ON MATHEMATICAL MODELLING OF THE SELF-HEATING OF CELLULOSIC MATERIALS

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ABSTRACT

This thesis considers mathematical modelling of self-heating of cellulosic materials, and in particular the effects of moisture on the heating characteristics. Following an introductory chapter containing a literature review, Chapter 2 presents some preliminary results and an industrial case study. The case study, which discusses a 'dry' body self-heating on a hot surface, investigates the following questions: (i) how hot can the surface get before ignition is likely? (ii) how well does the (slab-like) body approximate to an infinite slab? and (iii) how valid is the Frank-Kamenetskii approximation for the source term? It is shown that the minimal steady state temperature profile is stable when the temperature of the hot surface is below a certain critical value, and bounds for the higher steady state profile are derived. Chapter 3 presents the thermodynamic derivation of a reaction-diffusion model for the self-heating of a moist cellulosic body, including the effects of direct chemical oxidation as well as those of a further exothermic hydrolysis reaction and the evaporation and condensation of water. The model contains three main variables: the temperature of the body, the liquid water concentration in the body, and the water vapour concentration in the body. Chapter 4 investigates the limiting case of the model equations as the thermal conductivity and diffusivity of the body become large. In particular it is shown that, in this limiting case, the model can have at least twenty-five distinct bifurcation diagrams, compared with only two for the well known model without the effects of moisture content. In Chapter 5 the maximum principle and the methods of upper and lower solutions are used to derive existence, uniqueness and multiplicity results for the steady state solutions of the spatially distributed model. Finally, in Chapter 6, existence and uniqueness results for the time dependent spatially distributed model are derived.

I would like to express my gratitude to my supervisors Professor Graeme Wake and Mr Adrian Swift for their unfailing help and enthusiasm throughout my work. Thanks also to Dr Alex McNabb and Mr Aroon Parshotam for many helpful comments, Mr Richard Rayner for his help in producing the graphics, Miss Fiona Davies for her typing of this thesis, Joanne for her constant support, and Patricia for her friendship.

CONTENTS

CHAPTER 1

Introduction

1.1 Physical background

A body is said to be 'self-heating' when its temperature rises due to a process occurring inside the body itself. Under certain conditions this temperature rise may be sufficiently large so as to induce the body to thermally ignite. 'Spontaneous ignition' or 'spontaneous combustion' has then occurred.

Fires due to spontaneous combustion arising in practice can generally be placed into one of two categories, the common denominator being an internal exothermic process. The first category is where a 'small' body of material such as a sack, small pile or dust layer is stored subject to high ambient conditions (for example on a hot surface) and/or at a high initial temperature (for example chemicals from a drying process). Generally these fires are induced over quite a small time scale, sometimes a matter of hours or days. Typical scenarios for fires occurring in this category would include: the last batch of laundry from an industrial cleaning process catching fire in the early hours of the morning, or forest litter, for example gum leaves, igniting due to the proximity of a barbecue fire, or a woodchip/oil dust layer igniting on a hot fibreboard press. The second category is associated with fires that occur over far longer time scales, sometimes months, and at lower ambient conditions, sometimes room temperature - the spontaneous combustion of large stockpiles of material. Typical materials would include hay, woodchips, wool and bagasse (bagasse being the fibrous residue of the extraction of sugar from sugar cane). The economic importance of the study of spontaneous combustion can be placed in perspective by analysing the following table from Bowes [1], which summarizes statistics of building fires in the United Kingdom between 1970-1973.

Year	1970	1971	1972	1973	1970	1971	1972	1973
Number of fires	90412	89310	100081	105323				
Supposed cause	Proportion of all fires assigned to given cause				Proportion of all fires assigned to given cause which were also large(3)			
Electrical appliances and installations	28.5	29.5	29.8	31.2	0.53	0.51	0.48	0.54
Primary fuel burning appliances and installations (1)	20.3	19.3	19.2	18.5	0.35	0.39	0.31	0.46
Children playing with fire, eg matches	8.5	9.1	9.9	9.5	0.14	0.34	0.31	0.36
Smoker's materials	8.7	8.0	7.7	8.3	0.73	0.77	0.81	1.00
Malicious or intentional ignition	4.1	5.9	7.0	7.8	3.2	3.3	3.3	3.6
Spontaneous combustion	0.61	0.55	0.47	0.41	1.8	2.9	3.2	2.5
Other known causes (2)	15.9	14.6	14.4	13.5	0.65	0.67	0.67	0.85
Unknown	13.4	13.0	11.7	11.0	4.5	5.5	6.2	6.1

(1) Solid fuel, oil, gas, LPG, acetylene

(2) Listed and unlisted, excluding rubbish burning and including 'other and unspecified fires'. less than 5 per cent of total fires assigned to each

(3) Direct loss in excess of £10 000.

Figure 1.1 Building fire statistics 1970-1973.

These statistics indicate that spontaneous combustion is second only behind 'malicious or intentional damage' as the most common of the assigned causes of large fires.

In terms of the mathematical modelling of self-heating bodies, then, the three main areas of interest, which of course are closely related, are:

(i) **Critical size.** What is the 'largest' size of stockpile in which we can safely store a given material at a given ambient temperature and initial temperature?

(ii) **Critical ambient temperature.** What is the hottest storage temperature we can safely apply to a given stockpile at a given initial temperature?

(iii) **Critical initial temperature.** To what temperature should we allow a body to cool before storing it in a stockpile of given dimensions and given ambient temperature?

The mathematical analysis of most incidences of fires caused by spontaneous combustion can be reduced to a consideration of one of the above three factors.

1.2 Formulation of the model for self-heating by a single exothermic reaction

We shall assume that the thermal conductivity of the self-heating body is constant and that reactant consumption does not significantly inhibit the rate of the exothermic reaction. An energy balance between the heat generated in unit volume of a body by a single exothermic reaction (typically a chemical oxidation reaction) and the heat lost from that volume by thermal conduction gives the differential equation

$$k\nabla^2 T + q(T) = C\frac{\partial T}{\partial \hat{t}} \quad \text{in the region } \hat{r} \in \hat{\Omega} \subseteq \mathbb{R}^3,\ \hat{t} > 0 \tag{1.1a}$$

with boundary conditions

$$k\frac{\partial T}{\partial n} + h(T - T_a) = 0 \quad \text{on} \quad \partial\hat{\Omega}, \quad \text{(Newtonian Cooling)} \tag{1.1b}$$

or

$$T = T_a \quad \text{on} \quad \partial\hat{\Omega}, \quad \text{(perfect heat transfer)} \tag{1.1c}$$

and initial conditions

$$T(\hat{r}, \hat{t} = 0) = T_0(\hat{r}), \quad \hat{r} \in \bar{\hat{\Omega}}, \tag{1.1d}$$

where

T = absolute temperature,

T_a = absolute ambient temperature,

T_0 = initial temperature profile,

k	=	thermal conductivity,
$q(T)$	=	rate of heat production per unit volume at temperature T,
h	=	heat transfer coefficient,
$\frac{\partial}{\partial n}$	=	outward normal derivative at the boundary,
$\hat{t}$	=	time,
C	=	specific heat capacity.

The steady state, spatially uniform (that is the solution in the limit $k \to \infty$) case of this model was first studied by Semenov [2], and the solution for finite k and high activation energy was obtained in the infinite slab by Frank-Kamenetskii [3]. Both these authors assumed that the rate of the exothermic reaction varies in accordance with the Arrhenius law

$$q(T) = Q\,\rho Z \exp\left(\frac{-E}{RT}\right), \tag{1.2}$$

where

Q	=	exothermicity of the oxidation reaction,
ρ	=	density,
Z	=	pre-exponential factor of the Arrhenius equation (also known as a frequency factor),
E	=	activation energy of the oxidation reaction,
R	=	gas constant.

As we will see later in the discussion of the application of this theory to the prediction of safe storage regimes for dry bodies, the Arrhenius law has proved to be accurate over the practical parameter range, and indeed has been used by the majority of authors since its first formulation. Frank-Kamenetskii's [3] work on the infinite slab with perfect heat transfer on the boundary, used the dimensionless temperature rise over the ambient as

$$\theta = \frac{E}{RT_a^2}(T - T_a)\,, \tag{1.3}$$

so the steady state problem becomes, in dimensionless coordinates

$$\frac{d^2\theta}{dr^2} + \delta \exp\left[\frac{\theta}{(1+\varepsilon_a\theta)}\right] = 0, \qquad -1 < r < 1, \tag{1.4a}$$

with

$$\theta = 0, \qquad \text{at} \qquad r = \pm\, 1, \tag{1.4b}$$

where

$$\left.\begin{aligned} a_0 &= \text{half-width of the body,} \\ \varepsilon_a &= \frac{RT_a}{E}, \\ \delta &= \frac{\rho Q a_0^2\, E\, Z \exp\left(\frac{-E}{RT_a}\right)}{kRT_a^2}, \\ r &= \text{dimensionless length}\left(=\frac{\hat{r}}{a_0}\right). \end{aligned}\right\} \tag{1.4c}$$

The parameter δ is often referred to as the Frank-Kamenetskii parameter. Frank-Kamenetskii observed that, provided $\frac{E}{RT_a} >> 1$ (i.e. $\varepsilon_a << 1$), and θ is not too large, the problem reduces to the equation

$$\frac{d^2\theta}{dr^2} + \delta \exp\theta = 0, \qquad -1 < r < 1, \tag{1.5a}$$

with

$$\theta = 0, \qquad \text{at} \qquad r = \pm\, 1, \tag{1.5b}$$

which has the well-known closed form solution

$$\theta(r) = \ell nF - 2\ell n(\cosh(r \cosh^{-1}\sqrt{F})), \tag{1.6a}$$

where F is the solution of the transcendental equation

$$F = \cosh^2 \sqrt{\frac{\delta F}{2}}. \tag{1.6b}$$

The assumption $\varepsilon_a << 1$ is known as the Frank-Kamenetskii approximation, and is the most commonly used, but not the only such approximation, in the literature. For example Gray and Harper |4| introduced a quadratic approximation to the Arrhenius term i.e.

$$\exp\left(\frac{-E}{RT}\right) \approx \exp\left(\frac{-E}{RT_a}\right)(b_1 + b_2\theta + b_3\theta^2) \tag{1.7}$$

where $b_1 = 1$, $b_2 = e-2$, $b_3 = 1$.

The merits and consequences of the Frank-Kamenetskii approximation will be discussed again in Chapter 2.

1.3 Interpretation

It is well-known (the verification involves simple calculus) that for $\delta < 0.88$ two solutions to (1.6a, b) exist, the lower of which is stable (in a time sense) and the higher of which is unstable. But for $\delta > 0.88$ no solutions exist. Frank-Kamenetskii identified this transition with the onset of thermal ignition, since for $\delta > 0.88$ no stable steady state profile will exist and the temperature of the body will rise in an unbounded manner with time. The value $\delta = 0.88$ is referred to as δ_{crit} for the infinite slab. This behaviour in the δ, $\|\theta\|_0$ space, where $\|\theta\|_0 = \max_{r \in \Omega} |\theta(r)|$, is summarised in Figure 1.2 below

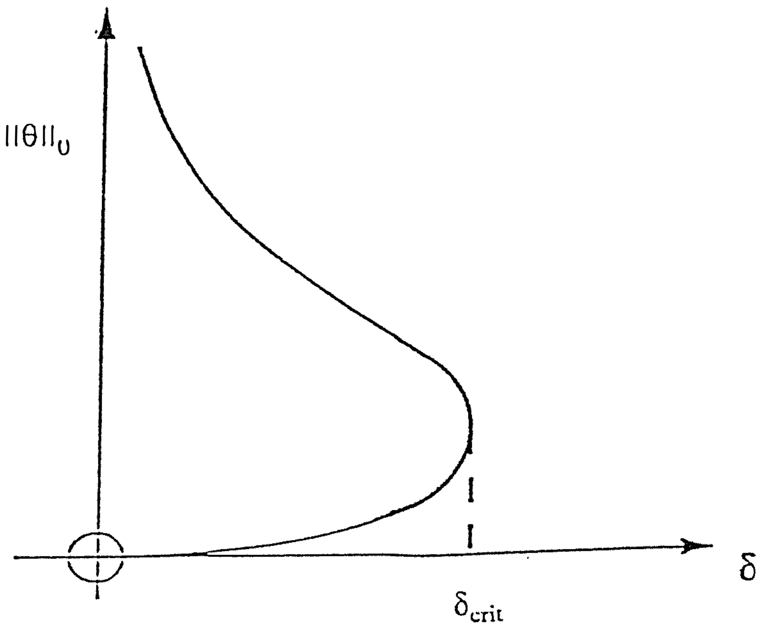

Figure 1.2 Typical δ, $||\theta||_0$ bifurcation diagram for the infinite slab with the Frank-Kamenetskii approximation.

For the infinite cylinder and unit sphere, δ_{crit} = 2.00, 3.32 respectively. For more general shapes (cubes, finite cylinders etc.) Boddington, Gray and Harvey [5] have introduced the concept of a root-mean-square 'Frank-Kamenetskii' radius, r_0, of a body, and it is this approach that is used by experimentalists in laboratory scale tests.

Several variations of this basic model have been studied, both with and without the Frank-Kamenetskii approximation. For example: a model with reactant consumption (Boddington et al [6]), criticality with variable thermal conductivity (Wake [7]), ignition of a self-heating body subject to asymmetric boundary conditions (Thomas and Bowes [8], Shoumann and Donaldson [9] and Sisson, Swift and Wake [10]), and a model for an exothermic reaction sustained by a single diffusing reactant (Burnell et al [11]). In 1989 Burnell et at [12] presented a paper questioning the appropriateness of the classical Frank-Kamenetskii formulation, particularly the use of the ambient temperature in the non-dimensionalization of the body temperature. They suggested an alternative formulation for the non-dimensionalization of the system i.e.

$$u = \frac{RT}{E}, \qquad (1.8a)$$

$$U = \frac{RT_a}{E}. \qquad (1.8b)$$

This gives the dimensionless form of the parabolic system (1.1a, b, c, d), (1.2) as

$$\nabla^2 u + \eta \exp\left(\frac{-1}{u}\right) = \frac{\partial u}{\partial t}, \quad r \in \Omega, \quad t > 0, \qquad (1.9a)$$

with

$$\frac{\partial u}{\partial n} + Bi\,(u - U) = 0, \quad r \in \partial\Omega, \qquad (1.9b)$$

(Newtonian cooling)

or

$$u = U, \quad r \in \partial\Omega, \qquad (1.9c)$$

(perfect heat transfer)

and

$$u(r, t = 0) = u_0(r), \qquad (1.9d)$$

where

$\eta = \dfrac{\rho Q Z R a_0^2}{kE}$,

a_0 = an appropriate characteristic length such as the half-width of the body,

Bi = dimensionless Biot number $= \dfrac{h a_0}{k}$,

$t = \dfrac{\hat{t} k}{a_0^2 C}$,

$r = \dfrac{\hat{r}}{a_0}$,

and Ω, $\partial\Omega$ are the scaled representations of $\hat{\Omega}$, $\partial\hat{\Omega}$ respectively.

The steady states of this system are given by

$$\nabla^2 u + \eta \exp\left(\frac{-1}{u}\right) = 0, \qquad r \in \Omega, \tag{1.9e}$$

with the same boundary conditions (1.9b) or (1.9c).

Their basic idea was that in most practical situations (and laboratory scale tests) T_a, the ambient temperature, is the most accessible control parameter, and hence U (the dimensionless representation of T_a) is the natural bifurcation, or 'distinguished', parameter. In the Frank-Kamenetskii formulation T_a appears in θ, δ and ε_a, whereas in the new formulation T_a appears only in U. As Burnell et al explain this means that for a bifurcation diagram in U, $\|u\|_0$ space, $T_{a,\,crit}$, the critical value of the ambient temperature, can be observed directly from the graph $\left(\text{as } U_{crit} = \frac{RT_{a,\,crit}}{E}\right)$. For the Frank-Kamenetskii formulation, however, an iterative process must be used to find $T_{a,\,crit}$ from the δ, $\|\theta\|_0$ bifurcation diagram as follows:

(i) use a trial value of $T_{a,\,crit}$ which gives $\varepsilon_a = \frac{RT_{a,\,crit}}{E}$;

(ii) record δ_{crit} from the δ, $\|\theta\|_0$ plot;

(iii) from this value of δ_{crit} calculate the next approximation to $T_{a,\,crit}$.

Also since the Frank-Kamenetskii approximation in effect sets $\varepsilon_a = \frac{RT_a}{E} = 0$, this approximation is obviously inappropriate in the new formulation. In their 1990 paper, Wake et al [13] presented existence, uniqueness and multiplicity results for the steady states of the model using this new dimensionless formulation. For the analysis of the model in this thesis we will use the new formulation of Burnell et al [12] and the full

Arrhenius representation of the heat balance equation, i.e. we will refrain from using the Frank-Kamenetskii approximation.

In the chemical literature the most common approach in analysing safe storage regimes for particular materials is to invoke the Frank-Kamenetskii approximation and the concept of Frank-Kamenetskii radius and then extrapolate to results for practical stockpiles from those obtained from laboratory scale tests. Using the Frank-Kamenetskii approximation the heat balance equation (1.1a), (1.2) for a system with one characteristic dimension (a_0) becomes

$$\frac{d^2\theta}{dr^2} + \frac{j}{r}\frac{d\theta}{dr} + \delta(a_0)\exp\theta = 0 \qquad (1.10)$$

where j is a shape factor and δ is as given in (1.4c). Boddington et al [5] give the shape factor j and the critical value of the parameter δ for non-standard shapes as

$$j = \left(\frac{3r_0^2}{r_S^2}\right) - 1, \qquad (1.11a)$$

where $r_s = \frac{3V}{S}$,

r_0 = the root mean-square radius,

V = volume of the body,

S = surface area of the body,

and

$$\delta_{crit} = 3(2j+6) / (j+7). \qquad (1.11b)$$

The values of r_0, j and δ_{crit} are given for various shapes, taken from Gray, Griffiths and Hasko [14], in Figure 1.3 below.

Shape	r_0	r_s	j	$\delta_{crit}(r_0)$
Cube $(2a_0)^3$	$1.194a_0$	$1.000a_0$	3.275	3.663
Equicylinder (Diam. $2a_0 \times$ length $2a_0$)	$1.115a_0$	$1.000a_0$	2.729	3.531
'Squat'cylinder (Diam. $2a_0 \times$ length $1.8a_0$)	$1.081a_0$	$0.965a_0$	2.762	3.541
'Long'cylinder (Diam. $2a_0 \times$ length $14a_0$)	$1.225a_0$	$1.500a_0$	1.000	2.999

Figure 1.3 Parameters for some non-standard shapes.

Eigeban et al [15] have shown that a good approximation to the critical value of the Frank-Kamenetskii parameter δ is then

$$\delta_{crit}(r_o) = \frac{\rho\, Q\, r_0^2\, EZ \exp\left(\frac{-E}{RT_a}\right)}{kRT_{a,\,crit}{}^2}, \tag{1.12}$$

or equivalently

$$\ell n\left(\frac{\delta_{crit}\, T_{a,\,crit}{}^2}{r_0^2\, \rho}\right) = \ell n\left(\frac{ZQE}{kR}\right) - \frac{E}{RT_{a,\,crit}}. \tag{1.13}$$

The idea behind this approach is that $T_{a,\,crit}$ can be measured in the laboratory by slowly heating various small piles (low r_0 values) at very high ambient temperatures. Then a plot of $\ell n\left(\frac{\delta_{crit}\, T_{a,\,crit}{}^2}{r_0^2\, \rho}\right)$ against $\left(\frac{1}{T_{a,\,crit}}\right)$ should give a straight line with slope $\frac{-E}{R}$, from which the activation energy, E, can be estimated. Figure 1.4 below shows an example of one such plot for barbecue fuel (Jones [16]).

