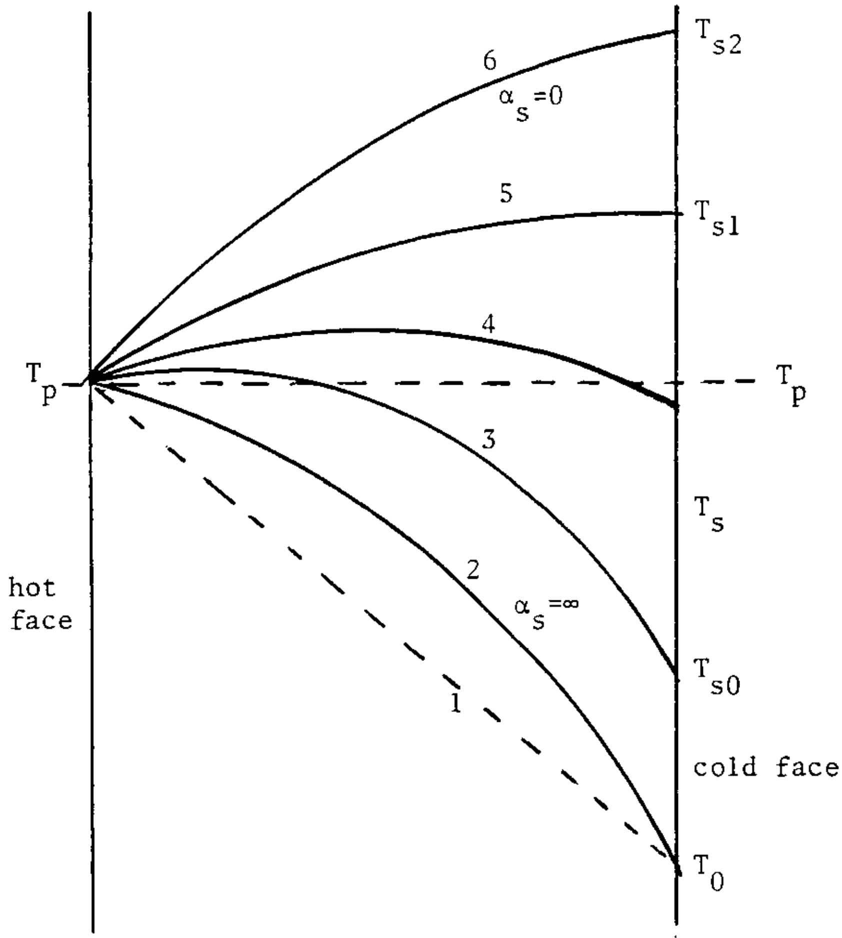


Figure 1.7: Temperature profiles for asymmetrically-heated slab; ($\alpha_p=\infty$, $0 \leqslant \alpha_s \leqslant \infty$).

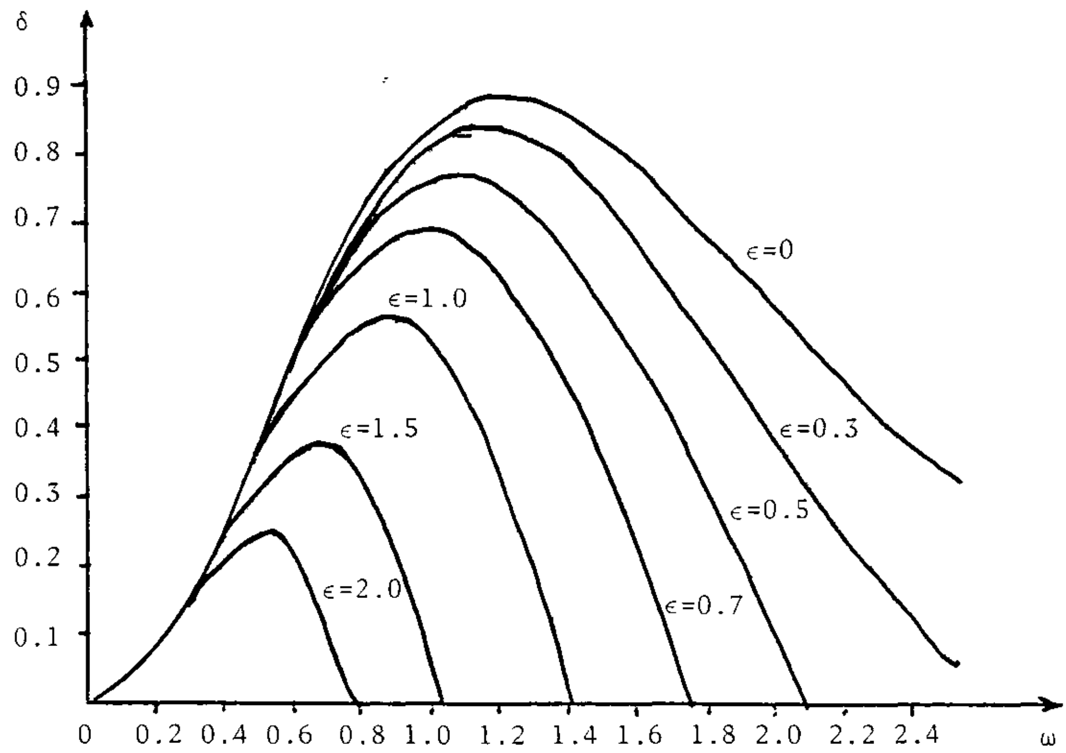


Figure 1.8: Adler [20] curves of δ against ω for specified values of ϵ.

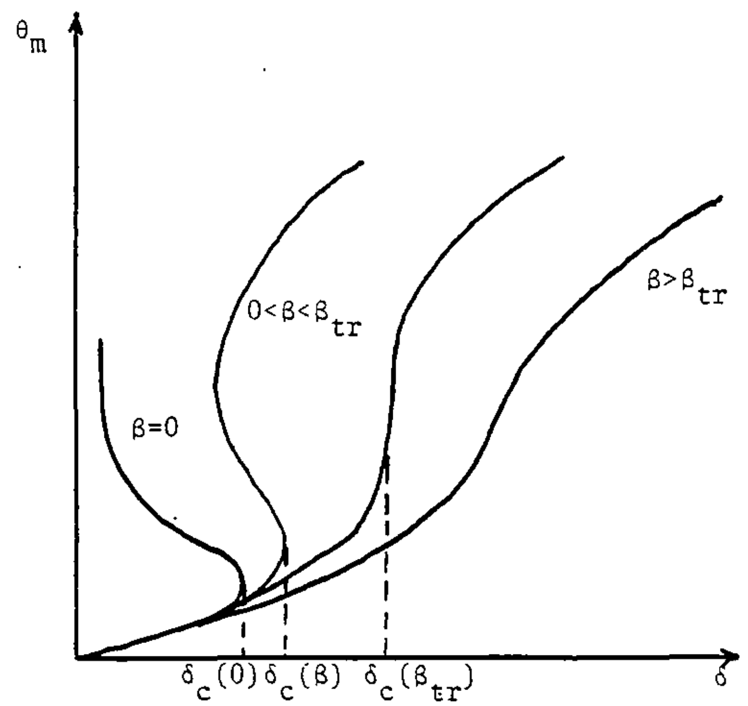


Figure 1.9: Graph of the maximum dimensionless temperature excess θ_m against δ exhibiting typical behaviour of reacting medium for various β values. β_{tr} corresponds to the transition region. For $\beta > \beta_{tr}$ reactant no longer exhibits ignition phenomena ($\delta_c \equiv \delta_{crit}$).

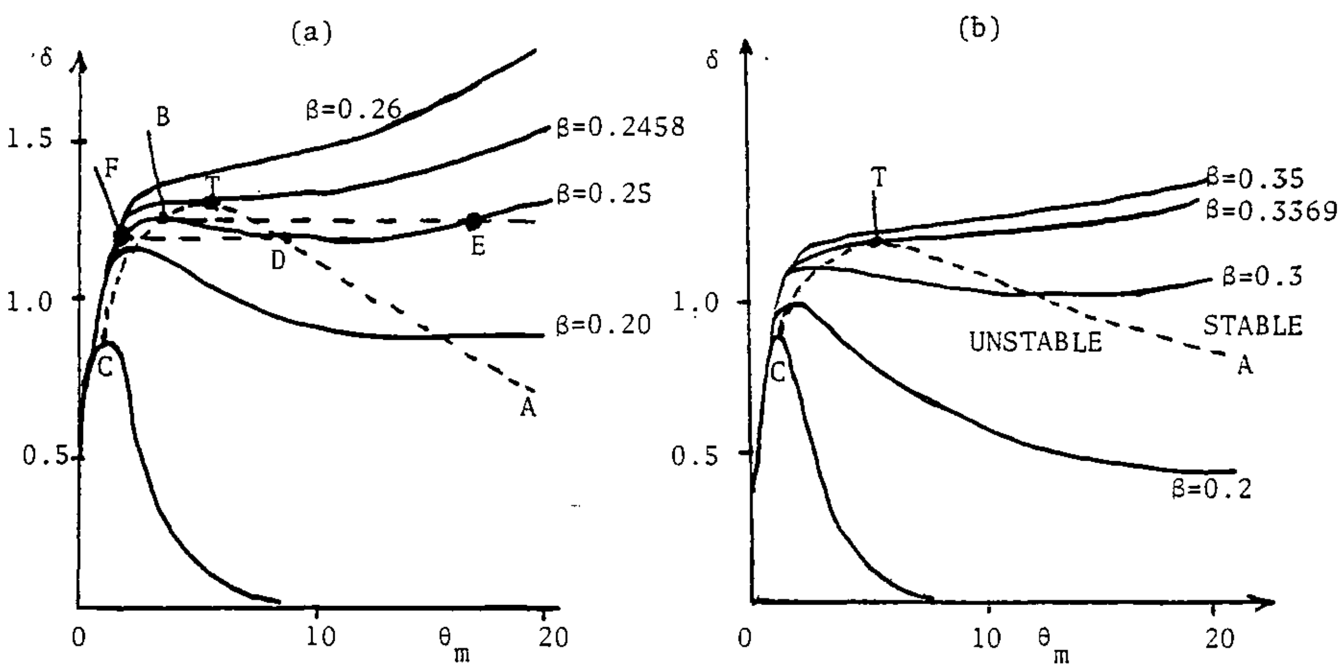


Figure 1.10: The curves for Biot number $\alpha = \infty$. The β effect on the slab with (a) Arrhenius rate law (b) Bimolecular law. Curve CT is the ignition locus and DA the extinction locus. T corresponds to the transition point, Point C represents Frank-Kamenetskii's classical solution. $B \to E$ and $D \to F$ represent typical ignition and extinction jumps respectively. Curve from [25].

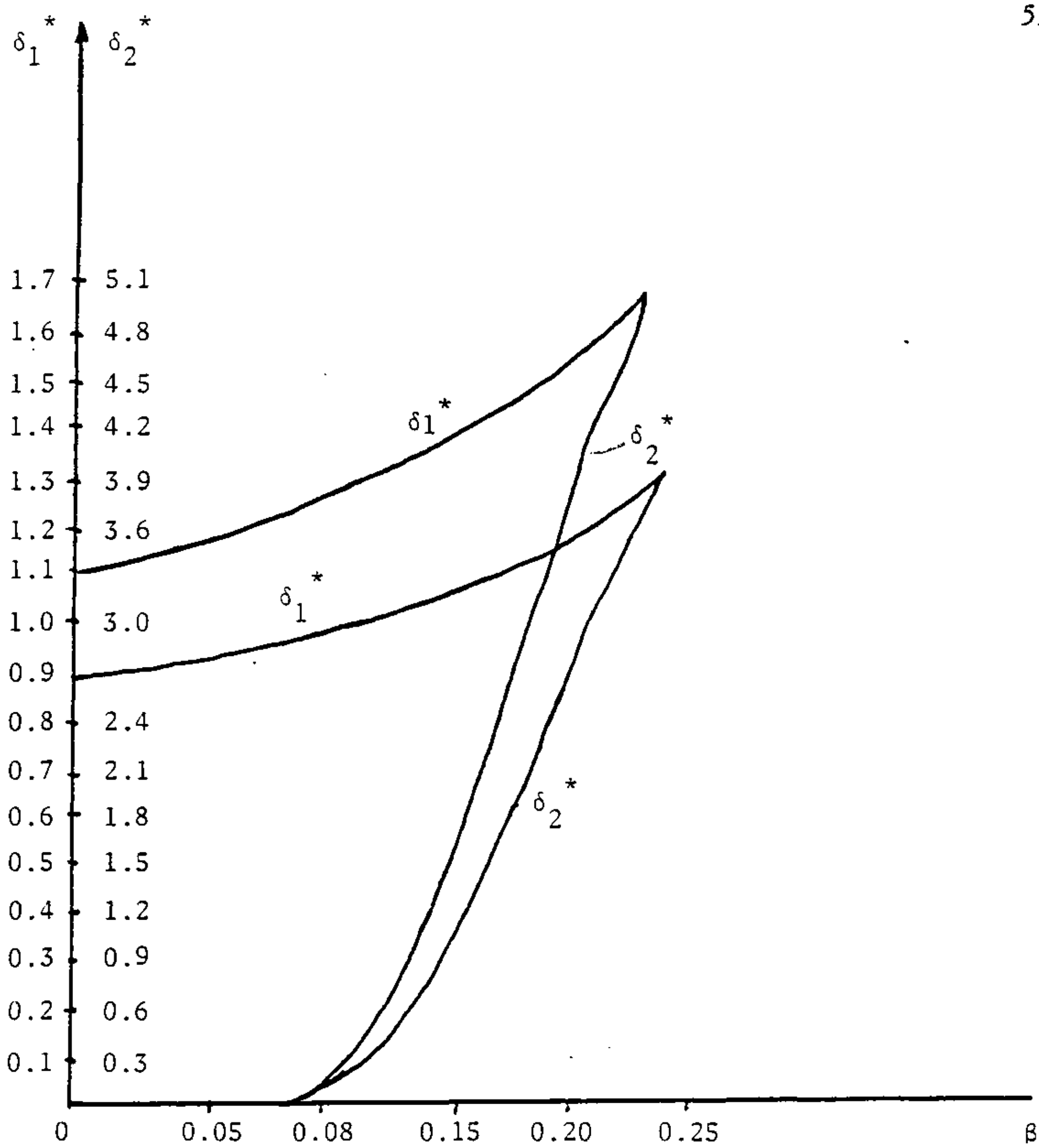


Figure 1.11: Curves obtained from [26]. Curves represent the dependence of the critical parameters of self-ignition δ_1^* and extinction δ_2^* for the slab and the sphere on parameter β .

TABLE 1: Values of δ_{crit} for various geometries; table reproduced from [3]

BODY	'EXACT'	COLLOCATION	SERIES	VARIATIONAL (1)	VARIATIONAL (2)
Slab	0.88	0.90	0.86	0.89	0.88
Cylinder	2	2.10	2	2.06	2
Sphere	3.32	3.47	3.32	3.42	3.32
Cube	2.52	2.36	2.57	2.54	2.45
Square Rod	1.70	-	1.72	1.73	1.69
Equicylinder	2.77	2.78	2.84	2.77	2.77
Right Cone	3.09	3.25	-	2.88	-

TABLE 2: Critical-continuity transition data from [25]

FRANK-KAMENETSKII ($\alpha=\infty$)

Parameters	Arrhenius	Bimolecular
β_{tr}	0.2458	0.3369
$\delta_{crit}(\beta_{tr})$	1.3074	1.1677
$\theta_{m,crit}(\beta_{tr})$	4.897	5.101
$\delta_{crit}(\beta=0)$	0.8758	
$\theta_{m,crit}(\beta=0)$	1.18	

SEMENOV ($\alpha=0$)

Parameters	Arrhenius	Bimolecular
β_{tr}	0.25	0.34315
$(Se)_{tr}$	0.5413	0.48113
$\bar{\theta}_{tr}$	4	4.121
$(Se)_{crit}(\beta=0)$	0.36788	
$\bar{\theta}_{crit}(\beta=0)$	1	

$(Se) \equiv (\delta/\alpha)$

CHAPTER TWO: REACTIVE SLAB WITH PARTIAL SURFACE INSULATION

2.0 INTRODUCTION

We consider modelling the thermally stability of buildings constructed on thermal active sites. These sites are covered by surface soil containing active organic material (refuse). The mass is usually slowly reacting and in thermal equilibrium with its surroundings. Of interest to us is the effect that the insulation provided by the buildings has on the thermal balance. Any meaningful analysis can only be considered for an idealised model of the physical problem.

Thus in some cartesian frame of reference $Ox'y'z'$, we consider a symmetrically heated exothermically reacting slab with the steady temperature distribution being a function of x' and y' only. The slab surface is partially covered by parallel insulation strips of length 2ℓ at $y' = \pm a$, with the remainder of the surface maintained at temperature T_0, the ambient temperature. We are then interested in determining the critical Frank-Kamenetskii parameter, δ_c, as a function of the insulation length, 2ℓ, the slab thickness $2a$, etc., for the steady-state thermal explosion theory. We make use of the same assumptions as in Chapter One, namely

(i) Zero order reaction

(ii) constant physical properties

(iii) Frank-Kamenetskii approximation in the reduced Arrhenius rate law, namely the case $\beta = 0$.

Thus the two-dimensional Fourier equation in temperature becomes

$$\frac{\partial^2 T}{\partial x'^2} + \frac{\partial^2 T}{\partial y'^2} + \frac{QZ_0}{\lambda} \exp\left(\frac{-E}{RT}\right) = 0,$$

where

$T(x',y')$	:	absolute temperature distribution within the slab
E	:	the overall activation energy
λ	:	thermal conductivity
R	:	universal gas constant
Z_0	:	frequency factor
Q	:	heat of reaction.

We conveniently choose our axes $0x'y'z'$ such that the temperature $T(x',y')$ is symmetrical about $0x'$ and $0y'$ (see Figure 2.0). Hence we only need to consider the region $0 \leqslant y' \leqslant a$, $x' \geqslant 0$. The boundary conditions are:-

$$y' = 0 \quad : \quad \frac{\partial T}{\partial y'} = 0, \qquad \forall x' \geqslant 0 \;,$$

$$y' = a \quad : \quad \frac{\partial T}{\partial y'} = 0, \qquad \forall x' < \ell \;,$$

$$: \quad T(x',a) = T_0, \qquad \forall x' > \ell \;,$$

$$x' = 0 \quad : \quad \frac{\partial T}{\partial x'} = 0, \quad \text{for} \quad 0 \leq y' \leq a \,.$$

If the temperature $T(x',y')$ is to be unique, we need to specify the boundary condition as $x' \to \infty$.

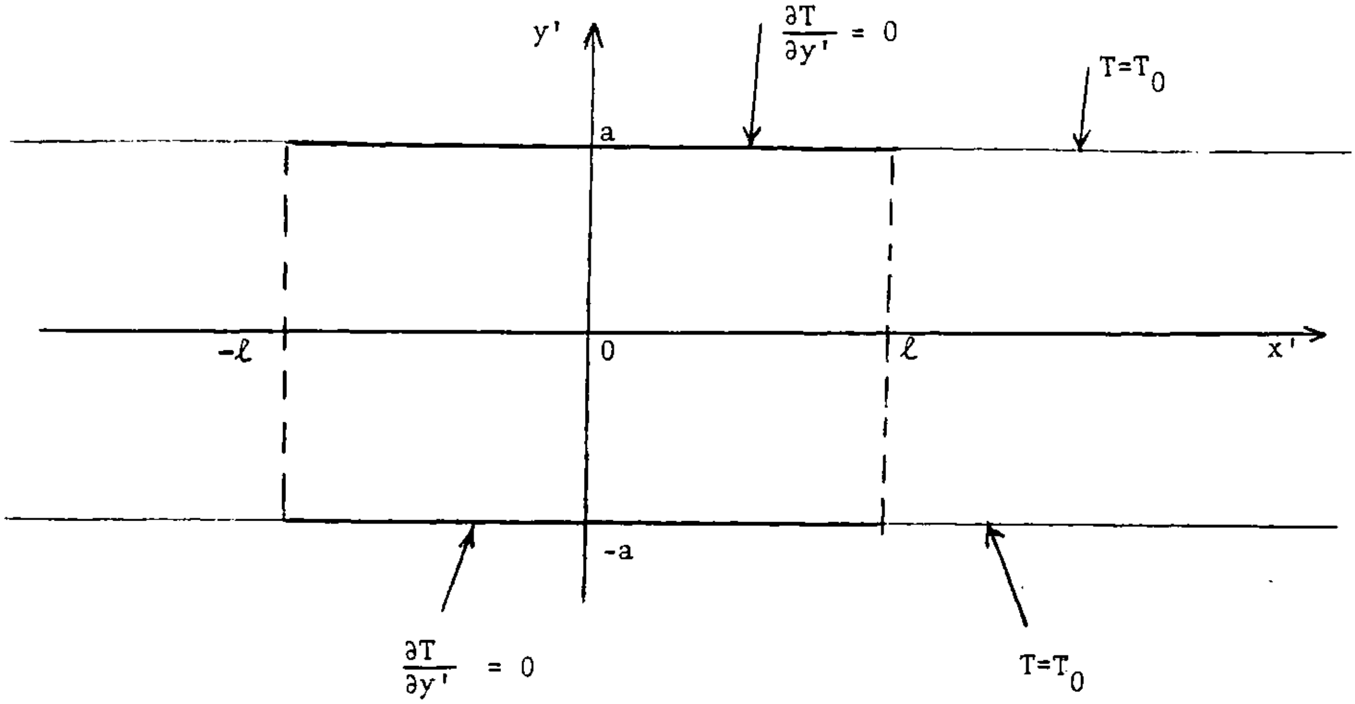


Figure 2.0: Schematic diagram for the reactive slab with the convenient choice of Ox'y' axes.

However, the equation can be made dimensionless by defining new auxilliary variables

$$x = \frac{x'}{a}, \quad y = \frac{y'}{a} \quad \epsilon = \frac{\ell}{a},$$

with $\theta = \frac{E}{RT_0^2}(T-T_0)$,

$$\beta = \frac{RT_0}{E},$$

and $\delta = (\frac{Q}{\lambda}) Z_0 a^2 (\frac{E}{RT_0^2}) \exp(-\frac{E}{RT_0})$. The choices for θ, β and δ are consistent with the definitions in Chapter One. Hence the energy equation together with boundary conditions reduces to

$$\frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial y^2} + \delta \exp[\frac{\theta}{(1+\beta\theta)}] = 0,$$

$$\begin{aligned}
y = 0 \quad &: \quad \frac{\partial\theta}{\partial y} = 0 \qquad \forall x \geqslant 0 \ , \\
y = 1 \quad &: \quad \frac{\partial\theta}{\partial y} = 0 \quad \text{for} \quad 0 \leqslant x < \epsilon \ , \\
&: \quad \theta(x,1) = 0 \qquad \forall x > \epsilon \ , \\
x = 0 \quad &: \quad \frac{\partial\theta}{\partial x} = 0 \quad \text{for} \quad 0 \leq y \leq 1 \ .
\end{aligned} \tag{2.0.0}$$

In general $\beta \ll 1$, hence we shall make the usual Frank-Kamenetskii approximation in the exponential term of the Arrhenius rate law, namely $\beta = 0$. When $\epsilon = 0$ (the case for zero insulation), θ becomes a function of y only and the solution is known (1.2.5). In this case $\theta \equiv \theta_{\epsilon=0}(y)$ such that

$$\theta_{\epsilon=0}(y) = 2 \log(\frac{\cosh \sigma}{\cosh \sigma y}) \quad ,$$

and $$\delta = 2\sigma^2 \text{sech}^2\sigma. \tag{2.0.1}$$

The curve of δ versus σ in Figure 2.1, shows that real solutions exist only for $0 \leqslant \delta \leqslant \delta_c(0)$, where $\delta_c(0) = 0.878$ with $\sigma_c \cong 1.2$.

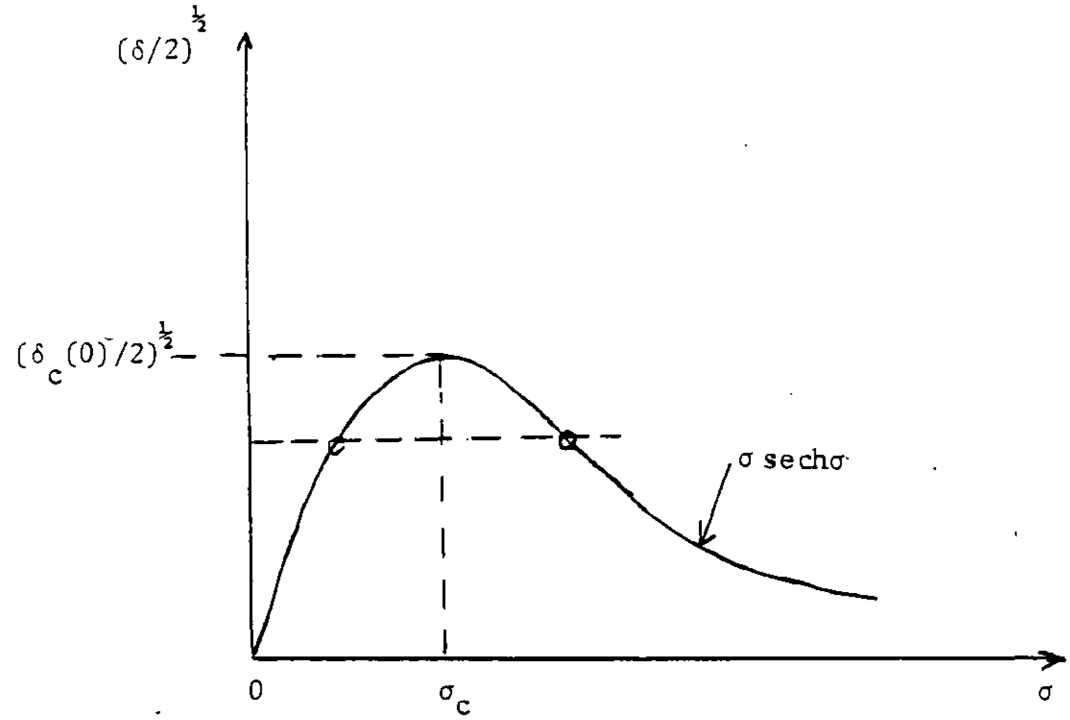


Figure 2.1: Graph of $(\delta/2)^{\frac{1}{2}}$ vs σ for $\sigma \geqslant 0$. The curve is symmetrical about the $(\delta/2)^{\frac{1}{2}}$ axis.

However, when $\epsilon \neq 0$, we seek to determine the critical Frank-Kamenetskii parameter $\delta_c(\epsilon)$ as a function of ϵ. We also note that the boundary condition at $x \to \infty$, is now given by $\theta(\infty, y) = \theta_{\epsilon=0}(y)$ with $\sigma = \sigma(\epsilon)$.

2.1 The Case $\epsilon \ll 1$.

When the surface insulation length is small, $\epsilon \ll 1$, we expect the critical Frank-Kamenetskii parameter $\delta_c(\epsilon)$, to differ slightly from $\delta_c(0)$. Hence we consider the perturbation about

$\sigma = \sigma_c$, namely

$$\sigma = \sigma_c - s \tag{2.1.0}$$

where $s \ll 1$. Substituting σ into the δ equation, we get

$$\delta = 2(\sigma_c - s)^2 \text{ sech}^2(\sigma_s - s).$$

Expanding δ as a Taylor series in powers of s, we get the critical parameter $\delta_c(s)$ as a function of s, thus

$$\delta_c(s) = \delta_c(0) + s\,\delta_c^{(1)}(0) + \frac{s^2}{2}\delta_c^{(2)}(0) + \frac{s^3}{6}\delta_c^{(3)}(0) + \ldots$$

where

$$\delta_c(0) = 2\sigma_c^2 \text{sech}^2\sigma_c \quad (\equiv 0.878)$$

$$\delta_c^{(1)}(0) = 4\sigma_c \text{sech}^2\sigma_c . (1 - \sigma_c \tanh\sigma_c)$$

$$\equiv 0$$

note: $\sigma_c \tanh\sigma_c = 1$ [see equations (1.2.15) and (1.2.16)].

Similarly it can easily be shown that

$$\delta_c^{(2)}(0) = -2\delta_c(0),$$

$$\delta_c^{(3)}(0) = -\frac{4}{\sigma_c}\delta_c(0), \text{ etc.}$$

Therefore

$$\delta_c(s) = \delta_c(0)[1 - s^2 - \frac{2}{3\sigma_c}s^3 + \ldots] \tag{2.1.1}$$

Outer Problem

We consider the critical solution in the slab far from the insulation, that is, as $x \to \infty$, where $\theta(\infty, y) \to \theta_{\epsilon=0}(y)$.

Replacing σ by σ_c-s in (2.0.1) and expanding $\theta(\infty,y)$ as Taylor series in powers of s, we have

$$\theta_c(\infty,y) = 2\log\left[\frac{\cosh(\sigma_c-s)}{\cosh(\sigma_c-s)y}\right]$$

$$= \theta_c^{\,0}(y) + s\theta_1^{\,0}(y) + s^2\theta_2^{\,0}(y) + s^3\theta_3^{\,0}(y) + \ldots$$

where

$$\theta_c^{\,0}(y) = 2\log\left(\frac{\cosh\sigma_c}{\cosh\sigma_c y}\right) \quad ,$$

$$\theta_1^{\,0}(y) = -\,2(\tanh\sigma_c - y\tanh\sigma_c y) \quad ,$$

$$\theta_2^{\,0}(y) = \mathrm{sech}^2\sigma_c - y^2\mathrm{sech}^2\sigma_c y \quad , \qquad (2.1.2)$$

$$\theta_3^{\,0}(y) = \frac{2}{3}\,(\mathrm{sech}^2\sigma_c\tanh\sigma_c - y^3\mathrm{sech}^2\sigma_c y\tanh\sigma_c y) \quad ,$$

etc.

In order to express $\delta_c(s)$ as a function of ϵ, we need to determine the relation between s and ϵ. To determine this relationship, it is imperative that we solve the energy equation in the neighbourhood of the insulation length, that is, when $x = O(\epsilon)$, and $y = O(1)$. Hence, we need to rescale the cartesian coordinates. However, the scaling terms will themselves depend on the relationship between s and ϵ. By assuming, $\epsilon = O(s^\alpha)$, we put

$$\eta = \frac{1-y}{s^\alpha} \quad \text{and} \quad \xi = \frac{x}{s^\alpha} \qquad (2.1.3)$$

where $\alpha > 0$.

We now expand the component functions of $\theta_c(\infty,y)$ [see equation (2.1.2)] about y = 1 to enable us to deal with the inner region where insulation is of importance. It can be shown that the dominant term of each component function is $O(s^{\alpha})$. Hence the dominant term for $\theta_c(\infty,\eta)$ is the $O(s^{\alpha})$ contribution from $\theta_c^{\,0}(\eta)$.

Note:

$$\begin{aligned}\log\cosh\sigma_c y &= \log\cosh[\sigma_c-\sigma_c(1-y)] \\ &= \log\cosh(\sigma_c-\sigma_c s^{\alpha}\eta) \\ &= \log\cosh\sigma_c-\sigma_c\tanh\sigma_c s^{\alpha}\eta+\ldots\end{aligned}$$

Therefore

$$\theta_c^{\,0}(\eta) = 2s^{\alpha}\eta + O(s^{2\alpha})$$

Thus $\theta_c(\infty,\eta)$ becomes

$$\theta_c(\infty,\eta) = 2s^{\alpha}\eta + \text{ smaller terms} \tag{2.1.4}$$

Inner Solution

Through the introduction of the auxiliary variables (2.1.3), the energy equation becomes

$$\frac{\partial^2\theta_c(\xi,\eta)}{\partial\xi^2} + \frac{\partial^2\theta_c(\xi,\eta)}{\partial\eta^2} + \delta_c(0)s^{2\alpha}\left(1-s^2+\frac{2s^3}{3\sigma_c}+\ldots\right)e^{\theta_c(\xi,\eta)} = 0 \tag{2.1.5a}$$

with the boundary conditions;

$$\begin{aligned} \eta = 0 \quad &: \quad \frac{\partial\theta_c}{\partial\eta} = 0 \qquad |\xi| < \frac{\epsilon}{s^{\alpha}}\ , \\ &: \quad \theta_c(\xi) = 0 \qquad |\xi| > \frac{\epsilon}{s^{\alpha}}\ , \\ \xi = 0 \quad &: \quad \frac{\partial\theta_c}{\partial\xi} = 0 \qquad \forall\eta\ , \end{aligned} \tag{2.1.5b}$$

$$\xi \to \infty \qquad : \quad \theta_c(\infty,\eta) = 2s^{\alpha}\eta \quad . \qquad (2.1.5c)$$

We now put

$$\theta_c(\xi,\eta) = s^{\alpha}\theta_{\alpha}(\xi,\eta) + \text{ smaller terms}, \qquad (2.1.6)$$

to represent the temperature solution in the inner region. Expansion (2.1.6) takes into account the dependence of $\theta_c(\xi,\eta)$ on powers of s as $\xi \to \infty$. Since we have assumed $\epsilon = 0(s^{\alpha})$, we now define ξ_1 by

$$\xi_1 = \frac{\epsilon}{s^{\alpha}} \quad ,$$

with ξ_1 assumed to be 0(1). On substituting $\theta_c(\xi,\eta)$ in (2.1.6) into (2.1.5) and then equating coefficients of powers of s^{α}, we have the dominant equation

$$\frac{\partial^2\theta_{\alpha}(\xi,\eta)}{\partial\xi^2} + \frac{\partial^2\theta_{\alpha}(\xi,\eta)}{\partial\eta^2} = 0 \qquad (2.1.7)$$

Writing $\Phi_{\alpha}(\xi,\eta) = \theta_{\alpha}(\xi,\eta) - 2\eta$, equation (2.1.7) reduces to

$$\nabla^2\Phi_{\alpha}(\xi,\eta) = 0,$$

with the boundary conditions

$$\begin{aligned} \eta = 0 \qquad &: \quad \frac{\partial\Phi_{\alpha}}{\partial\eta} = -2 \qquad |\xi| < \xi_1 \, , \\ &: \quad \Phi_{\alpha}(\xi,0) = 0 \qquad |\xi| > \xi_1 \, , \qquad (2.1.8) \\ \xi = 0 \qquad &: \quad \frac{\partial\Phi_{\alpha}}{\partial\xi} = 0 \qquad \forall\eta \, , \\ \xi,\eta \to \infty \quad &: \quad \Phi_{\alpha} \to 0 \quad . \end{aligned}$$

The solution of (2.1.8) is expressible in terms of the Weber-Schafheitlin discontinuous integral [28], namely

$$\Phi_\alpha(\xi,\eta) = 2\xi_1 \int_0^\infty \frac{J_1(\lambda_0\xi_1)}{\lambda_0} \cos\lambda_0\xi \; e^{-\lambda_0\eta} \, d\lambda_0 \qquad (2.1.9)$$

Therefore

$$\theta_c(\xi,\eta) = \theta_c(\infty,\eta) + 2\xi_1 s^\alpha \int_0^\infty \frac{J_1(\lambda_0\xi_1)}{\lambda_0} \cos\lambda_0\xi \; e^{-\lambda_0\eta} \, d\lambda_0$$

$$+ \text{ smaller terms}$$

Writing the inner solution in terms of the outer variables, we have,

$$\theta_c(x,y) = \theta_c(\infty,y) + 2\xi_1 s^\alpha \int_0^\infty \frac{J_1(\lambda_0\xi_1)}{\lambda_0} \cos(\lambda_0 x s^{-\alpha}) . e^{-\lambda_0(1-y)s^{-\alpha}} d\lambda_0$$

$$+ \text{ smaller terms.}$$

We now put

$$\mu = \lambda_0 s^{-\alpha} ,$$

thus $\theta_c(x,y)$ becomes

$$\theta_c(x,y) = \theta_c(\infty,y) + 2\xi_1 s^\alpha \int_0^\infty \frac{J_1(\mu\xi_1 s^\alpha)}{\mu} \cos\mu x \; e^{-\mu(1-y)} d\mu$$

$$+ \text{ smaller terms} \qquad (2.1.10)$$

<u>Intermediate problem</u>

We seek to determine the solution valid away from the insulation but which has the limiting form of (2.1.10). Making the substitution

$$\theta_c(x,y) = \theta_c(\infty,y) + s^{\alpha}\Psi_{\alpha}(x,y) + \text{smaller terms} \qquad (2.1.11)$$

in the energy equation and then equating the coefficients of powers of s, and noting that $\theta_c(\infty,y)$ satisfies the equation

$$\theta_c''(\infty,y) + \delta_c(\epsilon)\, e^{\theta_c(\infty,y)} = 0 .$$

We also obtain

$$\nabla^2\Psi_{\alpha} + \delta_c(\epsilon)e^{\theta_c(\infty,y)}.\Psi_{\alpha}(x,y) = 0,$$

etc.

We note that $\delta_c(\epsilon)\, e^{\theta_c(\infty,y)} = 2\sigma^2\text{sech}^2\sigma y$. Therefore the equation for Ψ_{α} is

$$\nabla^2\Psi_{\alpha} + 2\sigma^2\text{sech}^2\sigma y.\Psi_{\alpha}(x,y) = 0,$$

with the boundary conditions;

$$\begin{aligned} y = 0 \quad &: \quad \frac{\partial\Psi_{\alpha}}{\partial y} = 0 \ , \\ y = 1 \quad &: \quad \Psi_{\alpha}(x,1) = 0 \ , \qquad (2.1.12) \\ x \to \infty \quad &: \quad \Psi_{\alpha} \to 0 \ . \end{aligned}$$

Several attempts to determine the solution of (2.1.12) proved unsuccessful. However, Adler [29] suggests the following procedure for determining Ψ_{α};

Adler's Scheme

If H(x,y) is a harmonic function, a solution of (2.1.12) may be written

$$\tilde{\Psi}_\alpha(x,y) = \frac{\partial H}{\partial y} - \sigma\tanh\sigma y \cdot H(x,y) \qquad (2.1.13)$$

which is easily verified on substitution. Taking

$$H(x,y) = A(\mu)\cos\mu x \sinh\mu y,$$

the required solution of (2.1.12) becomes

$$\Psi_\alpha(x,y) = \int_0^\infty \tilde{\Psi}_\alpha(x,y)d\mu$$

$$= \int_0^\infty A(\mu)(\mu\cosh\mu y - \sigma\tanh\sigma y.\sinh\mu y)\cos\mu x \; d\mu \qquad (2.1.14)$$

Comparing equations (2.1.10) and (2.1.14), at y = 1, we have

$$A(\mu)(\mu\cosh\mu - \sigma\tanh\sigma\sinh\mu) = \frac{2\xi_1}{\mu} J_1(\mu\xi_1 s^\alpha)$$

Therefore

$$A(\mu) = \frac{2\xi_1 J_1(\mu\xi_1 s^\alpha)}{\mu(\mu\cosh\mu - \sigma\tanh\sigma.\sinh\mu)} \qquad (2.1.15)$$

Finally equation (2.1.11) becomes

$$\theta_c(x,y) = \theta_c(\infty,y) + 2\xi_1 s^\alpha \int_0^\infty \frac{J_1(\mu\xi_1 s^\alpha)(\mu\cosh\mu y - \sigma\tanh\sigma y.\sinh\mu y)\cos\mu x \; d\mu}{\mu(\mu\cosh\mu - \sigma\tanh\sigma.\sinh\mu)}$$

$$+ \text{ smaller terms} \qquad (2.1.16)$$

Adler further assumed that because of symmetry the maximum temperature should occur at the centre of the slab, that is at (0,0), and should be equal to $\theta_c^{\,0}(0)$. In fact $\theta_c^{\,0}(0)$ is in some sense a "critical temperature".

Thus at (0,0), we have

$$\log \cosh\sigma_c \cong \log \cosh\sigma + \epsilon \int_0^\infty \frac{J_1(\epsilon\mu)d\mu}{(\mu\cosh\mu - \sigma\tanh\sigma.\sinh\mu)} \qquad (2.1.17)$$

However, this assumption violates the condition $\frac{d\theta_c^{\ 0}(0)}{d\delta} = \infty$ at criticality. Adler justifies this departure as due to insulating the slab surface. By substituting $\sigma = \sigma_c - s$ into (2.1.17), Adler was able to determine the relationship between ϵ and s, namely $s \cong \epsilon^{\frac{1}{2}}$ with $\xi_1 = 1$ and $\alpha = 2$. Hence the critical Frank-Kamenetskii parameter, $\delta_c(\epsilon)$ becomes

$$\delta_c(\epsilon) = \delta_c(0)\ (1-\epsilon - (2/3\sigma_c).\epsilon^{3/2} + \ldots)$$

$$= 0.878(1-\epsilon - 0.56\epsilon^{3/2} + \ldots) \qquad (2.1.18)$$

Adler also showed that

$$\Phi_\alpha(\xi,\eta) = 2\xi_1 \mathrm{Re}[(1-z^2)^{\frac{1}{2}} + iz]$$

where $z = \frac{1}{\xi_1}(\xi + i\eta)$.

Hence the critical temperature distribution near the surface of the slab is

$$\theta_c(\xi,\eta) = \theta_c(\infty,\eta) + 2s^2\mathrm{Re}[(1-z^2)^{\frac{1}{2}} + iz]$$

$$- 3s^2\sigma_c\mathrm{Re}[(1-z^2)^{\frac{1}{2}} + iz] + \text{smaller terms} \qquad (2.1.19)$$

Equation (2.1.19) forms a basis for numerical computation.

2.2 The Case $\epsilon \gg 1$

We expect for $\epsilon \gg 1$, that the temperature distribution within the slab $\theta_c(x,y) \to 0$ and $\delta_c(\epsilon) \to 0$, where $\theta_c(x,y)$ is the limiting case corresponding to $\delta_c(\epsilon)$. The energy equation for $\theta(x,y)$ is

$$\frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial y^2} + \delta\, e^{\theta} = 0, \qquad 0 \leqslant x \leqslant \infty, \qquad 0 \leqslant y \leqslant 1$$

with the boundary conditions;

$$\begin{aligned}
y = 1 \quad &: \quad \frac{\partial\theta}{\partial y} = 0, \qquad |x| < \epsilon\ , \\
&: \quad \theta(x,1) = 0, \quad |x| > \epsilon\ , \\
y = 0 \quad &: \quad \frac{\partial\theta}{\partial y} = 0, \qquad \forall x, \\
x \to \infty \quad &: \quad \theta \to \theta(\infty,y) = \theta_{\epsilon=0}(y), \qquad \forall y, \\
x = 0 \quad &: \quad \frac{\partial\theta}{\partial x} = 0, \qquad \forall y\ .
\end{aligned} \tag{2.2.0}$$

As $\epsilon \to \infty$, we expect the temperature distribution within the reacting slab to be almost uniform except in the regions near the edges of the insulation where the slab loses its heat to the surroundings. Thus we expect the temperature within the slab to vary sufficiently slowly in the y-direction for the process to be dominated by the heat conduction in the x-direction. However, difficulties arise when we try to solve the one-dimensional equation in x, since the boundary condition at $x = \epsilon$ ($\epsilon \Rightarrow \infty$) is unknown. This difficulty can be overcome by solving the equation when the surface is completely insulated, $\epsilon = \infty$, with a zero heat reservoir at

$x = \epsilon$. This assumption is consistent with our expectation of $\theta_c(x,y) \to 0$ and $\delta_c(\epsilon) \to 0$ as $\epsilon \to \infty$. Physically, this assumption will yield an upper bound on $\delta_c(\epsilon)$, since the temperature at $x = \epsilon$ $(\epsilon \to \infty)$ will be small but non-zero for the idealised model. Therefore, the energy equation, neglecting the y-dependence of the temperature, becomes

$$\theta''(x) + \delta\, e^{\theta} = 0 \ , \qquad 0 \leqslant x \leqslant \epsilon \quad (\epsilon = \infty) \ ,$$

with boundary conditions;

$$\begin{aligned} x &= 0 \qquad \theta'(0) = 0 \\ x &= \epsilon \qquad \theta(\epsilon) = 0 \end{aligned} \tag{2.2.1}$$

We rescale equation (2.2.1) by setting

$$\xi = \frac{x}{\epsilon} \ , \qquad \delta = \frac{\tilde{\delta}}{\epsilon^2} \ ,$$

to get

$$\theta''(\xi) + \tilde{\delta}\, e^{\theta} = 0 \ , \qquad 0 \leqslant \xi \leqslant 1, \tag{2.2.2}$$

with the boundary conditions;

$$\begin{aligned} \xi &= 0 \quad : \quad \theta'(0) = 0 \\ \xi &= 1 \quad : \quad \theta(1) = 0 \end{aligned} \tag{2.2.3}$$

Therefore the solution of (2.2.2) is

$$\theta_0(\xi) = 2\log\left(\frac{\cosh p}{\cosh p\xi}\right) \ ,$$

and
$$\begin{aligned} \tilde{\delta} &= 2p^2 \operatorname{sech}^2 p \\ &= \epsilon^2 \delta \end{aligned} \tag{2.2.4}$$

The limiting $\delta_c(\epsilon)$ is determined by maximizing p in (2.2.4), namely $p = \sigma_c$ and hence

$$\delta_c(\epsilon) \cong \delta_c(0)/\epsilon^2 \tag{2.2.5}$$

and $$\theta_c(x) = 2\log\{\cosh\sigma_c/\cosh(\sigma_c x/\epsilon)\} \tag{2.2.6}$$

Equations (2.2.5) and (2.2.6) represent the upper bounds on $\delta_c(\epsilon)$ and $\theta_c(x)$ respectively. However, for the case $\epsilon \gg 1$ $(\epsilon \neq \infty)$, the true boundary condition as $x \to \infty$ is given by $\theta_c(x,y) \to \theta_{c,\epsilon=0}(y)$, where

$$\theta_{\epsilon=0}(y) = 2\log\left(\frac{\cosh\sigma}{\cosh\sigma y}\right),$$

and $$\delta = 2\sigma^2 \operatorname{sech}^2\sigma \; . \tag{2.2.7}$$

The boundary condition (2.2.7) is consistent with our assumption of zero heat reservoir for the case $\epsilon \to \infty$, since $\sigma \to 0$ as $\epsilon \to \infty$. The effect of this boundary condition is that it introduces the y-dependence on the lower order terms of the temperature distribution within the slab for $\epsilon \gg 1$ $(\epsilon \neq \infty)$. Physically (2.2.7) modifies solution (2.2.6) to take into account the temperature changes that occur at the edges of the insulation. Expanding δ in (2.2.7) in powers of σ, we get

$$\begin{aligned}\delta &= 2\sigma^2\left(1 + \frac{\sigma^2}{2} + \frac{\sigma^4}{24} + \frac{\sigma^6}{720} + \ldots\right)^{-2} \\ &= 2\sigma^2\left(1-\sigma^2 + \frac{2}{3}\sigma^4 + \ldots\right)\end{aligned} \tag{2.2.8}$$

Comparison of equations (2.2.5) and (2.2.8), gives

$$2\sigma^2\left(1-\sigma^2 + \frac{2}{3}\sigma^4 + \ldots\right) = \frac{\delta_c(0)}{\epsilon^2} \quad ,$$

hence, since $\sigma \ll 1$,

$$\sigma \cong \frac{1}{\epsilon}\,(\delta_c(0)/2)^{\frac{1}{2}}$$

or (2.2.9)

$$\sigma\epsilon \cong (\delta_c(0)/2)^{\frac{1}{2}}$$

$$= O(1)$$

Equation (2.2.9) represents the relationship that exists between σ and ϵ when we ignore the temperature changes that occur at the edges of the insulation. Of importance to us is that (2.2.9) gives the rescaling required for the inner problem for the case $\epsilon \gg 1$ ($\epsilon \neq \infty$) and $x < \epsilon$. Thus for the inner region we rescale the variables by putting

$$\xi = \left(\frac{2}{\kappa}\right)^{\frac{1}{2}} \sigma x \quad \text{and} \quad \eta = \left(\frac{2}{\kappa}\right)^{\frac{1}{2}} \sigma y \qquad (2.2.10)$$

where $\kappa = O(1)$. However, the critical solution in the outer region, where $x \gg \epsilon$, is given by equation (2.2.7), namely

$$\theta_c(\infty,y) = \theta_{\epsilon=0}(y)$$

$$= 2\log\left(\frac{\cosh\sigma}{\cosh\sigma y}\right) \quad .$$

Writing the outer solution in terms of the rescaled inner variables we obtain

$$\theta_c(\infty,\eta) = 2\log\left(\frac{\cosh\sigma}{\cosh\left(\frac{\kappa}{2}\right)^{\frac{1}{2}}\eta}\right) \quad . \qquad (2.2.11)$$

Consider the Inner Region $(x \ll \epsilon)$

From the analysis in above sections, we expect the dominant term of the temperature solutions to be a function of ξ only. Using the auxiliary variables of (2.2.10), the energy equation becomes

$$\frac{\partial^2\theta_c}{\partial\xi^2} + \frac{\partial^2\theta_c}{\partial\eta^2} + \kappa(1-\sigma^2 + \frac{2}{3}\sigma^4 + \ldots)e^{\theta_c} = 0 \qquad (2.2.12)$$

we now put

$$\theta_c(\xi,\eta) = \theta_0(\xi) + \sigma^\alpha\theta_1(\xi,\eta) + \text{smaller terms}$$

where $\alpha > 0$.

Hence equation (2.2.12) becomes

$$\theta_o''(\xi) + \nabla^2(\sigma^\alpha\theta_1+\ldots) + \kappa e^{\theta_0}(1+\sigma^\alpha\theta_1+\ldots) = 0 \quad .$$

On equating the coefficients of the powers of σ, we get

$$\theta_0''(\xi) + \kappa e^{\theta_0} = 0 \qquad (2.2.13)$$

$$\nabla^2\theta_1 + \kappa e^{\theta_0}.\theta_1(\xi,\eta) = \begin{cases} 0 & \alpha \neq 2 \\ \kappa e^{\theta_0} & \alpha = 2 \end{cases} \qquad (2.2.14)$$

etc. We note that (2.2.13) satisfies the boundary condition,

$$\xi = 0 \qquad \theta'(0) = 0 \quad .$$

Frank-Kamenetskii (Ref. [2](i) page 379) gives the solution of equation (2.2.13) satisfying the boundary conditions as

$$e^{\theta_0} = \frac{A}{\cosh^2\{(\frac{A\kappa}{2})^{\frac{1}{2}}\xi\}} \quad .$$

The relationship that exists between the constants A and κ can be determined if we know the temperature within the slab at the point $x = \epsilon$. We hope this temperature can be evaluated by matching the inner solution with the solution of the outer region. However, we put

$$p = \left(\frac{A\kappa}{2}\right)^{\frac{1}{2}} \quad ,$$

hence θ_0 becomes

$$e^{\theta_0(\xi)} = \frac{(2p^2/\kappa)}{\cosh^2 p\xi} \quad . \tag{2.2.15}$$

Thus the equation for $\theta_1(\xi,\eta)$ becomes

$$\nabla^2\theta_1 + 2p^2\operatorname{sech}^2 p\xi . \theta_1 = \begin{cases} 0 & , \quad \alpha \neq 2 \\ 2p^2\operatorname{sech}^2 p\xi & , \quad \alpha = 2 \end{cases} \tag{2.2.16}$$

with the boundary conditions;

$$\begin{aligned} \xi = 0 \quad &: \quad \frac{\partial\theta_1}{\partial\xi} = 0 \quad , \qquad \forall\eta \ , \\ \eta = 0 \quad &: \quad \frac{\partial\theta_1}{\partial\eta} = 0 \quad , \qquad \forall\xi \ , \\ \eta = \left(\frac{2}{\kappa}\right)^{\frac{1}{2}}\sigma \ &: \quad \frac{\partial\theta_1}{\partial\eta} = 0 \quad , \qquad \xi < \left(\frac{2}{\kappa}\right)^{\frac{1}{2}}\sigma\epsilon \end{aligned} \tag{2.2.17}$$

If $H(\xi,\eta)$ is a harmonic function, it can easily be verified that $\hat{\theta}_1(\xi,\eta)$ is a solution of (2.2.16), where

$$\left.\begin{array}{ll}\hat{\theta}_1(\xi,\eta) & \alpha \neq 2 \\ [\hat{\theta}_1(\xi,\eta)-1] & \alpha = 2\end{array}\right\} = \frac{\partial H}{\partial \xi} - p\tanh p\xi . H(\xi,\eta) \tag{2.2.18}$$

Attempts to determine $H(\xi,\eta)$ present difficulties since the appropriate conditions are difficult to deduce from (2.2.17).

2.3 Conclusions

Attempts to determine the intermediate region to match the solution in the region $x < \epsilon$ with (2.2.11) were unsuccessful. However, it is hoped that the solution of (2.2.16) might suggest the nature of scaling required in the intermediate region, since we expect the solution as $x \to \infty$ to interact with θ_1 to give a smooth temperature solution in the intermediate region.

CHAPTER THREE: SLAB WITH VARIABLE SURFACE TEMPERATURE

3.0 INTRODUCTION

We consider a symmetrically heated exothermically reacting slab occupying the region $-1 \leqslant y \leqslant 1$, $-\infty < x < \infty$ with respect to some suitable dimensionless frame of reference Oxyz as in Chapter Two. The same assumptions as in Chapter Two, including Frank-Kamenetskii's approximation ($\beta \equiv 0$) to the Arrhenius rate law, are still considered to be valid for this problem.

The energy conservation equation is then considered for the situation in which there is a variable surface temperature distribution. The surface temperature at $x \to \infty$ is considered to be slightly higher than that at $x \to -\infty$. Thus the energy equation is

$$\frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial y^2} + \delta e^{\theta} = 0, \qquad -1 \leqslant y \leqslant 1, \quad -\infty < x < \infty \tag{3.0.0}$$

where θ and δ correspond to the dimensionless excess temperature and the Frank-Kamenetskii parameter respectively. The temperature $\theta(x,y)$, is symmetrical about $y = 0$ and satisfies the boundary conditions;

$$\begin{aligned} y = 0 \quad &: \quad \frac{\partial\theta}{\partial y} = 0 \\ y = 1 \quad &: \quad \theta(x,1) = \epsilon f(x), \qquad 0 < \epsilon \ll 1 \end{aligned} \tag{3.0.1}$$

where $f(x)$ is a smooth monotonic function with the following characteristics at $x \to \pm\infty$:

$$f(x) \to 0 \quad \text{as} \quad x \to -\infty$$
$$f(x) \to 1 \quad \text{as} \quad x \to +\infty \qquad (3.0.2)$$

A typical example of $f(x)$ is:

(i) $$f(x) = \frac{1}{2}(1+\tanh x).$$

We seek to determine the critical Frank-Kamenetskii parameter, $\delta_c(\epsilon)$ as a function of ϵ and the corresponding critical temperature $\theta_c(x,y)$. We now consider the regions $x \to \pm\infty$, where θ is expected to be a function of y only.