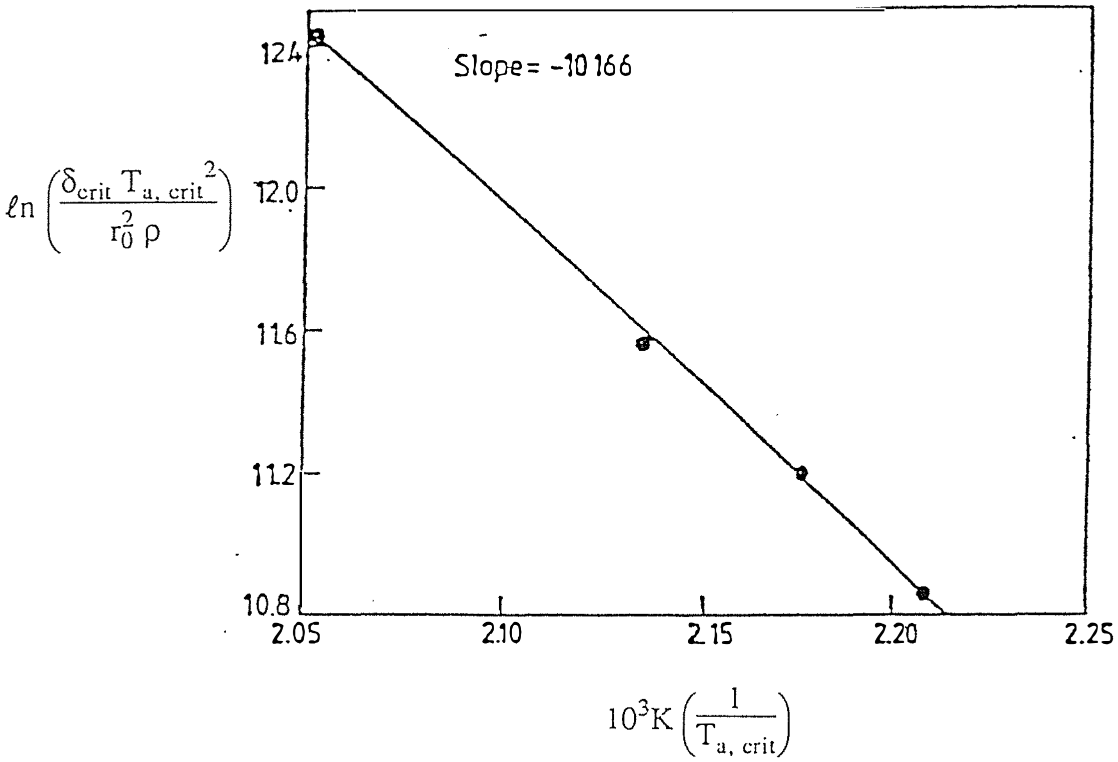

Figure 1.4 Frank-Kamenetskii plot for barbecue fuel.

Extrapolations can also be made from these graphs to practical values of T_a (say 20–40°), to predict the corresponding r_0 values, and so estimate the safe storage sizes at these temperatures. The $T_{a,\, crit}$ values for laboratory scale tests are measured by plotting temperature excess/time graphs for various oven temperatures. An example of one of these diagrams (bagasse pith in a squat cylinder, taken from Gray, Griffiths and Hasko [14]), is given in Figure 1.5 below.

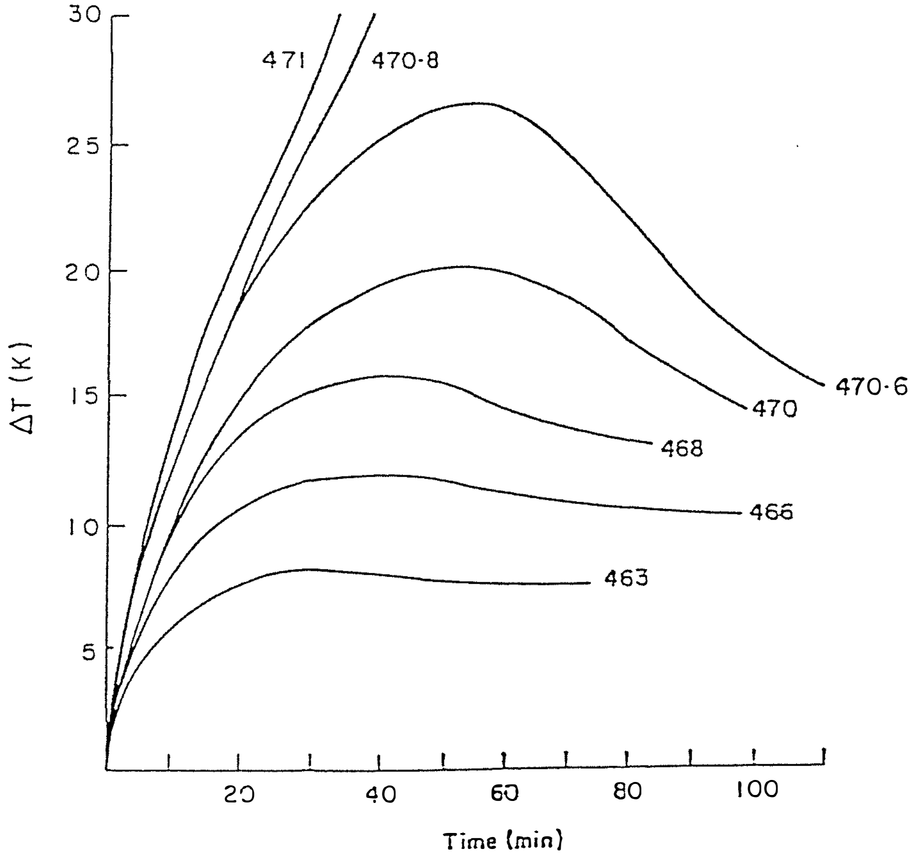

Figure 1.5 Temperature excess/time graphs for bagasse pith in a squat cylinder, for varying oven temperatures.

It can be seen from Figure 1.5 that there is a marked difference between the subcritical and the supercritical behaviour of the body. For oven temperatures above 470.8K, the body temperature continues to rise until (ultimately) ignition occurs. But for oven temperatures below 470.6K the temperature excess achieves a maximum then falls as reactant is consumed. Thus on the basis of this diagram, $T_{a,\ crit}$ for this particular body is 470.7K ± 0.1K. Figures 1.6, 1.7 and 1.8 below show some typical apparatus used in these laboratory scale tests (at the School of Chemistry, Macquarie University, Sydney, Australia).

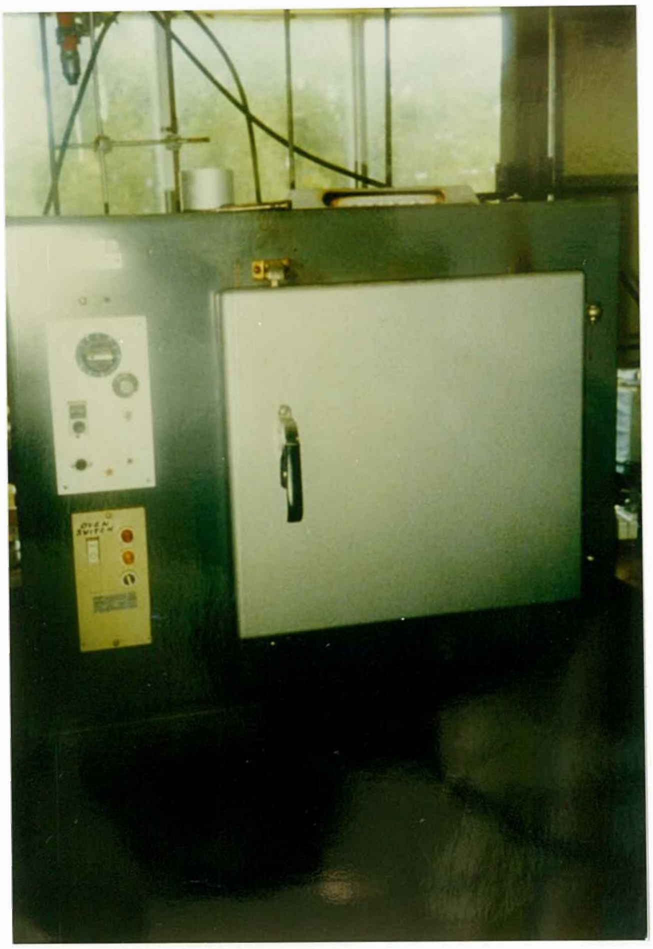

Figure 1.6 Oven for regulating high ambient temperatures.

Figure 1.7 Cylinder in oven.

Figure 1.8 Size range of vessels for laboratory scales tests.

This technique of extrapolation from laboratory scale tests has been applied to a wide range of materials. Results from the literature are summarized in Figure 1.9 below.

MATERIAL	STORAGE CONDITIONS ambient temperatures in °C critical heights in metres			REFERENCE		COMMENT ON MOISTURE FACTORS?
WOOL	Amb. temp. Crit. height	40 6.6		Jones	[17]	YES
QUEENSLAND BAGASSE	Amb. temp. Crit. height	40 66	20 276	Gray et al	[14]	YES
HOPS	Amb. temp. Crit. height	40 2.9		Jones and Raj	[18]	NO
EUCALYPTUS LEAVES	Amb. temp. Crit. height	40 3.9	25 6.9	Jones and Raj	[19]	NO
FIJIAN BAGASSE	Amb. temp. Crit. height	40 16.3	25 37.4	Raj and Jones	[20]	YES
FIJIAN HARDWOOD FLAKES	Amb. temp. Crit. height	40 39	25 95	Raj and Jones	[20]	YES
NSW WOOD SHAVINGS	Amb. temp. Crit. height	40 48.5	25 126	Jones and Raj	[19]	NO*
NSW RICE HUSKS	Amb. temp. Crit. height	40 25.5	25 63	Raj and Jones	[20]	YES
CHEMICALLY ACTIVATED CARBON	Amb. temp. Crit. height	40 2.5	30 4.8	Bowes and Cameron	[21]	YES

Figure 1.9 Table of storage predictions from the literature.

* in effect this is a 'yes' since Jones and Raj state that this result 'corresponds well with the value for Queensland bagasse'.

In more than half of these references the authors acknowledge that the bounds on the safe storage heights obtained at realistic ambient temperatures were something of an overestimation. For example Raj and Jones [20] state

> "all test materials show satisfactory conformity to the predictions of thermal ignition theory when heated in baskets ... When the results are extrapolated to outdoor temperatures, all test materials gave surprisingly high values of the calculated maximum stockpile height".

Gray, Griffiths and Hasko [14] conjectured that this discrepancy is due to the effects of moisture content in the real-sized stockpiles. It appears to be a major fault in the process outlined above that, since typical oven temperatures are above 100°C, after an initial period during which water evaporated from the system, the laboratory scale tests can only measure the amount of heat produced by 'dry' materials. Any data on the heat produced by ancillary reactions associated with the presence of water in the body e.g. hydrolysis or microbial factors, is bound to be lost. This is acknowledged by Jones [16]

> "...however, as has been pointed out more than once to the author, such extrapolations may require caution. It may happen that processes are occurring in the 'real' stockpile which are absent from the laboratory test, for example moisture effects and creation of reactive new surface by breakage on handling. In such circumstance the extrapolation would be of doubtful meaning".

This would also explain why the laboratory scale tests correspond so well to the Frank-Kamenetskii model (see Figure 1.4), which only accounts for heat produced by a dry material. It is thought by many authors, hence the comments on moisture content mentioned in Figure 1.9, that it is this underestimation of the amount of heat being produced inside the self-heating stockpiles that is the cause of the overestimation of the safe stockpiling sizes.

In a 1973 paper Smith [22] summarised the causes of self-heating in wet wood chips as

(i) the metabolism of living wood parenchyma cells in fresh wood chips;

(ii) the metabolism of bacteria and fungi;

(iii) direct chemical oxidation;

(iv) acid hydrolysis of cellulose.

We will assume these to be the main heat producing components in all stockpiles of cellulosic materials. Factor (i) will only be present if the material in the stockpile has been cut fairly recently. It can also be ignored if, for example, the material has gone through an industrial refining process prior to stockpiling. Factors (ii) and (iv) can only occur if there is moisture present in the body. We will look at the data for the production of heat by the metabolism of bacteria and fungi in a particular material (bagasse) later in this introduction. Factor (iii) is the classical exothermic process of the Frank-Kamenetskii model, which can occur whether or not moisture is present in the stockpile. The effects of moisture on the chemical/physical processes occurring in stockpiled cellulosic materials have been discussed by Gray, Griffiths and Hasko [14].

(i) evaporation and loss of water can confer an endothermicity which tends to stabilise the system;

(ii) completely dry cellulosic materials are hygroscopic. The rate of heat release which is due to condensation of water vapour and evolution of its latent heat can be sufficient to cause self-heating and thermal ignition;

(iii) when movement of water through a mass takes place by evaporation and condensation, no net thermal effect will result when the two rates balance. The overall heat release from the system will then approximate to that of dry material at the same temperature;

(iv) balanced internal rates of evaporation and condensation do not lead to identical conditions for criticality of wet and dry masses. The thermal diffusivity within wet material is greater than that within dry material and the stability of the wet mass is enhanced because of this;

(v) When a net loss of water occurs from the system, there is a gradual decrease in thermal diffusivity;

(vi) as long as water remains in the system, liquid-phase oxidations and acid hydrolysis of hemicellulose (an isomer of cellulose) may take place, making additional contributions to the heat release rate.

It is clear that, as well as taking into account the amount of heat produced by the extra exothermic reactions due to moisture content per se, any mathematical model for 'self-heating with moisture content' must also include the exothermic process of water vapour condensation, and the endothermic process of liquid water evaporation.

In the light of the obvious over estimation of safe storage regimes for bagasse, as seen in Figure 1.9, and in an attempt to gain further insight into the reasons for this discrepancy, some experimental work has recently been carried out at the Sugar Research Institute at Mackay, Queensland. Trials were conducted on various stockpiles including identical stockpiles with and without added H_2SO_4 (the presence of H_2SO_4 kills microbes in the stockpile). The results were given in Dixon [23] and are summarised below.

(i) the dry bagasse reaction alone is not sufficient to cause spontaneous combustion in full size stockpiles;

(ii) microbiological heat generation can be of little significance in initial bagasse stockpile temperature increases;

(iii) there must exist one or more low temperature reactions which generate rapid initial chemical heating in bagasse stockpiles;

(iv) preliminary micro-calorimetric investigations with bagasse at low temperature (60°C) show considerably enhanced heat generation in the presence of water;

(v) the relative importance of wet cellulose oxidation and aqueous phase oxidation of microbiological and hydrolysis by-products has not been established;

(vi) little change will occur in the total moisture content of the bulk of the bagasse stockpile during normal heating.

Work by Gray and Scott [24] showed that the initial bagasse storage temperature, typically 50-70°C, would not be sufficient to induce thermal ignition in stockpiled dry bagasse. Gray and Scott calculated that for dry bagasse an initial temperature greater than 90°C would be required for ignition in practical stockpile sizes and in the usual ambient temperature range. In comparison with the dry model, very little theoretical work has been done on the self-heating of damp stockpiles.

In 1939 Henry [25] published a paper on work arising from the analysis of the uptake of moisture by cotton bales. He considered the diffusion of one substance through another in the pores of a solid body which could absorb and immobilise some of the diffusing substance. Due to the small size of the pores encountered in these stockpiles and the fact that many of them are filled with liquid, Henry neglected the influence of convection in the model. There was also no account made of the influence of heat production by oxidation or hydrolysis reactions within the body. As Bowes [1], page 296, states

> "The transient diffusion of heat and moisture through porous hygroscopic materials was considered theoretically by Henry with particular reference to temperature and moisture changes in bales of textile fibres ... He suggested that the analysis might

be extended to include simultaneous heat generation by other processes but did not pursue this interesting possibility".

In the 1970's, Walker and co-workers (e.g. Walker and Harrison [26], Walker and Jackson [27], Walker and Manssen [28]) proceeded by essentially using the Frank-Kamenetskii model, but by operating at lower oven temperatures (80-92°C), they were able to include some of the effect of the moisture content. This model had the fault that it 'lumped' two, essentially distinct, reactions in the same Arrhenius term. Also no account was made of the evaporation or condensation of water. In 1990, Gray and Wake [29] considered a spatially uniform model, analysing the effects of condensation/evaporation of water in conjunction with the exothermic oxidation reaction. In their analysis Gray and Wake used the quadratic approximation (1.7) to the Arrhenius term. However as they state in their paper

"... we will assume that there are no extra self-heating reactions in the aqueous phase, although there undoubtedly are for some materials, such as bagasse".

Finally, again in 1990, Gray [30] presented a spatially uniform model which unified all the main factors thought to be involved in the self-heating of moist cellulosic stockpiles i.e.

(i) the heat produced by the oxidation reaction;
(ii) the heat produced by the hydrolysis reaction;
(iii) the endothermic evaporation process;
(iv) the exothermic condensation process;
(v) the heat lost due to Newtonian cooling.

Gray also included a term to represent the water consumed by the hydrolysis reaction. We have decided to ignore this term in our analysis. We do this for two reasons: (a) on the grounds of consistency, in that the model also 'neglects' the consumption of the other two reactants i.e. cellulose and oxygen, and (b) because steady state analysis with non-trivial concentrations of each species requires that all reactant consumption is 'neglected' (otherwise as $t \rightarrow \infty$ the water content will tend to zero which contradicts observation (vi) of Dixon [23] mentioned earlier). 'Neglect of reactant consumption' in this context means that we will assume that the consumption of the reactants does not effect the rates of any of the reactions in any way, i.e. there is always 'enough' of the reactants to fully sustain all the reactions. This model was formulated in the wake of the Sugar Research Institute's comment on the minimal effects of microbes on the self-heating of bagasse. How well the neglect of the heat produced by microbes can be justified for materials other than bagasse is an open question to a certain extent. However it seems reasonable to assume that, since all cellulosic materials have basically very similar chemical constituents, the heat produced by the hydrolysis reaction is the dominant factor when considering ancillary exothermic reactions due to moisture effects. It is the mathematical analysis of this slight variant of Gray's model, and the corresponding spatially distributed model, that we shall be mainly considering in this thesis.

Before embarking on this we will consider a case study involving self-heating by a single exothermic reaction of a (dry) body on a hot surface. This example will illustrate the power of steady state ignition theory in practical circumstances and introduces some further important concepts such as the maximum principle and the method of upper and lower solutions. We also introduce some new results on the stability of the minimal steady state solution, and on bounds for the higher steady state reached beyond criticality.

CHAPTER 2

Preliminary results and a Case Study

2.1 Preliminary results

We shall firstly define several important function spaces. We follow the definitions used by Ladyzenskaja, Solonnikov and Ural'ceva [31].

Definition 2.1.1

Suppose S denotes a bounded, open, connected set of points in n-dimensional real space $\mathbb{R}^n$, $\overline{S}$ is the closure of S and $0 < \alpha < 1$. Then

(i) A function $g : \overline{S} \to \mathbb{R}^n$ satisfies a Hölder condition with exponent α on $\overline{S}$ (i.e. g is of class C^α on $\overline{S}$) if $<g>_S^\alpha$ is finite, where

$$<g>_S^\alpha = \sup_{\substack{x,\, y \in \overline{S} \\ x \neq y}} \frac{|g(x) - g(y)|}{|x-y|^\alpha} .$$

(ii) Suppose k is a nonnegative integer and g is a C^k function on $\overline{S}$. Then set

$$<g>_S^k = \sum_{|\ell| = k} \sup_{x \in \overline{S}} |D_x^\ell \, g(x)| ,$$

where $\ell = (\ell_1, \ldots, \ell_n)$ is an n-tuple of nonnegative integers,

$$|\ell| = \ell_1 + \ldots + \ell_n, \qquad D_x^\ell f = \frac{\partial^{|\ell|} f}{\partial x_1^{\ell_1}, \ldots, \partial x_n^{\ell_n}} ,$$

and $\sum_{|\ell| = k}$ denotes summation over all derivatives of a given order k.

Also let $\|g\|_k = \sum_{j=0}^{k} <g>_S^j$.

(iii) If k is a nonnegative integer then g is of class $C^{k+\alpha}$ on $\bar{S}$ if each partial derivative of order $j \leq k$ exists and is of class C^{α} on $\bar{S}$. Then set

$$\|g\|_{k+\alpha} = \|g\|_k + \sum_{j=0}^{k} \sum_{|\ell| = j} \langle D_x^{\ell} g \rangle_S^{\alpha}.$$

Definition 2.1.2

Suppose k is a nonnegative integer, S is an open bounded set in $\mathbb{R}^n$ and $0 < \alpha < 1$. Then ∂S is of class $C^{k+\alpha}$ if at each point $x_0 \in \partial S$ there is a ball A, centre x_0, and a one-to-one mapping ψ of A onto an open set $D \subseteq \mathbb{R}^n$ such that

(i) $\psi(A \cap S) \subseteq \mathbb{R}_t^n = \{(x_1, \ldots, x_n) \in \mathbb{R}^n : x_i > 0\}$;

(ii) $\psi(A \cap \partial S) \subseteq \partial \mathbb{R}_t^n$;

(iii) ψ and ψ^{-1} are respectively class $C^{k+\alpha}$ on $\bar{A}$ and $\bar{D}$.

Definition 2.1.3

Suppose $S \subseteq \mathbb{R}^n$ is a bounded, open, connected set and $(a, b) \subseteq \mathbb{R}$ is an open interval. Further suppose that k is a nonnegative integer, $0 < \alpha < 1$ and $g : \bar{S} \times [a, b] \to \mathbb{R}^n$. Then g is of class $C^{2k+\alpha}$ on $\bar{S} \times [a, b]$ if $\|g\|_{2k+\alpha}$ is finite where

$$\|g\|_{2k+\alpha} = \sum_{i=0}^{2k} \sum_{|\ell| + 2j = i} [\|D_x^{\ell} D_t^{j} g\|_0 + \|D_x^{\ell} D_t^{j} g\|_{\alpha}]$$

here ℓ is as in (2.1.1) (ii), subscripts x and t represent partial derivatives with respect to the first and second variables of g respectively, and for any function $f : \bar{S} \times [a, b] \to \mathbb{R}^n$,

$$\|f\|_\alpha = \sup_{\substack{(x,t),\ (y,v) \in \bar{S} \times [a,\ b] \\ (x,t) \neq (y,v)}} \frac{|f(x,t) - f(y,v)|}{|(x,t) - (y,v)|^\alpha},$$

$$\|f\|_0 = \sup_{(x,t) \in \bar{S} \times [a,\ b]} |f(x,t)|.$$

Definition 2.1.4

Suppose $S \subseteq \mathbb{R}^n$ is a bounded, open, connected set of points. For any real $p \geq 1$, we define the Banach space $L_p(S)$ in the usual way to be the space consisting of all real measurable functions on S with finite norm

$$\|g\|_{p,\,S} = \left\{ \int_S |g(x)|^p \, dV \right\}^{1/p}$$

2.1.5 The maximum principle

One of the most important results we shall use in this thesis is the maximum principle for the solutions of differential equations. We shall use the maximum principle for the solutions of elliptic differential equations in the following two complementary forms $\boxed{A}$ and $\boxed{B}$.

$\boxed{A}$ Suppose that D is an open bounded set satisfying the interior sphere property of Sperb [32] in $\mathbb{R}^n$ and h is a continuous non-positive function. Suppose also that w_1 is a class C^2 function on D and is piecewise continuous on ∂D, and satisfies

$$\nabla^2 w_1 + h w_1 \geq 0, \quad \text{in D.}$$

Then

(i) if $h = 0$, the maximum of w_1 over $\bar{D}$ is obtained on ∂D ;

(ia) if $h = 0$ and w_1 attains a maximum of M at some point $r' \in D$, then $w_1 \equiv M$ in D ;

(ii) if ∂D is of class $C^{2+\tau}$ for some $\tau \in (0, 1)$, $h = 0$, and w_1 achieves its maximum at $r' \in \partial D$, with $w_1(r') > w_1(r)$ for all $r \in \partial D$, then $\frac{\partial w_1}{\partial n}$ (if it exists) at r' satisfies $\frac{\partial w_1}{\partial n}(r') > 0$;

(iii) if w_1 satisfies either

(a) $w_1 \leq 0$, on ∂D,

or (b) for some $\mu > 0$, $\frac{\partial w_1}{\partial n} + \mu w_1 \leq 0$, on ∂D,

then $w_1 \leq 0$ in $\bar{D}$, and $w_1(r) < 0$ for all $r \in D$ unless $\nabla^2 w_1 + hw_1 = 0$ in D and either (for (a)) $w_1 = 0$ on ∂D, or (for (b)) $\frac{\partial w_1}{\partial n} + \mu w_1 = 0$ on ∂D.

$\boxed{B}$ Suppose that D and h are as in $\boxed{A}$. Suppose also that w_2 is a class C^2 function on D and is piecewise continuous on ∂D and satisfies

$$\nabla^2 w_2 + hw_2 \leq 0, \quad \text{in } D.$$

Then

(i) if $h = 0$, then the minimum of w_2 over $\bar{D}$ is obtained on ∂D ;

(ia) if $h = 0$ and w_2 attains a minimum of m at some point $r' \in D$, $w_2 \equiv m$ in D ;

(ii) if ∂D is of class $C^{2+\tau}$ for some $\tau \in (0, 1)$, $h = 0$, and w_2 achieves its minimum at $r' \in \partial D$, with $w_2(r') < w_2(r)$ for all $r \in \partial D$, then $\frac{\partial w_2}{\partial n}$ (if it exists) at r′ satisfies $\frac{\partial w_2}{\partial n}(r') < 0$;

(iii) if w_2 satisfies either

(a) $w_2 \geq 0$, on ∂D,

or (b) for some $\mu > 0$, $\frac{\partial w_2}{\partial n} + \mu w_2 \geq 0$, on ∂D,

then $w_2 \geq 0$ on $\bar{D}$, and $w_2(r) > 0$ for all $r \in D$ unless $\nabla^2 w_2 + h w_2 = 0$ in D and either (for (a)) $w_2 = 0$ on ∂D, or (for (b)) $\frac{\partial w_2}{\partial n} + \mu w_2 = 0$ on ∂D.

■

For a fuller discussion of the various maximum principles see Sperb [32] and Gilbarg and Trudinger [33].

We shall now define the terms 'upper' and 'lower' solutions for the general elliptic differential equation, which includes a non-local term, that we shall be discussing in this work.

Definition 2.1.6

Consider the nonlinear elliptic boundary value problem

$$\nabla^2 u + f\left(r,\ u,\ \int_\Omega g(u)dV\right) = 0, \quad r \in \Omega, \tag{2.1}$$

$$Bu = q, \quad r \in \partial\Omega, \tag{2.2}$$

where B is one of the boundary operators

$$Bu \equiv u,$$

or

$$Bu \equiv \frac{\partial u}{\partial n} + \mu u,$$

Ω is an open bounded set satisfying the interior sphere property of Sperb [32], and, for the purposes of this thesis, q is either zero or a piecewise continuous positive function.

The function $\phi(r)$ is an upper solution for (2.1), (2.2) if ϕ is of class C^2 in $\bar{\Omega}$ and satisfies

$$\nabla^2\phi + f\left(r, \phi, \int_\Omega g(\phi)dV\right) \leq 0, \qquad r \in \Omega,$$

$$B\phi \geq q, \qquad r \in \partial\Omega.$$

Similarly the function $\psi(r)$ is a lower solution for (2.1), (2.2) if ψ is of class C^2 in $\bar{\Omega}$ and satisfies

$$\nabla^2\psi + f\left(r, \psi, \int_\Omega g(\psi)dV\right) \geq 0, \qquad r \in \Omega,$$

$$B\psi \leq q, \qquad r \in \partial\Omega.$$

∎

The existence of upper and lower solutions can be combined with the maximum principle to show that elliptic boundary value problems of the form (2.1), (2.2) have a solution. The result we will use here can be considered to be a generalization of Sattinger's [34] result concerning the case $g(u) \equiv 0$. The proof we will use is similar to that of Sattinger's except a Frèchet derivative is introduced to extend the results to non-zero g(u). The proof is given in detail both for the sake of completeness and as it illustrates the method of monotone iteration inherent in many of the results in this thesis.

Theorem 2.1.7

Suppose there exists an upper solution $\phi_0(r)$ of (2.1), (2.2) and a lower solution $\psi_0(r)$ of (2.1), (2.2) with $\phi_0(r) \geq \psi_0(r)$ for $r \in \Omega$. Then there exists a regular solution u(r) of (2.1), (2.2) such that

$$\psi_0 \leq u \leq \phi_0, \qquad r \in \Omega.$$

Proof

We will assume that we can find a positive constant Θ so that the function

$$F\left(r, u, \int_\Omega g(u)\, dV\right) \equiv f\left(r, u, \int_\Omega g(u)\, dV\right) + \Theta u,$$

is an increasing function of u.

Now $F\left(r, u, \int_\Omega g(u)\, dV\right)$ will be an increasing function of u if the corresponding Frèchet derivative is positive. To explain what is mean by the Frèchet derivative of F, we will consider the non-local term in the function which maps $u \to \int_\Omega g(u)\, dV$ to be given by

$$k(u) = \int_\Omega g(u)\, dV.$$

The Frèchet derivative of f(r, u, k(u)) for a small positive perturbation h(r) is defined to be J(u)(h) where

$$f(r, u+h, k(u+h)) - f(r, u, k(u)) = J(u)(h) + o(\|h\|).$$

Now

$$J(u)(h) = \frac{\partial f}{\partial u}(r, u, k)\, h + \frac{\partial f}{\partial k}(r, u, k)\, K(u)(h),$$

where K(u)(h) is a 'complementary' Frèchet derivative satisfying

$$k(u+h) - k(u) = K(u)(h) + o(\|h\|),$$

i.e.

$$K(u)(h) = \int_\Omega \frac{\partial g}{\partial u} h \, dV.$$

Obviously if $g(u) \equiv 0$, the requirement on Θ reduces to

$$\frac{\partial f}{\partial u}(r, u) + \Theta > 0, \qquad \text{(c.f. Sattinger [34])},$$

otherwise it is sufficient that Θ satisfies, for all small positive perturbations h,

$$J(u)(h) + \Theta h > 0, \qquad r \in \Omega.$$

Having found such a Θ, define a mapping $T : \psi = T\phi$ if

$$(\nabla^2 - \Theta)\, \psi = -\left[f\left(r, \phi, \int_\Omega g(\phi)\, dV\right) + \Theta\, \phi \right], \qquad r \in \Omega,$$

$$B\psi = q, \qquad r \in \partial\Omega.$$

Now T is completely continuous and monotone, i.e. $\phi \le \psi$ implies $T\phi < T\psi$ for $\min\psi_0 \le \phi, \psi \le \max \phi_0$. To show this monotonicity consider $\phi \le \psi$, then

$$(\nabla^2 - \Theta)T\phi = -\left[f\left(r, \phi, \int_\Omega g(\phi)\, dV\right) + \Theta\phi \right], \quad r \in \Omega,$$

$$(\nabla^2 - \Theta)T\psi = -\left[f\left(r, \psi, \int_\Omega g(\psi)\, dV\right) + \Theta\psi \right], \quad r \in \Omega,$$

$$BT\phi = BT\psi = q, \quad r \in \partial\Omega.$$

So

$$\left.\begin{aligned} (\nabla^2 - \Theta)\,(T\psi - T\phi) = -\Big[f\left(r, \psi, \int_\Omega g(\psi)\, dV\right) - f\left(r, \phi, \int_\Omega g(\phi)\, dV\right) \\ + \Theta(\psi - \phi) \Big], \quad r \in \Omega \\ B(T\psi - T\phi) = 0, \quad r \in \partial\Omega. \end{aligned}\right\} \quad (2.3)$$

If we now define

$$F\left(r, u, \int_\Omega g(u)\, dV\right) = f\left(r, u, \int_\Omega g(u)\, dV\right) + \Theta u,$$

then F has a positive Frèchet derivative and so is increasing in u. So the terms in the square brackets on the right hand side of (2.3) combine to form

$$F\left(r, \psi, \int_\Omega g(\psi)\, dV\right) - F\left(r, \phi, \int_\Omega g(\phi)\, dV\right) \ge 0.$$

This implies

$$(\nabla^2 - \Theta)w \leq 0, \qquad r \in \Omega,$$

$$Bw = 0, \qquad r \in \partial\Omega,$$

where $w = T\psi - T\phi$. So by the maximum principle $\boxed{B}$, $w > 0$ in Ω, and hence $T\psi > T\phi$ in Ω.

Now define $\phi_1 = T\phi_0$ and $\psi_1 = T\psi_0$ (where ϕ_0, ψ_0 are respectively the upper and lower solutions of (2.1), (2.2)). We will now show that $\phi_1 < \phi_0$ and $\psi_1 > \psi_0$. We have

$$(\nabla^2 - \Theta)\, \phi_1 = -\left[f\left(r, \phi_0, \int_\Omega g(\phi_0)\, dV\right) + \Theta\, \phi_0\right], \qquad r \in \Omega,$$

$$B\phi_1 = q, \qquad r \in \partial\Omega,$$

so

$$(\nabla^2 - \Theta)(\phi_1 - \phi_0) = -f\left(r, \phi_0, \int_\Omega g(\phi_0)\, dV\right) - \Theta\phi_0 - \nabla^2\phi_0 + \Theta\phi_0,$$

$$= -\left[\nabla^2\phi_0 + f\left(r, \phi_0, \int_\Omega g(\phi_0)\, dV\right)\right],$$

$$\geq 0, \qquad r \in \Omega,$$

and

$$B(\phi_1 - \phi_0) = q - B\phi_0 \leq 0, \qquad r \in \partial\Omega.$$

Therefore by the maximum principle $\boxed{A}$, $\phi_1 < \phi_0$ in Ω. Furthermore since $\psi_0 \leq \phi_0$ it follows by the monotone property of T that $T\psi_0 < T\phi_0$ in Ω, that is, $\psi_1 < \phi_1$.

So we have

$$\psi_0 < \psi_1 < \phi_1 < \phi_0.$$

Now define $\phi_2 = T\phi_1$. Since $\phi_1 < \phi_0$, we have $T\phi_1 < T\phi_0$ in Ω, that is $\phi_2 < \phi_1$. Also if we define $\psi_2 = T\psi_1$, then $\psi_2 > \psi_1$ in Ω. Since $\psi_1 < \phi_1$ it follows that $T\psi_1 < T\phi_1$ in Ω, so $\psi_2 < \phi_2$. So we have

$$\psi_0 < \psi_1 < \psi_2 < \phi_2 < \phi_1 < \phi_0.$$

Continuing in this manner we obtain the sequences $\{\phi_i\}$, $\{\psi_i\}$ satisfying

$$\psi_0 < \psi_1 < \psi_2 < \ldots < \phi_2 < \phi_1 < \phi_0.$$

Since the sequences $\{\phi_i\}$, $\{\psi_i\}$ are monotone and bounded, both converge pointwise. Let these limits be $\tilde{\phi}(r)$ and $\tilde{\psi}(r)$ respectively where

$$\tilde{\phi}(r) = \lim_{i\to\infty} \phi_i(r)\,, \quad \tilde{\psi}(r) = \lim_{i\to\infty} \psi_i(r).$$

The operator T is a composition of the nonlinear operation $\phi \longmapsto f\left(r, \phi, \int_\Omega g(\phi)\, dV\right) + \Theta\phi$ with the inversion of the linear, inhomogeneous elliptic boundary value problem $\chi \longmapsto \psi$ defined by

$$(\nabla^2 - \Theta)\,\psi = \chi, \qquad r \in \Omega$$

$$B\psi = q, \qquad r \in \partial\Omega$$

For ϕ and $f\left(r, \phi, \int_\Omega g(\phi)\, dV\right)$ bounded on the range of ϕ, the first operation takes bounded pointwise convergent sequences into pointwise convergent sequences. The operation $\chi \mapsto \psi$ takes $L_p(\Omega)$ continuously into the Sobolev space $W_{2,\,p}(\Omega)$ for all p, $1 < p < \infty$ (by the L_p estimates of Agmon et al [35]). So since $\phi_i = T\phi_{i-1}$ and since $\{\phi_i\}$ is a bounded pointwise convergent sequence, it converges also in $W_{2,\,p}$. By the embedding lemma [35], $W_{2,\,p}$ is embedded continuously into $C^{1+\alpha}$, and by the classical Schauder estimates for regular elliptic boundary value problems $\{\phi_i\}$ then also converges in $C^{2+\alpha}$. So we have

$$\tilde{\phi}(r) = \lim_{i\to\infty} \phi_i(r) = \lim_{i\to\infty} T\phi_{i-1}(r) = T \lim_{i\to\infty} \phi_{i-1}(r) = T\tilde{\phi}(r),$$

and similarly

$$\tilde{\psi}(r) = \lim_{i\to\infty} \psi_i(r) = \lim_{i\to\infty} T\,\psi_{i-1}(r) = T \lim_{i\to\infty} \psi_{i-1}(r) = T\,\tilde{\psi}(r).$$

So $\tilde{\phi}$ and $\tilde{\psi}$ are fixed points of the mapping T, and are of class $C^{2+\alpha}(\Omega)$ for $0 < \alpha < 1$. Thus $\tilde{\phi}$ and $\tilde{\psi}$ are solutions of (2.1), (2.2). Therefore (2.1), (2.2) has at least one solution between ϕ_0 and ψ_0. This completes the proof.

■

We shall make use throughout this thesis of the function w(r) which satisfies:

$$\left.\begin{array}{ll} \nabla^2 w + 1 = 0, & r \in \Omega \subseteq \mathbb{R}^3, \\ \text{with either} & \\ \dfrac{\partial w}{\partial n} + \mu w = 0, & r \in \partial\Omega, \\ \text{(where } \partial\Omega \text{ is of class } C^{2+\tau} \text{ for some } \tau \in (0,1)), & \\ \text{or} & \\ w = 0, & r \in \partial\Omega. \end{array}\right\} \quad (2.4)$$

Theorem 2.1.8

Suppose the function w(r) satisfies (2.4) in Ω.

Then

(i) $w(r) > 0, \quad r \in \Omega,$

(ii) $\dfrac{\partial w(r)}{\partial n} < 0, \quad r \in \partial\Omega.$

Proof

Directly from the maximum principle $\boxed{B}$.

Theorem 2.1.9

Consider the problems

(a)
$$\nabla^2 w_s + 1 = 0, \quad r \in S \subseteq \mathbb{R}^3,$$
$$w_s = 0, \quad r \in \partial S,$$

and

(b)
$$\nabla^2 w_d + 1 = 0, \quad r \in D \subseteq \mathbb{R}^3,$$
$$w_d = 0, \quad r \in \partial D,$$

where S, D are regions satisfying the interior sphere property of Sperb [32].

Then if $S \subseteq D$, i.e. S is wholly enclosed by D,

$$w_d \geq w_s, \quad r \in S.$$

Proof

Assume there exist points in S such that $w_s > w_d$. Then, since w_d and w_s are positive in S by Theorem 2.1.8, there exists a positive constant $k < 1$ such that

$$kw_s < w_d \quad \text{for} \quad r \in S/r', \tag{2.5}$$

$$kw_s = w_d \quad \text{at} \quad r = r' \in S, \tag{2.6}$$

(if there exists more than one such point r', we choose just one of these points in the following argument). Therefore $kw_s - w_d$ has a maximum of zero at $r = r'$. But $\nabla^2(kw_s - w_d) = -k + 1 > 0$ everywhere in S and in particular at $r = r'$, so by the maximum principle $\boxed{A}$, $kw_s - w_d \equiv 0$ for all $r \in S$. This is a contradiction of inequality (2.5). Therefore $w_d \geq w_s$, $r \in S$.