Solution as $x \to -\infty$

The temperature within the slab at $x \to -\infty$, satisfies the equation

$$\theta'' + \delta e^{\theta} = 0, \qquad 0 \leqslant y \leqslant 1$$

with the boundary conditions;

$$y = 0 \quad : \quad \frac{\partial\theta}{\partial y} = 0 \quad , \qquad (3.0.3)$$

$$y = 1 \quad : \quad \theta(-\infty,1) = 0.$$

The solution of (3.0.3) is given by

$$\theta(-\infty,y) = 2\log\left(\frac{\cosh\sigma}{\cosh\sigma y}\right),$$

and $$\delta = 2\sigma^2\operatorname{sech}^2\sigma . \qquad (3.0.4)$$

Solution as $x \to +\infty$

The energy equation in this region becomes

$$\theta'' + \delta e^{\theta} = 0, \qquad 0 \leqslant y \leqslant 1 \ ;$$

with the boundary conditions:

$$y = 0 \quad : \quad \frac{d\theta}{dy} = 0 \tag{3.0.5}$$

$$y = 1 \quad : \quad \theta(\infty,1) = \epsilon$$

We now put

$$\theta = \epsilon + \phi(y) \text{ and } \Lambda = \delta e^{\epsilon} \ .$$

On substituting θ and δ into equation (3.0.5), we get an equation in $\phi(y)$, namely

$$\phi'' + \Lambda e^{\phi} = 0, \qquad 0 \leqslant y \leqslant 1 \ ,$$

with boundary conditions:

$$y = 0 \quad : \quad \frac{d\phi}{dy} = 0 \tag{3.0.6}$$

$$y = 1 \quad : \quad \phi(1) = 0 \ .$$

Finally the solution of (3.0.5) is

$$\theta(\infty,y) = \epsilon + 2\log\left(\frac{\cosh \rho}{\cosh \rho y}\right) \ , \tag{3.0.7}$$

and $\qquad \delta = 2\rho^2 e^{-\epsilon} \operatorname{sech}^2 \rho$

3.1 Perturbation Analysis about the Criticality

On comparing the solutions (3.0.4) and (3.0.7), it is apparent that the criticality conditions for thermal ignition will first occur in the region $x \to \infty$. The asymptotic solution can then be determined by replacing ρ in (3.0.7) by σ_c, where σ_c is the critical parameter for the slab solution. Thus we get

$$\theta_c(\infty,y) = \epsilon + 2\log\left(\frac{\cosh \sigma_c}{\cosh \sigma_c y}\right) , \qquad (3.1.0)$$

and $\delta_c(\epsilon) = \delta_c(0)e^{-\epsilon}$,

where $\delta_c(0) = 2\sigma_c^{\,2}\text{sech}^2\sigma_c$

$\cong 0.878$

with $\sigma_c \cong 1.2$.

In order for us to evaluate the asymptotic solution as $x \to -\infty$, we put $\sigma = \sigma_c - s$, where $0 < s \ll 1$.

<u>Consider $x \to -\infty$</u>

On substituting $\sigma = \sigma_c - s$ into equation (3.0.4), we get

$$\delta_c(s) = 2(\sigma_c - s)^2\text{sech}^2(\sigma_c - s) \quad .$$

Expanding $\delta_c(s)$ as a Taylor series in powers of s, we obtain

$$\delta_c(s) = \delta_c(0)[1 - s^2 - \frac{2s^3}{3\sigma_c} + \ldots] \qquad (3.1.1a)$$

[Note: see equations (2.1.0) and (2.1.1)]

Comparison of (3.1.0) and (3.1.1a) shows that $s \cong \epsilon^{\frac{1}{2}}$; thus σ and $\delta_c(s)$ become

$$\sigma = \sigma_c - \epsilon^{\frac{1}{2}}$$

$$\text{and} \qquad \delta_c(\epsilon) = \delta_c(0)[1-\epsilon - \frac{2}{3\sigma_c}\epsilon^{3/2} + \ldots] \quad . \qquad (3.1.1b)$$

This expansion for $\delta_c(\epsilon)$ is valid to $0(\epsilon)$. We now seek to determine the solution of (3.0.3) δ replaced by $\delta_c(0)\, e^{-\epsilon}$. Thus the energy equation becomes

$$\theta'' + \delta_c(0)e^{-\epsilon}\exp\theta = 0, \qquad 0 \leqslant y \leqslant 1;$$

with the boundary conditions

$$y = 0 \quad : \quad \frac{d\theta}{dy} = 0 \quad , \qquad (3.1.2)$$

$$y = 1 \quad : \quad \theta(-\infty, 1) = 0.$$

Writing the solution of (3.1.2) in powers of ϵ, we put

$$\theta \equiv \theta_c(-\infty, y) = \theta_c{}^0(y) + \epsilon^{\frac{1}{2}}\theta_1{}^0(y) + \epsilon\theta_2{}^0(y) + \ldots \qquad (3.1.3)$$

Therefore

$$\delta_c(\epsilon)\ \exp\theta = \delta_c(0)e^{\theta_c{}^0}(1-\epsilon+\ldots)[1+\epsilon^{\frac{1}{2}}\theta_1{}^0 + \epsilon\{\theta_2{}^0 + \tfrac{1}{2}(\theta_1^0)^2 - 1\} + \ldots]$$

Equation (3.1.2) now becomes

$$\frac{d^2}{dy^2}[\theta_c{}^0 + \epsilon^{\frac{1}{2}}\theta_1{}^0 + \epsilon\theta_2{}^0 + \ldots] + \delta_c(0)e^{\theta_c{}^0}[1+\epsilon^{\frac{1}{2}}\theta_1{}^0 + \epsilon\{\theta_2{}^0 + \tfrac{1}{2}(\theta_1{}^0)^2 - 1\} + \ldots]$$

$$= 0$$

On equating the coefficients of powers of ϵ, we obtain

$$\frac{d^2\theta_c^{\,0}}{dy^2} + \delta_c(0)e^{\theta_c^{\,0}} = 0 \quad ,$$

$$\frac{d^2\theta_1^{\,0}}{dy^2} + \delta_c(0)e^{\theta_c^{\,0}} \,.\, \theta_1^{\,0} = 0 \quad , \tag{3.1.4}$$

$$\frac{d^2\theta_2^{\,0}}{dy^2} + \delta_c(0)e^{\theta_c^{\,0}}\{\theta_2^{\,0} + \frac{1}{2}(\theta_1^{\,0})^2\} = 0,$$

etc.

Equations (3.1.4) give the expansion $\theta_c(-\infty,y)$ to $O(\epsilon)$. However, the functions $\theta_1^{\,0}(y)$, $\theta_2^{\,0}(y)$ etc., can be obtained directly from (3.0.4) by expanding $\theta(-\infty,y)$ about the point $\sigma = \sigma_c - \epsilon^{\frac{1}{2}}$, in powers of ϵ. Note this expansion will only lead to identical results with solutions of (3.1.4) up to $O(\epsilon)$. Hence

$$\theta_c(-\infty,y) = 2\log\{\cosh(\sigma_c-\epsilon^{\frac{1}{2}})/\cosh(\sigma_c-\epsilon^{\frac{1}{2}})y\} \tag{3.1.5}$$

Taylor series expansion of (3.1.5) in powers of $\epsilon^{\frac{1}{2}}$ gives

$$\theta_c(-\infty,y) = \theta_c^{\,0}(y) + \epsilon^{\frac{1}{2}}\theta_1^{\,0}(y) + \epsilon\theta_2^{\,0}(y) + \ldots$$

where

$$\theta_c^{\,0}(y) = 2\log\left(\frac{\cosh\sigma_c}{\cosh\sigma_c y}\right) \quad ,$$

$$\theta_1^{\,0}(y) = -2(\tanh\sigma_c - y\tanh\sigma_c y) \quad , \tag{3.1.6}$$

$$\theta_2^{\,0}(y) = \operatorname{sech}^2\sigma_c - y^2\operatorname{sech}^2\sigma_c y \quad , \quad \text{etc.}$$

Intermediate Region

We seek to determine a solution of the temperature distribution within the slab as a function of x and y, which has the asymptotic form of (3.0.7) and (3.1.6). Noting the dependence of the asymptotic solutions on the powers of $\epsilon^{\frac{1}{2}}$, we consider the following expansion for the intermediate region, namely

$$\theta(x,y) \equiv \theta_c(x,y) = \theta_c^{\,0}(y) + \epsilon^{\frac{1}{2}}\theta_1(x,y) + \epsilon\theta_2(x,y) + \ldots$$

and $$\delta_c(\epsilon) = \delta_c(0)[1-\epsilon+ \ldots] \qquad (3.1.7)$$

Therefore

$$\delta\exp\theta = \delta_c(0)e^{\theta_c^{\,0}}(1-\epsilon + \ldots)[1+\epsilon^{\frac{1}{2}}\theta_1 + \epsilon(\theta_2 + \tfrac{1}{2}\theta_1^{\,2}-1)+\ldots]$$

but

$$\delta_c(0)e^{\theta_c^{\,0}} = 2\sigma_c^{\,2}\operatorname{sech}^2\sigma_c y$$

Hence the energy equation becomes

$$\nabla^2(\theta_c^{\,0}+\epsilon^{\frac{1}{2}}\theta_1+\epsilon\theta_2+\ldots) + 2\sigma_c^{\,2}\operatorname{sech}^2\sigma_c y[1+\epsilon^{\frac{1}{2}}\theta_1+\epsilon(\theta_2+\tfrac{1}{2}\theta_1^{\,2}-1)+\ldots] = 0$$

Equating the coefficients of the powers of ϵ, we get

$$\frac{d^2\theta_c^{\,0}}{dy^2} + \delta_c(0)e^{\theta_c^{\,0}} = 0,$$

$$\nabla^2\theta_1 + 2\sigma_c^{\,2}\operatorname{sech}^2\sigma_c y.\theta_1 = 0\ , \qquad (3.1.8)$$

$$\nabla^2\theta_2 + 2\sigma_c^{\,2}\operatorname{sech}^2\sigma_c y.(\theta_2+\tfrac{1}{2}\theta_1^{\,2}-1) = 0,$$

etc.

where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$$

with boundary conditions

$$\begin{aligned} y = 0 \quad &: \quad \frac{\partial \theta_1}{\partial y} = \frac{\partial \theta_2}{\partial y} = 0 \ , \\ y = 1 \quad &: \quad \theta_1(x,1) = 0, \quad \theta_2(x,1) = f(x) \end{aligned} \tag{3.1.9}$$

and asymptotic conditions

$$\begin{aligned} x \to \infty \quad &: \quad \theta_1 \to 0 \ , \qquad \theta_2 \to 1 \ , \\ x \to -\infty \quad &: \quad \theta_1 \to \theta_1^{\,0}(y) \ , \quad \theta_2^{\,0} \to \theta_2^{\,0}(y), \text{ etc.} \end{aligned} \tag{3.1.10}$$

Solution of the θ_1-equation

We use the following result:

If ψ_1 is a harmonic function, a solution of the equation

$$\nabla^2\theta_1 + 2\sigma_c^{\,2}\operatorname{sech}^2\sigma_c y.\theta_1 = 0 \ ,$$

is

$$\theta_1(x,y) = \frac{\partial \psi_1}{\partial y} - \sigma_c \tanh\sigma_c y.\psi_1 \tag{3.1.11}$$

which can be easily verified on substitution. Below we now consider the equation

$$\nabla^2\psi_1(x,y) = 0 \ , \tag{3.1.12}$$

with ψ_1 appropriately chosen at $x = \pm\infty$ and at $y = 0,1$.

3.2 Determination of the Appropriate Boundary Conditions to Equation (3.1.12)

$$\theta_1(x,y) = \frac{\partial\psi_1}{\partial y} - \sigma_c \tanh\sigma_c y.\psi_1(x,y) \quad . \qquad (3.2.0)$$

The boundary conditions satisfied by $\psi_1(x,y)$ can be obtained from equations (3.1.9) and (3.1.10).

$\underline{x \to -\infty}$

$$\theta_1{}^0 = -2(\tanh\sigma_c - y \tanh\sigma_c y)$$

$$= -\frac{2}{\sigma_c}(1-\sigma_c y\tanh\sigma_c y)$$

note: $\sigma_c \tanh\sigma_c = 1$.

Therefore $\theta_1{}^0(y) = \frac{\partial}{\partial y}\left(-\frac{2y}{\sigma_c}\right) - \sigma_c \tanh\sigma_c y.\left(-\frac{2y}{\sigma_c}\right)$

but $\theta_1{}^0(y) = \frac{\partial}{\partial y}\psi_1(-\infty,y) - \sigma_c \tanh\sigma_c y.\psi_1(-\infty,y)$.

Hence as $x \to -\infty, \psi_1 \to -\frac{2y}{\sigma_c}$.

$\underline{x \to +\infty}$

$$\frac{\partial}{\partial y}\psi_1(\infty,y) - \sigma_c \tanh\sigma_c y.\psi_1(\infty,y) = 0$$

integrating with respect to y, equation becomes

$$\int \frac{d\psi_1(\infty,y)}{\psi_1(\infty,y)} = \sigma_c \int \tanh\sigma_c y \; dy$$

Thus $\psi_1(\infty,y) = A \cosh\sigma_c y$

but $\nabla^2\psi_1 = 0$, hence $A = 0$ (ψ_1 is harmonic everywhere). Thus as $x \to \infty$ $\psi_1 \to 0$.

Also

$$\frac{\partial \theta_1}{\partial y} = \frac{\partial^2 \psi_1}{\partial y^2} - \sigma_c \tanh\sigma_c y \,.\, \frac{\partial \psi_1}{\partial y} - \sigma_c{}^2 \operatorname{sech}^2\sigma_c y . \psi_1$$

$$= - \frac{\partial^2 \psi_1}{\partial x^2} - \sigma_c \tanh\sigma_c y .\, \frac{\partial \psi_1}{\partial y} - \sigma_c{}^2 \operatorname{sech}^2\sigma_c y . \psi_1$$

but at $y = 0$ $\frac{\partial \theta_1}{\partial y} = 0.$

Therefore

$$\frac{\partial^2}{\partial x^2} \psi_1(x,0) + \sigma_c{}^2 \psi_1(x,0) = 0$$

which gives

$$\psi_1(x,0) = A_2 \sin\sigma_c x + B_2 \cos\sigma_c x \quad .$$

However, the asymptotic conditions at $x \to \pm\infty$ show that $A_2 = B_2 = 0$. Hence $\psi_1(x,0) = 0$. The problem for ψ_1 becomes

$$\nabla^2\psi_1(x,y) = 0, \quad 0 \leq y \leq 1, \qquad -\infty < x < \infty \; ;$$

with boundary conditions;

$$\begin{aligned} y = 0 \quad &: \quad \psi_1(x,0) = 0 \\ y = 1 \quad &: \quad \frac{\partial \psi_1}{\partial y} - \psi_1(x,1) = 0 \\ x \to +\infty \quad &: \quad \psi_1 \to 0 \\ x \to -\infty \quad &: \quad \psi_1 \to -\frac{2y}{\sigma_c} \, , \end{aligned} \tag{3.2.1}$$

with $\psi_1(x,y)$ as a smooth function of x (so as to exclude $\psi_1 = -\frac{2y}{\sigma_c}$ for $x < 0$, and $\psi_1 = 0$ for $x > 0$, which is a possibility but non-physical solution). We now put

$$\psi_1(x, y) = -\frac{y}{\sigma_c} + \phi_1(x,y)$$

Therefore

$$\phi_1 \to -\frac{y}{\sigma_c} \text{ as } x \to -\infty$$

$$\phi_1 \to \frac{y}{\sigma_c} \text{ as } x \to +\infty \qquad \text{and } \nabla^2\phi_1 = 0.$$

Hence

$$\phi_1(-x,y) = -\phi_1(x,y)$$

On setting $x = 0$, we get

$$\phi_1(0,y) = 0$$

The problem then reduces to

$$\nabla^2\psi_1(x,y) = 0, \qquad 0 \leqslant y \leqslant 1, \qquad 0 \leqslant x < \infty ;$$

with boundary conditions

$$\begin{aligned} x = 0 \quad &: \quad \psi_1(0,y) = -\frac{y}{\sigma_c} \\ x \to \infty \quad &: \quad \psi_1 \to 0 \\ y = 0 \quad &: \quad \psi_1(x.0) = 0 \\ y = 1 \quad &: \quad \frac{\partial\psi_1}{\partial y} - \psi_1(x,1) = 0 \end{aligned} \qquad (3.2.2)$$

Attempts to solve equation (3.2.2) leads to failure. Consequently we conclude that there is no solution for the intermediate region for the case when the region $x \to \infty$ is critical. The result is astonishing since the solutions at $x \to \pm \infty$ are well defined. We seek to overcome this paradox by determining:-

(i) the temperature excess θ when the whole slab is in a stable non-critical state.

(ii) By invoking the method of "adiabatic invariants", which has been used to resolve corresponding difficulties in electrical and mechanical systems [30].

3.3 Perturbation Analysis for the Non-Critical State

We consider the problem

$$\frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial y^2} + \delta e^{\theta} = 0, \quad 0 \leqslant y \leqslant 1, \quad -\infty < x < \infty$$

with boundary conditions

$$y = 0 \quad : \quad \frac{\partial\theta}{\partial y} = 0$$

$$y = 1 \quad : \quad \theta(x,1) = \epsilon f(x)$$

where f(x) has the same properties as in section 3.0. A particular case is:

(i) $f(x) = \frac{1}{2}(1+\tanh x)$

Asymptotic Solutions

$$\text{As } x \to \infty: \quad \theta \equiv \theta_{\infty}(y) = \epsilon + 2\log\left(\frac{\cosh\rho}{\cosh\rho y}\right)$$
$$\text{and} \quad \delta = 2\rho^2 e^{-\epsilon}\operatorname{sech}^2\rho \;. \tag{3.3.1}$$

$$\text{As } x \to -\infty: \quad \theta \equiv \theta_{-\infty}(y) = 2\log\left(\frac{\cosh\sigma}{\cosh\sigma y}\right)$$
$$\text{and} \quad \delta = 2\sigma^2\operatorname{sech}^2\sigma. \tag{3.3.2}$$

We seek to find an expression for σ as a function of ϵ and ρ. Comparing the δ's in equations (3.3.1) and (3.3.2), we get

$$2\sigma^2\operatorname{sech}^2\sigma = 2\rho^2 e^{-\epsilon}\operatorname{sech}^2\rho$$

Therefore

$$\sigma\operatorname{sech}\sigma = \rho e^{-(\epsilon/2)}\operatorname{sech}\rho \;. \tag{3.3.3}$$

We now consider expressing σ as function of ρ in powers of ϵ by putting

$$\sigma = \rho + \sigma_1\epsilon^{\tau} + \sigma_2\epsilon^{2\tau} + \sigma_3\epsilon^{3\tau} + \dots \;.$$

Expanding $\sigma\operatorname{sech}\sigma$ as a Taylor series in powers of ϵ^{τ}, we get

$$\sigma\ \mathrm{sech}\sigma = \rho\ \mathrm{sech}\rho + (\sigma_1\epsilon^{\tau}+\sigma_2\epsilon^{2\tau}+\ldots)\ (1-\rho\tanh\rho)\mathrm{sech}\rho$$

$$+\frac{1}{2}\ (\sigma_1\epsilon^{\tau}+\sigma_2\epsilon^{2\tau}+\ldots)^2(\rho\tanh\rho-2\tanh\rho-\rho\,\mathrm{sech}^2\rho)\mathrm{sech}\rho$$

$$+\ \ldots \tag{3.3.4}$$

From equation (3.3.3)

$$\sigma\ \mathrm{sech}\sigma = \rho\mathrm{sech}\rho\left[1-\left(\frac{\epsilon}{2}\right)+\frac{1}{2}\left(\frac{\epsilon}{2}\right)^2-\frac{1}{6}\left(\frac{\epsilon}{2}\right)^3+\ldots\right] \tag{3.3.5}$$

Comparison of equations (3.3.4) and (3.3.5) gives

$$\sigma = \rho-[\rho/2(1-\rho\tanh\rho)]\epsilon+[\rho(1+\rho^2\mathrm{sech}^2\rho)/8(1-\rho\tanh\rho)^3]\epsilon^2$$

$$+\ O(\epsilon^3)\ . \tag{3.3.6}$$

Expansion of log(coshσy) as a Taylor series in powers of ϵ gives

$$\log\cosh\sigma y = \log\cosh\rho y + (\sigma_1\epsilon+\sigma_2\epsilon^2+\ldots)y\tanh\rho y$$

$$+\frac{1}{2}(\sigma_1^{\,2}\epsilon^2+2\sigma_1\sigma_2\epsilon^3+\sigma_2^{\,2}\epsilon^4+\ldots)y^2\mathrm{sech}^2\rho y$$

$$-\frac{1}{3}(\sigma_1^{\,3}\epsilon^3+\ldots)y^3\mathrm{sech}^2\rho y\ \tanh\rho y+\ldots$$

Therefore

$$\theta_{-\infty}(y) = \phi_0^{\ 0}(y)+\epsilon\phi_1^{\ 0}(y)+\epsilon^2\phi_2^{\ 0}(y)+\epsilon^3\phi_3^{\ 0}(y)+\ldots \tag{3.3.7}$$

where

$$\phi_0^{\ 0}(y) = 2\log\left(\frac{\cosh\rho}{\cosh\rho y}\right)\quad ,$$

$$\phi_1^{\ 0}(y) = 2\sigma_1(\tanh\rho-y\tanh\rho y)\quad ,$$

$$\phi_2^{\ 0}(y) = 2\sigma_2(\tanh\rho-y\tanh\rho y)+\sigma_1^{\,2}(\mathrm{sech}^2\rho-y^2\mathrm{sech}^2\rho y)\quad ,$$

$$\phi_3^{\,0} = 2\sigma_3(\tanh\rho - y\tanh\rho y) + 2\sigma_1\sigma_2(\mathrm{sech}^2\rho - y^2\mathrm{sech}^2\rho y)$$

$$- \frac{2}{3}\sigma_1^{\,3}(\mathrm{sech}^2\rho\tanh\rho - y^3\mathrm{sech}^2\rho y\ \tanh\rho y),$$

etc.

The Intermediate Problem

We seek solution $\theta(x,y)$ which satisfies the asymptotic solutions (3.3.1) and (3.3.7), taking into consideration the powers of ϵ, we put

$$\theta(x,y) = \phi_0^{\,0}(y) + \epsilon\phi_1(x,y) + \epsilon^2\phi_2(x,y) + \ldots$$

and $$\delta = 2\rho^2 e^{-\epsilon}\mathrm{sech}^2\rho \tag{3.3.8}$$

Therefore

$$\delta \exp\theta(x,y) = 2\rho^2 e^{\phi_0^{\,0}}\mathrm{sech}^2\rho\{(1-\epsilon+\frac{\epsilon^2}{2}+\ldots)$$
$$[1+(\epsilon\phi_1+\epsilon^2\phi_2)+\ldots+\frac{1}{2}(\epsilon\phi_1+\epsilon^2\phi_2)^2+\ldots]\}$$

but $$2\rho^2 e^{\phi_0^{\,0}}\mathrm{sech}^2\rho = 2\rho^2\mathrm{sech}^2\rho y\ .$$

Hence

$$\delta \exp\theta(x,y) = 2\rho^2\mathrm{sech}^2\rho y\{1-(1-\phi_1)\epsilon+[\phi_2-\phi_1+\frac{1}{2}(1+\phi_1^{\,2})]\,\epsilon^2\ldots]$$

Thus equation (3.3.0) becomes

$$\nabla^2(\phi_0^{\,0}+\epsilon\phi_1+\epsilon^2\phi_2+\ldots)+2\rho^2\mathrm{sech}^2\rho y\{1-(1-\phi_1)\epsilon+[\phi_2-\phi_1$$
$$+\frac{1}{2}(1+\phi_1^{\,2})]\epsilon^2+\ldots\} = 0$$

On equating the coefficients of the powers of ϵ, we get

$$\frac{d^2\phi_0^{\,0}}{dy^2} + 2\rho^2\mathrm{sech}^2\rho y = 0\quad ,$$

$$\nabla^2\phi_1 - 2\rho^2\text{sech}^2\rho y.(1-\phi_1) = 0 \quad ,$$
$$\nabla^2\phi_2 + 2\rho^2\text{sech}^2\rho y.[(\phi_2-\phi_1) + \frac{1}{2}(1+\phi_1^2)] = 0 \quad , \tag{3.3.9}$$

with boundary conditions

$$\begin{aligned} y = 0 \quad &: \quad \frac{\partial\phi_1}{\partial y} = \frac{\partial\phi_2}{\partial y} = 0 \quad , \\ y = 1 \quad &: \quad \phi_1(x,1) = f(x), \quad \phi_2(x,1) = 0 \; , \\ x \to -\infty \quad &: \quad \phi_1 \to \phi_1{}^0(y), \quad \phi_2 \to \phi_2{}^0(y), \\ x \to \infty \quad &: \quad \Phi_1 \to 1 \; , \qquad \phi_2 \to 0 \; . \end{aligned} \tag{3.3.10}$$

<u>Consider the $\phi_1(x,y)$ equation</u>

$$\nabla^2\phi_1(x,y) - 2\rho^2\text{sech}^2\rho y.(1-\phi_1) = 0, \quad 0 \leqslant y \leqslant 1, \quad -\infty < x < \infty$$

with boundary conditions

$$\begin{aligned} y = 0 \quad &: \quad \frac{\partial\phi_1}{\partial y} = 0 \\ y = 1 \quad &: \quad \phi_1(x,1) = f(x) \\ x \to \infty \quad &: \quad \phi_1 \to 1 \\ x \to -\infty \quad &: \quad \phi_1 \to \phi_1{}^0(y) \end{aligned} \tag{3.3.11}$$

We put $\xi_1(x,y) = 1-\phi_1(x,y)$ and hence the equation for ξ_1 is

$$\nabla^2\xi_1(x,y) + 2\rho^2\text{sech}^2\rho y.\xi_1(x,y) = 0, \quad 0 \leqslant y \leqslant 1, \quad -\infty < x < \infty \tag{3.3.12}$$

with boundary conditions

$$y = 0 \quad : \quad \frac{\partial \xi_1}{\partial y} = 0 \ ,$$

$$y = 1 \quad : \quad \xi_1(x,1) = 1-f(x) \ ,$$

$$x \to \infty \quad : \quad \xi_1 \to 0 \ ,$$

$$x \to -\infty \quad : \quad \xi_1 \to 1-\phi_1{}^0(y) \ .$$

The solution of equation (3.3.12) is given by

$$\xi_1(x,y) = \frac{\partial \psi_1}{\partial y} - \rho \tanh\rho y . \psi_1(x,y)$$

where $\nabla^2 \psi_1 = 0$. To determine $\psi_1(x,y)$ we consider the appropriate boundary conditions from the conditions on $\xi_1(x,y)$:

(i) when $x \to \infty$: $\xi_1 \to 0$

Therefore

$$0 = \frac{\partial \psi_1}{\partial y} - \rho \tanh\rho y . \psi_1(\infty,y)$$

$\psi_1(\infty,y) = c \cosh\rho y$ satisfies the above equation, but $\nabla^2 \psi_1 = 0$ (everywhere), hence $c = 0$. Thus as $x \to \infty$ $\psi_1 \to 0$.

(ii) when $x \to -\infty$: $\xi_1 \to 1 - \phi_1{}^0(y)$

but $\phi_1{}^0(y) = - \dfrac{\rho(\tanh\rho - y \tanh\rho y)}{(1-\rho\tanh\rho)}$.

Thus

$$\xi_1(-\infty,y) = 1 + \left[\frac{\rho(\tanh\rho - y \tanh\rho y)}{(1-\rho\tanh\rho)}\right]$$

$$= \frac{\partial}{\partial y}\left(\frac{y}{1-\rho\tanh\rho}\right) - \rho\tanh\rho y\left(\frac{y}{1-\rho\tanh\rho}\right)$$

Hence as $x \to -\infty$ $\psi_1 \to \dfrac{y}{(1-\rho\tanh\rho)}$.