Theorem 2.1.10

Let $D \subseteq \mathbb{R}^3$ be any convex shape with ∂D of class $C^{2+\tau}$ for some $\tau \in (0, 1)$, and S be a sphere (of radius a) wholly enclosed by D. If we consider the problems

(a) $\quad \nabla^2 v + 1 = 0, \qquad r \in D,$

$$\frac{\partial v}{\partial n} + \mu v = 0, \qquad r \in \partial D,$$

and

(b) $\nabla^2 w_s + 1 = 0, \qquad r \in S,$

$$\frac{\partial w_s}{\partial n} + \mu w_s = 0, \qquad r \in \partial S,$$

with $\mu > 0$,

then $v \geq w_s, \qquad r \in S.$

Proof

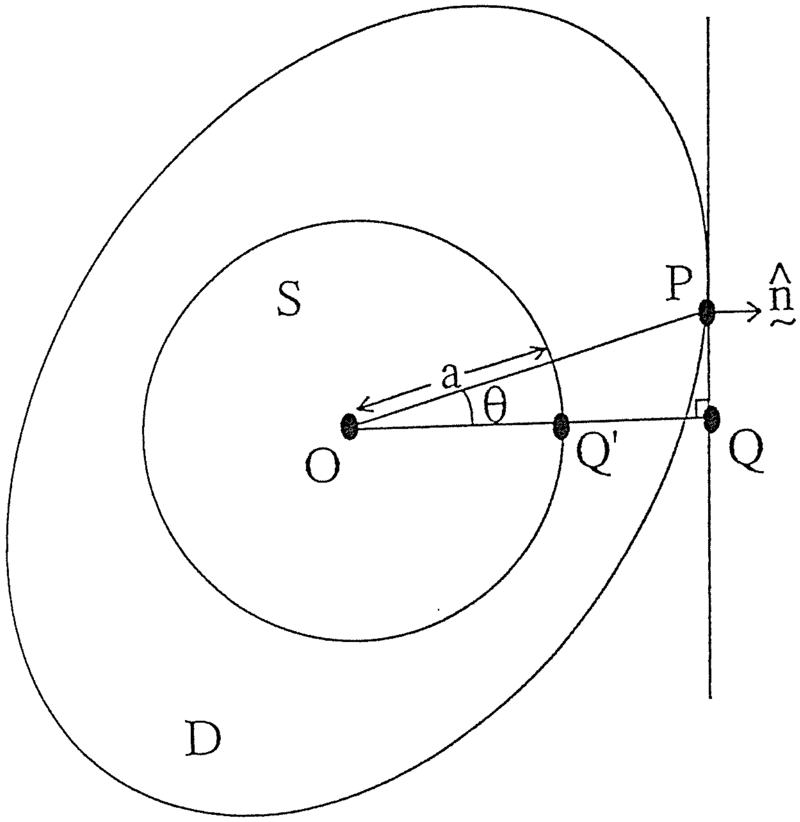

Figure 2.1 Convex shape with enclosed sphere

Let O be the centre of the sphere, P be a point on ∂D, Q be on the tangent to ∂D at P such that PQ is perpendicular to OQ, Q′ be a point on OQ which is also on ∂S, and let θ be the angle between OQ and OP. It is well-known that the solution to (b) is

$$w_s(r) = \frac{a^2 - r^2}{6} + \frac{a}{3\mu}, \quad r \in S. \tag{2.7}$$

Now we can easily extend w_s's domain to D, as w_s satisfies the same equation i.e. $\nabla^2 w_s + 1 = 0$. Consider the new boundary value

$$\left(\frac{\partial w_s}{\partial n} + \mu w_s\right)\bigg|_p .$$

Now at P,

$$\frac{\partial w_s}{\partial r} = \frac{-OP}{3}, \quad w_s = \frac{a^2 - OP^2}{6} + \frac{a}{3\mu},$$

and

$$\frac{\partial w_s}{\partial n} = \frac{\partial w_s}{\partial r}\cos\theta.$$

So

$$\left(\frac{\partial w_s}{\partial n} + \mu w_s\right)\bigg|_p = \frac{-OP}{3}\cos\theta + \frac{a}{3} + \mu\left(\frac{a^2 - OP^2}{6}\right)$$

$$= \frac{-OP}{3}\frac{OQ}{OP} + \frac{a}{3} + \mu\left(\frac{a^2 - OP^2}{6}\right)$$

but $OQ \geq a$, (for all P since D is a convex shape and $OQ \geq OQ' = a$)

and $OP \geq a$,

which gives

$$\left(\frac{\partial w_s}{\partial n} + \mu w_s\right)\bigg|_p \leq 0, \quad \forall\, P \in \partial D.$$

We finally consider the function $v - w_s$ (again extending w_s's domain to D),

$$\nabla^2(v - w_s) = 0, \qquad r \in D,$$

$$\frac{\partial(v - w_s)}{\partial n} + \mu(v - w_s) \geq 0, \qquad r \in \partial D,$$

which gives, by the maximum principle $\boxed{B}$, $v \geq w_s$, $r \in D$, and in particular

$$v \geq w_s, \qquad r \in S.$$

■

Corollary 2.1.11

For the region D and function v defined in Theorem 2.1.10, there exists an $\varepsilon > 0$ such that

$$v \geq \varepsilon, \qquad \text{for all } r \in \bar{D}.$$

Proof

Considering the vector $\underset{\sim}{r}$ to be a position vector in 3-space, define the sphere S_δ with centre $\underset{\sim}{r}_s$ to be

$$S_\delta = \{\underset{\sim}{r} : |\underset{\sim}{r} - \underset{\sim}{r}_s| < \delta\}.$$

Now as D is convex, there is a $\delta > 0$ such that $\forall \underset{\sim}{r} \in \bar{D}$, there exists a sphere S_δ such that $\underset{\sim}{r} \in \bar{S}_\delta$. Then by (2.7) and Theorem 2.1.10,

$$v \geq \frac{\delta}{3\mu} > 0, \qquad \forall \underset{\sim}{r} \in \bar{D}.$$

■

The result stated below may well be a standard result from differential equation theory, but we present a proof here for completeness.

Theorem 2.1.12

Suppose there exists a function ϕ which is of class C^2 on a region $\Omega \subseteq \mathbb{R}^3$ and satisfies

$$\nabla^2\phi < 0, \quad \text{at} \quad r = r' \in \Omega.$$

Then ϕ cannot have a local minimum at $r = r'$.

Proof

For the purposes of this argument we will write $r \in \Omega$ as the position vector $\underset{\sim}{r} = (X_1, X_2, X_3)$ in a suitable cartesian coordinate system.

Suppose $\phi(\underset{\sim}{r})$ does have a minimum at $\underset{\sim}{r} = \underset{\sim}{r}'$, and $\nabla^2\phi(\underset{\sim}{r}') < 0$. The Taylor series expansion of $\phi(\underset{\sim}{r})$ about $\underset{\sim}{r} = \underset{\sim}{r}'$ is

$$\phi(\underset{\sim}{r}) = \phi(\underset{\sim}{r}') + (\underset{\sim}{r}-\underset{\sim}{r}')^T \,\nabla\phi(\underset{\sim}{r}') + \frac{1}{2}(\underset{\sim}{r}-\underset{\sim}{r}')^T \,A(\underset{\sim}{r}-\underset{\sim}{r}') + o(\|\underset{\sim}{r}-\underset{\sim}{r}'\|^2),$$

where A is the Hessian matrix of ϕ given by

$$A_{ij} = \frac{\partial^2\phi}{\partial X_i \partial X_j}(\underset{\sim}{r}').$$

This gives (as $\nabla\phi(\underset{\sim}{r}') = \underset{\sim}{0}$),

$$\phi(\underset{\sim}{r}) - \phi(\underset{\sim}{r}') = \frac{1}{2}(\underset{\sim}{r}-\underset{\sim}{r}')^T \,A(\underset{\sim}{r}-\underset{\sim}{r}') + o(\|\underset{\sim}{r}-\underset{\sim}{r}'\|^2) \geq 0,$$

hence A is a semi-positive definite matrix with

$$\text{trace}(A) = \nabla^2\phi(\underset{\sim}{r}') \geq 0.$$

This contradicts our original statement regarding the sign of $\nabla^2\phi(\underset{\sim}{r}')$ and so completes the proof.

2.2 Industrial Case Study

2.2.1 Background

In this section we will consider in detail the investigation of a particular industrial fire caused by spontaneous ignition. By using the experimentally measured physical parameters of the materials involved, we shall predict a safe storage (or in this case, cleaning) regime which should prevent similar fires from occurring in the same environment. The fire in question was caused by the self-heating to ignition of a wood fibre dust layer on a hot factory press. Since the typical press operating temperature was approximately 200°C, this fire comes under the first of the two categories of spontaneous combustion fires outlined in the introduction i.e. where a small body of material is stored subject to high ambient conditions. Since the hot surface temperature is above 100°C we will assume that there is no moisture and there are no microbes present in the self-heating dust layer (the maximum temperature commonly recognised as an upper limit for living processes is 75 - 79°C (Kempner [36])). Therefore we will assume the self-heating of the body is due to a single exothermic process i.e. direct chemical oxidation, so that the analysis of the model can proceed by the single Arrhenius term approach. The problem can be treated as a self-heating body subject to asymmetric boundary conditions. We will compare the results obtained using three different approaches, all of which solve for the steady states ($\partial T/\partial \hat{t} = 0$) of the classical problem (1.1a, b, c), (1.2). Firstly by the method of Thomas and Bowes [8], which uses the Frank-Kamenetskii approximation to the Arrhenius term and assumes the dust layer can be approximated by an infinite slab. Secondly by a method which retains the full Arrhenius kinetics but also assumes the body is an infinite slab. For this method we use the new dimensionless formulation of Burnell et al [12], this approach has also been studied by Shoumann and Donaldson [9] using the classical Frank-Kamenetskii dimensionless formulation. Finally we shall use a method which solves the full problem: full Arrhenius kinetics in the three dimensional domain. By these comparisons we hope to answer some of the following questions that arise in practical situations using ignition theory.

(i) how well does the Frank-Kamenetskii approximation behave in practice?

(ii) when does the infinite slab approximation for a rectangular block fail to be valid in ignition theory?

(iii) what are the upper and lower bounds for the steady state temperature profile beyond criticality for models retaining the full Arrhenius kinetics?

We will comment on the suitability of Newtonian cooling versus perfect heat transfer boundary conditions for this particular problem. Finally we shall show that the minimal positive solutions for $U_p < U_{p,\,crit}$ for both the full Arrhenius term models is stable. We shall do this by a non-trivial extension of the approach of Keller and Cohen [37]. We must make this adaptation since, unlike Keller and Cohen's [37] system, our bifurcation parameter U_p occurs in the boundary conditions for the model. This work has been published, see Sisson, Swift and Wake [10].

At this stage we shall give a more detailed outline of the conditions in the factory under which the fire occurred.

A New Zealand company which produces medium density fibreboard from pine woodchips noticed several unexplained fires occurring on the presses in their factory (on average two per year). Figures 2.2 - 2.4 below show, respectively, the fibreboard processing machine within the factory, the fibreboard press itself, and the finished product - medium density fibreboard.

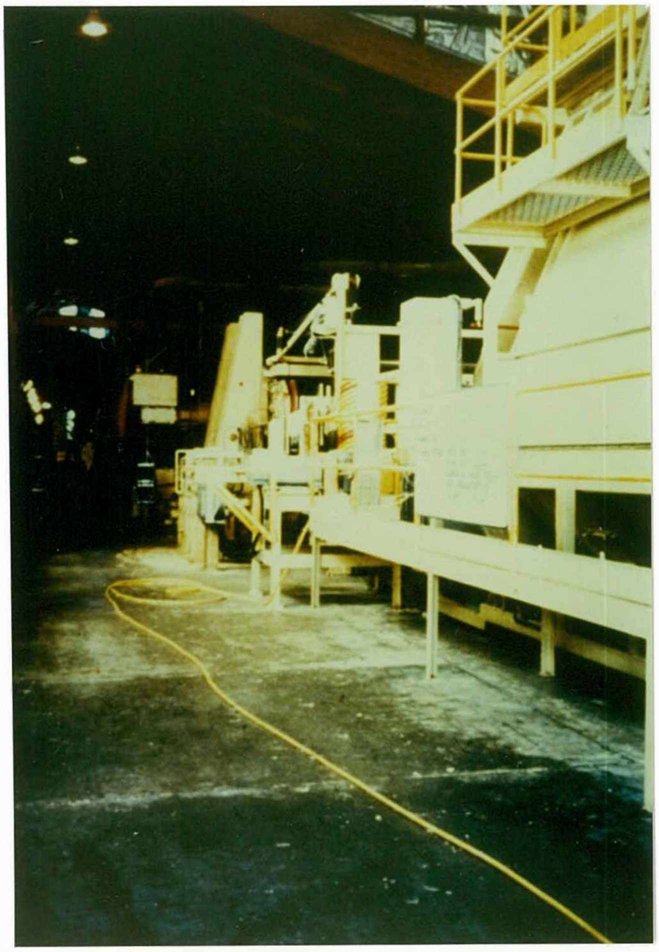

Figure 2.2 Fibreboard processing machine

Figure 2.3 Fibreboard press

Figure 2.4 Medium density fibreboard

Figure 2.5 below gives a schematic representation of the press operation in the factory.

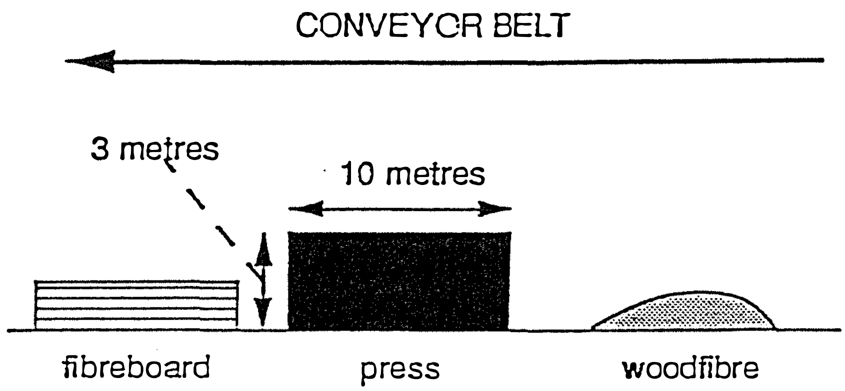

Figure 2.5 Schematic diagram of fibreboard press

The press itself was heated by thermal oil usually at a temperature of 200°C (subject to fluctuations). During its normal operation deposits of mixed fibre and oil built up as dust layers on various parts of the press. The company required the possible cause of the fires due to spontaneous ignition of these dust layers to be investigated, given that the normal 'ignition temperature' of the fibre/oil substance was well in excess of 200°C. The results would be used to implement efficient cleaning procedures (the press operated 24 hours per day, being shut down only for cleaning). On a visit to the factory made by one of the team of investigators, it was observed that the fibre/oil mixture was escaping from the conveyor belt and building up on shelves inside the press casing. The largest of these dust layers is shown in Figure 2.6 below.

Figure 2.6 Largest dust layer

This dust layer was observed to be a rectangular block of fixed base 50cm × 100cm. The height of the dust layer (a_h) was measured to be a maximum of 20cm on the day of the visit. The block is shown schematically in Figure 2.7 below.

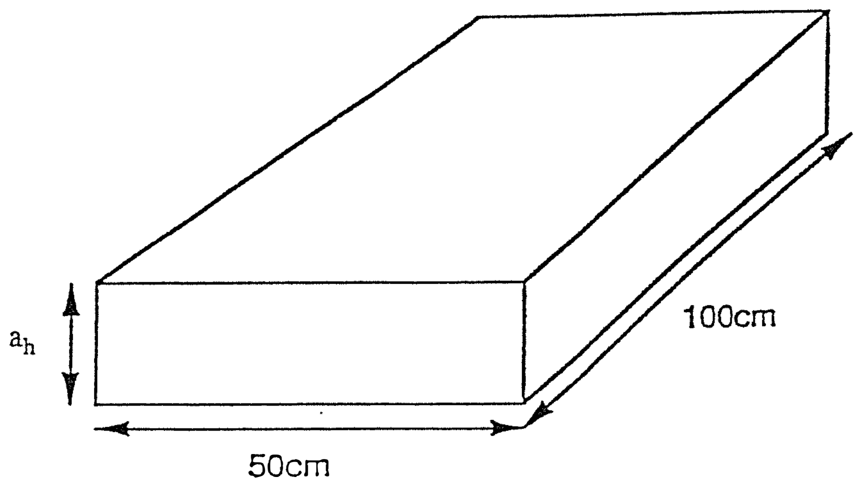

Figure 2.7 Schematic diagram of largest dust layer

The problem then, is to estimate the maximum height of the rectangular block (as a function of the press temperature), such that the dust layer is not likely to self-heat to ignition.

2.2.2 Boundary conditions

The block shown in Figure 2.7 does not satisfy the 'interior sphere' property (see Sperb [32]). So in order to use maximum principle $\boxed{B}$ (part (ii)) we consider a similar block with 'rounded corners'. This will have negligible effect on the nature of the bifurcation diagrams and the results that follow (see e.g. Fradkin and Wake [38]).

In this section we will consider the suitable boundary conditions for the press/dust layer interface. The boundary conditions for the dust layer/air interface will be discussed further in a later section in this Chapter. If, provisionally, Newtonian cooling boundary conditions are taken at each interface, then the boundary conditions become

$$k_2 \frac{\partial T}{\partial n} + h_1 (T - T_p) = 0, \quad \text{at the press/dust layer interface,} \tag{2.8}$$

$$k_2 \frac{\partial T}{\partial n} + h_2 (T - T_a) = 0, \quad \text{at the dust layer/air interface,} \tag{2.9}$$

where

k_2 = thermal conductivity of the fibre/oil dust layer,

h_1 = heat transfer coefficient for the press/dust layer interface,

h_2 = heat transfer coefficient for the dust layer/air interface,

T_p = absolute temperature of the press,

T_a = absolute ambient temperature in the factory (taken as a fixed 300K),

also

k_1 = thermal conductivity of the press,

k_3 = thermal conductivity of air.

In their paper Thomas and Bowes [8] assumed perfect heat transfer between the hot surface and the slab body, that is $h_1 \to \infty$. This gives the boundary condition at the press/dust layer interface as

$$T = T_p. \tag{2.10}$$

Actual values of k_1 and k_2 are unavailable, but typical values (Jones [39]) would be

$$k_1 = 47\ \mathrm{Wm}^{-1}\ \mathrm{K}^{-1},$$

$$k_2 = 0.103\ \mathrm{Wm}^{-1}\ \mathrm{K}^{-1},$$

also

$$k_3 = 0.026\ \mathrm{Wm}^{-1}\ \mathrm{K}^{-1}.$$

Given that $k_1 >> k_2$, and h_1 is dependent on the ratio of these, Thomas and Bowes' assumption seems to be valid for this model. Thus we will also use (2.10) as the boundary condition at the press/dust layer interface. The difference between k_2 and k_3 however, and so the appropriate boundary condition at the dust layer/air interface, is less well defined.

2.2.3 Outline of Thomas and Bowes' method

The application of the paper of Thomas and Bowes [8] assumes that two important simplifications can be made to the model: (a) the rectangular block can be approximated by an infinite slab; (b) it is valid to make the Frank-Kamenetskii approximation based on the press temperature T_p, i.e.

$$\exp\left(\frac{-E}{RT}\right) \approx \exp\left(\frac{-E}{RT_p}\right)\exp\left(\frac{E(T-T_p)}{RT_p^{\,2}}\right).$$

Under these assumptions the equation for the steady states of (1.1a), (1.2) with the boundary conditions (2.9), (2.10) becomes

$$\left.\begin{aligned} &\frac{d^2\theta}{dX^2} + \delta \exp\theta = 0, && 0 < X < 2, \\ &\theta = 0, && \text{at } X = 0, \\ &\frac{d\theta}{dX} + \mu(\theta-\theta_a) = 0, && \text{at } X = 2, \end{aligned}\right\} \qquad (2.11)$$

where (using the Frank-Kamenetskii like dimensionless formulation)

$$\left.\begin{aligned}
&\theta = \frac{E}{RT_p^{\,2}}(T-T_p), \qquad && \theta_a = \frac{E}{RT_p^{\,2}}(T_a-T_p),\\
&\mu = \frac{h_2\left(\frac{a_h}{2}\right)}{k_2}, && X = \frac{x}{\left(\frac{a_h}{2}\right)},\\
&\delta = \frac{QZ\rho E\left(\frac{a_h}{2}\right)^2}{kRT_p^{\,2}}\exp\left(\frac{-E}{RT_p}\right) &&
\end{aligned}\right\} \qquad (2.12)$$

The analysis of (2.11) proceeds in a similar manner to that of the corresponding model with symmetric boundary conditions outlined between equations (1.5a) - (1.6b) of Chapter 1. The δ, $\|\theta\|_0$ space bifurcation diagram can also be summarised as in Figure 1.2. In their paper Thomas and Bowes tabulate δ_{crit} against θ_a, from which the critical value of the height a_h can be estimated, for a particular T_p, via (2.12). These results (once we have chosen the appropriate boundary condition at the dust layer/air interface), and the effect of the above simplifications on the predictions for the critical dust layer heights, will be shown later.