(iii) $y = 0$: $\dfrac{\partial}{\partial y}\xi_1(x,0) = 0$

Therefore

$$\frac{\partial^2}{\partial x^2}\psi_1(x,0) + \rho^2\psi_1(x,0) = 0$$

with $\psi_1(x,0) = B_1 \cos \rho x + B_2 \sin \rho x$. However, we are seeking a decaying solution as $x \to \pm\infty$, consequently $B_1 = B_2 \equiv 0$. Hence at $y = 0$ $\psi_1(x,0) = 0$. The problem then reduces to

$$\nabla^2\psi_1(x,y) = 0, \qquad 0 \leqslant y \leqslant 1, \qquad -\infty < x < \infty, \qquad (3.3.13)$$

with boundary conditions

$y = 0$: $\psi_1(x,0) = 0$

$y = 1$: $1-f(x) = \dfrac{\partial}{\partial y}\psi_1(x,1) - \rho\tanh\rho . \psi_1(x,1)$

$x \to \infty$: $\psi_1 \to 0$

$x \to -\infty$: $\psi_1 \to \dfrac{y}{(1-\rho\tanh\rho)}$, with ψ_1

being a smooth function of x (so as to exclude non-physical solutions for example $\psi_1 = 0$ for $x > 0$ and $\psi_1 = y/(1-\rho\tanh\rho)$ for $x < 0$).

We put

$$\overline{\phi}_1(x,y) = \psi_1(x,y) - \frac{1}{2}\,\frac{y}{(1-\rho\tanh\rho)}$$

Thus as

$x \to \infty$: $\overline{\phi}_1 \to -\frac{1}{2}[y/(1-\rho\tanh\rho)]$

and as

$$x \to -\infty \quad : \quad \overline{\phi}_1 \to \frac{1}{2}[y/(1-\rho\tanh\rho)] .$$

Hence $\overline{\phi}_1(x,y) = -\overline{\phi}_1(-x,y)$

setting $x = 0$, we get

$$\overline{\phi}_1(0,y) = 0 \quad .$$

We now replace the boundary conditions at $x = \pm\infty$ of (3.3.13) by

$$x = 0 \quad : \quad \psi_1(0,y) = \frac{1}{2}[y/(1-\rho\tanh\rho)]$$

$$x \to \infty \quad : \quad \psi_1 \to 0 .$$

We then consider the modified problem

$$\nabla^2\psi_1(x,y) = 0 \; ; \qquad 0 \leqslant y \leqslant 1 \; , \qquad 0 \leqslant x < \infty . \tag{3.3.14}$$

with boundary conditions

$$y = 0 \quad : \quad \psi_1(x,0) = 0$$

$$y = 1 \quad : \quad 1-f(x) = \frac{\partial\psi_1}{\partial y} - \rho\tanh\rho . \psi(x,1)$$

$$x = 0 \quad : \quad \psi_1(0,y) = \frac{1}{2}[y/(1-\rho\tanh\rho)]$$

and the asymptotic condition

$$x \to \infty \quad : \quad \psi_1 \to 0.$$

In order to solve problem (3.3.14) we apply a Fourier-Sine transform and solve the transformed problem. We define:

$$\Psi_1(\gamma,y) \equiv F_s\{\psi_1(x,y)\} = \sqrt{\frac{2}{\pi}} \int_0^\infty \psi_1(x,y)\ \sin\gamma x \ \ dx$$

and its inverse transform

$$\psi_1(x,y) = \sqrt{\frac{2}{\pi}} \int_0^\infty \Psi_1(\gamma,y)\ \sin\gamma x \ \ d\gamma$$

$$\equiv F_s^{-1}\{\Psi_1(\gamma,y)\} \quad .$$

Thus

$$F_s \ \{\frac{\partial^2\psi}{\partial x^2}\} = \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{\partial^2\psi_1}{\partial x^2} \ \sin\gamma x \ \ dx$$

$$= \sqrt{\frac{2}{\pi}} \ . \ \gamma\psi_1(0,y) \ - \ \gamma^2\Psi_1(\gamma,y) \ .$$

Taking the Fourier-Sine transform of equation (3.3.14) we obtain

$$\frac{\partial^2}{\partial y^2} \ \ \Psi_1(\gamma,y) + \frac{\gamma y}{\sqrt{2\pi}(1-\rho\tanh\rho)} \ - \gamma^2\Psi_1(\gamma,y) = 0$$

The $\Psi_1(\gamma,y)$ solution is given by

$$\Psi_1(\gamma,y) = A\ \cosh\gamma y + B\ \sinh\gamma y + [\ \frac{y}{\sqrt{2\pi}\ \gamma(1-\rho\tanh\rho)}] \tag{3.3.15}$$

at $y = 1$:

$$1-f(x) = \frac{\partial\psi_1}{\partial y} - \rho\tanh\rho . \psi_1(x.1) .$$

We consider the case (i) $f(x) = \frac{1}{2}(1+\tanh x)$ and taking the F_s of the boundary condition when $y = 1$, we get

$$F_s\{1-f(x)\} = \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{1}{2}(1-\tanh x)\sin\gamma x \, dx$$

$$= \frac{1}{\sqrt{2\pi}} \left[\gamma - \frac{\pi}{2}\operatorname{cosech}\left(\frac{\gamma}{2}\right)\right]$$

[Note: $\int_0^\infty (1-\tanh x)\sin\gamma x \, dx = \gamma - \frac{\pi}{2}\operatorname{cosech}(\frac{\gamma}{2})$, see[31].]

Hence when $y = 1$

$$\frac{\partial}{\partial y}\Psi_1(\gamma,1) - \rho\tanh\rho.\Psi_1(\gamma,1) = \frac{1}{\sqrt{2\pi}} \left[\gamma - \frac{\pi}{2}\operatorname{cosech}\left(\frac{\gamma}{2}\right)\right] .$$

At $y = 0$: $\psi_1(x,0) = 0$, hence $\Psi_1(\gamma,0) = 0$.

Therefore $A \equiv 0$. Equation (3.3.15) becomes

$$\Psi_1(\gamma,y) = B\sinh\gamma y + \frac{y}{\sqrt{2\pi}\,\gamma(1-\rho\tanh\rho)} .$$

Differentiating Ψ_1 with respect to y, we get

$$\frac{\partial\Psi_1(\gamma,y)}{\partial y} = B\gamma\cosh\gamma y + \frac{1}{\sqrt{2\pi}\,\gamma(1-\rho\tanh\rho)}$$

when $y = 1$, we obtain

$$\frac{1}{\sqrt{2\pi}}[\gamma-(\pi/2)\operatorname{cosech}(\gamma/2)] = B\gamma\cosh\gamma + \frac{1}{\sqrt{2\pi}\,\gamma(1-\rho\tanh\rho)}$$

$$- B\rho\tanh\rho\sinh\gamma - \frac{\rho\tanh\rho}{\sqrt{2\pi}\,\gamma(1-\rho\tanh\rho)}$$

Therefore

$$B = \frac{1}{\sqrt{2\pi}} \quad \frac{[\gamma-(1/\gamma)-(\pi/2)\operatorname{cosech}(\gamma/2)]}{(\gamma\cosh\gamma-\rho\tanh\rho\ \sinh\gamma)}$$

Thus $\Psi_1(\gamma,y)$ becomes

$$\Psi_1(\gamma,y) = \frac{1}{\sqrt{2\pi}} \left\{ \frac{\gamma-(1/\gamma)-(\pi/2)\operatorname{cosech}(\gamma/2)}{(\gamma\cosh\gamma-\rho\tanh\rho.\sinh\gamma)} \right\} \sinh \gamma y$$

$$+ \frac{y}{\sqrt{2\pi}\ \gamma(1-\rho\tanh\rho)} \qquad (3.3.16)$$

Hence

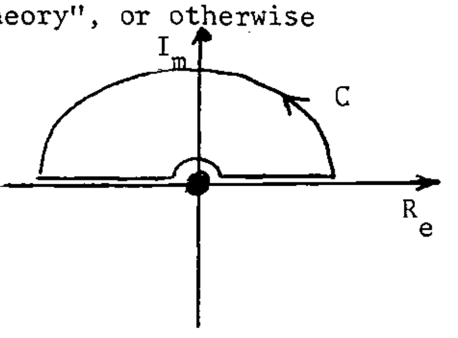
$$\psi_1(x,y) = \frac{1}{\pi} \int_0^\infty \left[\frac{\gamma-(1/\gamma)-(\pi/2)\operatorname{cosech}(\gamma/2)}{(\gamma\cosh\gamma-\lambda\ \sinh\gamma\ )} \right] \sinh\gamma y.\sin\gamma x \quad d\gamma$$

$$+ \frac{1}{\pi} \int_0^\infty \frac{y\ \sin\gamma x}{(1-\lambda)\gamma}\, d\gamma \qquad (3.3.17)$$

where $\lambda = \rho\tanh\rho$.

Note: $\int_0^\infty \frac{\sin z}{z}\, dz = \frac{\pi}{2}$, from the "Residue Theory", or otherwise consider

$$\frac{1}{2\pi i} \int_C \frac{e^{iz}}{z}\, dz$$



Therefore $\int_{-\infty}^{0} \frac{e^{iz}}{z}\, dz + \int_0^\infty \frac{e^{iz}}{z}\, dz = \pi i$

Hence

$$\frac{1}{2i} \int_0^\infty \left(\frac{e^{iz}-e^{-iz}}{z} \right) dz = \frac{\pi}{2}$$

Equation (3.3.17) becomes

$$\psi_1(x,y) = \frac{1}{\pi} \int^{\infty} \left[\frac{\gamma-(1/\gamma)-(\pi/2)\text{cosech}(\gamma/2)}{(\gamma\cosh\gamma-\lambda\sinh\gamma)} \right] \sinh\gamma y.\sin\gamma x \;\; d\gamma$$

$$- \frac{y}{2(1-\lambda)} \qquad (3.3.18)$$

We now put $F(\gamma) = \frac{1}{\sqrt{2\pi}} [\gamma - \frac{\pi}{2}\text{cosech}(\frac{\gamma}{2})]$ (3.3.19)

Hence

$$\psi_1(x,y) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} \frac{F(\gamma)\sinh\gamma y.\sin\gamma x}{(\gamma\cosh\gamma-\lambda\sinh\gamma)} d\gamma + \frac{y}{2(1-\lambda)}$$

$$- \frac{1}{\pi} \int_0^{\infty} \frac{\sinh\gamma y \; \sin\gamma x \; d\gamma}{\gamma(\gamma\cosh\gamma-\lambda\sinh\gamma)} \qquad (3.3.20)$$

Note: $\int_0^{\infty} (1-\tanh x)\sin\gamma x \;\; dx = \gamma - \frac{\pi}{2}\text{cosech}(\frac{\gamma}{2})$

$$= \sqrt{2\pi}\, F(\gamma)$$

but $1-f(x) = 1-\frac{1}{2}(1+\tanh x)$

$$= \frac{1}{2}(1-\tanh x)$$

Therefore $2\int_0^{\infty} [1-f(x)]\sin\gamma x \; dx = \sqrt{2\pi}\, F(\gamma)$ (3.3.21)

We consider a function $G(\tau)$ such that

$$G(\tau) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} \frac{\sin\gamma\tau\sin\gamma x \; \sinh\gamma y}{(\gamma\cosh\gamma-\lambda\sinh\gamma)} \; d\gamma \qquad (3.2.22)$$

Thus we have

$$\frac{\sin\gamma x \;\; \sinh\gamma y}{(\gamma\cosh\gamma-\lambda\sinh\gamma)} = \sqrt{\frac{2}{\pi}} \int_0^{\infty} G(\tau)\sin\gamma\tau \; d\tau \qquad (3.3.23)$$

The first integral in (3.3.20) becomes

$$\sqrt{\frac{2}{\pi}} \int_0^\infty \frac{F(\gamma)\sin\gamma x \sinh\gamma y}{(\gamma\cosh\gamma-\lambda\sinh\gamma)} d\gamma = \sqrt{\frac{2}{\pi}} \int_0^\infty G(\tau)d\tau \sqrt{\frac{2}{\pi}} \int_0^\infty F(\gamma)\sin\gamma\tau \, d\gamma \tag{3.3.24}$$

but from equation (3.3.21)

$$[1-f(x)] = \sqrt{\frac{2}{\pi}} \int F(\gamma)\sin\gamma x \, d\gamma$$

Therefore

$$[1-f(\tau)] = \sqrt{\frac{2}{\pi}} \int_0^\infty F(\gamma)\sin\gamma\tau \, d\gamma$$

Hence equation (3.3.24) reduces to

$$\sqrt{\frac{2}{\pi}} \int_0^\infty \frac{F(\gamma)\sin\gamma x \sinh\gamma y}{(\gamma\cosh\gamma-\lambda\sinh\gamma)} d\gamma = \sqrt{\frac{2}{\pi}} \int_0^\infty [1-f(\tau)]G(\tau) \, d\tau \tag{3.3.25}$$

Also

$$\frac{1}{\pi} \int_0^\infty \frac{\sin\gamma x \sinh\gamma y}{\gamma(\gamma\cosh\gamma-\lambda\sinh\gamma)} d\gamma = \frac{1}{\pi} \int_0^\infty G(\tau)d\tau \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{\sin \gamma\tau}{\gamma} d\gamma$$

$$= \frac{1}{\sqrt{2\pi}} \int_0^\infty G(\tau)d\tau \tag{3.3.26}$$

Using equations (3.3.26) and (3.3.25) equation (3.3.20) becomes

$$\psi_1(x,y) = \sqrt{\frac{2}{\pi}} \int_0^\infty [1-f(\tau)]G(\tau)d\tau - \frac{1}{\sqrt{2\pi}} \int_0^\infty G(\tau)d\tau + \frac{y}{2(1-\lambda)} \tag{3.3.27}$$

We define the complex variable $z = x + iy$ and hence $I_m[\cos z] = -\sinh y \sin x, \ldots$ where $I_m[\ ]$ refers to the imaginary part. It can be easily shown that

$$-G(\tau) = I_m[\sqrt{\frac{2}{\pi}} \int_0^\infty \frac{\sin\gamma\tau \cos\gamma z}{(\gamma\cosh\gamma - \lambda\sinh\gamma)} d\gamma]$$

$$= I_m[\frac{1}{\sqrt{2\pi}} \int_0^\infty \frac{\sin\gamma(z+\tau)}{(\gamma\cosh\gamma-\lambda\sinh\gamma)} d\gamma - \frac{1}{\sqrt{2\pi}} \int_0^\infty \frac{\sin\gamma(z-\tau)\, d\gamma}{(\gamma\cosh\gamma-\lambda\sinh\gamma)}]$$

(3.3.28)

Note: $\phi_1(x,y) = 1-\xi_1(x,y)$

$$= 1 - \frac{\partial\psi_1}{\partial y} + \rho\tanh\rho y . \psi_1(x,y) \qquad (3.3.29a)$$

Substituting $\psi_1(x,y)$ from (3.3.27) into equation (3.3.29a) gives the solution for ϕ_1. We now seek to determine if the integral of (3.3.18) is well defined for all positive values of x and γ. We now put

$$I = \int_0^\infty [\frac{\gamma^2\sinh(\gamma/2)-\sinh(\gamma/2)-(\pi/2)\gamma}{\gamma\sinh(\gamma/2)[\gamma\cosh\gamma-\lambda\sinh\gamma]}] \sinh\gamma y \sin\gamma x\, d\gamma$$

Note: $\sinh x = x + \frac{x^3}{3!} + \frac{x^5}{5!} + \ldots \qquad \forall x$

$\cosh x = 1 + \frac{x^2}{2!} + \frac{x^4}{4!} + \ldots \qquad \forall x$

<u>when $\gamma \to 0$</u>

$$\gamma^2\sinh(\gamma/2)-\sinh(\gamma/2) - \frac{\pi}{2}\gamma = \gamma^2(\frac{\gamma}{2} + \frac{\gamma^3}{48} + \ldots)$$

$$-(\frac{\gamma}{2} + \frac{\gamma^3}{48} + \dots) - \frac{\pi\gamma}{2}$$

$$\cong -2.1\gamma + 0.48\,\gamma^3 + \dots$$

Similarly

$$\sinh(\frac{\gamma}{2})[\gamma\cosh\gamma - \lambda\sinh\gamma]$$

$$= (\frac{\gamma}{2} + \frac{\gamma^3}{48} + \dots)\{\gamma(1 + \frac{\gamma^2}{2} + \frac{\gamma^4}{24} + \dots) - \lambda(\gamma + \frac{\gamma^3}{6} + \dots)\}$$

$$= \frac{\gamma^2}{2}(1-\lambda) + \frac{\gamma^4}{48}(13-\lambda)$$

Hence put

$$I_0(\gamma) = \{\frac{\gamma^2\sinh(\gamma/2) - \sinh(\gamma/2) - (\pi/2)\gamma}{\gamma\sinh(\gamma/2)[\gamma\cosh\gamma - \lambda\sinh\gamma]}\} \sinh\gamma y \sin\gamma x$$

$$\cong [\frac{-2.1 + 0.48\gamma^2}{\frac{\gamma^2}{2}(1-\lambda) + \frac{\gamma^4}{48}(13-\lambda)}] \sinh\gamma y \quad \sin\gamma x$$

$$\cong \frac{(-4.2 + 0.96\gamma^2)(y + \frac{\gamma^2}{6}y^3 + \dots)}{[\gamma(1-\lambda) + \frac{\gamma^3}{24}(13-\lambda)]} \sin\gamma x$$

In the limit $x \to \infty$; $\gamma x \to 0(1)$. Hence the integrand is divergent since $I_0(\gamma)$ becomes

$$\lim_{x\to\infty} I_0(\gamma) \to -\frac{4.2\,y}{\gamma(1-\lambda)}$$

when $x \to 0$; $\gamma x \to 0$ and hence $I_0(\gamma)$ becomes

$$\operatorname{limit}_{x\to 0} I_0 \to -\frac{4.2\,yx}{(1-\lambda)}$$

Hence the integrand is finite for vanishing values of γ.

When $\gamma \to \infty$:

$$\gamma^2 \sinh(\gamma/2) - \sinh(\gamma/2) - \frac{\pi\gamma}{2}$$

$$\cong + \frac{1}{2}\gamma^2 e^{(\gamma/2)}[1 - \frac{\pi}{\gamma} e^{-\gamma/2} - \frac{1}{\gamma^2}]$$

$$\cong \frac{1}{2}\gamma^2 e^{(\gamma/2)}[1 - \frac{\pi}{\gamma} e^{-\gamma/2}] \; .$$

$$(\gamma\cosh\gamma - \lambda\sinh\gamma)\sinh(\gamma/2)$$

$$\cong \tfrac{1}{2} e^{(\gamma/2)} [\tfrac{1}{2}\gamma e^{\gamma} - \tfrac{1}{2}\lambda e^{\gamma}]$$

$$\cong \tfrac{1}{4} e^{(3\gamma/2)} (\gamma - \lambda) \; .$$

Hence

$$I_0(\gamma) \cong \frac{2\gamma^2(1 - \frac{\pi}{\gamma} e^{-(\gamma/2)})}{\gamma e^{\gamma}(\gamma-\lambda)} e^{\gamma y} \sin \gamma x$$

Note: at criticality $\lambda_{max} = 1$ and hence for the subcritical slab solution $\lambda < 1$. Therefore

$$I_0(\gamma) \cong 2[\gamma - (\tfrac{\pi}{\gamma}) e^{-(\gamma/2)}] e^{-\gamma(1-y)}$$

$$\lim_{\gamma \to \infty} I_0(\gamma) \to \frac{1}{e^{\gamma(1-y)}}$$

when $y = 1$ the integrand is singular. However for $y < 1$, $I_0(\gamma)$ tend to zero as γ approaches infinity.

3.4 Method of "Adiabatic Invariants": Resolution of paradox

In order to resolve the paradox of section 3.2, we reconsider the formulation of the surface temperature for the slab. We insist that the temperature gradient with respect to x is negligible in comparison to the surface temperature. Thus we now put

$$\theta(x,1) = \epsilon F(\epsilon x),$$

where $\frac{\partial\theta}{\partial x}(x,1) = \epsilon^2 F'(\epsilon x) \ll \theta(x,1)$. Putting $X = \epsilon x$, and substituting into equation (3.0.0), the energy equation becomes

$$\epsilon^2 \frac{\partial^2\theta}{\partial X^2} + \frac{\partial^2\theta}{\partial y^2} + \delta e^\theta = 0, \qquad 0 \leqslant y \leqslant 1, \quad -\infty < X < \infty \tag{3.4.0a}$$

with boundary conditions

$$\begin{aligned} y = 0 \quad &: \quad \frac{\partial\theta}{\partial y} = 0 \\ y = 1 \quad &: \quad \theta(X,1) = \epsilon F(X). \end{aligned} \tag{3.4.0b}$$

where

$$F(X) \to 0 \quad \text{as} \quad X \to -\infty,$$

$$F(X) \to 1 \quad \text{as} \quad X \to \infty.$$

Equation (3.4.0) implies that the surface temperature varies sufficiently slowly for the conductive forces to become quasi-one dimensional. Thus at each X, the surface temperature is nearly constant and the dominant conduction process is in the y direction. Hence for $\epsilon \ll 1$, the energy equation reduces to

$$\frac{\partial^2\theta}{\partial y^2} + \delta e^{\theta} = 0, \qquad 0 \leqslant y \leqslant 1 \ , \qquad \forall X$$

with boundary conditions

$$y = 0 \quad : \quad \frac{\partial\theta}{\partial y} = 0 \ , \qquad\qquad (3.4.1)$$

$$y = 1 \quad : \quad \theta(X,1) = \epsilon F(X).$$

The solution of equation (3.4.1) is given by

$$\theta(X,y) = \epsilon F(X) + 2\log\left(\frac{\cosh\ \sigma(X)}{\cosh\ \sigma(X)y}\right) \ ,$$

and (3.4.2)

$$\delta e^{\epsilon F(X)} = 2\sigma^2(X)\operatorname{sech}^2\sigma(X)$$

However, in the limit when the conditions at $x = \infty$ are critical,

$$\delta = \delta_c(0)e^{-\epsilon} \qquad \text{(see section 3.1, equation(3.1.0))}$$

Substituting this value of δ into (3.4.2) we obtain an expression for $\sigma(X)$ in powers of ϵ, namely

$$2\sigma^2(X)\operatorname{sech}^2\sigma(X) = \delta_c(0)e^{-\epsilon[1-F(X)]}$$

It can be shown (section 3.2) that

$$\sigma(X) = \sigma_c - \epsilon^{\frac{1}{2}}[1-F(X)]^{\frac{1}{2}}$$

Expanding $\theta \equiv \theta_c(X,y)$ in powers of $\epsilon^{\frac{1}{2}}$, we get

$$\theta_c(X,y) = \theta_c^{\ 0}(y) + \epsilon^{\frac{1}{2}}[1-F(X)]^{\frac{1}{2}}\ \theta_1^{\ 0}(y)$$

$$+ \ \epsilon\{F(X)+[1-F(X)]\theta_2^{\ 0}(y) \ + \ \ldots \qquad (3.4.3)$$

and

$$\delta_c(\epsilon) = \delta_c(0)\exp(-\epsilon)$$

Equation (3.4.3) represents the critical solution everywhere in the slab with $\theta_c(X,y)$ expansion valid to $0(\epsilon)$. Functions $\theta_c{}^0(y)$, $\theta_1{}^0(y)$, etc., are the same as defined in section 3.1, equation (3.1.6). The asymptotic properties of (3.1.0) and (3.1.6) follow directly from (3.4.0) and (3.4.3).

3.5 Conclusion

Attempts to express the critical Frank-Kamenetskii parameter $\delta_c(\epsilon)$ as a function of ϵ for an arbitrary surface temperature f(x), as defined in equation (3.0.2) proved unsuccessful. This difficulty arose in failing to determine a physically realistic solution for the intermediate region satisfying both the boundary conditions and the asymptotic conditions, even though the problem is well defined as $x \to \pm \infty$. However, this paradox was resolved by using the method of "Adiabatic Invariants", where limitations were imposed on the gradient with respect to x of the surface temperature, namely $\theta_x(x,1) \ll \theta(x,1)$.

By seeking to determine the non-critical slab solution in section 3.3, we hoped to ascertain the behaviour of the temperature solution as $\rho \to \sigma_c$. Infact our solution (3.3.18) will become singular as $\rho \to \sigma_c$ due to the term $(1-\rho\tanh\rho)^{-1}$.

Consequently, these observations and our failure to solve the critical case directly as in section 3.1 lead us to doubt the existence of a critical solution for the slab with an arbitrary surface temperature $f(x)$ as defined in (3.0.1) and (3.0.2).

CHAPTER FOUR: FINITE DIFFERENCE FORMULATION OF THE INSULATED SLAB

4.0 INTRODUCTION

In numerical solutions of partial differential equations, one normally employs the finite-difference grid system, such that the numerical solution, to a required degree of accuracy, corresponds to the continuous system it represents. The choice of the number of points and the grid interval are normally dictated by practical considerations, for example, computer time and the domain of solution. However, normally uniform grid intervals are chosen in a given direction, with spatial derivatives usually represented by central differences. The central differences for the uniform grid intervals give accuracy of $O(h^2)$ for the spatial derivatives, where h is the interval in the direction of coordinate differentiation. Although finite-differences schemes that use uniform grids are the simplest and most accurate, they are unsatisfactory for problems with boundary layers. If the number of grid points in the boundary layer is not large enough, then the numerical solution is apt to have gross errors even in the region outside the boundary layer. Increasing the number of grid points will result in unacceptably large computational time. However, this problem can be resolved by the introduction of an irregular grid with smaller spacing near the boundary layer. In fact, a non-uniform grid interval can be constructed which gives the same order of accuracy as the uniform grid when the derivatives are represented by central differences.

4.1 Generation of non-uniform grid points

In the insulated slab problem, we expect singular behaviour in the temperature profile near the region $y = 1$ and $x = \epsilon$. Thus it is imperative to develop a non-uniform grid in the y-direction with smaller grid spacing in the region $y \sim 1$. However, in the x-direction, we have an additional requirement, namely our domain of interest is semi-infinite in length. We expect the temperature to be almost uniform for values of $x \gg \epsilon$. Thus once again it is important to develop an irregular grid system to maximize efficient use of computational time.

To develop this non-uniform grid system, suppose the range $(0,L)$ of the independent variable z is divided into N intervals of non-constant length as indicated in Figure 4.0. We number the grid points $i(i=1$ to $i=N+1)$ and represent the value of z at the point i by z_i, so that $z_1 = 0$ and $z_{n+1} = L$. The grid interval between z_i and z_{i+1} is represented by h_i

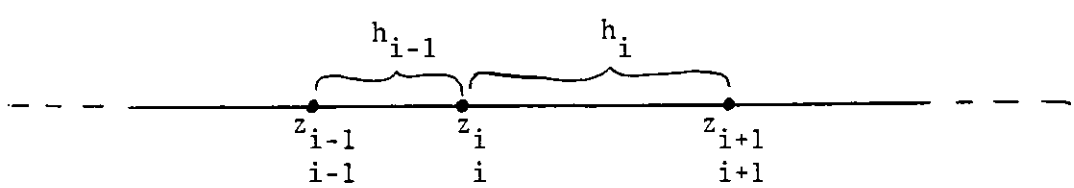


Figure 4.0: Finite difference scheme with irregular grid interval $h_i=z_{i+1}-z_i$ and $h_{i-1}=z_i-z_{i-1}$.

Now consider an analytic function $f(z)$ in the range $0 \leqslant z \leqslant L$, with $f_i = f(z_i)$. In order to express the derivatives as finite difference approximations, we expand f_{i+1} and f_{i-1} as Taylor series about the point $z = z_i$ to derive

$$f_{i+1} = f_i + h_i f_i^{(1)} + \frac{h_i^2}{2} f_i^{(2)} + \frac{h_i^3}{6} f_i^{(3)} + \frac{h_i^4}{24} f_i^{(4)} + \ldots. \qquad (4.1.0)$$

$$f_{i-1} = f_i - h_{i-1} f_i^{(1)} + \frac{h_{i-1}^2}{2} f_i^{(2)} - \frac{h_{i-1}^3}{6} f_i^{(3)} + \frac{h_{i-1}^4}{24} f_i^{(4)} + \ldots. \qquad (4.1.1)$$

Since we generally want $f_i^{(1)}$ and $f_i^{(2)}$, we assume that higher derivatives are negligible. Thus to solve for $f_i^{(1)}$, take $h_{i-1}^2 \times(4.1.0) - h_i^2 \times(4.1.1)$, we get

$$(h_i h_{i-1}^2 + h_i^2 h_{i-1}) f_i^{(1)} = h_{i-1}^2 f_{i+1} - h_i^2 f_{i-1} - (h_{i-1}^2 - h_i^2) f_i$$
$$- \frac{1}{6}(h_i^3 h_{i-1}^2 + h_i^2 h_{i-1}^3) f_i^{(3)} + \ldots.$$

Finally, we obtain

$$f_i^{(1)} = \frac{f_{i+1} - \left(\frac{h_i}{h_{i-1}}\right)^2 f_{i-1} - \left[1 - \left(\frac{h_i}{h_{i-1}}\right)^2\right] f_i}{h_i \left[1 + \left(\frac{h_i}{h_{i-1}}\right)\right]}$$
$$- \frac{h_i h_{i-1}}{6} f_i^{(3)} + \ldots \qquad (4.1.2)$$

To solve for $f_i^{(2)}$, we have $h_{i-1} \times(4.1.0) + h_i \times(4.1.1)$, to get

$$\frac{1}{2}(h_i^2 h_{i-1} + h_i h_{i-1}^2) f_i^{(2)} = h_{i-1} f_{i+1} + h_i f_{i-1} - (h_{i-1}^2 - h_i^2) f_i$$

$$- \frac{1}{6}(h_i^3 h_{i-1}^2 + h_i^2 h_{i-1}^3) f_i^{(3)} + \dots$$

On further simplication $f_i^{(2)}$ becomes

$$f_i^{(2)} = \frac{2\{f_{i+1} + (\frac{h_i}{h_{i-1}}) f_{i-1} - [1 + (\frac{h_i}{h_{i-1}})] f_i\}}{h_i h_{i-1} [1 + (\frac{h_i}{h_{i-1}})]}$$

$$+ \frac{1}{3} h_{i-1} [1 - (\frac{h_i}{h_{i-1}})] f_i^{(3)} - \frac{(h_i^3 + h_{i-1}^3) f_i^{(4)}}{12 h_{i-1} [1 + (\frac{h_i}{h_{i-1}})]} + \dots$$

(4.1.3)

Equations (4.1.2) and (4.1.3) give $f_i^{(1)}$ and $f_i^{(2)}$ correct to $O(h_i h_{i-1})$ and $O(h_i - h_{i-1})$ respectively. However, for a regular grid, $f_i^{(1)}$ and $f_i^{(2)}$ can be determined directly by putting $h = h_i = h_{i-1}$ into equations (4.1.2) and (4.1.3) respectively. Hence for the uniform grid spacing we obtain

$$f_i^{(1)} = \frac{f_{i+1} - f_{i-1}}{2h} - \frac{h^2}{6} f_i^{(3)} + \dots$$

$$f_i^{(2)} = \frac{f_{i+1} + f_{i-1} - 2f_i}{h^2} - \frac{h^2}{12} f_i^{(4)} + \dots \qquad (4.1.4)$$

Thus the finite-difference representations in (4.1.4) give an error bound of $O(h^2)$ for the derivatives. This error bound is normally acceptable in numerical solution of partial differential equations. However, equation (4.1.3) gives the expression for $f_i^{(2)}$ correct to $O(h_i - h_{i-1})$, a first order error term. To obtain second order error term for $f_i^{(2)}$, we choose the grid spacing such that

$$h_i - h_{i-1} = O(h_{i-1}^2) \quad . \tag{4.1.5}$$

Thus, to construct irregular grid intervals, with the same order of accuracy as a regular grid, we are restricted in our choice of h_i and h_{i-1}, as in equation (4.1.5). In the paper by Sundquist, H and Veronis, G., [32], they choose h_i, namely

$$h_1 = h$$

$$h_i = h_{i-1}\{1 + \frac{\gamma h_{i-1}}{L}\} \qquad i=2,\ldots \tag{4.1.6}$$

where γ is a constant of $O(1)$. By using (4.1.6), the error terms for the derivatives in equations (4.1.2) and (4.1.3) are now of $O(h_{i-1}^2)$ and $O(\gamma h_{i-1}^2)$ respectively. Consequently $f_i^{(1)}$ and $f_i^{(2)}$ have the same order of accuracy for both the regular and irregular grid systems. However Sandquist and Veronis found their choices of γ lead to unacceptably large errors in the region outside the boundary layer for the theoretical model of wind-driven ocean circulation proposed by Stommel (1948). To overcome this difficulty γ was modified such that

$$\gamma = \frac{\alpha}{z_0} \left(\frac{z_0 - z_1}{z_0}\right)^{\tau}$$

where α and τ are constants, with α being of order unity and $\tau > 0$. z_0 represents the region in which the grid-spacing is largest. This choice of γ resulted in considerable reduction in numerical errors in the region near $z = z_0$. Hence for the non-regular grid system we get

$$h_1 = h$$
$$h_i = h_{i-1}[1+ \frac{\alpha}{z_0} \left(\frac{z_0-z_1}{z_0} \right)^{\tau} h_{i-1}] \tag{4.1.7}$$

This choice of h_i also reduces the grid density in the boundary layer, namely $z \cong 0$. Numerical tests of the Stommel (1948) model were carried out for $\alpha = 1,2,3,4$ and $\tau = 1,2,3,4$ for twenty grid points and with $z_0 = \pi$. The best results were obtained for $\alpha = 4$ and $\tau = 1$, which gave 2.5% error near $z = \pi$. This was a significant improvement compared to 3.4% error obtained for the original choice of $\gamma = 2$ in (4.1.6).

However, the major difficulty in implementing this choice of h_i is the cumbersome way of determining the optimum values of α, τ and number of grid points. In two-dimensional problems, this difficulty will result in considerable computational effort to get the appropriate optimum values for the non-regular grid system. This difficulty can be resolved by using a system of stretched coordinates. This method involves the transformation of the region of differentiation into a region where a regular grid will be used. The regular grid in the transformed region is infact equivalent to a non-regular grid interval in the original z-plane, see Figure 4.1

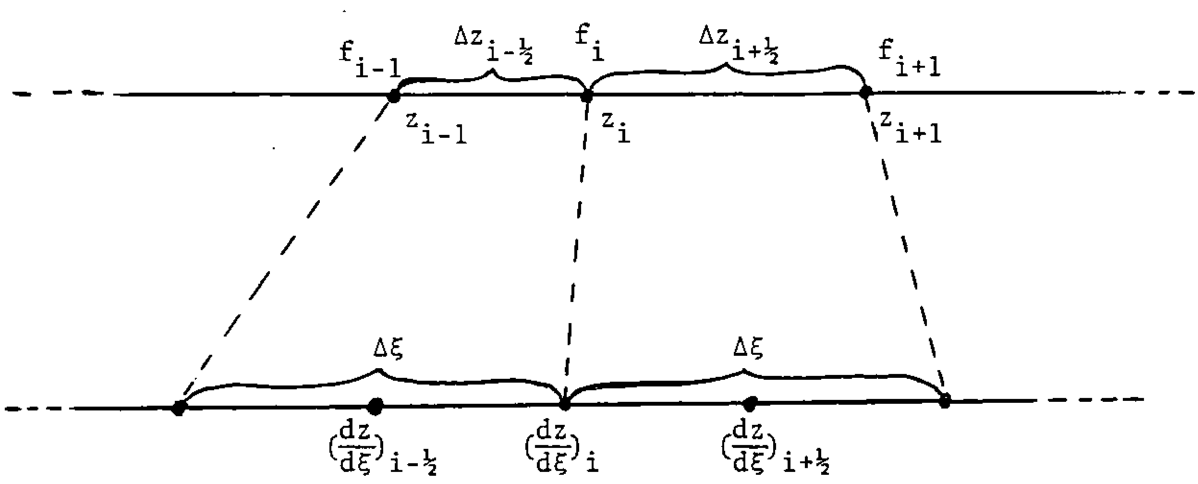


Figure 4.1: Non-uniform grid defined through use of coordinate stretching.

The idea in the use of stretched coordinates is to reduce the error bound on the derivatives by making the grid interval $\Delta\xi$ in the transformed plane as small as possible. Thus to obtain first order error in finite-difference approximation of $f_i^{(1)}$, subtract equation (4.1.1) from (4.1.0) to obtain

$$f_i^{(1)} = \frac{f_{i+1}-f_{i-1}}{(h_i+h_{i-1})} - \frac{1}{2}(h_i-h_{i-1})f_i^{(2)} + \ldots \qquad (4.1.8)$$

Replacing h_i and h_{i-1} by $\Delta z_{i+\frac{1}{2}}$ and $\Delta z_{i-\frac{1}{2}}$ respectively in equations (4.1.8) and (4.1.3), we get

$$f_i^{(1)} = \frac{f_{i+1}-f_{i-1}}{(\Delta z_{i+\frac{1}{2}}+\Delta z_{i-\frac{1}{2}})} + 0(\Delta z_{i+\frac{1}{2}}-\Delta z_{i-\frac{1}{2}})f_i^{(2)}$$

$$\cong \frac{f_{i+1}-f_{i-1}}{(\Delta z_{i+\frac{1}{2}}+\Delta z_{i-\frac{1}{2}})} \qquad (4.1.9)$$

and

$$f_i^{(2)} = \frac{2}{(\Delta z_{i+\frac{1}{2}}+\Delta z_{i-\frac{1}{2}})}\left\{\frac{f_{i+1}-f_i}{\Delta z_{i+\frac{1}{2}}} - \frac{f_i-f_{i-1}}{\Delta z_{i-\frac{1}{2}}}\right\}$$

$$+ 0(\Delta z_{i+\frac{1}{2}} - \Delta z_{i-\frac{1}{2}})$$

$$\cong \frac{2}{(\Delta z_{i+\frac{1}{2}} + \Delta z_{i-\frac{1}{2}})} \left\{ \frac{f_{i+1}-f_i}{\Delta z_{i+\frac{1}{2}}} - \frac{f_i-f_{i-1}}{\Delta z_{i-\frac{1}{2}}} \right\} \tag{4.1.10}$$

We now define a stretched coordinate ξ, such that

$$z = z(\xi)$$

and its inverse

$$\xi = \xi(z)$$

Thus $f(z) = f(z(\xi(z)))$.

Differentiating $f(z)$ with respect to z, we obtain

$$\frac{df}{dz} = \frac{df}{d\xi} \frac{d\xi(z)}{dz} \tag{4.1.11}$$

also note

$$\xi(z(\xi)) = \xi$$

therefore $$\frac{d\xi}{dz}(z(\xi)) \frac{dz}{d\xi}(\xi) = 1 . \tag{4.1.12}$$

Substituting (4.1.12) into (4.1.11) we get

$$\frac{df(z(\xi))}{dz} = [\frac{df(z(\xi))}{d\xi} / \frac{dz(\xi)}{d\xi}] \tag{4.1.13}$$

Using central difference approximation in the numerator we obtain

$$(\frac{df}{dz})_i \cong \frac{f_{i+1} - f_{i-1}}{2\Delta\xi(\frac{dz}{d\xi})_i} \tag{4.1.14}$$

Also we have

$$\frac{d^2 f(z(\xi))}{dz^2} = \frac{d}{dz}\ \frac{df(z(\xi))}{dz}$$

$$= \frac{d}{d\xi}\ \{ \frac{df(z(\xi))}{dz} \} / \ \frac{dz(\xi)}{d\xi}$$

$$= [\ \frac{d}{d\xi}\ \{ \frac{df(z(\xi))}{d\xi} / \frac{dz(\xi)}{d\xi}\ ] / \frac{dz(\xi)}{d\xi} \qquad (4.1.15)$$

Discretizing equation (4.1.15)

(i) Using the central difference in the numerator

(ii) and using the central difference approximation for $\frac{df}{d\xi}$, we obtain

$$\frac{d^2 f(z(\xi))}{dz^2} \cong \frac{1}{\Delta\xi} \left\{ \frac{\frac{f_{i+1}-f_i}{\Delta\xi}}{(\frac{dz}{d\xi})_{i+\frac{1}{2}}} - \frac{\frac{f_i - f_{i-1}}{\Delta\xi}}{(\frac{dz}{d\xi})_{i-\frac{1}{2}}} \right\} \bigg/ (\frac{dz}{d\xi})_i$$

$$\cong \frac{f_{i+1}}{(\Delta\xi)^2 (z_\xi)_{i+\frac{1}{2}} (z_\xi)_i}$$

$$+ \frac{f_{i-1}}{(\Delta\xi)^2 (z_\xi)_{i-\frac{1}{2}} (z_\xi)_i}$$

$$- \frac{1}{(\Delta\xi)^2 (z_\xi)_i} [\ \frac{1}{(z_\xi)_{i+\frac{1}{2}}} + \frac{1}{(z_\xi)_{i-\frac{1}{2}}}\ ] + O(\Delta\xi^2) \qquad (4.1.16)$$

For details of the error terms in the finite-difference formulation of the derivatives in equations (4.1.14) and (4.1.16), see Ref. [32]. However, it suffices to note the following properties of $z(\xi)$;

(i) $\frac{dz}{d\xi}$ should be finite throughout the whole interval. However, if $\frac{dz}{d\xi}$ is infinite, then the mapping will give poor resolution since $\Delta z \approx (\frac{dz}{d\xi}).\Delta\xi$. Thus the resolution cannot be improved even if we increase the number of grid points.

(ii) On the other hand, if $(\frac{dz}{d\xi}) = 0$, at $z = 0$, higher resolution will be obtained near $z = 0$. This condition is true if $z_1 = 0$.

The finite-difference approximations for the derivatives can be simplified by a convenient choice of the function of z, namely $z(\xi) = P_n(\xi)$, where $P_n(\xi)$ is a polynomial of degree greater than unity. In the paper [33] by Eugena K. de Rivas, comparisons were made between the method of stretched coordinates with the method used by Sundquist-Veronis. Although the method of coordinate stretching gave higher error values, there is no tendency for the relative errors to grow for $z \to 0$ for the Stommel (1948) model. However, the major advantage of this method is the ease with which grid-spacings are immediately known once the number of the grid points have been decided whereas for the method used by Sundquist-Veronis would require considerable effort in determining α and τ in (4.1.7). Consequently in our computational work on the insulated slab, we employed the method of coordinate stretching as defined by equations (4.1.14) and (4.1.16).

4.2 Grid-System in y-direction

As afore mentioned, we expect the temperature within the slab to vary rapidly as y approaches unity. Hence we seek to determine a function $y = y(\eta)$ as shown in Figure 4.2. For y values approaching unity, we require the grid-intervals to become very small to cope with rapid changes in temperatures. We impose the following conditions on $y(\eta)$, namely

(i) $y(0) = 0, \quad y(1) = 1, \quad \text{with} \quad 0 \leqslant \eta \leqslant 1$

(ii) $\left(\frac{dy}{d\eta}\right)_{\eta=0} = 1 \quad \text{and} \quad \left(\frac{dy}{d\eta}\right)_{\eta=1} = \gamma \quad \text{where} \quad 0 < \gamma \ll 1$

(4.2.0)

To satisfy the conditions (4.2.0), we require a cubic polynomial function of $y(\eta)$, namely

$$y = a_0 + a_1\eta + a_2\eta^2 + a_3\eta^3 \quad .$$

On imposing the condition (4.2.0) we have

$$y = \eta \{1 + (1-\gamma)(1-\eta)\eta\}$$

OR

$$y = \eta + (1-\gamma)\eta^2 - (1-\gamma)\eta^3 \quad .$$

Although choosing $\left(\frac{dy}{d\eta}\right)_{\eta=0} = 0$, would give high resolution near $y = 0$, we anticipate difficulties since we have to generate an extra grid point because of the Neumann boundary condition at $x = 0$, since $\frac{\partial\theta(0,y)}{\partial x} = 0$. Hence the convenience of choosing $\left(\frac{dy}{d\eta}\right)_{\eta=0} = 1$ becomes more apparent. By an appropriate choice of γ, the overall truncation error can be reduced with a view of obtaining small grid spacing near $y = 1$.

4.3 Grid-spacing in the x-direction

Our choice of the irregular grid is dictated by two main considerations;

(i) We expect the temperature within the slab to change rapidly in the region $x \sim \epsilon$ and $y \sim 1$. Hence we require very small grid intervals in this region. Infact the mapping of the insulation in ξ-plane covers a region of length $\overline{\xi}$ as shown in Figure 4.3. The mapping function $x = x(\xi)$ is chosen such that we have uniform grid intervals in the region $0 \leqslant x \leqslant 2\epsilon$, or $0 \leqslant \xi \leqslant 2\overline{\xi}$. This choice of region with uniform grid allows the temperature to settle down before the introduction of irregular grid spacing.

(ii) The temperature profiles for large values of x, namely $x \gg \epsilon$, are dominated by heat conduction in the y-direction, hence in this region large computer time savings can be obtained by using a finite-difference scheme with irregular grid intervals, with intervals largest as $x \to \infty$. For numerical computational purposes, the point $x \to \infty$, is defined to be equal to X_∞.

The difficulty of choosing a continuous function $x(\xi)$ with the above constraints was resolved by taking separate mappings of x into ξ-plane, namely

(a) $X_I(\xi)$ $\quad 0 \leqslant x \leqslant 2\epsilon \quad$ or $\quad 0 \leqslant \xi \leqslant 2\overline{\xi}$

(b) $X_{II}(\xi)$ $\quad 2\epsilon \leqslant x \leqslant X_\infty \quad$ or $\quad 2\overline{\xi} \leqslant \xi \leqslant 1.0$

We then imposed constraints on $X_I(\xi)$ and $X_{II}(\xi)$ with a view of minimizing interpolation errors in the derivatives $f_i^{(1)}$ and $f_i^{(2)}$. We therefore consider

Region I: $0 \leqslant \xi \leqslant 2\bar{\xi}$

We put $X_I(\xi) = \frac{\epsilon}{\bar{\xi}}\xi$

Region II:

At $x = 2\epsilon$ or $\xi = 2\bar{\xi}$, we at least expect X_I and X_{II} to equal each other. However, the nature of the continuity in the derivatives for the two mappings is dictated by the degree of accuracy we require in the finite-difference formulation of the spatial derivatives of the temperature within the slab (see below). Accepting errors in spatial derivatives of $0(\Delta\xi)^2$, we insist that $X_I(\xi)$ and $X_{II}(\xi)$ have the following properties;

at $\xi = 2\bar{\xi}$

(i) $$X_{II}(2\bar{\xi}) = X_I(\bar{\xi}) \equiv 2\epsilon$$

(ii) $$\left.\frac{dX_{II}}{d\xi}\right|_{\xi=2\bar{\xi}} = \left.\frac{dX_I}{d\xi}\right|_{\xi=2\bar{\xi}} \equiv \frac{\epsilon}{\bar{\xi}}$$

(iii) $$\left.\frac{d^2X_{II}}{d\xi^2}\right|_{\xi=2\bar{\xi}} = \left.\frac{d^2X_I}{d\xi^2}\right|_{\xi=2\bar{\xi}} \equiv 0$$

(iv) $$\left.\frac{d^3X_{II}}{d\xi^3}\right)_{\xi=2\overline{\xi}} = \left.\frac{d^3X_I}{d\xi^3}\right)_{\xi=2\overline{\xi}} \equiv 0 \qquad (4.3.1)$$

We also impose a bound on ξ such that $0 \leqslant \xi \leqslant 1$, with $\xi = 1$, being equivalent to $x = X_\infty$ in the x-plane. Thus at $\xi = 1$, we put

$$X_{II}(1) = X_\infty$$
$$\left.\frac{dX_{II}}{d\xi}\right)_{\xi=1} = \beta_0 \qquad (4.3.2)$$

Hence we can vary the grid intervals by altering β_0 thereby controlling the size and spread of grid intervals in the region $x > 2\epsilon$, with a view of minimizing the errors on the spatial derivatives as defined in equations (4.1.14) and (4.1.16). To satisfy the conditions (4.3.1) and (4.3.2) we choose the mapping function $X_{II}(\xi)$ such that

$$X_{II}(\xi) = a_0 + a_1\xi + a_2\xi^2 + a_3\xi^3 + a_4\xi^4 + a_5\xi^5$$

where a_i's are constants, $i = 0(5)$. (4.3.3)

By substituting equations (4.3.0) and (4.3.3) into equations (4.3.1) and (4.3.2), we obtain a system of equations in a_i's. From these system of equations, a_i's can be expressed in terms of β_0. ϵ and X_∞. (For the details of a_i's see Appendix).

4.4 Computational Molecule and the finite-difference of Equations for the slab problem

We now replace the energy equation (2.0.0) with the finite-difference system of equations. The Neumann boundary conditions are approximated by the use of equation (4.1.14). Thus we need to generate extra grid points to take into account this approximation to the first derivatives of the temperature. The computational molecule at the point (i,j) for the Laplacian operator becomes

$$
\begin{aligned}
\nabla^2\theta &= \frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial y^2} \\
&= \frac{\theta_{i+1,j}}{(\Delta\xi)^2(x_\xi)_{i+\frac{1}{2}}(x_\xi)_i} + \frac{\theta_{i,j+1}}{(\Delta\eta)^2(y_\eta)_{j+\frac{1}{2}}(y_\eta)_j} \\
&+ \frac{\theta_{i-1,j}}{(\Delta\xi)^2(x_\xi)_{i-\frac{1}{2}}(x_\xi)_i} + \frac{\theta_{i,j-1}}{(\Delta\eta)^2(y_\eta)_{j-\frac{1}{2}}(y_\eta)_i} \\
&- \frac{1}{(\Delta\xi)^2}\left\{ \frac{1}{(x_\xi)_i}\left[\frac{1}{(x_\xi)_{i+\frac{1}{2}}} + \frac{1}{(x_\xi)_{i-\frac{1}{2}}}\right] + \right. \\
&\qquad \left. \left(\frac{\Delta\xi}{\Delta\eta}\right)^2 \frac{1}{(y_\eta)_j}\left[\frac{1}{(y_\eta)_{j+\frac{1}{2}}} + \frac{1}{(y_\eta)_{j-\frac{1}{2}}}\right]\right\}\theta_{i,j} \\
&+ O[(\Delta\xi)^2, (\Delta\eta)^2]
\end{aligned}
\tag{4.4.0}
$$

where $i = 1,2,\ldots N$

$j = 1,2,\ldots,(M-1), M \qquad \forall\xi \leqslant \bar{\xi}$

$j = 1,2,\ldots,(M-2),(M-1). \qquad \forall\xi > \bar{\xi}$.

M and N represents the number of grid points in the η and ξ spatial directions. Thus

$$\Delta\xi = (1/N)$$

$$\Delta\eta = 1/(M-1).$$

Boundary conditions:

Accepting errors of $O(\Delta\xi)^2$ or $O(\Delta\eta)^2$, therefore using equation (4.1.14), we have

(i) $x = 0$ $\quad \frac{\partial\theta}{\partial x} = 0$

but $\quad \frac{\partial\theta}{\partial x} \cong \frac{\theta_{i+1,j} - \theta_{i-1,j}}{2(\Delta\xi)(x_\xi)_i}$

hence at $x = 0$ $\quad i = 1$

$$\theta_{2,j} = \theta_{0,j} \qquad j = 1(M).$$

(ii) $y = 0$ $\quad \frac{\partial\theta}{\partial y} = 0$

but $\quad \frac{\partial\theta}{\partial y} \cong \frac{\theta_{i,j+1} - \theta_{i,j-1}}{2(\Delta\eta)(y_\eta)_j}$

thus at $y = 0$

$$\theta_{i,2} = \theta_{i,0} \qquad i = 1(N).$$

(iii) $y = 1$ $\quad \frac{\partial\theta}{\partial y} = 0 \qquad x \leqslant \epsilon \quad$ or $\quad \xi \leqslant \bar{\xi}$

Let N_s represent the number of grid points in the region covered by insulation, therefore at $y = 1$; $j = M$.

$$\theta_{i,M+1} = \theta_{i,M} \qquad i = 1(N_s).$$

N_s can be determined from the following relationship, namely

$$\bar{\xi} = \Delta\xi(N_s - 1).$$

$$\text{or} \qquad N_s = N\bar{\xi} + 1 \qquad (4.4.1)$$

(iv) at $x = X_\infty$, $\xi = 1$

$$\theta(X_\infty, y) = 2\log\left(\frac{\cosh\sigma}{\cosh\sigma y}\right)$$

with $\delta = 2\sigma^2 \mathrm{sech}^2\sigma$.