2.2.4 Outline of full Arrhenius, infinite slab model

To assess the validity of the Frank-Kamenetskii approximation we shall also solve the problem by retaining the full Arrhenius kinetics and also approximating the block by an infinite slab. Using the dimensionless formulation of Burnell et al [12] the steady state problem becomes

$$\left.\begin{array}{lr} \dfrac{d^2u}{dX^2} + \eta \exp\left(\dfrac{-1}{u}\right) = 0, & 0 < X < 1, \\[2ex] u = U_p, & \text{at } X = 0, \\[2ex] \dfrac{du}{dX} + Bi(u - U_a) = 0, & \text{at } X = 1 \end{array}\right\} \tag{2.13}$$

where

$$\left.\begin{array}{lll} u = \dfrac{RT}{E}, & U_p = \dfrac{RT_p}{E}, & U_a = \dfrac{RT_a}{E}, \\[2ex] \eta = \dfrac{\rho QAR(a_h)^2}{kE}, & X = \dfrac{x}{a_h}, & Bi = \dfrac{h_2 a_h}{k_2} \end{array}\right\} \tag{2.14}$$

Here η is a constant (for a given a_h) and the bifurcation (distinguished) parameter is taken as U_p, the dimensionless temperature of the press. No exact solution is known for (2.13) so it must be solved by numerical means. The numerical algorithm used is similar to that outlined for the three dimensional model in Section 2.2.8 later in this Chapter. A schematic example of a typical bifurcation diagram in U_p, β space (where β is the temperature of a typical point in the domain) for a model which retains the full Arrhenius kinetics is given below in Figure 2.8.

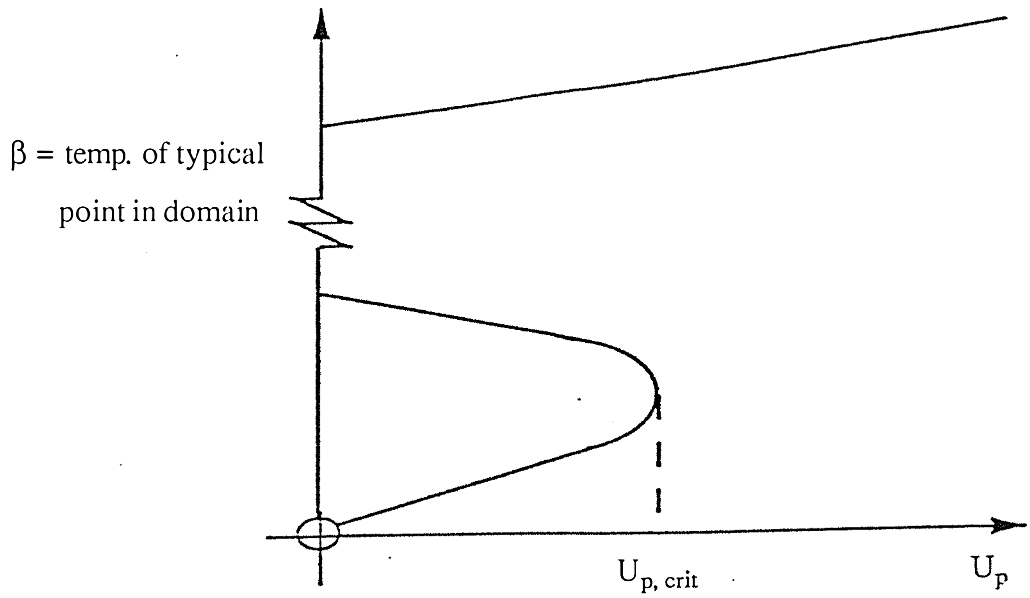

Figure 2.8 Schematic diagram of a typical U_p, β bifurcation diagram for the full Arrhenius, infinite slab model

For $U_p > U_{p,\,crit}$ there exists a high temperature steady state profile. This bifurcation diagram can be compared with that of Thomas and Bowes [8] (Figure 1.2) which predicts no steady state solutions beyond criticality. This larger steady state is 'lost' due to the Frank-Kamenetskii approximation to the Arrhenius term. Later in this chapter we shall verify that this steady state is so large that ignition will have occurred 'long' before it is ever reached in a time sense.

2.2.5 Measurement of physical constants related to the model

Experimental analysis was performed on samples of the fibre/oil material (Smedley [40]) using methods similar to those outlined in the introduction. This analysis yielded

$$\frac{\rho QAR}{kE} = 4.23 \times 10^{14} \text{ m}^{-2},$$

$$\frac{E}{R} = 16220 \text{ K}.$$

The actual value of the dust layer/air heat transfer coefficient was unavailable, but, given that a typical value of a wall/air heat transfer coefficient in still air is 8.3 $\mathrm{Wm^{-1}K^{-1}}$ (Jones [39]) we will take

$$\frac{h_2}{k_2} \sim 80\text{m}^{-1}.$$

2.2.6 The boundary condition at the dust layer/air interface

In section 2.2.2 above we justified the boundary condition $T = T_p$ at the press/dust layer interface. Here we will test the hypothesis that $h_2 \to \infty$ is also a valid assumption for the model, i.e. that the boundary condition at the dust layer/air interface can be taken as

$$T = T_a. \tag{2.15}$$

We will use the method in section 2.2.4 (infinite slab, full Arrhenius model) with

(a) $h_2 \to \infty$,

i.e. $T = T_a$ at the dust layer/air interface,

and

(b) $\dfrac{h_2}{k_2} = 80m^{-1}$,

i.e. $\dfrac{dT}{dx} + 80(T-T_a) = 0$ at the dust layer/air interface,

and compare the results.

Figure 2.9 below shows the comparison of the graphs of a_h vs critical temperature of the press for (a) and (b).

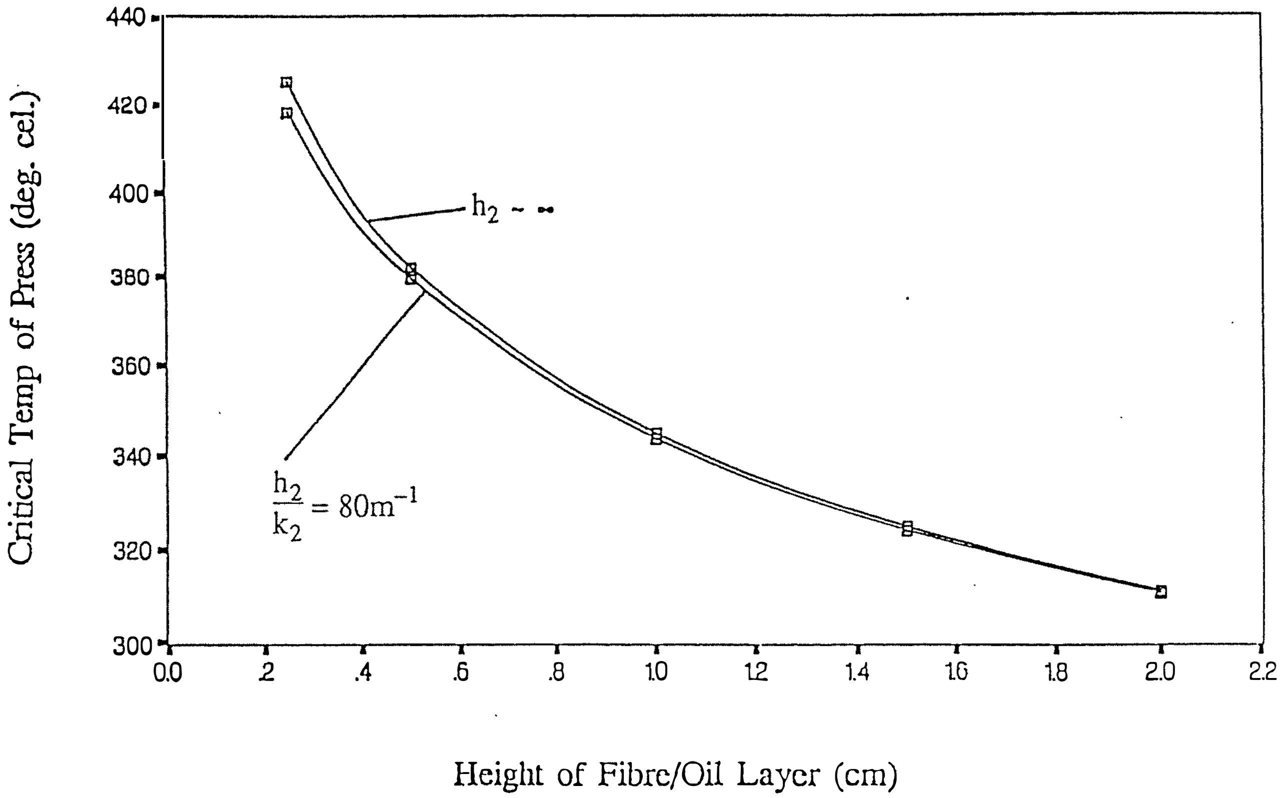

Figure 2.9 Comparison of critical press temperatures for given dust layer heights for $h_2 \rightarrow \infty$ and $h_2/k_2 = 80m^{-1}$.

The comparison suggests that for the practical range of a_h ($\geq$ 2cm) and T_p (<573K) the critical press temperatures corresponding to the two boundary conditions are indistinguishable. The tabulated results in Thomas and Bowes paper also indicate that $h_2 \to \infty$ is a good approximation for this model. Consequently our final steady state model on which the analysis of all three methods will be based is the steady states of (1.1a), (1.2) with the boundary conditions (2.10), (2.15).

2.2.7 Existence of solutions to the full Arrhenius model

In this section we will verify the existence of at least one solution for all $U_p > 0$ (in particular $U_p > U_{p,\,crit}$) for the models which retain the full Arrhenius kinetics (i.e. both the infinite slab and the full three dimensional domains). We will also show, using the maximum principle, that any solution of the model must occur between the constructed bounds.

Theorem 2.2.1

Consider the problem

$$\left.\begin{array}{ll} \nabla^2 u + \eta \exp\left(\dfrac{-1}{u}\right) = 0, & \text{in } \Omega, \\[2ex] u(\partial\Omega') = U_a, & \\ u(\partial\Omega'') = U_p, & \partial\Omega' \cup \partial\Omega'' = \partial\Omega, \\[2ex] \text{with} \quad U_p > U_a > 0, & \eta > 0. \end{array}\right\} \qquad (2.16)$$

There exists a solution u to this problem for all $U_p > U_a > 0$, satisfying

$$U_a \leq u \leq U_p + \eta w,$$

where w satisfies (2.4) with $w(\partial\Omega) = 0$.

Proof

Let
$$\psi(r) \equiv U_a \quad r \in \Omega,$$

then
$$\nabla^2\psi + \eta \exp\left(\frac{-1}{\psi}\right) = \eta \exp\left(\frac{-1}{U_a}\right) \quad \text{in } \Omega,$$
$$\geq 0,$$

and
$$\psi(r) = U_a \leq \min(U_a, U_p) \quad \text{on } \partial\Omega.$$

So $\psi(r) = U_a$ is a lower solution of (2.16).

Also let
$$\phi(r) = U_p + \eta w(r), \quad r \in \Omega,$$

then
$$\nabla^2\phi + \eta \exp\left(\frac{-1}{\phi}\right) = -\eta \left(1 - \exp\left(\frac{-1}{\phi}\right)\right), \quad \text{in } \Omega,$$
$$\leq 0,$$

and
$$\phi(r) = U_p \geq \max(U_a, U_p) \quad \text{on } \partial\Omega.$$

So $\phi(r) = U_p + \eta w(r), \quad r \in \Omega,$ is an upper solution of (2.16).

Also since $U_p > U_a$, $\phi(r) > \psi(r)$ in Ω. So by Theorem 2.1.7, there exists a solution u of (2.16) with
$$U_a \leq u \leq U_p + \eta w.$$

Corollary 2.2.2

Setting $\phi = U_p + \eta w - u$ and $\psi = u - U_a$, and applying the maximum principle $\boxed{B}$, it can easily be shown that $\phi \geq 0$ and $\psi \geq 0$ in Ω. Therefore any solution u of (2.16) must satisfy

$$U_a \leq u \leq U_p + \eta w, \quad \text{in } \Omega.$$

2.2.8 Three dimensional model and outline of the numerical algorithm

Again using the dimensionless formulation of Burnell et al [12], the three dimensional version of the steady state problem becomes

$$\left.\begin{aligned} &\frac{\partial^2 u}{\partial X^2} + \frac{\partial^2 u}{\partial Y^2} + \frac{\partial^2 u}{\partial Z^2} + \eta \exp\left(\frac{-1}{u}\right) = 0, \quad \text{in } \Omega, \\ &\text{with} \\ &U = U_a, \quad \text{on the dust layer/air interface,} \\ &U = U_p, \quad \text{on the dust layer/press interface.} \end{aligned}\right\} \qquad (2.17)$$

The dimensionless variables are defined as in (2.14) with the additions

$$Y = \frac{y}{a_h}, \quad Z = \frac{z}{a_h}. \qquad (2.18)$$

Using three term difference approximations to the second derivatives in the three coordinate directions, and a suitable three dimensional finite difference mesh to represent the domain, (2.17) reduces to a system of non-linear equations of the form

$$\underset{\sim}{F}(\underset{\sim}{a}, \beta) = \underset{\sim}{0}, \qquad (2.19)$$

where $\underset{\sim}{a}$ is the vector of unknown temperatures at the internal mesh points (excluding β), and β (which will take the role of a path following parameter) is the temperature at an arbitrarily chosen mesh point in the domain. This system is solved (for a particular a_h) by defining β to be some given β_0 and then solving the resulting well-posed system for the unknown temperature vector $\underset{\sim}{a} = \underset{\sim}{a}(\beta_0)$ by a Newton-Raphson method (which involves the calculation of the Jacobian matrix for $\underset{\sim}{F}$). We can then solve (2.19) for $\underset{\sim}{a}(\beta_0+\Delta\beta)$ by a combined Euler predictor and Newton corrector scheme. This approach is similar to that used by Abbot [41]. In particular U_p is thus calculated for a range of values of β. As β can be thought of as a characterisation value for the domain temperature profile, a plot in $U_p(\beta)$, β space will represent a steady state bifurcation diagram for the system for a particular a_h. The graph is plotted in this manner since physically U_p is the control variable and β the response. The critical value of U_p, i.e. $U_{p,\,crit}$ can then be observed from the graph in the usual way. It is expected on physical grounds that the value of $U_{p,\,crit}$ should be independent of the point at which we choose to define β, but we have been unable to find a rigorous proof of this.

2.2.9 Existence and bounds for higher steady state

In this section we will prove the existence of, and derive bounds for, the higher steady state solution the temperature will approach (in a time sense) beyond criticality. We will do this for the two models which retain the full Arrhenius term. Our aim is to show that this 'passage of U_p through criticality' is sufficient to induce thermal ignition in the body. We achieve this by showing that the steady state temperature a typical point in the body will approach is very high indeed ($> 10^{10}$ °C).

It is obvious that in most physical situations ignition will occur long before this higher steady state is attained; thus in terms of physically observed behaviour predicted beyond criticality, there is no difference between these models and the Thomas and Bowes model (which predicts no higher steady state beyond criticality), in realistic situations. However, although this steady state is not physically realizable, it is an important factor for the set of different initial conditions, which arise in, for example, the question of hot assembly (see Gray and Wake [42]).

2.2.9.1 Existence

It can be shown, using methods similar to those used by Wake et al [13] for the symmetrical heating case, that for η 'sufficiently large' (2.16) has

(i) an upper solution $\phi = U_p + \eta w$,

(ii) a lower solution $\psi = U_a + \exp(Aw\, \ell n\eta) - 1$,

with $\phi \geq \psi$ in Ω,

where w is the solution of (2.4) with $w(\partial\Omega) = 0$, and $A = \dfrac{1}{2\|w\|_0}$.

In this context, η 'sufficiently large' corresponds to η satisfying the following inequalities

$$\left.\begin{array}{ll}
\text{(i)} & \ell n\eta > \dfrac{1}{Ak_1}, \\[2ex]
\text{(ii)} & \exp(A\ell_1\, \ell n\eta) > 2, \\[2ex]
\text{(iii)} & \sqrt{\eta} > Ae\, \ell n\eta, \\[2ex]
\text{(iv)} & \eta > \dfrac{\sqrt{\eta}-1}{\|w\|_0},
\end{array}\right\} \tag{2.20}$$

where k_1, ℓ_1 are constants satisfying

$$|\nabla w|^2 \geq k_1 > 0 \quad \text{in } \Omega_{k_1},$$

$$w \geq \ell_1 > 0 \quad \text{in } \bar{\Omega}_{\ell_1},$$

with
$$\Omega_{k_1} \cup \bar{\Omega}_{\ell_1} = \Omega.$$

We will not give the details of this result at this stage, as this approach will be used again later in this thesis, and these inequalities will then be derived fully, (in Chapter 5).

By Theorem 2.1.7 there then exists, for η satisfying the inequalities (2.20), a solution u of (2.16) with

$$U_a + \exp(Aw\,\ell n\eta) - 1 \leq u \leq U_p + \eta w, \quad \text{in } \Omega. \tag{2.21}$$

This solution corresponds to the very high steady state. To obtain bounds for this steady state, or at least for a typical point in the profile, we must solve (2.4) (with $w(\partial\Omega) = 0$) in the particular domain.

2.2.9.2 Bounds on the higher steady state for the full Arrhenius, infinite slab model

To derive bounds for the higher steady state for an infinite slab of height a_h we must solve the one dimensional linear ordinary differential equation

$$\frac{d^2w}{dX^2} = -1, \quad 0 < X < 1,$$

$$w = 0, \quad \text{at } X = 0,$$
$$w = 0, \quad \text{at } X = 1.$$

This has the simple analytic solution

$$w(X) = X(1-X)/2. \tag{2.22}$$

Now, since

$$\eta = 4.23 \times 10^{14}(a_h)^2 \ m^{-2} \quad .$$

for a_h in the range of interest, i.e. $a_h \geq 5$cm, we can assume

$$\eta \geq 1.05 \times 10^{12}. \tag{2.23}$$

For w given in (2.22), that is with

$$\|w\|_0 = 0.125, \quad A = 4, \tag{2.24}$$

we can choose Ω_{k_2}, $\bar{\Omega}_{\ell_2}$ such that

$$\left.\begin{array}{ll} |\nabla w|^2 \geq k_2 = 0.23, & \text{in } \Omega_{k_2} \\ \\ w \geq \ell_2 = 0.01, & \text{in } \bar{\Omega}_{\ell_2}. \end{array}\right\} \tag{2.25}$$

Substituting these values into the inequalities (2.20) we see that all are satisfied since

(i) $27.67 > 1.09$,

(ii) $3.02 > 2$,

(iii) $1.02 \times 10^6 > 301$,

(iv) $1.05 \times 10^{12} > 8.2 \times 10^6$.

So, indeed, for the range of a_h of interest, and for w given in (2.22), η is sufficiently large so that ϕ and ψ given in section 2.2.9.1 are upper and lower solutions respectively for the infinite slab, full Arrhenius model. Now let us define β^* (in degrees Celsius) to be the temperature which the (dimensionless) temperature β of the typical point in the domain approaches for $U_p > U_{p,\,crit}$.