Note that

$$y = \eta + (1-\gamma)\eta^2 - (1-\gamma)\eta^3 . \qquad \text{(see section 4.2)}$$

On using the boundary conditions, the finite-difference scheme results in $[M.N_s + (M-1).(N-N_s)]$ system of nonlinear equations which can be expressed in matrix form as

$$A\underset{\sim}{\theta} = \underset{\sim}{d} \qquad (4.4.1)$$

where $\underset{\sim}{\theta}$ is a vector representing the unknown temperature at the grid points within the region (see Figure 4.4), such that

$$\underset{\sim}{\theta} = (\theta_{1,1},\ldots,\theta_{1,M};\ldots;\theta_{N_s,1},\ldots,\theta_{N_s,M};\theta_{N_s+1,1},\ldots,\theta_{N_s+1,M-1};\ldots;\theta_{N,1},\ldots,\theta_{N,M-1})^T$$

Writing

$$\underset{\sim}{d} = \underset{\sim}{d}_1 + \underset{\sim}{d}_2$$

where $\underset{\sim}{d}_1$ and $\underset{\sim}{d}_2$ contains the contributions due to the nonlinear terms and boundary conditions (at $x = X_\infty$) respectively, namely

$$\underset{\sim}{d} = -(\Delta\xi)^2\delta \begin{bmatrix} e^{\theta_{1,1}} \\ \vdots \\ e^{\theta_{1,M}} \\ \hline \approx \\ \hline e^{\theta_{N_s,1}} \\ \vdots \\ e^{\theta_{N_s,M}} \\ \hline e^{\theta_{N_s+1,1}} \\ \vdots \\ e^{\theta_{N_s+1,M-1}} \\ \hline \approx \\ \hline e^{\theta_{N,1}} \\ \vdots \\ e^{\theta_{N,M-1}} \end{bmatrix} - \begin{bmatrix} 0 \\ \hline \approx \\ \hline 0 \\ \hline 0 \\ \hline \approx \\ \hline \phi_1 \\ \vdots \\ \phi_{M-1} \end{bmatrix}$$

where $\phi \equiv \theta(X_\infty, y)$, the boundary condition at $x = X_\infty$

$$= \theta_{N+1,j} \qquad j = 1(M-1).$$

However, A is the coefficient matrix of the form

$$A = \begin{bmatrix} B_1 & C_1 & & & & & & & & \\ G_2 & B_2 & C_2 & & & & & & & \\ & \cdot & \cdot & \cdot & & & & & & \\ & & \cdot & \cdot & \cdot & & & & & \\ & & & G_{N_s} & B_{N_s} & C_{N_s} & & & & \\ & & & & G_{N_s+1} & B_{N_s+1} & C_{N_s+1} & & & \\ & & & & & \cdot & \cdot & \cdot & & \\ & & & & & & \cdot & \cdot & \cdot & \\ & & & & & & & G_{N-1} & B_{N-1} & C_{N-1} \\ & & & & & & & & G_N & B_N \end{bmatrix}$$

where $\underset{\sim}{B}_\kappa$'s are tri-diagonal matrices of order $(M \times M)$ for $1 \leqslant \kappa \leqslant N_s$ and of order $[(M-1)\times(M-1)]$ for $N_s < \kappa \leqslant N$, namely

$$\underset{\sim}{B}_\kappa = \begin{bmatrix} b^\kappa_{1,1} & b^\kappa_{1,2} & & & & \\ b^\kappa_{2,1} & b^\kappa_{2,2} & b^\kappa_{2,3} & & & \\ & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ & & & b^\kappa_{j-1,j-2} & b^\kappa_{j-1,j-1} & b^\kappa_{j-1,j} \\ & & & & b^\kappa_{j,j-1} & b^\kappa_{j,j} \end{bmatrix}$$

with

$$b^{\kappa}_{j,j} = -\left\{\frac{1}{(x_\xi)_\kappa}\left[\frac{1}{(x_\xi)_{\kappa+\frac{1}{2}}} + \frac{1}{(x_\xi)_{\kappa-\frac{1}{2}}}\right] + \left(\frac{\Delta\xi}{\Delta\eta}\right)^2 \frac{1}{(y_\eta)_j}\left[\frac{1}{(y_\eta)_{j+\frac{1}{2}}} + \frac{1}{(y_\eta)_{j-\frac{1}{2}}}\right]\right\}$$

$$j = \begin{cases} 1(M) & \text{for} \quad 1 \leqslant \kappa \leqslant N_s \\ 1(M-1) & \text{for} \quad N_s < \kappa \leqslant N \end{cases}$$

$$b^{\kappa}_{1,2} = \left(\frac{\Delta\xi}{\Delta\eta}\right)^2 \frac{1}{(y_\eta)_2}\left[\frac{1}{(y_\eta)_{3/2}} + \frac{1}{(y_\eta)_{\frac{1}{2}}}\right] \quad \forall \kappa \geqslant 1$$

$$b^{\kappa}_{j,j+1} = \left(\frac{\Delta\xi}{\Delta\eta}\right)^2 \frac{1}{(y_\eta)_j (y_\eta)_{j+\frac{1}{2}}}$$

where

$$j = \begin{cases} 2(M-1) & \text{for} \quad 1 \leqslant \kappa \leqslant N_s \\ 2(M-2) & \text{for} \quad N_s < \kappa \leqslant N \end{cases}$$

$$b^{\kappa}_{j,j-1} = \left(\frac{\Delta\xi}{\Delta\eta}\right)^2 \frac{1}{(y_\eta)_j (y_\eta)_{j-\frac{1}{2}}} \qquad \begin{matrix} j = 2(M-1) & 1 \leqslant \kappa \leqslant N_s \\ j = 2(M-2) & \kappa > N_s \end{matrix}$$

$$b^{\kappa}_{p,p-1} = \left(\frac{\Delta\xi}{\Delta\eta}\right)^2 \frac{1}{(y_\eta)_p}\left[\frac{1}{(y_\eta)_{p+\frac{1}{2}}} + \frac{1}{(y_\eta)_{p-\frac{1}{2}}}\right]$$

with

$$p = \begin{cases} M & \text{for} \quad 1 \leqslant \kappa \leqslant N_s \\ M-1 & \text{for} \quad N_s < \kappa \leqslant N \end{cases}$$

C_κ's represent diagonal matrices with all the elements equal to $C^{(\kappa)}$ such that

$$C^{(\kappa)} = \begin{bmatrix} c^{(\kappa)} & & \\ & c^{(\kappa)} & \\ & & c^{(\kappa)} \end{bmatrix}$$

with

$$c^{(1)} = \frac{1}{(x\ )_1} \left[\frac{1}{(x\ )_{3/2}} + \frac{1}{(x\ )_{1/2}} \right]$$

and

$$c^{(\kappa)} = \frac{1}{(x_\xi)_\kappa \ (x_\xi)_{\kappa+\frac{1}{2}}} \qquad \kappa = 2(N-1)$$

$G_{\kappa+1}$'s represent the sub-diagonal matrices of A such that

$$G^{(\kappa)} = \begin{bmatrix} g^{(\kappa)} & & & \\ & \cdot & & \\ & & \cdot & \\ & & & \cdot \\ & & & & g^{(\kappa)} \end{bmatrix}$$

with $$g^{(\kappa)} = \frac{1}{(x_\xi)_{\kappa+1} (x_\xi)_{\kappa+\frac{1}{2}}} \qquad \kappa = 1(N-1).$$

Note that dimensions of C_κ's and $G_{\kappa+1}$'s are given by

(i) $(M \times M)$ for $1 \leqslant \kappa \leqslant (N_s-1)$

(ii) $(M-1)\times(M-1)$ for $N_s \leqslant \kappa \leqslant (N-1)$

4.5 Conclusions

The finite-difference scheme developed in this chapter is applicable to any partial differential equation with spatial coordinates. However, in our case, emphasis has been on developing the system of equations for the slab problem with insulation. Details of the computational procedure and the nature and form of the grid spacing in both the y and x directions will be discussed in Chapter Five. It is apparent that more analysis of the finite-difference equations is required in order to obtain the solution.

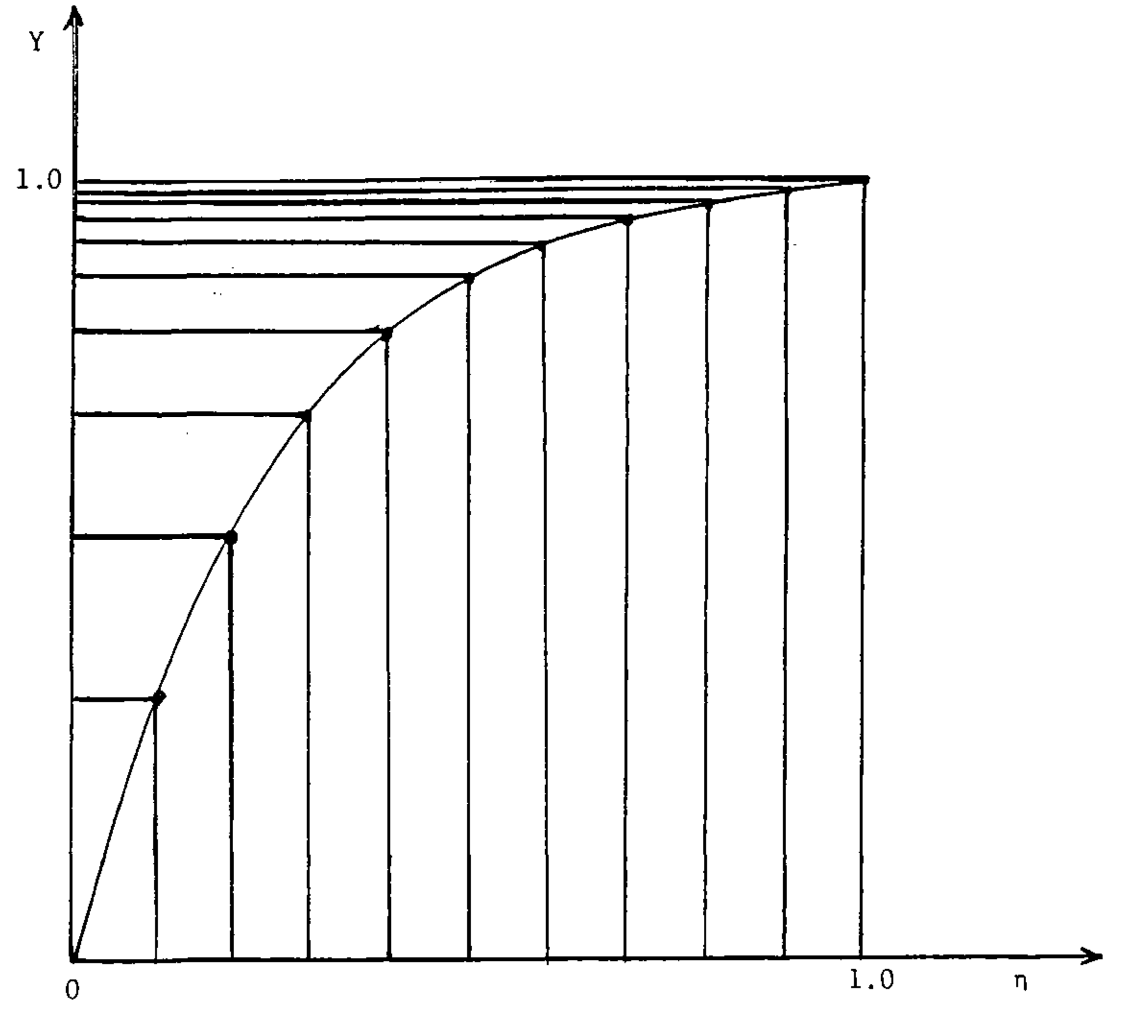


Figure 4.2: Distribution of grid points required in Y-direction

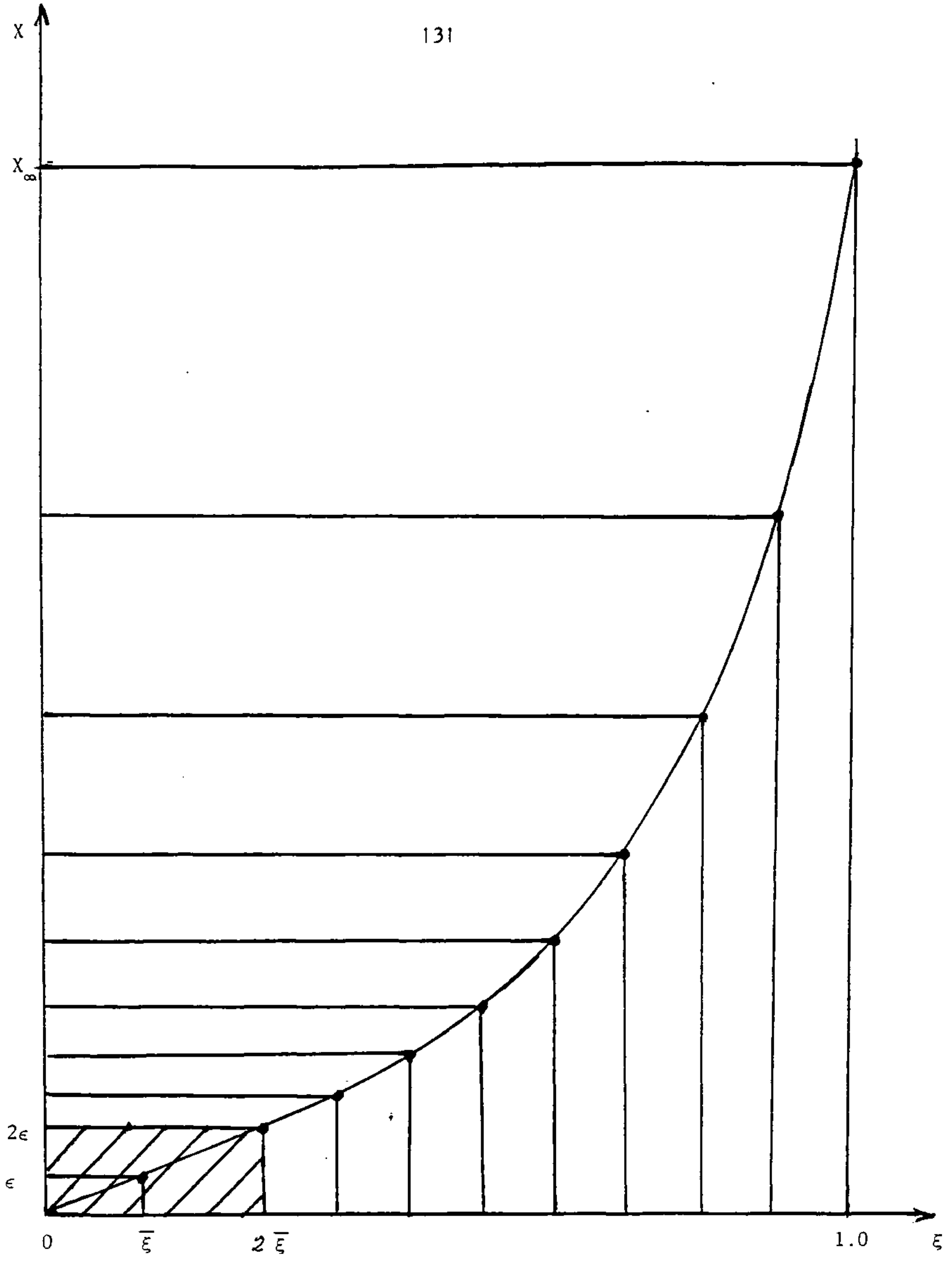


Figure 4.3: The required grid distribution in the X-direction with $0 \leqslant \xi \leqslant \bar{\xi}$ being in the region in the ξ-plane occupied by the insulation. The shaded region represents regular grid intervals in the X-direction.

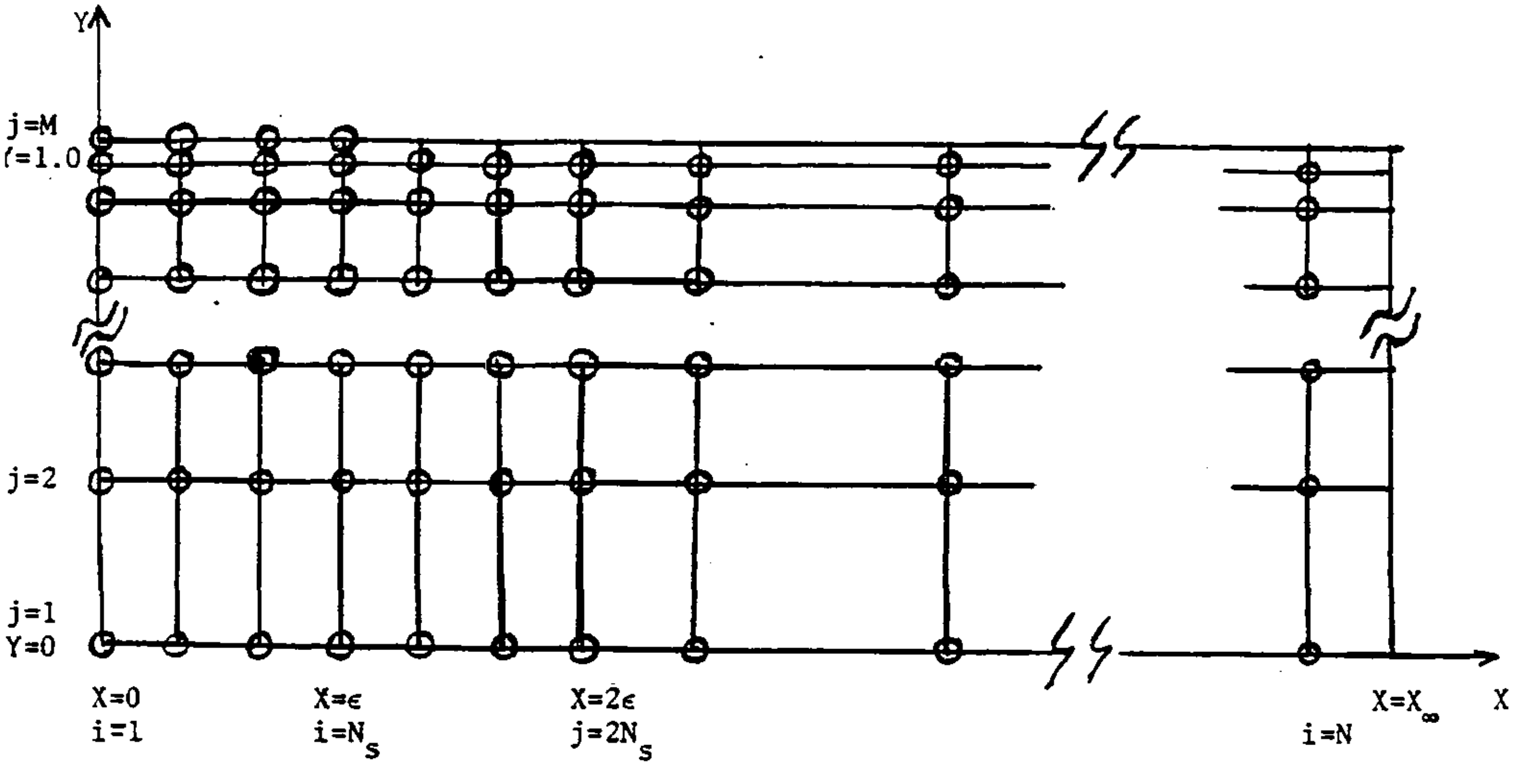


Figure 4.4: The circled points in the domain of differentiation represent the nature and form of the grid points in the X-Y plane. Extra grid points are generated to take into account the Neumann boundary conditions at

(i) $y = 1, \quad x < \epsilon$

(ii) $y = 0, \quad \forall x$

(iii) $x = 0, \quad \forall y$

CHAPTER FIVE: NUMERICAL SOLUTION OF THE FINITE DIFFERENCE SYSTEM OF EQUATIONS

5.0 INTRODUCTION

We seek to determine numerically the critical conditions for the onset of thermal instability of the slab defined in Chapter Two. Using the finite-difference system of equations developed in Chapter Four, we want to obtain the critical Frank-Kamenetskii parameter $\delta_c(\epsilon)$ as a function of ϵ, the dimensionless insulation length. Normally Newtonian methods have been used to solve similar systems of equations. Of importance to us, is the determination of the relationship between $\delta_c(\epsilon)$ and ϵ, especially for $\epsilon \cong 0(1)$, since no perturbation analysis is possible for ϵ of this order of magnitude. However, computational results for $\delta_c(\epsilon)$ for $\epsilon \ll 1$ and $\epsilon \gg 1$, will provide comparisons with the predictions of the perturbation analysis given in Chapter Two.

5.1 Direct Newtonian Method

We now consider the finite-difference formulation contained in Chapter Four by putting

$$\underline{f}(\underline{\theta}) \equiv A\underline{\theta} - \underline{d} = 0 \qquad (5.1.1)$$

where A and $\underline{d}$ are matrices as defined in section 4.4.

In order for us to employ a Newtonian scheme, we need to define a correction vector $\Delta\underline{\theta}^n$, namely

$$\Delta\underline{\theta}^n = \underline{\theta}^{n+1} - \underline{\theta}^n \tag{5.1.2}$$

where n denotes the n^{th} iteration. On combining equations (5.1.1) and (5.1.2), we get

$$\underline{f}(\underline{\theta}^n + \Delta\underline{\theta}^n) = 0 \tag{5.1.3}$$

Expanding equation (5.1.3) as a Taylor series in powers of $\Delta\underline{\theta}^n$, we obtain

$$\underline{f}(\underline{\theta}^n) + \underline{f}'(\underline{\theta}^n).\Delta\underline{\theta}^n + \ldots = 0 \tag{5.1.4}$$

where

$$\underline{f}'(\theta) = \left[\frac{\partial f_p}{\partial \theta_q}(\underline{\theta})\right]$$

$$= \begin{bmatrix} \frac{\partial f_1}{\partial \theta_1} & \frac{\partial f_1}{\partial \theta_2} & \cdots\cdots & \frac{\partial f_1}{\partial \theta_r} \\ \frac{\partial f_2}{\partial \theta_1} & \frac{\partial f_2}{\partial \theta_2} & & \frac{\partial f_2}{\partial \theta_r} \\ \vdots & \vdots & & \vdots \\ \frac{\partial f_r}{\partial \theta_1} & \frac{\partial f_r}{\partial \theta_2} & \cdots\cdots & \frac{\partial f_r}{\partial \theta_r} \end{bmatrix}$$

where r corresponds to the number of the equations. If a_{pq} denotes the elements of the coefficient matrix A, then

$$f_p(\theta_q) = \sum_q a_{pq}\theta_q - d_p(\theta_q) ,$$

and hence

$$\frac{\partial f_p(\underline{\theta})}{\partial \theta_q} = a_{pq} - \delta_{pq} \frac{\partial}{\partial \theta_q} (d_p(\underline{\theta})$$

where δ_{pq} is the normal Kronecker delta, namely,

$$\delta_{pq} = \begin{cases} 1 & \text{if} \quad p = q \\ 0 & \text{if} \quad p \neq q \end{cases}$$

Using the definition of $\underline{d}$ in section 4.4, we obtain

$$\frac{\partial f_p(\underline{\theta})}{\partial \theta_q} = a_{pq} + (\Delta\xi)^2 \delta \exp(\theta_p)$$

Finally equation (5.1.4) becomes

$$J(\underline{\theta}^n)\Delta\underline{\theta}^n = - \underline{f}(\underline{\theta}^n) \tag{5.1.5}$$

where the Jacobian matrix $J(\underline{\theta})$ is given by

$$J(\underline{\theta}) = A + (\Delta\xi)^2 \delta \, \mathrm{diag}[\exp(\underline{\theta})]$$

where 'diag[exp($\underline{\theta}$)]' defines a diagonal matrix with elements equal exp(θ). We note that the non-linear terms of the energy equation (4.1.4) only occur in the principal diagonal of the Jacobian matrix, $J(\underline{\theta})$. Consequently the elements of $J(\theta)$ are equal to the elements of the coefficient matrix A except for principal diagonal elements which now become

$$b^{\kappa}_{i,i} = (\Delta\xi)^2 \delta \exp(\theta_{\kappa,i}) - \frac{1}{(x_\xi)_\kappa} \left[\frac{1}{(x_\xi)_{\kappa+\frac{1}{2}}} + \frac{1}{(x_\xi)_{\kappa-\frac{1}{2}}} \right]$$

$$- \left(\frac{\Delta\xi}{\Delta\eta}\right)^2 \frac{1}{(y_\eta)_i} \left[\frac{1}{(y_\eta)_{i+\frac{1}{2}}} + \frac{1}{(y_\eta)_{i-\frac{1}{2}}} \right]$$

$$\text{with} \qquad i = \begin{cases} 1(M) & \text{for} \quad 1 \leqslant \kappa \leqslant N_s \\ 1(M-1) & \text{for} \quad N_s < \kappa \leqslant N \end{cases}$$

(see Section 4.4 for details).

The critical condition for the onset of thermal instability occurs when the Jacobian matrix, $J(\underline{\theta})$, becomes singular. Ideally we seek a solution of (5.1.5) for the case when the determinant, D, of the Jacobian matrix vanishes. However, at criticality, the inverse of the Jacobian matrix is undefined and hence the Newtonian scheme will lead to failure in computation. To avoid this difficulty, we instead seek to solve (5.1.5) with δ chosen as close as possible to the critical δ but with $J(\underline{\theta})$ remaining non-singular. Thus by a Block Tri-diagonal solver or computer library facility we determine the approximate solution to (5.1.5) and consequently we then evaluate the determinant D. Hence for various values of δ we compute the corresponding determinants and from a plot of D versus δ, seek to approximate the critical values of δ corresponding to the case when $D \equiv 0$.

Computational Procedure:-

For small values of the insulation length, say, $\epsilon \ll 1$, we expect $\delta_c(\epsilon)$ to be approximated by $\delta_c(0)$, where $\delta_c(0) = 0.878$. Hence for $\epsilon \ll 1$, say $\epsilon = 0.01$, we consider the following procedure for numerical computation of the critical Frank-Kamenetskii parameter,

(1) At $\delta = 0$, the inert problem, after computing the approximate $\underline{\theta}$ solution, we evaluate the corresponding determinant, say D_0.

(2) Next we choose $\delta = \delta_1$ such that δ_1 is as close as possible to the critical δ but at the same time $J(\underline{\theta})$ remaining non-singular. Choosing $\delta_1 = 0.8$, we compute D_1, the corresponding determinant.

(3) Increasing δ_1 by a small increment $\Delta\delta$, we get δ_2 and finally D_2. Because of instability problems during computation, we select $\Delta\delta$ such that $\Delta\delta = 0.0025$. Thus $\delta_2 = 0.8025$.

(4) Similarly $\delta_3 = 0.805$ and hence the corresponding determinant is D_3.

(5) From a plot of D vs. δ , the critical conditions for thermal instability can be approximated by passing through these points a simple quadratic polynomial of the form

$$\delta = a_0 + a_1\overline{D} + a_2\overline{D}^2 ,$$

where $\overline{D} = (D/D_0)$. The determinants D_1, D_2 and D_3 were scaled by D_0 to overcome 'over-flow' problems in computations on the computer due to the large magnitudes of the determinants.

On fitting the curve through these points, see Figure 5.1, we obtain the suspected critical δ, namely $\delta_c^{(1)}(\epsilon)$, the value corresponding to the value $\delta(\overline{D} = 0) = a_0$. This value $\delta_c^{(1)}(\epsilon)$, is the value of δ that results in a singular Jacobian matrix, and hence the limit for the convergence of the iterative scheme.

Taking an appropriate weighting between $\delta_c^{(1)}(\epsilon)$ and δ_3, we evaluate δ_4 and consequently we compute the scaled determinant $\overline{D}_4$. Through these points, in the $\overline{D}$ - δ plane, we fit a cubic polynomial of the form

$$\delta = a_0 + a_1\overline{D} + a_2\overline{D}^2 + a_3\overline{D}^3 \quad ,$$

and we label $\delta_c^{(2)}(\epsilon)$ this new value of a_0. Again taking the weighting between $\delta_c^{(2)}(\epsilon)$ and δ_4, we obtain δ_5. The above procedure is repeated until a desired criterion of convergence is met, namely

$$|\delta_c^{(n)}(\epsilon) - \delta_{n+2}| < 10^{-\alpha} \quad , \quad \alpha > 0$$

α represents the degree of accuracy required.

Discussion of the Direct Newton's Method

The afore-mentioned computational procedure for determining $\delta_c(\epsilon)$ can be repeated for different ϵ values. This method offers a relatively simple and easy procedure for determining the critical Frank-Kamenetskii parameter corresponding to a singular Jacobian matrix, $J(\underline{\theta})$. The main advantage of this curve fitting scheme is that it is both simple and easy to implement. For a well behaved curve of $\overline{D}$ vs. δ, the method can be cheap, since few points will be enough to achieve the desired accuracy of $\delta_c(\epsilon)$.

However, in the neighbourhood of the critical δ, the computations tend to become unstable. This difficulty is partially resolved by choosing successively smaller increments of δ. Unfortunately, in our case, the computations became unstable even for δ values far away from the critical δ. For example for $\epsilon = 0.01$, the computation became unstable for $\delta > 0.6$, whereas the critical δ is expected to be close to $\delta_c(0)$. Attempts to resolve this difficulty by reducing further the step size of δ resulted in the computed determinants remaining almost unchanged despite changes in δ. These small changes in $\overline{D}$'s make curve fitting both unreliable and expensive in predicting the critical δ. Infact, we anticipate for moderate values of ϵ and large number of grid points, the scheme will result in unacceptable large computing time. We however note that this scheme, for $\epsilon = 0.01$, gives results for the critical δ of the correct order of magnitude.

5.2 Quasi-Newtonian Methods

In order for us to solve equation (5.1.5), and simultaneously avoid the singular behaviour exhibited at criticality by the Jacobian matrix in (5.1.5), we consider the following modified system of equations,

$$\underline{F}(\underline{\theta},\delta) = \begin{bmatrix} \underline{g}(\underline{\theta},\delta) \\ f(\underline{\theta},\delta) \end{bmatrix} = 0 \qquad (5.2.0)$$

with

$$\underline{F} : \mathbb{R}^{n+m} \rightarrow \mathbb{R}^{n+m}$$
$$\underline{f} : \mathbb{R}^{n} \rightarrow \mathbb{R}^{n-m}$$
$$\underline{g} : \mathbb{R}^{m} \rightarrow \mathbb{R}^{m}$$

where m represents the number of singularities of $\underline{f}(\underline{\theta},\delta)$. However, since we are dealing with a simple turning point problem (see Figure 1.2), we expect the system of equations to exhibit one singularity at $\delta = \delta_c(\epsilon)$. Hence m is equal to unity. The function $\underline{g}(\underline{\theta},\delta)$, here represents an auxiliary condition, required so that the Jacobian matrix of $\underline{F}(\underline{\theta},\delta)$ will remain non-singular for all values of δ including $\delta = \delta_c(\epsilon)$.

We now define the correction vector $\Delta\underline{\theta}^{\kappa}$ and $\Delta\delta^{\kappa}$ by putting

$$\Delta\underline{\theta}^{\kappa} = \underline{\theta}^{\kappa+1} - \underline{\theta}^{\kappa}$$

and (5.2.1)

$$\Delta\delta^{\kappa} = \delta^{\kappa+1} - \delta^{\kappa}$$

where κ refers to the κ^{th} iteration. On combining equations (5.2.0) and (5.2.1), we obtain

$$\underline{F}(\underline{\theta}^{\kappa}+\Delta\underline{\theta}^{\kappa}, \delta^{\kappa}+\Delta\delta^{\kappa}) = 0 \quad .$$

Expanding $\underline{F}$ as a Taylor series in powers of $\Delta\underline{\theta}^{\kappa}$ and $\Delta\delta$, we get

$$\nabla_{\underline{\theta}} \underline{F}(\underline{\theta}^{\kappa},\delta^{\kappa})\Delta\underline{\theta}^{\kappa} + \nabla_{\delta} \underline{F}(\underline{\theta}^{\kappa},\delta^{\kappa})\Delta\delta^{\kappa} = - \underline{F}(\underline{\theta}^{\kappa},\delta^{\kappa}) \qquad (5.2.2)$$

Elaborating on equation (5.2.2), we obtain

$$[\underline{F}_{\underline{\theta},\delta}(\theta^K,\delta^K)]\ [\Delta\underline{\theta}^K,\Delta\delta^K]^T = -\ [g,\underline{f}]^T \qquad (5.2.3)$$

where $\underline{F}_{\underline{\theta},\delta}(\underline{\theta}^K,\delta^K)$ is given by

$$\underline{F}_{\underline{\theta},\delta}(\underline{\theta},\delta) = \begin{pmatrix} \nabla_{\underline{\theta}}{}^T g(\underline{\theta},\delta) & , & \nabla_\delta g(\underline{\theta},\delta) \\ \nabla_{\underline{\theta}}\underline{f}(\underline{\theta},\delta) & , & \nabla_\delta \underline{f}(\underline{\theta},\delta) \end{pmatrix}$$

Thus $\underline{F}_{\underline{\theta},\delta}(\underline{\theta},\delta)$ represents the overall (n+1) square Jacobian matrix of equation (5.2.0). Because vector $\underline{f}(\underline{\theta},\delta)$ is known explicitly its derivatives can be obtained analytically and are given by:-

$$\nabla_{\underline{\theta}}\underline{f}(\underline{\theta},\delta) \equiv J(\underline{\theta}) \quad ,$$

the original n-square matrix defined by the iterative scheme in equation (5.1.5). The elements of the n-vector $\nabla_\delta\underline{f}(\underline{\theta},\delta)$ are also explicitly known and are given by

$$\nabla_\delta\underline{f}(\underline{\theta},\delta) = -(\Delta\xi)^2 \exp(\underline{\theta}) + \frac{\partial}{\partial\delta}(\underline{d}_2) \quad .$$

We note from Chapter Four that all the elements of $\underline{d}_2$ are identically equal to zero except for the last row-block, representing the imposed boundary condition at $x = X_\infty$. (For details see Chapter Four).

Finally

$$\nabla_{\delta}\underline{f}(\underline{\theta},\delta) = -(\Delta\xi)^2 \begin{bmatrix} e^{\theta_{1,1}} \\ \vdots \\ e^{1,M} \\ \hline \vdots \\ \hline e^{\theta_{\kappa-1,1}} \\ \vdots \\ e^{\theta_{\kappa-1,M-1}} \\ \hline e^{\theta_{\kappa,1}} \\ \vdots \\ e^{\theta_{\kappa,M-1}} \end{bmatrix} - \begin{bmatrix} 0 \\ \hline \vdots \\ \hline 0 \\ \hline \nabla_{\delta}\phi_1 \\ \vdots \\ \nabla_{\delta}\phi_{M-1} \end{bmatrix}$$

with

$$\nabla_{\delta}\underline{\phi} = \frac{(\tanh\sigma - y\tanh\sigma y)}{2\sigma \operatorname{sech}^2\sigma(1-\sigma\tanh\sigma)} \quad . \qquad (5.2.4)$$

The suffixes κ and M represent the number of grid points in the x and y directions respectively.

Although the original Jacobian matrix, $\nabla_{\underline{\theta}}\underline{f}(\underline{\theta},\delta)$ becomes singular at criticality, we seek to choose an appropriate scalar function $g(\underline{\theta},\delta)$ such that the overall Jacobian matrix $\underline{F}_{\underline{\theta},\delta}(\underline{\theta},\delta)$ will remain non-singular throughout the entire computation for all values of δ including the critical value of δ. Hence we now put

$$g(\underline{\theta},\delta) = \det[\nabla_{\underline{\theta}}\ \underline{f}(\underline{\theta},\delta)] \qquad (5.2.5)$$

This choice of the auxiliary function $g(\underline{\theta},\delta)$ is both convenient and consistent with our definition of the vector $\underline{F}(\underline{\theta},\delta)$ in equation (5.2.0). This is because the determinant of the matrix $\nabla_{\underline{\theta}}\, \underline{f}(\underline{\theta},\delta)$ vanishes when δ equals to the critical value of the Frank-Kamenetskii parameter. Consequently the iterative scheme of equation (5.2.3) will yield the critical value of δ as part of its solution.

In solving equation (5.2.3), difficulties arise when we attempt to update the boundary condition at $x = X_\infty$. This is because the boundary condition is not known explicitly as a function δ but is instead given by

$$\theta(\infty,y) = 2\log\left(\frac{\cosh\sigma}{\cosh\sigma y}\right) \quad ,$$

with

$$\delta = 2\sigma^2 \operatorname{sech}^2\sigma \quad .$$

Further difficulties will arise when we seek to evaluate the elements of the vector $\nabla_{\delta}\underline{\phi}$ in equation (5.2.4). This is because, for small values of ϵ, $\sigma\tanh\sigma \sim 1$. To avoid these difficulties, we replace δ by σ as the unknown parameter in (5.2.3). Hence equation (5.2.3) becomes

$$[\underline{F}_{\underline{\theta},\sigma}(\underline{\theta}^K,\delta^K)][\Delta\underline{\theta}^K,\Delta\sigma^K]^T = -\,[g,\underline{f}]^T \qquad (5.2.6)$$

with $$\underline{F}_{\underline{\theta},\sigma}(\underline{\theta},\delta) = \begin{pmatrix} \nabla_{\underline{\theta}}{}^T g(\underline{\theta},\delta) & , & \nabla_\sigma g(\underline{\theta},\delta) \\ \nabla_{\underline{\theta}}\, \underline{f}(\underline{\theta},\delta) & , & \nabla_\sigma \underline{f}(\underline{\theta},\delta) \end{pmatrix} ,$$

and $$\nabla_\sigma \, \underline{f}(\underline{\theta},\delta) = -\,(\Delta\xi)^2 \exp(\underline{\theta}) \cdot \frac{d\delta}{d\sigma} + \frac{\partial}{\partial\sigma} \quad (\underline{d}_2)$$

$$= -\,(\Delta\xi)^2 \frac{d\delta}{d\sigma} \begin{bmatrix} e^{\theta_{1,1}} \\ \vdots \\ e^{\theta_{1,M}} \\ \hline \vdots \\ \hline e^{\theta_{\kappa-1,1}} \\ \vdots \\ e^{\theta_{\kappa-1,M-1}} \\ \hline e^{\theta_{\kappa,1}} \\ \vdots \\ e^{\theta_{\kappa,M-1}} \end{bmatrix} \quad \begin{bmatrix} 0 \\ \hline \vdots \\ \hline 0 \\ \hline \nabla_\sigma \phi_1 \\ \\ \nabla_\sigma \phi_{M-1} \end{bmatrix}$$

with $$\frac{d\delta}{d\sigma} = 4\sigma(1-\sigma\tanh\sigma)\operatorname{sech}^2\sigma,$$

and $$\nabla_\sigma \underline{\phi} = 2(\tanh\sigma - y\tanh\sigma y).$$

Equation (5.2.6) can be solved by using computer library facilities. For a given value of ϵ, we suggest the following computational procedure:-

(1) We choose our starting vector $(\underline{\theta}^0,\sigma^0)$ with $(\underline{\theta}^0,\sigma^0)$ being close to the expected critical region.

(2) We then compute the elements of the vector $\underline{\lambda}(\underline{\theta}^0,\sigma^0)$, such that

$$\underline{\lambda}(\underline{\theta},\sigma) = \begin{pmatrix} \nabla_{\underline{\theta}}\, g(\underline{\theta},\sigma) \\ \\ \nabla_{\sigma}\, g(\underline{\theta},\sigma) \end{pmatrix} \tag{5.2.7}$$

- the elements of the differentiation of the determinant with respect to $\underline{\theta}$ and σ.

(3) Thus we now determine the elements of

$$\nabla_{\sigma}\, \underline{f}(\underline{\theta}^0,\sigma^0), \nabla_{\underline{\theta}}\, \underline{f}(\underline{\theta}^0,\sigma^0) \quad \text{and} \quad [g(\underline{\theta}^0,\sigma^0),\ \ \underline{f}(\underline{\theta}^0,\sigma^0)]^T$$

(4) Solution of (5.2.6) will yield the correction vectors $(\Delta\underline{\theta}^0,\Delta\sigma^0)$, and hence we obtain the new starting point $(\underline{\theta}^1,\sigma^1)$, where

$$\underline{\theta}^1 = \underline{\theta}^0 + \Delta\underline{\theta}^0 \quad \text{and} \quad \sigma^1 = \sigma^0 + \Delta\sigma^0 \ .$$

Or generally

$$\begin{aligned} \underline{\theta}^{j+1} &= \underline{\theta}^j + \Delta\underline{\theta}^j \\ \sigma^{j+1} &= \sigma^j + \Delta\sigma^j \end{aligned} \tag{5.2.8}$$

with $j = 0,1,2$, etc.

With the modified value of σ in (5.2.8), we now compare the coresponding value of the Frank-Kamenetskii parameter, namely

$$\delta^{j+1} = 2[\sigma^{j+1}\ \operatorname{sech}\sigma^{j+1}]^2 \ .$$

We now repeat the computational steps (2) to (4) with the vector $(\underline{\theta}^0,\sigma^0)$ now replaced by $(\underline{\theta}^{j+1},\sigma^{j+1})$. The above procedure is continually repeated until a desired criterion of convergence is met, say

$$|g_n/g_0| < 10^{-7}$$

where

$$g_n \equiv g(\underline{\theta}^n,\sigma^n), \qquad \text{[see equation (5.2.5)]} \quad .$$

It is of importance during the computation to check the values and behaviour of;

(i) $|\delta^{j+1}-\delta^j|$

(ii) $\|(g,\underline{f}^T)\|$

(iii) $|\theta^{j+1}-\theta^j|$.

Since the auxiliary function $g(\underline{\theta},\sigma)$ is not known explicitly, it is apparent that the elements of $\underline{\lambda}(\underline{\theta},\sigma)$ can only be determined by numerical differentiation. However, numerical differentiation is both a risky and expensive operation. Thus the computational effort required to evaluate $\underline{\lambda}(\underline{\theta},\sigma)$ will become unacceptably large since $\underline{\lambda}(\underline{\theta},\sigma)$ has to be updated for each and every iteration step. Hence we seek to overcome this difficulty by considering the following methods; Andreas 1 and Andreas 2.

Andreas 1:

In this method, we seek to reduce the computational effort in evaluating $\underline{\lambda}(\underline{\theta},\sigma)$ by using the Broyden's method (see Appendix) to update λ_j to λ_{j+1} by putting

$$\lambda_{j+1} = \lambda_j + (g_{j+1}-g_j-\lambda_j{}^T\binom{\Delta\underline{\theta}^j}{\Delta\sigma^j})\frac{((\Delta\underline{\theta}^j)^T,\Delta\sigma^j)}{\|((\Delta\underline{\theta}^j)^T,\Delta\sigma^j)\|^2} \qquad (5.2.9)$$

Andreas 2:

In this method, we seek to overcome the difficulties in determining the elements of $\underline{\lambda}(\underline{\theta},\sigma)$ in (5.2.7) by considering factorisation of the original Jacobian matrix $J(\underline{\theta})$ (see equation (5.1.5)) after a suitable row and column interchange. Thus we now consider the following factorisation

$$J(\underline{\theta},\delta) = \begin{pmatrix} L(\underline{\theta},\delta) & , & 0 \\ q^T(\underline{\theta},\delta) & , & 1 \end{pmatrix} \begin{pmatrix} R(\underline{\theta},\delta) & , & G(\underline{\theta},\delta) \\ \underline{0} & , & \omega(\underline{\theta},\delta) \end{pmatrix} \qquad (5.2.10)$$

where $R(\underline{\theta},\delta)$ and $L(\underline{\theta},\delta)$ are $(n-1)\times(n-1)$ upper and unitary lower triangular matrices respectively. On combining equations (5.2.10) and (5.2.5), we get

$$g(\underline{\theta},\delta) = \det\left[\begin{pmatrix} L(\underline{\theta},\delta) & , & 0 \\ q^T(\underline{\theta},\delta) & , & 1 \end{pmatrix}\right] \det\left[\begin{pmatrix} R(\underline{\theta},\delta) & , & G(\underline{\theta},\delta) \\ 0 & , & \omega(\underline{\theta},\delta) \end{pmatrix}\right] \qquad (5.2.11)$$

and hence the condition $g(\underline{\theta},\delta) \equiv 0$, implies that $\omega(\underline{\theta},\delta) \equiv 0$.

Hence we seek to solve the following (n+1) system of equations

$$\begin{aligned} \underline{f}(\underline{\theta},\delta) &= 0 \\ \omega(\underline{\theta},\delta) &= 0 \end{aligned} \qquad (5.2.12)$$

The above factorization of the original Jacobian matrix is suggested by Griewank [34]. The advantage in using the above factorization is that by an appropriate choice of null vectors, the scalar function $\omega(\underline{\theta},\delta)$ can be known explicitly and its gradient can then be determined by taking <u>one</u> divided difference. Furthermore, we do not have to do any Broyden updating (see equation (5.2.9)) but can obtain quadratic convergence at the expense of two evaluations of $\nabla_{\underline{\theta},\delta}\underline{f}(\underline{\theta},\delta)$ per step. In [34] Griewank approximates the null vectors by putting

$$u(\underline{\theta},\delta)^T = (-q(\underline{\theta},\delta)^T \, L^{-1}(\underline{\theta},\delta), \, 1), \qquad (5.2.13)$$

and

$$V(\underline{\theta},\delta)^T = (-G(\underline{\theta},\delta)^T \, R^{-T}(\underline{\theta},\delta) \, , \, 1), \qquad (5.2.14)$$

so that

$$\omega(\underline{\theta},\delta) = u(\underline{\theta},\delta)^T \, J(\underline{\theta},\delta) \, V(\underline{\theta},\delta) \qquad (5.2.15)$$

<u>Verification of (5.2.15):</u>

$$u(\underline{\theta},\delta)^T \, J(\underline{\theta},\delta) = [-q^T L^{-1}, 1] \begin{pmatrix} L & , & 0 \\ q^T & , & 1 \end{pmatrix} \begin{pmatrix} R & , & G \\ \underline{0} & , & \omega \end{pmatrix}$$

$$= [\underline{0}, 1] \begin{bmatrix} R & , & G \\ \underline{0} & , & \omega \end{bmatrix}$$

Therefore

$$u^T J(\underline{\theta},\delta)V = [\underline{0},1] \begin{bmatrix} R & , & G \\ \underline{0} & , & \omega \end{bmatrix} \begin{bmatrix} -R^{-1}G \\ 1 \end{bmatrix}$$

$$= [\underline{0},1] \begin{bmatrix} \underline{0} \\ \omega \end{bmatrix}$$

$$\equiv \omega$$

On using Newton's approximation on equation (5.2.11), we obtain

$$\begin{bmatrix} \nabla_{\underline{\theta}}{}^T \omega(\underline{\theta}^K,\delta^K) & , & \nabla_\sigma \omega(\underline{\theta}^K,\delta^K) \\ \nabla_{\underline{\theta}}\, \underline{f}(\underline{\theta}^K,\delta^K) & , & \nabla_\sigma \underline{f}(\underline{\theta}^K,\delta^K) \end{bmatrix} \begin{bmatrix} \Delta\underline{\theta}^K \\ \Delta\sigma^K \end{bmatrix} = - \begin{bmatrix} \omega(\underline{\theta}^K,\delta^K) \\ \underline{f}(\underline{\theta}^K,\delta^K) \end{bmatrix}$$

(5.2.16)

The elements of $\nabla_{\underline{\theta}}\, \underline{f}(\underline{\theta},\delta)$ and $\nabla_\sigma\, \underline{f}(\underline{\theta},\delta)$ are known and are as evaluated in above sections. However, the elements of $\nabla_{\underline{\theta}}\, \omega(\underline{\theta},\delta)$ and $\nabla_\sigma\, \omega(\underline{\theta},\delta)$ can be determined by differentiating equation (5.2.15).

Determination of the elements of $\nabla_{\underline{\theta},\sigma}\, \omega(\underline{\theta},\delta)$

On differentiating equation (5.2.15) with respect to $\underline{\theta}$ and σ, we obtain

$$\nabla_{\underline{\theta},\sigma} \omega = (\nabla_{\underline{\theta},\sigma} u^T)JV + u^T(\nabla_{\underline{\theta},\sigma}J)V + u^TJ(\nabla_{\underline{\theta},\sigma} V)$$

We note

$$J(\underline{\theta},\delta)\ V(\underline{\theta},\delta) = \begin{pmatrix} L & , & 0 \\ q^T & , & 1 \end{pmatrix} \begin{pmatrix} R & , & G \\ \underline{0} & , & \omega \end{pmatrix} \begin{pmatrix} -R^{-1} & G \\ & 1 \end{pmatrix}$$

$$= (\underline{0},\omega)^T$$

but

$$\nabla_{\underline{\theta},\sigma} u^T = [-(\nabla_{\underline{\theta},\sigma} q^TL^{-1}),\ 0]$$

and hence

$$(\nabla_{\underline{\theta},\sigma} u^T)\ J(\underline{\theta},\delta)\ V(\underline{\theta},\delta)$$

$$= [-(\nabla_{\underline{\theta},\sigma} q^TL^{-1}),0][\underline{0},\omega]^T$$

$$\equiv 0.$$

Similarly

$$u^T(\underline{\theta},\delta)\ J(\underline{\theta},\delta)\ (\nabla_{\underline{\theta},\sigma} V(\underline{\theta},\delta))$$

$$\equiv 0.$$

Therefore

$$\nabla_{\underline{\theta},\sigma} \omega(\underline{\theta},\delta) = u^T(\nabla_{\underline{\theta},\sigma}\ \nabla_{\underline{\theta}} \underline{f}(\underline{\theta},\sigma))\ V$$

$$= u^T[\nabla_{\underline{\theta}}(\nabla_{\underline{\theta},\sigma} \underline{f}(\underline{\theta},\delta))].V$$

We now put

$$\Lambda(\underline{\theta},\delta) = \nabla_{\underline{\theta},\sigma}\underline{f}(\underline{\theta},\delta)$$

and hence

$$\nabla_{\underline{\theta},\sigma}\ \omega(\underline{\theta},\delta) = u^T(\underline{\theta},\delta)\ (\nabla_{\underline{\theta}}\ \Lambda(\underline{\theta},\delta))\ V(\underline{\theta},\delta) \qquad (5.2.17)$$

but

$$(\nabla_{\underline{\theta}}\ \Lambda(\underline{\theta},\delta)).V(\underline{\theta},\delta) = \frac{d}{d\alpha}\ \Lambda(\underline{\theta}+\alpha V,\delta)\Big|_{\alpha=0}$$

Finally equation (5.2.17) becomes

$$\nabla_{\underline{\theta},\sigma}\ \omega(\underline{\theta},\delta) = u^T(\underline{\theta},\delta)\ \frac{d}{d\alpha}\ \Lambda(\underline{\theta}+\alpha V,\delta)\Big|_{\alpha=0}$$

$$= u^T(\underline{\theta},\delta)\ \frac{d}{d\alpha}\ (\nabla_{\underline{\theta},\sigma}\underline{f}(\underline{\theta}+\alpha V,\delta)\Big|_{\alpha=0}$$

Therefore

$$\nabla_{\underline{\theta}}\ \omega(\underline{\theta},\delta) = u^T(\underline{\theta},\delta)\ \frac{d}{d\alpha}\ \nabla_{\underline{\theta}}\underline{f}(\underline{\theta}+\alpha V,\delta)\Big|_{\alpha=0} \qquad (5.2.18a)$$

and

$$\nabla_{\sigma}\ \omega(\underline{\theta},\delta) = u^T(\underline{\theta},\delta)\ \frac{d}{d\alpha}\ \nabla_{\sigma}\underline{f}(\underline{\theta}+\alpha V,\delta)\Big|_{\alpha=0} \qquad (5.2.18b)$$

On taking one divided difference, we obtain

$$\nabla_{\underline{\theta}}\ \omega(\underline{\theta},\delta) \cong u^T[\nabla_{\underline{\theta}}\ \underline{f}(\underline{\theta}+\mu V,\delta) - \nabla_{\underline{\theta}}\underline{f}(\underline{\theta},\delta)]/(\mu\|V\|)$$

We note

$$u^T(\underline{\theta},\delta)\ \nabla_{\underline{\theta}}\underline{f}(\underline{\theta},\delta) = (\underline{0},\omega)^T$$

Therefore

$$\nabla_{\underline{\theta}}\ \omega(\underline{\theta},\delta) \cong \{u^T J(\underline{\theta}+\mu V,\delta) - \omega(\underline{\theta},\delta)e_n{}^T\}/(\mu\|V\|) \qquad (5.2.19)$$

where $(\omega(\underline{\theta},\delta)\ e_n{}^T)$ is the nth entry and μ is a small parameter, say $\|\underline{\theta}\|$ multiplied by the square root of the machine precision.

$\nabla_\sigma\ \omega(\underline{\theta},\delta)$ now becomes

$$\nabla_\sigma\ \omega(\underline{\theta},\delta) \cong u^T\{\nabla_\sigma\ \underline{f}(\underline{\theta}+\mu V,\delta) - \nabla_\sigma\ \underline{f}(\underline{\theta},\delta)\}/(\mu\|V\|) \qquad (5.2.20)$$

However, from equation (5.2.6) $\nabla_\sigma\ \underline{f}(\underline{\theta},\delta)$ is given by

$$\nabla_\sigma\ \underline{f} = -\ (\Delta\xi)^2\ \frac{d\delta}{d\sigma}\ .\ \exp(\underline{\theta}) + \frac{\partial}{\partial\sigma}\ [d_2(\sigma,y)]$$

Therefore equation (5.2.20) becomes

$$\nabla_\sigma\ \omega(\underline{\theta},\delta) \cong -\ (\Delta\xi)^2\ \frac{d\delta}{d\sigma}\ .\ \exp(\underline{\theta})[\exp(\mu V)-1]/(\mu\|V\|)$$

or

$$\nabla_\sigma\ \omega(\underline{\theta},\delta) \cong -\ (\Delta\xi)^2[\mu V+\frac{1}{2}\ (\mu V)^2+\ \ldots]\ \exp(\underline{\theta})\ .\ \frac{d\delta}{d\sigma}$$

$$\cong -\ (\Delta\xi)^2(\mu V)\ \frac{d\delta}{d\sigma}\exp(\underline{\theta}) + 0(\mu^2) \qquad (5.2.21)$$

Summary of Andreas 2:

(1) We start our computation from the point $(\underline{\theta}^0, \sigma^0)$, with $(\underline{\theta}^0, \sigma)$ being close to the expected critical condition $(\underline{\theta}_c(\epsilon), \sigma(\epsilon))$.

(2) We then factorize the original Jacobian matrix $J(\underline{\theta}, \delta)$ ($= \nabla_{\underline{\theta}} \; \underline{f}(\underline{\theta}, \delta)$) after a suitable row and column interchange. Thus we have

$$J(\underline{\theta},\delta) = \begin{pmatrix} L(\underline{\theta},\delta) & , & 0 \\ q^T(\underline{\theta},\delta) & , & 1 \end{pmatrix} \begin{pmatrix} R(\underline{\theta},\delta) & , & G(\underline{\theta},\delta) \\ \underline{0} & , & \omega(\underline{\theta},\delta) \end{pmatrix}$$

(3) We now compute the null vectors $u(\underline{\theta}, \delta)$, $V(\underline{\theta}, \delta)$ and the scalar function $\omega(\underline{\theta}, \delta)$, namely

$$u^T(\underline{\theta},\delta) = (-q^T L^{-1}, 1)$$

$$V^T(\underline{\theta},\delta) = (-G^T R^{-T}, 1)$$

and $$\omega(\underline{\theta},\delta) = u^T(\underline{\theta},\delta) J(\underline{\theta},\delta) V(\underline{\theta},\delta)$$

(4) Using equation (5.2.19), we compute the elements of the gradient of $\omega(\underline{\theta}, \delta)$ with respect to the n-vector $\underline{\theta}$ as follows:

When we evaluate the original Jacobian matrix, $J = \nabla_{\underline{\theta}} \underline{f}$, at the neighbouring point $(\underline{\theta} + \mu V, \delta)$, we accumulate the n-vector $u^T(\underline{\theta}, \delta) J(\underline{\theta} + \mu V, \delta)$ and then subtract $\omega(\underline{\theta}, \delta)$ from its last component. On dividing by $(\mu \, \| V \|)$, we obtain the elements of $\nabla_{\underline{\theta}} \, \omega(\underline{\theta}, \delta)$ up to the term of $O(\mu^2)$.

(5) We then evaluate the elements of $\underline{f}(\underline{\theta},\delta)$. The gradient of $\omega(\underline{\theta},\delta)$ with respect to the σ parameter is determined by (5.2.21), namely

$$\nabla_{\sigma}\ \omega(\theta,\delta) = -\ (\Delta\xi)^2 \frac{d\delta}{d\sigma} \cdot [\exp(\underline{\theta})] \cdot (\mu V) \quad ,$$

up to the term of $O(\mu^2)$.

(6) Using computer library facilities, but remembering to exploit the factorization of $J(\underline{\theta},\delta)$, we compute the correction vectors $(\Delta\underline{\theta},\Delta\sigma)$, namely we solve

$$\begin{pmatrix} \nabla_{\underline{\theta}}{}^{T}\omega & , & \nabla_{\sigma}\omega \\ \nabla_{\underline{\theta}}\underline{f} & & \nabla_{\sigma}\underline{f} \end{pmatrix} \begin{pmatrix} \Delta\underline{\theta} \\ \Delta\sigma \end{pmatrix} = - \begin{pmatrix} \omega \\ \underline{f} \end{pmatrix}$$

or

$$\begin{bmatrix} \nabla_{\underline{\theta}}{}^{T}\omega(\underline{\theta},\delta) & , & \nabla_{\sigma}\omega \\ \begin{pmatrix} L & , & 0 \\ q^{T} & , & 1 \end{pmatrix} \begin{pmatrix} R & , & G \\ 0 & , & \omega \end{pmatrix} & , & \nabla_{\sigma}\underline{f} \end{bmatrix} \quad [\Delta\underline{\theta},\Delta\sigma]^{T} = -[\omega,\underline{f}]^{T}$$

(7) After updating $\underline{\theta}$, σ and δ, we repeat steps (2) to (6). This process is repeated until a desired criterion of convergence is met.

5.3 Discussion on the Quasi-Newtonian Methods

Andreas 1:

This method was designed to determine the critical conditions for the onset of thermal ignition for the problem defined in Chapters Two and Four whilst avoiding the pitfalls encountered in implementing the Direct Newton's iterative scheme (5.1.5). However, before we considered implementing Andreas 1 to determine the solution to (5.1.1), we sought to solve a simple but well-known thermal ignition problem such that the corresponding system of finite-difference equations $\underline{f}_1(\underline{\theta},\delta)$ exhibited the same essential characteristics as $\underline{f}(\underline{\theta},\delta)$, namely at the critical value of δ, $\nabla_{\underline{\theta}}\underline{f}_1(\underline{\theta},\delta)$ becomes singular. Infact extensive computational work was done for the one-dimensional self-heating slab problem defined in equation (1.2.5). This problem is equivalent to (5.1.1) when the slab surface is free of insulation, namely the case $\epsilon \equiv 0$.