Then, for example, for an infinite slab of height 5cm, and a typical point chosen at the 'centre' of the slab (i.e. X = 0.5), this approach gives the following bounds on β^*

$$1.65 \times 10^{10}\ ^\circ C \le \beta^* \le 2.12 \times 10^{15}\ ^\circ C.$$

2.2.9.3 Bounds on higher steady state for full Arrhenius, three dimensional domain model.

Obtaining bounds via (2.20) involves solving the equation

$$\nabla^2 w = -1, \quad \text{in } \Omega,$$

$$w(\partial\Omega) = 0,$$

where Ω is a 'brick' of base 50cm $\times$ 100cm and height a_h. Given that we must simply show that the lower bound is sufficiently large to induce ignition, an acceptable method of obtaining bounds for this problem can be found by using the solutions for w in the inscribed and escribed spheres for the domain Ω. This has the effect of modifying the bounds in (2.21).

The inscribed and escribed spheres for the brick are defined respectively by the regions Ω_2 and Ω_1. These regions are illustrated in Figure 2.10 below.

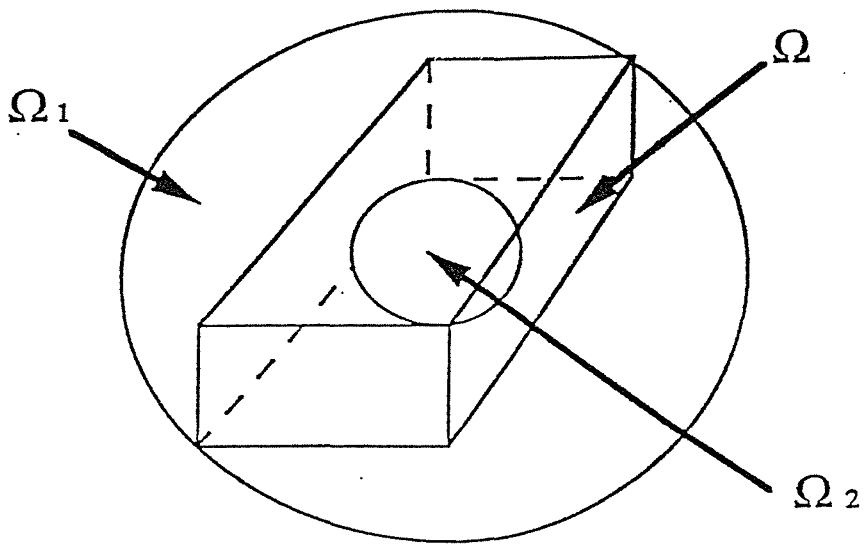

Figure 2.10 Inscribed and escribed spheres for the brick

We shall make use of the functions w_1, w_2 which are, respectively, the unique solutions to the problems

$$\left.\begin{aligned} &\nabla^2 w_1 + 1 = 0, && \text{in } \Omega_1, \\ &w_1 = 0, && \text{on } \partial\Omega_1, \end{aligned}\right\} \tag{2.26}$$

and

$$\left.\begin{array}{ll} \nabla^2 w_2 + 1 = 0, & \text{in } \Omega_2, \\ w_2 = 0, & \text{on } \partial\Omega_2, \end{array}\right\} \qquad (2.27)$$

and also of the following Theorem.

Theorem 2.2.3

If w, with $w(\partial\Omega) = 0$, w_1 and w_2 are respectively the solutions of (2.4), (2.26) and (2.27) then

$$w_1(r) \geq w(r) \geq w_2(r), \qquad r \in \Omega_2.$$

Proof

Simple application of Theorem 2.1.9.

By Theorem 2.2.1 and Corollary 2.2.2 the solution u of (2.15), and in particular the portion of the u profile inside Ω_2, exists and satisfies

$$\nabla^2 u + \eta \exp\left(\frac{-1}{u}\right) = 0, \qquad r \in \Omega_2$$

with

$$U_a \leq u(r) \leq U_p + w(r), \qquad r \in \partial\Omega_2.$$

Now consider the solution of

$$\left.\begin{aligned} &\nabla^2 u + \eta\, \exp\left(\frac{-1}{u}\right) = 0, \qquad r \in \Omega_2, \\ &u(r) = q_1(r), \qquad r \in \partial\Omega_2, \\ &U_a \le q_1(r) \le U_p + w(r), \qquad r \in \partial\Omega_2. \end{aligned}\right\} \tag{2.28}$$

where $q_1(r)$ is an unspecified function satisfying

We will show that

$$\phi = U_p + \eta w_1, \qquad r \in \Omega_2,$$

is an upper solution of (2.28).

Now

$$\nabla^2\phi + \eta\, \exp\left(\frac{-1}{\phi}\right) = \eta\left[-1 + \exp\left(\frac{-1}{\phi}\right)\right],$$

$$\le 0, \qquad r \in \Omega_2,$$

and

$$\phi(r) = U_p + \eta w_1(r) \ge U_p + w(r) \ge q_1(r), \qquad r \in \partial\Omega_2.$$

so indeed ϕ is an upper solution.

Also

$$\psi = U_a + \exp(A_2 w_2 \,\ell n\eta) - 1, \qquad r \in \Omega_2,$$

is a lower solution of (2.28) for the part of u inside Ω_2, where $A_2 = \dfrac{1}{2\|w_2\|_0}$ and η is sufficiently large so that it satisfies the following inequalities

$$\left.\begin{array}{ll} \text{(i)} & \ell n\eta > \dfrac{1}{A_2 k_3}, \\[2ex] \text{(ii)} & \exp(A_2 \ell_3 \,\ell n\eta) > 2, \\[2ex] \text{(iii)} & \sqrt{\eta} > A_2 e \,\ell n\eta, \\[2ex] \text{(iv)} & \eta > \dfrac{\sqrt{\eta} - 1}{\|w_2\|_0}, \end{array}\right\} \qquad (2.29)$$

and where k_3, ℓ_3 are constants satisfying

$$|\nabla w_2|^2 \geq k_3 > 0, \qquad \text{in } \Omega_{k_3},$$

$$w \geq \ell_3 > 0, \qquad \text{in } \bar{\Omega}_{\ell_3},$$

with
$$\Omega_{k_3} \cup \bar{\Omega}_{\ell_3} = \Omega_2.$$

Again, the details for the verification of this lower solution will be given later in the thesis. It should be noted that ψ satisfies the correct boundary inequality to be a lower solution since, on $\partial\Omega_2$

$$\psi(r) = U_a \leq q_1(r) \qquad r \in \partial\Omega_2.$$

In the inscribed sphere of radius $\frac{1}{2}$, (2.27) reduces to

$$\frac{d^2w_2}{dr^2} + \frac{2}{r}\frac{dw_2}{dr} + 1 = 0, \qquad 0 < r < \frac{1}{2},$$

$$w_2'(0) = 0,$$

$$w_2\left(\frac{1}{2}\right) = 0,$$

which has the analytic solution

$$w_2 = \frac{1}{24}(1 - 4r^2). \tag{2.30}$$

In the escribed sphere, which has radius $\sqrt{\frac{1}{4}\left(1 + \frac{5}{4\underline{a}_h^{\,2}}\right)}$, (2.26) reduces to

$$\frac{d^2w_1}{dr^2} + \frac{2}{r}\frac{dw_1}{dr} + 1 = 0, \qquad 0 < r < \sqrt{\frac{1}{4}\left(1 + \frac{5}{4\underline{a}_h^{\,2}}\right)},$$

$$w_1'\left(0\right) = 0,$$

$$w_1\left(\sqrt{\frac{1}{4}\left(1 + \frac{5}{4\underline{a}_h^{\,2}}\right)}\right) = 0,$$

which has the analytic solution

$$w_1 = \frac{1}{24}\left(1 + \frac{5}{4\underline{a}_h^{\,2}} - 4r^2\right), \tag{2.31}$$

where $\underline{a}_h$ is the dimensionless length of a_h.

Now (2.30) gives $\|w_2\|_0 = \frac{1}{24}$, $A_2 = 12$ and we can choose $\ell_3 = 0.01$, $k_3 = 0.0211$, hence η satisfies all the inequalities (2.29). Choosing the typical point β to be the centre of the escribed sphere, we obtain the following bounds for β^* (i.e. the temperature of the typical point in degrees celcius) for the three dimensional brick with dust layer height 5cm.

$$1.65 \times 10^{10}\,°C \le \beta^* \le 3.55 \times 10^{17}\,°C.$$

These results can be used to derive bounds for the higher steady state for any point within Ω_2, and they indicate that the higher steady state solution is indeed sufficiently large in magnitude to induce ignition in the body.

2.2.10 Example steady state bifurcation diagrams

In the example steady state bifurcation diagrams given below, the bold sections have been computer generated and the broken sections correspond to the higher steady state the system will approach for $U_p > U_{p,\,crit}$ (derived by appealing to the bounds in section 2.2.9). Figure 2.11 corresponds to the steady state bifurcation diagram obtained for the full Arrhenius, infinite slab model for a 5cm high dust layer with typical point β chosen at the 'centre' of the infinite slab. Figure 2.12 corresponds to the bifurcation diagram obtained for the full Arrhenius, three dimensional for the dust layer of height 5cm, with β chosen at the centre of the inscribed sphere.

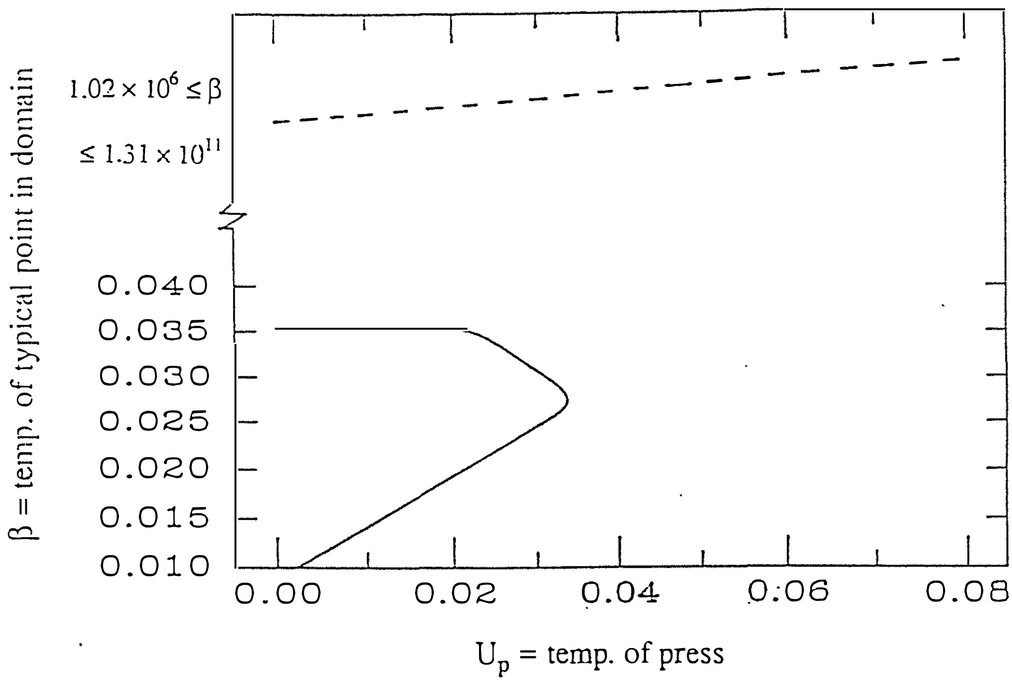

Figure 2.11 Steady state bifurcation diagram for full Arrhenius, infinite slab model (a_h = 5cm)

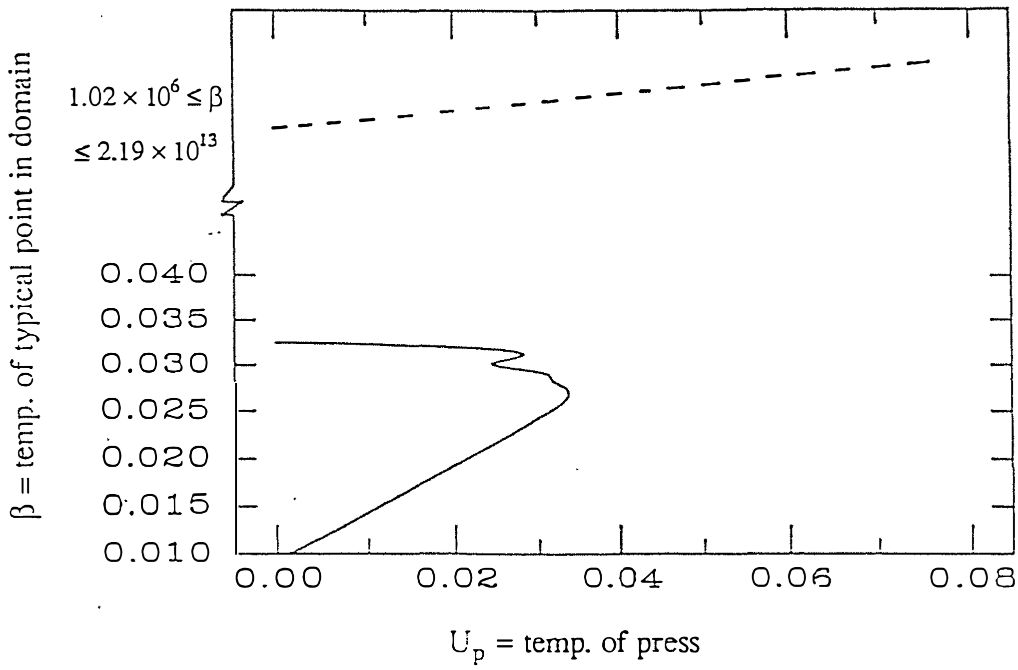

Figure 2.12 Steady state bifurcation diagram for full Arrhenius, three dimensional domain model (a_h = 5cm)

2.2.11 Stability

In this section we shall show that the minimal solution of (2.16) is stable for $U_p < U_{p,\,crit}$. We shall do this by using a similar method to that outlined in Keller and Cohen [37]. Keller and Cohen considered equations of the form

$$Lu = \lambda f(r, u), \qquad r \in \Omega, \tag{2.32}$$

where L is an elliptic, self-adjoint, second order operator and λ is the bifurcation parameter. The difference between this work and our model is that in our problem the bifurcation parameter U_p occurs in the boundary conditions, not in the equation itself. Thus our system cannot be transformed into a bifurcation problem of the form (2.32). We will follow a similar route to that of Keller and Cohen and only explain in detail the differences between the two sets of results.

We are considering solutions $u_1(r, t, U_p)$ of the parabolic problem

$$\left.\begin{aligned} \nabla^2 u_1 + \eta \exp\left(\frac{-1}{u_1}\right) &= \frac{\partial u_1}{\partial t}, \qquad r \in \Omega, \qquad t > 0, \\ u_1 &= U_a, \qquad r \in \partial\Omega', \qquad t > 0, \\ u_1 &= U_p, \qquad r \in \partial\Omega'', \qquad t > 0, \qquad \partial\Omega' \cup \partial\Omega'' = \partial\Omega, \end{aligned}\right\} \tag{2.33}$$

with $\qquad u_1(r, 0, U_p) = u_0(r), \qquad r \in \bar{\Omega},$

and the solution $u(r, U_p)$ of the corresponding steady state problem (2.16). We shall transform these systems so we are dealing with a modified problem with homogeneous boundary conditions.

Let

$$v_1(r, t, U_p) = u_1(r, t, U_p) - h(r, U_p), \tag{2.34}$$

$$v(r, U_p) = u(r, U_p) - h(r, U_p), \tag{2.35}$$

where $h(r, U_p)$ is the solution of the linear problem with inhomogeneous boundary conditions

$$\left.\begin{aligned} \nabla^2 h &= 0, && r \in \Omega, \\ h &= U_a, && r \in \partial\Omega', \\ h &= U_p, && r \in \partial\Omega'', \qquad \partial\Omega' \cup \partial\Omega'' = \partial\Omega, \\ \text{with} & && \qquad\qquad U_p > U_a > 0. \end{aligned}\right\} \tag{2.36}$$

The systems (2.16), (2.33) transform respectively to

$$\left.\begin{aligned} \nabla^2 v + \eta \exp\left(\frac{-1}{v + h}\right) &= 0, && r \in \Omega, \\ v &= 0, && r \in \partial\Omega, \end{aligned}\right\} \tag{2.37}$$

and

$$\left.\begin{aligned} \nabla^2 v_1 + \eta \exp\left(\frac{-1}{v_1 + h}\right) &= \frac{\partial v_1}{\partial t}, && r \in \Omega, \quad t > 0, \\ v_1 &= 0, && r \in \partial\Omega, \\ \text{with} \quad v_1(r, 0, U_p) &= u_0(r) - h(r, Up), && r \in \bar{\Omega}. \end{aligned}\right\} \tag{2.38}$$

We will now focus our attention on these related problems.

Lemma 2.2.4 Positivity Lemma

Let $\rho_1(r, U_p)$ be positive and continuous on Ω and let $\phi(r)$ be twice differentiable on Ω and satisfy

$$\nabla^2\phi + \rho_1(r, U_p)\phi < 0, \quad r \in \Omega,$$

$$\phi = 0, \quad r \in \partial\Omega.$$

Then $\phi(r) > 0$ on Ω if and only if $1 < \mu_1$, where μ_1 is the principle (lowest) eigenvalue of the problem

$$\nabla^2\psi + \mu\rho_1(r, U_p)\psi = 0, \quad r \in \Omega,$$

$$\psi = 0, \quad r \in \partial\Omega.$$

Proof

Similar to that of the Positivity Lemma (with $\lambda = 1$) of Keller and Cohen [37], page 1363.

We shall now state some of the properties of the function

$$f(r, v, h, U_p) = \exp\left(\frac{-1}{v + h}\right).$$

By applying the maximum principle $\boxed{\text{B}}$ to the problems (2.36), (2.37) we see that respectively $h > 0$, $v > 0$, $r \in \Omega$. This gives

$$f(r, v, h, U_p) > 0, \quad r \in \Omega. \tag{2.39}$$

we also have

$$\frac{\partial f}{\partial \phi}(r, \phi, h, U_p) > 0, \quad \text{and is continuous for } \phi > 0, \quad r \in \Omega, \tag{2.40}$$

$$\frac{\partial f}{\partial \psi}(r,\, v,\, \psi,\, U_p) > 0, \qquad \text{and is continuous for } \psi > 0, \qquad r \in \Omega. \tag{2.41}$$

We can also derive a further result concerning the monotonicity of f with respect to U_p. Consider the functions ϕ, ψ which are solutions respectively of

$$\begin{aligned} \nabla^2 \phi &= 0, && r \in \Omega, \\ \phi &= U_a, && r \in \partial\Omega', \\ \phi &= U_{p1}, && r \in \partial\Omega''. \end{aligned}$$

and

$$\begin{aligned} \nabla^2 \psi &= 0, && r \in \Omega, \\ \psi &= U_a, && r \in \partial\Omega', \\ \psi &= U_{p2}, && r \in \partial\Omega'', \end{aligned}$$

with
$$U_{p2} > U_{p1} \geq 0, \qquad \partial\Omega' \cup \partial\Omega'' = \partial\Omega.$$

Then the function $\phi - \psi$ satisfies

$$\begin{aligned} \nabla^2(\phi - \psi) &= 0, && r \in \Omega, \\ (\phi - \psi) &\geq 0, && r \in \partial\Omega. \end{aligned}$$

So by the maximum principle $\boxed{B}$, $\phi - \psi > 0$ in Ω, i.e. $\phi > \psi$ in Ω. This result combined with (2.41) gives

$$f(r,\, v,\, h(U_{p2}),\, U_{p2}) > f(r,\, v,\, h(U_{p1}),\, U_{p1}), \qquad r \in \Omega, \qquad \text{if } U_{p2} > U_{p1} \geq 0. \tag{2.42}$$

We will now give some further preliminary results which are needed before the main result on stability can be derived.