Details of the Numerical Analysis for the Simple Slab Problem

On using the same numerical analysis as in sections 5.1 and 5.2, we derive the corresponding system of equations for $\underline{f}_1(\underline{\theta},\delta)$. Infact these equations are equivalent to those for $\underline{f}(\underline{\theta},\delta)$ with $\underline{f}(\underline{\theta},\delta)$ now replaced $\underline{f}_1(\underline{\theta},\delta)$. Because of the simple boundary conditions (1.2.5), we can determine the critical value of the Frank-Kamenetskii parameter by either implementing (5.2.3) or (5.2.6). Hence we have

$$\{(\underline{F}_1)_{\underline{\theta},\delta}(\underline{\theta}^{\kappa},\delta^{\kappa})\}\,(\Delta\underline{\theta}^{\kappa},\delta^{\kappa})^T = -\,(g_1,\underline{f}_1)^T \tag{5.3.1}$$

or

$$\{(\underline{F}_1)_{\underline{\theta},\sigma}(\underline{\theta}^{\kappa},\delta^{\kappa})\}\quad(\Delta\underline{\theta}^{\kappa},\Delta\sigma^{\kappa})^T = -\,(g_1,\underline{f}_1)^T \tag{5.3.2}$$

where

$$(\underline{F}_1)_{\underline{\theta},\delta} = \begin{pmatrix} \nabla_{\underline{\theta}}{}^T g_1 & , & \nabla_{\delta} g_1 \\ \nabla_{\underline{\theta}}\underline{f}_1 & , & \nabla_{\delta}\underline{f}_1 \end{pmatrix}$$

or $$(\underline{F}_1)_{\underline{\theta},\sigma} = \begin{pmatrix} \nabla_{\underline{\theta}}{}^T g_1 & , & \nabla_{\sigma} g_1 \\ \nabla_{\underline{\theta}}\underline{f}_1 & , & \nabla_{\sigma}\underline{f}_1 \end{pmatrix}$$

index 'κ' refers to the κth iteration.

The vector function $\underline{f}_1(\underline{\theta},\delta)$ is given by

$$\underline{f}_1(\underline{\theta},\delta) = A_1\underline{\theta} + h^2\delta\exp(\underline{\theta}) \tag{5.3.3}$$
$$\equiv 0.$$

where h is the uniform grid spacing. The coefficient matrix A_1, is a tri-diagonal matrix of the form

$$A_1 = \begin{bmatrix} -2 & 2 & & & & & \\ 1 & -2 & 1 & & & & \\ & 1 & -2 & 1 & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & 1 & -2 & 1 \\ & & & & & 1 & -2 \end{bmatrix}$$

The Jacobian matrix from (5.3.3) is

$$\nabla_{\underline{\theta}}\underline{f}_1 = \begin{bmatrix} B_1 & 2 & & & & & \\ 1 & B_2 & 1 & & & & \\ & 1 & B_3 & 1 & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & 1 & B_{n-1} & 1 \\ & & & & & 1 & B_n \end{bmatrix}$$

where $B_j = -2 + h^2\ \delta\exp(\theta_j)\ \ j = 1(N)$ and N is the number of grid points.

Before computing the solution to (5.3.1) or (5.3.2), we seek to determine the elements of the (n+1) vector $\underline{\lambda}(\underline{\theta}^0,\sigma^0)$ at the starting point of the iteration, namely at the point $(\underline{\theta}^0,\sigma^0)$. These elements can be determined by numerical differentiation, but this is both expensive and risky. However, we note from analytical considerations that the elements of $\nabla_{\underline{\theta}} g_1(\underline{\theta}^0,\sigma^0)$ are of the form

$$\nabla_{\underline{\theta}}\ g_1(\underline{\theta},\sigma) = \underline{\mu}(\underline{\theta}) \cdot \delta^{\tau} \qquad (5.3.4)$$

where $\underline{\mu}(\underline{\theta})$ is a vector representing the exponential factors of $\underline{\theta}$ and τ is a positive integer such that $\tau = 1,2,\ldots,(n-1)$. Thus by conveniently starting our computation at $\delta = 0$, we reduce the computer effort required to obtain the $\underline{\lambda}(\underline{\theta}^0,\sigma^0)$ elements. Hence we only need to compute the scalar $\nabla_{\delta} g_1(\underline{\theta}^0,\sigma^0)$. We then use the Broyden Method to update the $\underline{\lambda}(\underline{\theta},\sigma)$ values at each and subsequent iteration step.

Computational Results for Problem (1.2.5)

With grid mesh sizes 1/4, 1/8, 1/16 and 1/32, the results of the computation are contained in Tables 5.1 and 5.2. We also note that during the computation, the scheme apparently seeks out first the 'critical' value of δ and then the value of the determinant of $\nabla_{\underline{\theta}} \underline{f}_1(\underline{\theta},\delta)$ drops rapidly with subsequent iterations. Infact, the value of determinant diminishes by a factor of 10^{12} within a small number of iteration steps whilst δ remained unchanged up to eight significant figures. The absolute value of $g_1(\underline{\theta},\delta)$ can never vanish during iteration due to the large magnitudes involved. However, we define the critical value of δ as the value of δ at which the determinant of $\nabla_{\underline{\theta}} \underline{f}_1(\underline{\theta},\delta)$ diminishes rapidly whilst δ remains unchanged. Infact at this 'critical' value of δ, the determinant did decrease in magnitude by a factor of order 10^{12}. As can be seen from Tables 5.1 and 5.2, the computed 'critical' value of δ compares favourably with the analytical result, namely $\delta_c = 0.878$.

5.4 Conclusion

Although Andreas 1 predicted the critical value of δ that compares favourably with the analytical result, difficulties arose when we considered the two-dimensional problem. These arose when we sought to determine the elements of $\underline{\lambda}(\underline{\theta}^0,\sigma^0)$ by numerical differentiation. To avoid this difficulty we sought to solve (5.2.6) by arbitrarily defining the elements of $\nabla_{\underline{\theta}} g(\underline{\theta}^0,\sigma^0)$. From the computational work on the one-dimensional problem (1.2.5), we noted that the elements of $\underline{\lambda}(\underline{\theta},\sigma)$ were of the same order of magnitude as $g(\underline{\theta},\sigma)$. Thus we put

$$\nabla_{\underline{\theta}}\, g(\underline{\theta}^0,\sigma^0) = \det[\nabla_{\underline{\theta}}\, \underline{f}(\underline{\theta}^0,\delta)]$$

We had hoped that the Broyden Method would correct the errors introduced in $\underline{\lambda}(\underline{\theta}^0,\sigma^0)$ during subsequent iterations. However, the computation oscillated about the critical δ. To ensure convergence of the iteration scheme it is necessary to consider line-search methods, namely we insist that $\|\underline{f}(\underline{\theta})\|^2 + \gamma^2 g^2 \ll 1$, where γ can be chosen such that $1/\gamma = g_0 \equiv \det\{\nabla_{\underline{\theta}}\, \underline{f}(\underline{\theta}^0,\sigma^0)\}$, the value of the determinant at the starting point of iteration. Infact Griewank [34] does suggest schemes that might ensure convergence of the iterative scheme. Furthermore, we can still obtain approximate critical values of δ for various ϵ values by using graphical method as in Section 5.1. We do not anticipate difficulties in determining the critical δ values since the computed δ and g values are in the neighbourhood of the critical region. The main disadvantage of the graphical method is that we no longer have control of the progress of the computation as in Section 5.1. However, the data obtained will be sufficient to determine the critical δ from a plot of g versus δ.

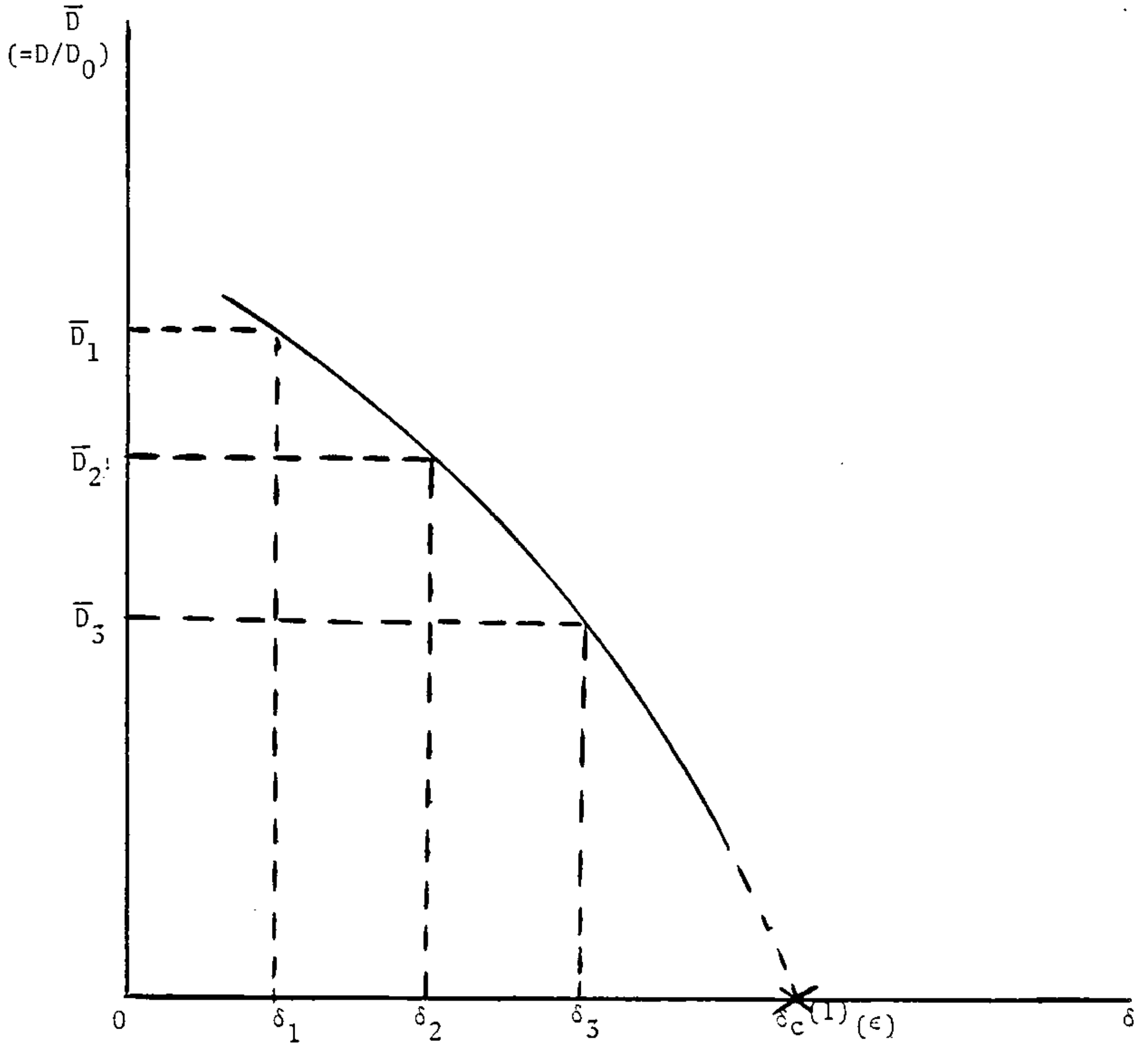
However, we hope that implementation of Andreas 2 will overcome the difficulties encountered in Andreas 1, since we no longer need to compute the $\underline{\lambda}(\underline{\theta},\sigma)$ elements.

Table 5.1: Values of the scaled determinant $\bar{g} = (g/g_0)$ for various grid mesh sizes.

NUMBER OF ITERATIONS	h = 1/4 $\bar{g}$	h = 1/8 $\bar{g}$	h = 1/16 $\bar{g}$	h = 1/32 $\bar{g}$
1	1.00	1.00	1.00	1.00
2	-0.66	-0.64	-0.64	-0.64
3	0.14	0.15	0.18	0.12
4	0.37	-0.11	0.74×10^{-1}	0.88×10^{-2}
5	0.25×10^{-1}	0.10×10^{-1}	-0.31×10^{-1}	-0.52×10^{-3}
6	0.23×10^{-1}	0.18×10^{-2}	-0.95×10^{-2}	0.65×10^{-4}
7	-0.29×10^{-1}	-0.23×10^{-3}	-0.32×10^{-3}	0.10×10^{-5}
8	-0.72×10^{-5}	0.73×10^{-6}	0.72×10^{-5}	-0.25×10^{-9}
9	0.59×10^{-6}	0.90×10^{-8}	0.25×10^{-6}	0.87×10^{-12}
10	0.75×10^{-7}	-0.87×10^{-10}	-0.39×10^{-9}	0.84×10^{-13}
11	-0.32×10^{-12}	0.85×10^{-13}		
12		-0.57×10^{-13}		
13				

Table 5.2

NUMBER OF ITERATIONS	COMPUTED δ VALUES h = 1/4	h = 1/8	h = 1/16	h = 1/32
1	2.0000	2.0000	2.0000	2.0000
2	1.2150	1.2543	1.3927	0.9531
3	0.9127	0.8700	0.8033	0.8843
4	0.9683	0.8847	0.8807	0.87840
5	0.8663	0.8767	0.8780	0.87835
6	0.8717	0.8767	0.8780	0.87835
7	0.8712	0.8767	0.8780	0.87835



$$\delta = a_0 + a_1\overline{D} + a_2\overline{D}^2$$

Figure 5.1: Graph of $\overline{D}$ vs. δ

APPENDIX

6.0 Coordinate Stretching in the x-direction

As discussed in Chapter Four, our choice of coordinate stretching in the x-direction is dictated by two main considerations:

(i) We expect rapid temperature changes to occur within the slab in the region $x \sim \epsilon$ and $y \sim 1$. Hence it is imperative to have very small grid intervals in this region. Consequently, we seek to determine the mapping function $x = X(\xi)$ such that we have uniform grid intervals in the region $0 \leqslant X \leqslant 2\epsilon$ or $0 \leqslant \xi \leqslant 2\bar{\xi}$, see Figure 4.3. This choice of the region with uniform grid spacings allows the temperature to settle down before the introduction of non-uniform grid intervals.

(ii) We expect for large values of x, $x \gg \epsilon$, that the temperature with the slab varies slightly with changes in x. However, significant changes occur in the y-direction. Consequently for efficient use of computer time, we will use irregular grid intervals in the region $2\epsilon \leqslant x \leqslant X_\infty$ or $2\bar{\xi} \leqslant \xi \leqslant 1$, with the intervals largest near $x \to X_\infty$.

The difficulty in choosing a continuous mapping function $x = X(\xi)$ with the above constraints was resolved by choosing separate mappings of x into ξ-plane, namely

$$X_I(\xi) \qquad 0 \leqslant x \leqslant 2\epsilon \qquad \text{or} \qquad 0 \leqslant \xi \leqslant 2\bar{\xi}$$

$$X_{II}(\xi) \qquad 2\epsilon \leqslant x \leqslant X_\infty \qquad \text{or} \qquad 2\bar{\xi} \leqslant \xi \leqslant 1$$

We then imposed constraints on $X_I(\xi)$ and $X_{II}(\xi)$ with a view to minimizing interpolation errors in the derivatives $f_i^{(1)}$ and $f_i^{(2)}$ (see Chapter Four). We therefore consider,

<u>Region I</u>: $0 \leqslant \xi \leqslant 2\bar{\xi}$

We put $$X_I(\xi) = \frac{\epsilon\xi}{\bar{\xi}} \tag{6.0.0}$$

<u>Region II</u>:

At $x = 2\epsilon$ and $\xi = 2\bar{\xi}$, we at least expect X_I and X_{II} to equal each other. However the nature of continuity of derivatives is dictated by the degree of accuracy we require in the finite-difference formulation of spatial derivatives of the temperature within the slab. Accepting errors in spatial derivatives of the $O(\Delta\xi^2)$, we insist that $X_I(\xi)$ and $X_{II}(\xi)$ have the following properties;

at $\xi = 2\bar{\xi}$

$$X_{II}(2\bar{\xi}) = X_I(2\bar{\xi}) = 2\epsilon$$

$$\left.\frac{d}{d\xi} X_{II}\right|_{\xi=2\bar{\xi}} = \left.\frac{d}{d\xi} X_I\right|_{\xi=2\bar{\xi}} \equiv \frac{\epsilon}{\bar{\xi}} \tag{6.0.1}$$

$$\left.\frac{d^2}{d\xi^2} X_{II}\right|_{\xi=2\bar{\xi}} = \left.\frac{d^2}{d\xi^2} X_I\right|_{\xi=2\bar{\xi}} \equiv 0$$

$$\left.\frac{d^3}{d\xi^3} X_{II}\right|_{\xi=2\bar{\xi}} = \left.\frac{d^3}{d\xi^3} X_I\right|_{\xi=2\bar{\xi}} \equiv 0 \tag{6.0.2}$$

We also impose a bound on ξ such that $0 \leqslant \xi \leqslant 1$, with $\xi = 1$ being equivalent to $x = X_\infty$ in the x-plane. Hence as $\xi = 1$, we put

$$X_{II}(1) = X_\infty$$
$$\frac{d}{d\xi} X_{II}\Big|_{\xi=1} = \beta_0 \qquad (6.0.3)$$

Thus the parameter β_0 can be used to control the size and spread of grid intervals in the region $\xi > 2\bar{\xi}$. To satisfy the conditions (6.1) to (6.3), we choose the mapping function $X_{II}(\xi)$ such that

$$X_{II}(\xi) = a_0 + a_1\xi + a_2\xi^2 + a_3\xi^3 + a_4\xi^4 + a_5\xi^5 \qquad (6.0.4)$$

On substituting equations (6.0.0) and (6.0.4) into (6.0.1), (6.0.2) and (6.0.3), we obtain the following system of equations in a_i's (i=0(5))

$$a_0 + 2\bar{\xi}a_1 + 4\bar{\xi}^2 a_2 + 8\bar{\xi}^3 a_3 + 16\bar{\xi}^4 a_4 + 32\bar{\xi}^5 a_5 = 2\epsilon$$
$$\bar{\xi}a_1 + 4\bar{\xi}^2 a_2 + 12\bar{\xi}^3 a_3 + 32\bar{\xi}^4 a_4 + 80\bar{\xi}^5 a_5 = \epsilon$$
$$2\bar{\xi}^2 a_2 + 12\bar{\xi}^3 a_3 + 48\bar{\xi}^4 a_4 + 160\bar{\xi}^5 a_5 = 0$$
$$6\bar{\xi}^3 a_3 + 48\bar{\xi}^4 a_4 + 240\bar{\xi}^5 a_5 = 0 \qquad (6.0.5)$$

$$a_0 + a_1 + a_2 + a_3 + a_4 + a_5 = 0$$
$$a_1 + 2a_2 + 3a_3 + 4a_4 + 5a_5 = \beta_0$$

On solving simultaneously the system of equations (6.5) and after tedious algebra we have expressions for a_i's (i=0 to 5), namely

$$a_0 = [1 - \frac{3\Phi_7\Psi_1}{4\Phi_2}\,(\frac{\Phi_4}{\Phi_3} + 16\Psi_7 - 320\bar{\xi}^2\Psi_4 + 640\bar{\xi}^3\Psi_3)].X_\infty$$

$$- [1 + \frac{1}{4\Phi_3}\{\Psi_1\Psi_5 + 4\Phi_6 - \Phi_8 - 5\Phi_4\Psi_1\Psi_5(1 + \frac{4\Phi_3}{\Phi_4}[\Psi_8 + 8\bar{\xi}^2\Psi_4 - 32\bar{\xi}^3\Psi_3])\}]\beta_0$$

$$+ \frac{1}{4\bar{\xi}\Phi_3}[4\Phi_6 - \Phi_8 + \frac{\Psi_1\Psi_6}{4}\,(\frac{\Phi_4}{\Phi_3} + 20\Psi_8 - 4\Psi_7 + 160\bar{\xi}^2\Psi_4 - 640\bar{\xi}^3\Psi_3)]\epsilon$$

$$a_1 = \frac{15\Phi_7\Psi_1}{\Phi_2}\,[1 - 24\bar{\xi}^2\Psi_3\,(1-(8\bar{\xi}/3)) - \frac{\Phi_4}{\Phi_3}\,(1-(3\bar{\xi}/2))].X_\infty$$

$$+ [1 + \frac{1}{\Phi_3}(\Phi_6 - \frac{5\Psi_1\Psi_5\Psi_8}{4})]\beta_0$$

$$- \frac{1}{\bar{\xi}\Phi_3}\,[\Phi_6 - \frac{5\Psi_1\Psi_6\Psi_8}{4}]\epsilon$$

$$a_2 = -\{\frac{480\bar{\xi}^3\Psi_1\Psi_7\Psi_3}{\Phi_2}.X_\infty + \frac{6\bar{\xi}^2}{\Phi_3}[1 - \frac{20\bar{\xi}\Psi_1\Psi_3\Psi_5}{3}]\beta_0$$

$$- \frac{6\bar{\xi}}{\Phi_3}[1 - \frac{20\bar{\xi}\Psi_1\Psi_3\Psi_6}{3}]\epsilon\}$$

$$a_3 = \frac{120\bar{\xi}^2\Psi_7\Psi_1\Psi_4}{\Phi_2}.X_\infty + \frac{2\bar{\xi}}{\Phi_3}[1 - 5\bar{\xi}\Psi_1\Psi_4\Psi_5]\beta_0$$

$$- \frac{2}{\Phi_3}[1 - 5\bar{\xi}\Psi_1\Psi_4\Psi_6]\epsilon$$

$$a_4 = \frac{15\Phi_7\Phi_4\Psi_1}{4\Phi_2\Phi_3} \cdot X_\infty - \frac{1}{4\Phi_3}\left[1+\frac{5\Phi_4\Psi_1\Psi_5}{4\Phi_3}\right]\beta_0$$

$$+ \frac{1}{4\overline{\xi}\Phi_3}\left[1+\frac{5\Phi_4\Psi_1\Psi_6}{4\Phi_3}\right]\epsilon$$

$$a_5 = -\left\{\frac{3\Phi_7\Psi_1}{\Phi_2} \cdot X_\infty - \frac{\Psi_1\Psi_5}{4\Phi_3}\beta_0 + \frac{\Psi_1\Psi_6}{4\Phi_3\overline{\xi}}\epsilon\right\}$$

where:

$$\Psi_1 = \frac{4\Phi_2\Phi_3}{8\Phi_1\Phi_3-5\Phi_2\Phi_4},$$

$$\Psi_3 = \left(1-\frac{3\Phi_4}{16\overline{\xi}\Phi_3}\right),$$

$$\Psi_4 = \left(1-\frac{\Phi_4}{4\overline{\xi}\Phi_3}\right),$$

$$\Psi_5 = \left(1-\frac{4\Phi_3^2}{\Phi_2}\right),$$

$$\Psi_6 = \left(1-\frac{8\Phi_3\Phi_5}{\Phi_2}\right),$$

$$\Psi_7 = \left(1-\frac{\Phi_4}{\Phi_3}\right),$$

$$\Psi_8 = 64\overline{\xi}^3\Psi_3 - 24\overline{\xi}^2\Psi_4 + \Psi_7,$$

with Φ_i (i=1 to 8) given by

Values of ϕ_i	=	COEFFICIENTS OF THE POWERS OF ξ ξ^0	ξ^1	ξ^2	ξ^3	ξ^4	ξ^5	ξ^6	ξ^7
ϕ_1	=	1	-9	24	20	-240	528	-512	192
ϕ_2	=	1	-12	60	-160	240	-192	64	0
ϕ_3	=	-1	6	-12	8	0	0	0	0
ϕ_4	=	-1	0	24	-64	48	0	0	0
ϕ_5	=	1	-3	0	4	0	0	0	0
ϕ_6	=	1	-6	12	0	0	0	0	0
ϕ_7	=	1	-4	4	0	0	0	0	0
ϕ_8	=	1	-8	24	0	0	0	0	0

6.1 Broyden's Method

Consider the following system of equations

$$\underline{g}(\underline{v}) = 0 \qquad \underline{g} : \mathbb{R}^n \to \mathbb{R}^m \tag{6.1.0}$$

Using Newton's approximations, we have

$$[\underline{g}(\underline{v}+\underline{s})]_i = \underline{g}_i(\underline{v}) + \sum_{j=1}^{M} \frac{\partial}{\partial s_j} g_i(\underline{v}) s_j \tag{6.1.1}$$

where g_i represents i^{th} equation of $\underline{g}$. Therefore

$$\underline{g}(\underline{v}+\underline{s}) - \underline{g}(\underline{v}) = \underline{\underline{J}}\ \underline{s} \tag{6.1.2}$$

$\underline{\underline{J}}$ is an (m × n) matrix and s is (n × 1).

Let $\underline{\underline{\lambda}}$ be an approximation to $\underline{\underline{J}}$ at $\underline{v}$. We now want to determine $\underline{\underline{\lambda}}^*$ at $\underline{v} + \underline{s}$. Hence we put

$$\underline{\underline{\lambda}}^* = \underline{\underline{\lambda}} + \Delta\underline{\underline{\lambda}}$$

and (6.1.3)

$$\Delta\underline{\underline{\lambda}} = \underline{v}\ \underline{p}^T$$

Imposing the quasi-Newton condition, equation (6.1.3) and (6.1.2) give

$$\underline{\underline{\lambda}}^* \underline{s} = \underline{g}(\underline{v} + \underline{s}) - \underline{g}(\underline{v})$$

$$= \underline{q}, \text{ say} \qquad (6.1.4)$$

and hence

$$(\underline{\underline{\lambda}} + \Delta\underline{\underline{\lambda}})\underline{s} = \underline{q}$$

$$(\underline{\underline{\lambda}} + \underline{v}\ \underline{p}^T)\underline{s} = \underline{q}$$

Thus

$$\underline{v}(\underline{p}^T\underline{s}) = \underline{q} - \underline{\underline{\lambda}}\underline{s}$$

Therefore

$$\underline{v} = \frac{\underline{q} - \underline{\underline{\lambda}}\ \underline{s}}{(\underline{p}^T\underline{s})} \qquad (6.1.5)$$

Combining equations (6.1.5) and (6.1.3), we get

$$\underline{\underline{\lambda}}^* = \underline{\underline{\lambda}} + \frac{(\underline{q} - \underline{\underline{\lambda}}\ \underline{s})}{\underline{p}^T\underline{s}}\ \underline{p}^T$$

we now put $\underline{s} = \underline{p}$ and hence

$$\underline{\underline{\lambda}}^* = \underline{\underline{\lambda}} + (\underline{q} - \underline{\underline{\lambda}}\,\underline{s}) \frac{\underline{s}^T}{\underline{s}^T\underline{s}} \tag{6.1.6}$$

substituting for $\underline{q}$ in (6.1.4) into (6.1.6), we obtain

$$\underline{\underline{\lambda}}^* = \underline{\underline{\lambda}} + [\underline{g}(\underline{v} + \underline{s}) - \underline{g}(\underline{v}) - \underline{\underline{\lambda}}\,\underline{s}] \frac{\underline{s}^T}{\underline{s}^T\underline{s}} .$$

In our particular case the value of M in equation (6.1.0) is equal to unity, and hence

$$\underline{\lambda}^* = \underline{\lambda} + (\underline{g}(\underline{v} + \underline{s}) - \underline{g}(\underline{v}) - \underline{\lambda}\,\underline{s}) \frac{\underline{s}^T}{\underline{s}^T\underline{s}} .$$

We now put $\underline{s} = (\Delta\underline{\theta}, \Delta\sigma)^T$. Therefore

$$\underline{\lambda}_{j+1} = \underline{\lambda}_j + [g^{j+1} - g^j - \underline{\lambda}_j^T \begin{pmatrix} \Delta\underline{\theta}^j \\ \Delta\sigma^j \end{pmatrix}] \frac{((\Delta\underline{\theta}^j)^T, \Delta\sigma^j)}{\|((\Delta\underline{\theta}^j)^T, \Delta\sigma^j)\|^2} \tag{6.1.7}$$

where j refers to the j^{th} iteration. Note the notation for θ and σ is as was used in Chapter Five.

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