Theorem 2.2.5

Let $F(r, \phi, h, U_p)$ satisfy

$$F(r, \phi, h, U_p) > f(r, \psi, h, U_p), \quad \text{on } \Omega, \text{ if } \phi > \psi \geq 0,$$

and suppose for some $U_p > 0$ a positive solution $\phi(r, U_p)$ exists for the problem

$$\nabla^2\phi + \eta F(r, \phi, h, U_p) = 0, \quad r \in \Omega,$$

$$\phi = 0, \quad r \in \partial\Omega.$$

Then the minimal positive solution $\mathbf{v}(r, U_p)$ of (2.37) satisfies

$$\mathbf{v}(r, U_p) \leq \phi(r, U_p)$$

Proof

Similar to proof of Theorem 3.3, Keller and Cohen [37] p1367.

Corollary 2.2.6

The minimal solution $\mathbf{v}(r, U_p)$ of (2.37) is an increasing function of U_p, on $0 < U_p < U_{p,\,crit}$.

Proof

For any fixed value of U_p in the interval $0 < U_p < U_p' < U_{p,\,crit}$, define

$$F(r, v, h, U_p) = f(r, v, h, U_p').$$

Then for this value of U_p, the hypothesis of Theorem 2.2.5 is satisfied, say with $\phi(r, U_p) \equiv \mathbf{v}(r, U_p')$.

So by Theorem 2.2.5,

$$\mathbf{v}(r, U_p) \le \mathbf{v}(r, U_p').$$

Also

$$\nabla^2(\mathbf{v}(r, U_p') - \mathbf{v}(r, U_p)) = -\eta(f(r, \mathbf{v}, h, U_p') - f(r, \mathbf{v}, h, U_p))$$

$$< 0, \quad r \in \Omega, \quad \text{by } (2.42),$$

and

$$\mathbf{v}(r, U_p') - \mathbf{v}(r, U_p) = 0, \quad r \in \partial\Omega.$$

So by the maximum principle $\boxed{B}$, $\mathbf{v}(r, U_p') > \mathbf{v}(r, U_p)$ in Ω. This completes the proof.

It is well-known (see e.g. Diekmann and Temme [43] p48) that the occurrence of criticality (i.e. $U_p = U_{p,\,crit}$) corresponds to the existence of a non-trivial solution of the linearized version of the system (2.37). In fact this result is just the contra-positive of the implicit function theorem. With this in mind, a mathematical definition of $U_{p,\,crit}$ is that it is the smallest value of U_p such that the system

$$\left.\begin{aligned} \nabla^2\psi + \eta \frac{\exp\left(\dfrac{-1}{\mathbf{v}+h}\right)}{(\mathbf{v}+h)^2}\,\psi = 0, \quad & r \in \Omega, \\ \psi = 0, \quad & r \in \partial\Omega, \end{aligned}\right\} \qquad (2.43)$$

has a non-trivial solution, where $\mathbf{v}$ is the minimal solution of (2.37). That is $U_{p,\,crit}$ is the smallest value of U_p such that $\mu_1(U_p) = 1$, where $\mu_1(U_p)$ is the principle eigenvalue of

$$\left.\begin{aligned} &\nabla^2\psi + \mu\eta\,\frac{\exp\left(\dfrac{-1}{\mathbf{v}+\mathrm{h}}\right)}{(\mathbf{v}+\mathrm{h})^2}\,\psi = 0, \quad r \in \Omega, \\ &\psi = 0 \quad r \in \partial\Omega. \end{aligned}\right\} \tag{2.44}$$

Theorem 2.2.7

Let U_p lie in the open interval $0 < U_p < U_{p,\,crit}$. Then each U_p in this interval must satisfy $1 < \mu_1(U_p)$ where $\mu_1(U_p)$ is the principle eigenvalue of (2.44).

Proof

As mentioned by Keller and Cohen [37] in the proof of Theorem 4.1 p1370, the function

$$\mathbf{m}(r, U_p) \equiv \frac{\partial \mathbf{v}}{\partial U_p}(r, U_p),$$

exists and is continuous in U_p on $0 < U_p < U_{p,\,crit}$ (see note below). The function $\mathbf{m}$ then satisfies

$$\left.\begin{aligned} &\nabla^2\mathbf{m} + \eta\,\frac{\partial f}{\partial v}(r, \mathbf{v}, h, U_p)\mathbf{m} = -\,\eta\,\frac{\partial f}{\partial h}(r, \mathbf{v}, h, U_p)\,\frac{\partial h}{\partial U_p}, \quad r \in \Omega, \\ &\mathbf{m} = 0, \quad r \in \partial\Omega. \end{aligned}\right\} \tag{2.45}$$

Now (2.40), (2.41) give $\dfrac{\partial f}{\partial v} > 0$, $\dfrac{\partial f}{\partial h} > 0$ respectively, and the function $n(r, U_p) \equiv \dfrac{\partial h}{\partial U_p}(r, U_p)$ satisfies

$$\nabla^2 n = 0, \qquad r \in \Omega$$

$$n(\partial\Omega') = 0,$$

$$n(\partial\Omega'') = 1, \qquad \partial\Omega' \cup \partial\Omega'' = \partial\Omega,$$

so a simple application of the maximum principle $\boxed{B}$ shows that n > 0 in Ω. We will now show that **m** is positive (strictly) in Ω. We have by Corollary 2.2.6 that **v** is an increasing function of U_p i.e. $\mathbf{m} \geq 0$ in Ω. If we assume there is a point $r' \in \Omega$ such that $\mathbf{m} = 0$ at r' then **m** has a local minimum of zero at r'. But then (2.45) gives

$$\nabla^2 \mathbf{m} = -\eta \frac{\partial f}{\partial h}(r', \mathbf{v}, h, U_p) \frac{\partial h}{\partial U_p}, \quad \text{at } r = r',$$

$$< 0,$$

and by Theorem 2.1.12 this means that m cannot have a local minimum at $r = r'$. Thus $\mathbf{m} > 0$ in Ω. We can now apply Lemma 2.2.4 to equation (2.45) with $\mathbf{m} > 0$ to show $1 < \mu_1(U_p)$ for $0 < U_p < U_{p,\,crit}$.

Note

There is a small error in Keller and Cohen's [37] Theorem 4.1 (which is the parallel of the result we have just proved here). The result stated by Keller and Cohen implies that $1 < \mu_1(U_p)$ for **all** $U_p > 0$. This is clearly untrue, since $1 = \mu_1(U_{p,\,crit})$ and a fold bifurcation must occur at an eigenvalue of the linearized problem. Also in their proof they imply that $\frac{\partial \mathbf{v}}{\partial U_p}$ is continuous for **all** $U_p > 0$, when in fact there is a discontinuity in $\frac{\partial \mathbf{v}}{\partial U_p}$ at $U_p = U_{p,\,crit}$. Thus the results in fact hold for $0 < U_p < U_{p,\,crit}$ **only**, as we have stated here.

By the standard approach of writing a solution of (2.38) in the form

$$v_1(r, t, U_p) = v(r, U_p) + \varepsilon\, \psi(r) \exp(-\alpha t) + O(\varepsilon^2), \tag{2.46}$$

where v is a solution of (2.37), we see to first order that ε, α and ψ must satisfy

$$\left.\begin{aligned} \nabla^2\psi + \left[\alpha + \eta\frac{\partial f}{\partial v}(r, v, h, U_p)\right]\psi = 0, \quad & r \in \Omega \\ \psi = 0, \quad & r \in \partial\Omega. \end{aligned}\right\} \tag{2.47}$$

So by (2.46) a solution is stable under a small perturbation if the principle eigenvalue, α_1, of (2.47) is positive and unstable if α_1 is negative.

These results can be combined to give the following result concerning stability.

Theorem 2.2.8

For $0 < U_p < U_{p,\,crit}$, the minimal positive solution $\mathbf{v}(r, U_p)$ of the problem (2.37) is stable.

Proof

This is similar to that given in Keller and Cohen [37], but we will give the details here for completeness. Let $\mathbf{v}(U_p, r)$ be the minimal positive solution of (2.37), and let $\alpha_1(U_p)$ be the principle eigenvalue of (2.47), then the variational characterization of $\alpha_1(U_p)$ gives

$$\alpha_1(U_p) = \min_{\phi(r) \in Q}\left[\frac{-\int_\Omega \phi\nabla^2\phi\, dV - \eta\int_\Omega \phi^2\frac{\partial f}{\partial v}\, dV}{\int_\Omega \phi^2\, dV}\right], \tag{2.48}$$

where Q is the set of admissible functions, i.e.

$$Q \equiv \left\{\phi(r) : \ \phi(r) > 0 \ \text{ on } \ \Omega, \quad \phi(r) \in C(\bar{\Omega}) \cap C^1(\Omega), \quad \phi(r) = 0 \ \text{ on } \partial\Omega\right\}.$$

We can also write, by the variational characterization of the principle eigenvalue of the problem (2.44),

$$\mu_1(U_p) = \min_{\phi(r) \in Q} \left[\frac{-\int_\Omega \phi \nabla^2 \phi \, dV}{\eta \int_\Omega \phi^2 \frac{\partial f}{\partial v} dV} \right],$$

which gives for any $\phi(r) \in Q$ and any U_p in $0 < U_p < U_{p,\,crit}$

$$-\int_\Omega \phi \nabla^2 \phi \, dV \geq \mu_1(U_p) \, \eta \int_\Omega \phi^2 \frac{\partial f}{\partial v} dV.$$

So $\alpha_1(U_p)$ satisfies

$$\alpha_1(U_p) \geq \min_{\phi(r) \in Q} \left[(\mu_1(U_p) - 1) \, \eta \frac{\int_\Omega \phi^2 \frac{\partial f}{\partial v} dV}{\int_\Omega \phi^2 \, dV} \right].$$

Now by Theorem 2.2.7, $\mu_1(U_p) - 1 > 0$.

Also $\phi(r) > 0$ in Ω, $\frac{\partial f}{\partial v} > 0$ in Ω, so $\alpha_1(U_p) > 0$ and the minimal solution $\mathbf{v}(r, U_p)$ is stable for $0 < U_p < U_{p,\,crit}$.

We are now finally in a position to give a stability result for the minimal solution $\mathbf{u}(r, U_p)$ of (2.16) as a corollary to Theorem 2.2.8.

Corollary 2.2.9

The minimal solution $\mathbf{u}(r, U_p)$ of (2.16) is stable for $0 < U_p < U_{p,\,crit}$.

Proof

Trivially, since there is a one-to-one correspondence between the problem for $\mathbf{v}$ given by (2.37) and the problem for $\mathbf{u}$ given by (2.16) i.e. $\mathbf{u} = h + \mathbf{v}$ where h is independent of time.

2.2.12 Comparison of critical press temperatures

A comparison of the critical press temperatures (in degrees Celsius) as a function of the dust layer height for the three methods is given in Figure 2.13 below.

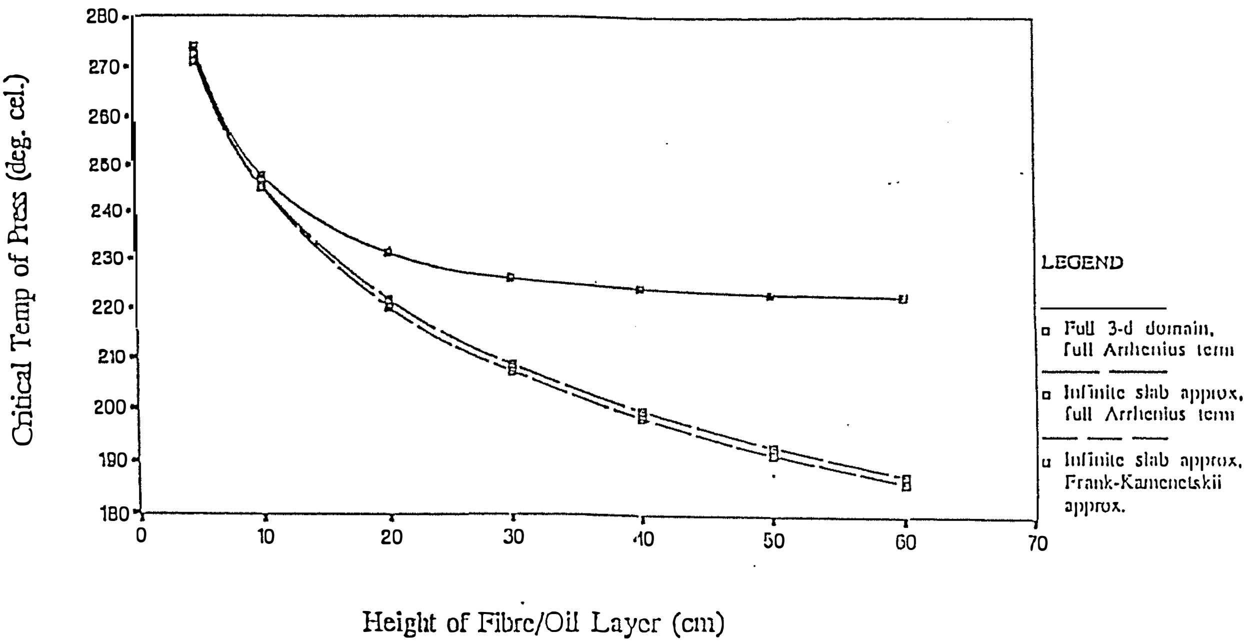

Figure 2.13 Graph of the height of the fibre/oil dust layer against the critical temperature of the press for the three models discussed in this Chapter.

2.2.12.1 Advice to the company

On the basis of the model which best approximates the physical situation, i.e. the Full Arrhenius term with full three dimensional domain model, spontaneous ignition of the fibre/oil layer will be likely when both the dust layer exceeds 20cm in height and the press temperature rises above 220°C. The company, therefore, should be advised to adjust their cleaning procedures accordingly and also to monitor the press temperatures.

2.2.12.2 Infinite slab approximation to the domain

As would be expected, for a_h < 10cm the domain approximates well to an infinite slab. However, for a_h > 10cm (the practical range of interest) the approximation becomes increasingly poor, with up to a 15% difference in the critical press temperatures for the range of a_h considered.

2.2.12.3 On the Frank-Kamenetskii approximation

For the range of dust layers and press temperatures considered, the Frank-Kamenetskii approximation seems to perform well in the infinite slab domain. However, it should be observed that even though we have retained the full Arrhenius term, the results for the infinite slab model are not independent of the Frank-Kamenetskii approximation. This is because the method outlined in Chapter 1 was used to derive the activation energy of the reaction and the physical constants for the model, and this uses the Frank-Kamenetskii approximation. So we are really comparing how the two equations in the infinite slab domain behave with the same physical constants. The true validity of the Frank-Kamenetskii approximation can therefore only be determined when an experimental method for the derivation of the relevant physical constants is developed that does not itself use the approximation.

2.2.12.2 Comment on plots as $a_h \to \infty$

On physical grounds, it is expected that the graph corresponding to the full three dimensional domain model should have a horizontal asymptote as $a_h \to \infty$, i.e. the critical temperature for the corresponding semi-infinite rod. For the models that use the infinite slab domain approximation, the whole upper half plane is filled as $a_h \to \infty$, thus it is expected that $T_{p,\,crit} \to 0$ as $a_h \to \infty$ for these models.

2.2.12.3 Multiplicity of steady states

The occurrence of a series of 'intermediate' steady state solutions (Figure 2.11) is only observed for the full three dimensional domain model. For the symmetrical heating case gross multiplicity of steady state solutions was first observed by Steggerda [44] in the unit sphere, and does not occur in the infinite slab. These observations suggest gross multiplicity of steady state solutions is a property of three dimensional regions in contrast with the situation for 'one dimensional' domains. This conjecture requires further investigation but is not of special relevance to the practical concerns of this Chapter.

CHAPTER 3

Thermodynamic derivation of a model for the self-heating of damp cellulosic materials

3.1 Heat producing reactions

Since this work was motivated by the study of bagasse, a material that goes through a refining process before storage, we shall ignore heat produced by the metabolism of living cells from freshly harvested materials. The chemical reactions outlined schematically below are likely to hold for most self-heating damp cellulosic bodies.

(i) CELLULOSE + OXYGEN $\rightarrow$ PRODUCTS + HEAT,
an exothermic oxidation reaction.

(ii) CELLULOSE + WATER + OXYGEN $\rightarrow$ PRODUCTS + HEAT,
an exothermic hydrolysis reaction.

(iii) MICROBES + SUGARS + WATER + OXYGEN $\rightarrow$ PRODUCTS + HEAT,
metabolism of bacteria and fungi, an exothermic process, ('sugars' would include glucose).

(iv) WATER VAPOUR $\rightarrow$ LIQUID WATER,
an exothermic condensation process.

(v) LIQUID WATER $\rightarrow$ WATER VAPOUR,
an endothermic evaporation process.

On the basis of the experimental work done on bagasse by Dixon |23| outlined in Chapter 1, we shall neglect the heat produced by (iii), i.e. by the action of microbes, in this thesis.

3.2 Assumptions

In the derivation of the mathematical model we shall make the following assumptions

(i) That reactant consumption, or the formation of reaction products, does not effect the rates of any of the reactions in the system. This is a parallel assumption to that made by the classical model for the self-heating of a body by a single exothermic reaction.

(ii) That there is no forced convection through the system. This is a reasonable assumption provided there is no applied pressure gradient.

(iii) That the thermal conductivity coefficient and the coefficient of diffusivity of water vapour through the system are constant.

(iv) That the dry air/water vapour mixture behaves as an ideal gas.

(v) That heat can travel through the system by conduction and also by the diffusion of water vapour. Liquid water remains static in the system until vaporized.

(vi) Heat is lost at the boundary by Newtonian cooling. No moisture is transferred across the boundary - this assumption is based on Dixon's [23] comments on bagasse, and is likely to be valid for other cellulosic substances, especially those stored under a cover.

(vii) As a result of assumptions (i) and (vi), total moisture content in the system is conserved.

(viii) Dry air concentration is constant in the body.

In our formulation of the equations we shall also include the effects of natural convection in the system for the sake of completeness. In our analysis of the resulting formulation however, we shall, for the same reasons outlined by Henry [25] in Chapter 1, ignore these convection effects.

3.3 Derivation of the equations

3.3.1 Conservation law

In the derivation of this model we will use the conservation equations for energy and mass. We will first derive the basic conservation equation we will be applying (see for example Aris [45] p50). Consider a quantity inside a closed region $\hat{\Omega}$ with boundary $\partial\hat{\Omega}$. Let the quantity have concentration $A(\hat{r}, \hat{t})$, $\hat{r} \in \hat{\Omega}$, $\hat{t} > 0$, and flux $\underset{\sim}{j}(\hat{r}, \hat{t})$, $\hat{r} \in \hat{\Omega}$, $\hat{t} > 0$, where $\underset{\sim}{j}$ is a vector such that the amount of the quantity per unit area per unit time that crosses an element with normal $\underset{\sim}{n}$ is $\underset{\sim}{j} \cdot \underset{\sim}{n}$.

Also let $g(\hat{r}, \hat{t})$, $\hat{r} \in \hat{\Omega}$, $\hat{t} > 0$ represent the rate of generation of the quantity in $\hat{\Omega}$. We will assume that A, $\underset{\sim}{j}$ and g are continuous functions of $\hat{r}$. If we now consider a region D where $D \subseteq \hat{\Omega}$, with boundary ∂D, and outward normal on the boundary $\underset{\sim}{n}$, then the rate of change of the amount of the quantity in D is

$$\frac{\partial}{\partial \hat{t}} \int_D A \, d\hat{V},$$

the rate at which the quantity crosses ∂D is

$$\int_{\partial D} \underset{\sim}{j} \cdot \underset{\sim}{n} \, d\hat{S},$$

and the rate of generation of the quantity within D is

$$\int_D g \, d\hat{V}.$$

Now by Green's theorem we can write

$$\int_{\partial D} \underset{\sim}{j} \cdot \underset{\sim}{n}\, d\hat{S} = \int_D \nabla \cdot \underset{\sim}{j}\, d\hat{V}\,,$$

so we can balance the three terms to give the conservation equation for the quantity as

$$\int_D \left(\frac{\partial A}{\partial \hat{t}} + \nabla \cdot \underset{\sim}{j} - g \right) d\hat{V} = 0\,.$$

Since this equation must hold for any region $D \subseteq \hat{\Omega}$, we have

$$\frac{\partial A}{\partial \hat{t}} + \nabla \cdot \underset{\sim}{j} = g, \quad \text{in } \hat{\Omega}, \tag{3.1}$$

as the basic conservation equation for any quantity in the region.

3.3.2 Enthalpy per unit volume of the body

Assuming the body consists of cellulosic solid, liquid water, water vapour, and dry air, then the following expressions are obtained for the enthalpy per unit volume of each of the constituent components of the body

enthalpy of cellulosic solid = H_s,

enthalpy of liquid water = XH_w,

enthalpy of water vapour = YH_v,

enthalpy of dry air = $\rho_a H_a$.

where

H_s = enthalpy of the cellulosic solid per unit volume,

H_w = partial molar enthalpy of liquid water,

H_v	=	partial molar enthalpy of water vapour = $H_w + L_v$,
L_v	=	latent molar heat of vaporization of liquid water,
H_a	=	partial molar enthalpy of dry air,
X	=	liquid water concentration per unit volume,
Y	=	water vapour concentration per unit volume,
ρ_a	=	dry air concentration per unit volume.

This gives the enthalpy per unit volume of the body as

$$E_h = XH_w + YH_v + \rho_a H_a + H_s. \tag{3.2}$$

Differentiation of (3.2) with respect to $\hat{t}$ gives

$$\frac{\partial E_h}{\partial \hat{t}} = \frac{\partial X}{\partial \hat{t}} H_w + X\frac{\partial H_w}{\partial \hat{t}} + \frac{\partial Y}{\partial \hat{t}} H_v + Y\frac{\partial H_v}{\partial \hat{t}} + \rho_a \frac{\partial H_a}{\partial \hat{t}} + \frac{\partial H_s}{\partial \hat{t}}.$$

We will assume H_w, H_v, H_a, H_s are functions of T only. In fact if we are dealing with an ideal gas we lose nothing by this assumption. Generally the H_i, i = 1, ..., 4, $\underset{\sim}{H} = (H_w, H_v, H_a, H_s)$ will also be functions of X, Y, p (where p = pressure), for example

$$\frac{\partial H_w}{\partial \hat{t}} = \frac{\partial H_w}{\partial T}\frac{\partial T}{\partial \hat{t}} + \frac{\partial H_w}{\partial X}\frac{\partial X}{\partial \hat{t}} + \frac{\partial H_w}{\partial Y}\frac{\partial Y}{\partial \hat{t}} + \frac{\partial H_w}{\partial p}\frac{\partial p}{\partial \hat{t}}.$$

However, if we assume the dry air/water vapour mixture is an ideal gas, then the last term vanishes. Also as Aris [45] observes, the sum of the contributions of the $\frac{\partial H_i}{\partial X}$, $\frac{\partial H_i}{\partial Y}$, i = 1, ..., 4 terms to the $\frac{\partial E_h}{\partial \hat{t}}$ expression is zero since the H_i, i = 1, ..., 4 are intensive thermodynamic properties.

This gives

$$\frac{\partial E_h}{\partial \hat{t}} = \left[X\frac{\partial H_w}{\partial T} + Y\frac{\partial H_v}{\partial T} + \rho_a\frac{\partial H_a}{\partial T} + \frac{\partial H_s}{\partial T} \right]\frac{\partial T}{\partial \hat{t}} + \frac{\partial X}{\partial \hat{t}} H_w + \frac{\partial Y}{\partial \hat{t}} H_v , \tag{3.3}$$

where the coefficient of $\frac{\partial T}{\partial \hat{t}}$ is the specific heat per unit volume of the system and will be written as C_s.

That is

$$C_s = X\frac{\partial H_w}{\partial T} + Y\frac{\partial H_v}{\partial T} + \rho_a\frac{\partial H_a}{\partial T} + \frac{\partial H_s}{\partial T} ,$$

giving

$$\frac{\partial E_h}{\partial \hat{t}} = C_s\frac{\partial T}{\partial \hat{t}} + \frac{\partial X}{\partial \hat{t}} H_w + \frac{\partial Y}{\partial \hat{t}} H_v . \tag{3.4}$$

3.3.3 Transport of heat and mass in the system

Heat and mass will be transported in the cellulose/liquid water/water vapour/dry air mixture by several means

(i) Conduction of heat due to temperature differences in the system.

(ii) Diffusion of water vapour due to concentration differences in the system.

(iii) Convection of water vapour through the system. In the absence of forced convection, this will be by natural convection arising from differences in the average density of the water vapour/dry air mixture.

The enthalpy flux $\underset{\sim}{F}_e$ will include contributions from each of the above three factors. In fact we can write

$$\underset{\sim}{F}_e = \underset{\sim}{F}_c + H_v \underset{\sim}{F}_v , \tag{3.5}$$

where $\underset{\sim}{F}_c$ is the contribution to the enthalpy flux by conduction of heat and $\underset{\sim}{F}_v$ is the mass flux due to the diffusion and convection of water vapour.

Mass flux

In the system we are considering, the only movement of mass is that associated with the diffusion and convection of water vapour. An important variable for describing convective effects in porous systems is the volume flux, also known as the superficial velocity, $\underset{\sim}{v}$. We will assume that this volume flux satisfies Darcy's law i.e.

$$\underset{\sim}{v} = -\frac{\kappa}{\mu} (\nabla p - (\rho_a + Y) \underset{\sim}{g}) , \tag{3.6}$$

where p is the pressure, κ is the permeability of the system, μ is the viscosity of the water vapour/dry air mixture and the vector $\underset{\sim}{g}$ represents gravitational effects. Assuming the water vapour/dry air mixture behaves as an ideal gas the pressure p is given by

$$p = RT\left(\frac{Y}{M_1} + \frac{\rho_a}{M_2} \right), \tag{3.7}$$

where M_1 is the molecular weight of water vapour and M_2 is the molecular weight of dry air. The mass flux can then be written as

$$\underset{\sim}{F}_v = -D\nabla Y + Y\underset{\sim}{v} , \tag{3.8}$$

where $-D\nabla Y$ is the contribution of diffusion of the water vapour and D is the diffusivity of water vapour in the system.

Enthalpy flux

Assuming the contribution of conduction of heat to the overall enthalpy flux is given by

$$\underset{\sim}{F}_c = -k\nabla T\,, \tag{3.9}$$

where k is the thermal conductivity of cellulose, we can combine equations (3.5) and (3.8) to give the total enthalpy flux as

$$\underset{\sim}{F}_e = -k\nabla T + H_v\,[\,-D\nabla Y + Y\underset{\sim}{v}\,]\,. \tag{3.10}$$

3.3.4 Rates of generation of heat and mass in the system

We will assume there are two exothermic chemical reactions occurring in the system, the classical oxidation reaction and an ancillary hydrolysis reaction due to the presence of water. We will further assume that the rate of the oxidation reaction is given by the Arrhenius law, so

$$\text{rate of heat production by the oxidation reaction} = Q\rho Z \exp\left(\frac{-E}{RT}\right), \tag{3.11}$$

where

Q = exothermicity per unit volume of the oxidation reaction,

Z = pre-exponential factor for the oxidation reaction,

E = activation energy of the oxidation reaction,

ρ = cellulose concentration per unit volume.

For the hydrolysis reaction we will follow Gray [30] in assuming that this reaction is first order in the liquid water and cellulose concentrations, and that the reaction rate obeys the Arrhenius law, i.e.

$$\text{rate of heat production by the hydrolysis reaction} = Q_w \rho Z_w X \exp\left(\frac{-E_w}{RT}\right), \quad (3.12)$$

where

Q_w = exothermicity per unit volume of the hydrolysis reaction,

Z_w = pre-exponential factor for the hydrolysis reaction,

E_w = activation energy of the hydrolysis reaction.

Although moisture can change between the liquid and vapour phases in the system, there is no net production or consumption of moisture in the body. Similarly there are no changes in the cellulose or air concentrations, so the rate of generation of mass in the system is zero.

3.3.5 The mass conservation equation

Applying the basic conservation equation (3.1) to the mass balance problem in the region $\hat{\Omega}$, with mass flux given by (3.8) gives

$$\frac{\partial(X+Y)}{\partial\hat{t}} + \nabla \,.\, \{ -D\nabla Y + T\underset{\sim}{v} \} = 0\,, \quad \hat{r} \in \hat{\Omega}\,,\ \hat{t} > 0. \quad (3.13)$$

Given that liquid water remains static in a unit volume of the body, the rate equation for the change in liquid water concentration in unit volume is given by

$$\frac{\partial X}{\partial\hat{t}} = \begin{array}{c}\text{rate of water vapour}\\ \text{condensation}\end{array} - \begin{array}{c}\text{rate of liquid water}\\ \text{evaporation}\end{array}.$$

Following Gray [30], we will assume:

(i) that the rate of the (exothermic) condensation reaction is independent of temperature and is first order with water vapour concentration,

(ii) that the evaporation of water is the rate determining step in transfer to the vapour phase, and that this is an endothermic reaction with an activation energy equal to the latent heat of vapourization of liquid water, and is first order with liquid water concentration.

This gives, again assuming Arrhenius kinetics,

rate of water vapour condensation = $Z_c Y$,

rate of liquid water evaporation = $Z_e X \exp\left(\frac{-L_v}{RT}\right)$,

where

Z_c = constant of proportionality for the condensation process (equivalent to a pre-exponential factor),

Z_e = pre-exponential factor for the evaporation process.

So we have the following rate equation for X

$$\frac{\partial X}{\partial \hat{t}} = Z_c Y - Z_e X \exp\left(\frac{-L_v}{RT}\right), \quad \hat{r} \in \hat{\Omega}, \quad \hat{t} > 0. \qquad (3.14)$$

Substituting this expression in (3.13) gives the rate equation for Y as

$$\frac{\partial Y}{\partial \hat{t}} = Z_e X \exp\left(\frac{-L_v}{RT}\right) - Z_c Y - \nabla \, . \, \{ -D\nabla Y + Y\underset{\sim}{v} \}, \quad \hat{r} \in \hat{\Omega}, \quad \hat{t} > 0. \qquad (3.15)$$

3.3.6 The energy conservation equation

Applying (3.1) to the energy conservation equation with enthalpy flux given by (3.10) and the rate of generation of heat given by (3.11) and (3.12) gives

$$C_s \frac{\partial T}{\partial \hat{t}} + \frac{\partial X}{\partial \hat{t}} h_w + \frac{\partial Y}{\partial \hat{t}} h_v + \nabla \,.\, \{ -k\nabla T + H_v [-D\nabla Y + Y\underset{\sim}{v}] \}$$

$$= Q\rho Z \exp\left(\frac{-E}{RT}\right) + Q_w \rho Z_w X \exp\left(\frac{-E_w}{RT}\right), \quad \hat{r} \in \hat{\Omega}, \quad \hat{t} > 0,$$

$\Rightarrow$ (as $H_v = H_w + L_v$ and by (3.13), (3.14))

$$C_s \frac{\partial T}{\partial \hat{t}} - L_v \left(Z_c Y - Z_c X \exp\left(\frac{-L_v}{RT}\right)\right) - \nabla \,.\, (k\nabla T) + [-D\nabla Y + Y\underset{\sim}{v}] \,.\, \nabla H_v$$

$$= Q\rho Z \exp\left(\frac{-E}{RT}\right) + Q_w \rho Z_w X \exp\left(\frac{-E_w}{RT}\right), \quad \hat{r} \in \hat{\Omega}, \quad \hat{t} > 0. \qquad (3.16)$$

The term $-D\nabla Y \,.\, \nabla H_v$ is usually neglected in models of this nature. As Aris [45] states

> "[this] term seldom appears in any derivation of such an equation and when it does appear is usually neglected without more ado. Amundson [46] has included it in his discussion of models of the fixed-bed reactor, but remarks that he knows no experimental or theoretical work that has been done to justify this neglect ... We also bow down in the house of Rimmon and sacrifice it to the demands of simplicity."

In his work on the coupled diffusion of heat and moisture in bulk wool, Heath [47] has stated that this term is small in comparison with $\nabla \,.\, (k\nabla T)$, with the ratio of order $10^{-2}\Delta Y$. In this thesis we will follow the lead of Aris and Heath and neglect the $-D\nabla Y \,.\, \nabla H_v$ term.

3.3.7 Boundary and initial conditions

As mentioned in section 3.2 we shall assume the temperature change across the boundary $\partial\hat{\Omega}$ is governed by Newtonian cooling and that no moisture crosses $\partial\hat{\Omega}$. This gives

$$k\frac{\partial T}{\partial n} + h(T-T_a) = 0, \quad \hat{r} \in \partial\hat{\Omega}, \quad \hat{t} > 0, \tag{3.17}$$

where h is the heat transfer coefficient between the body and its surroundings,

$$\frac{\partial Y}{\partial n} = 0, \quad \hat{r} \in \partial\hat{\Omega}, \quad \hat{t} > 0, \tag{3.18}$$

$$\frac{\partial X}{\partial n} = 0, \quad \hat{r} \in \partial\hat{\Omega}, \quad \hat{t} > 0. \tag{3.19}$$

We shall also take the variables $T(\hat{r}, \hat{t})$, $Y(\hat{r}, \hat{t})$, $X(\hat{r}, \hat{t})$ to have the initial profiles

$$T(\hat{r}, \hat{t} = 0) = T_1(\hat{r}) \geq 0, \quad \hat{r} \in \bar{\hat{\Omega}} \tag{3.20}$$

$$Y(\hat{r}, \hat{t} = 0) = Y_1(\hat{r}) \geq 0, \quad \hat{r} \in \bar{\hat{\Omega}} \tag{3.21}$$

$$X(\hat{r}, \hat{t} = 0) = X_1(\hat{r}) \geq 0, \quad \hat{r} \in \bar{\hat{\Omega}}. \tag{3.22}$$

3.3.8 Model equations with and without convection

Now

$$H_v = L_v + H_w = L_v + \int_{T_0}^{T} C_w \, dT,$$

where the standard state of water is liquid at temperature T_0, and C_w is the specific heat of liquid water. So

$$\nabla H_v = \nabla(L_Z + \int_{T_0}^{T} C_w \, dT) = C_w \nabla T. \tag{3.23}$$

Then assuming k and D are constants, the reaction/diffusion/convection system for the seven variables T, Y, X, $\underset{\sim}{v}$, p is

$$C_s \frac{\partial T}{\partial \hat{t}} = Q\rho Z \exp\left(\frac{-E}{RT}\right) + Q_w \rho \, Z_w X \exp\left(\frac{-E_w}{RT}\right) + L_v\left[Z_c Y - Z_c X \exp\left(\frac{-L_v}{RT}\right)\right]$$

$$+ k\nabla^2 T - C_w Y \underset{\sim}{v} \,.\, \nabla T, \quad \hat{r} \in \hat{\Omega}, \hat{t} > 0,$$

$$\frac{\partial Y}{\partial \hat{t}} = Z_c X \exp\left(\frac{-L_v}{RT}\right) - Z_c Y + D\nabla^2 Y - Y\nabla \,.\, \underset{\sim}{v} - \underset{\sim}{v} \,.\, \nabla Y, \quad \hat{r} \in \hat{\Omega}, \hat{t} > 0,$$

$$\frac{\partial X}{\partial \hat{t}} = Z_c Y - Z_c X \exp\left(\frac{-L_v}{RT}\right), \quad \hat{r} \in \hat{\Omega}, \hat{t} > 0,$$

$$\underset{\sim}{v} = -\frac{\kappa}{\mu}(\nabla p - (\rho_a + Y)\underset{\sim}{g}), \quad \hat{r} \in \hat{\Omega}, \hat{t} > 0,$$

$$p = RT\left(\frac{Y}{M_1} + \frac{\rho_a}{M_2}\right), \quad \hat{r} \in \hat{\Omega}, \hat{t} > 0,$$

with the boundary conditions (3.17) - (3.19) and initial conditions (3.20) - (3.22).

Neglecting natural convection, i.e. setting $\underset{\sim}{v} \equiv \underset{\sim}{0}$, the reaction/diffusion system for the three variables T, Y, X becomes

$$C_s \frac{\partial T}{\partial \hat{t}} = Q\rho Z \exp\left(\frac{-E}{RT}\right) + Q_w \rho\, Z_w X \exp\left(\frac{-E_w}{RT}\right)$$

$$+ L_v\left[Z_c Y - Z_e X \exp\left(\frac{-L_v}{RT}\right)\right] + k\nabla^2 T, \quad \hat{r} \in \hat{\Omega}, \hat{t} > 0, \tag{3.24}$$

$$\frac{\partial Y}{\partial \hat{t}} = Z_e X \exp\left(\frac{-L_v}{RT}\right) - Z_c Y + D\nabla^2 Y, \quad \hat{r} \in \hat{\Omega}, \hat{t} > 0, \tag{3.25}$$

$$\frac{\partial X}{\partial \hat{t}} = Z_c Y - Z_e X \exp\left(\frac{-L_v}{RT}\right), \quad \hat{r} \in \hat{\Omega}, \hat{t} > 0, \tag{3.26}$$

with the boundary conditions (3.17) - (3.19) and the initial conditions (3.20) - (3.22). For the reasons outlined earlier in this Chapter and in Chapter 1 it is the solution of the reaction/diffusion system (3.23) - (3.25) that we shall consider for the rest of this thesis.

3.4 Dimensionless formulation of the equations

3.4.1 Dimensionless formulation of the spatially distributed equations

Set

$$\left.\begin{array}{llll}
u = \dfrac{RT}{E}, & x = \dfrac{XV_l}{\int_{\hat{\Omega}}(Y_l(\hat{r}) + X_l(\hat{r}))d\hat{V}}, & y = \dfrac{YV_l}{\int_{\hat{\Omega}}(Y_l(\hat{r}) + X_l(\hat{r})d\hat{V}}, & \\
\alpha = \dfrac{L_v}{E}, & \alpha_w = \dfrac{E_w}{E}, & t = \dfrac{R\rho QZ\hat{t}}{C_s E}, & \\
\lambda = \dfrac{\int_{\hat{\Omega}}(Y_l(\hat{r}) + X_l(\hat{r}))d\hat{V}}{V_l \rho}, & \eta' = \dfrac{kE}{\rho QRZa_0^2}, & \varepsilon = \dfrac{R\rho Q}{C_s E}, & \gamma = \dfrac{D}{a_0^2 Z}, \\
r = \dfrac{\hat{r}}{a_0}, & h_w = \dfrac{Q_w}{Q}, & h_c = \dfrac{L_v}{Q}, & Q_w = \dfrac{\rho Z_w}{Z}, \\
Q_c = \dfrac{Z_c}{Z}, & Q_e = \dfrac{Z_e}{Z}, & &
\end{array}\right\} \tag{3.27}$$

where V_1 is the volume of the region $\hat{\Omega}$. Also let $\hat{\Omega}$ and $\partial\hat{\Omega}$ be mapped into Ω and $\partial\Omega$ respectively by the transformation $r = \hat{r}/a_0$. Here λ is a constant which represents the ratio of total moisture concentration to cellulose concentration in the body. Then the non-dimensioned representation of the equations (3.24) – (3.26) is

$$\frac{\partial u}{\partial t} = \exp\left(\frac{-1}{u}\right) + \lambda \left\{ h_w \,\phi_w \,x \exp\left(\frac{-\alpha_w}{u}\right) - h_c \,\phi_e \,x \exp\left(\frac{-\alpha}{u}\right) + h_c \,\phi_c \,y \right\}$$

$$+ \eta' \nabla^2 u, \quad r \in \Omega, \quad t > 0, \tag{3.28}$$

$$\varepsilon \frac{\partial y}{\partial t} = \phi_e \,x \exp\left(\frac{-\alpha}{u}\right) - \phi_c \,y + \gamma \nabla^2 y, \quad r \in \Omega, \quad t > 0, \tag{3.29}$$

$$\varepsilon \frac{\partial x}{\partial t} = \phi_c \,y - \phi_e \,x \exp\left(\frac{-\alpha}{u}\right), \quad r \in \Omega, \quad t > 0. \tag{3.30}$$

Also setting

$$\left.\begin{array}{lll} Bi = \dfrac{ha_0}{k}, & U = \dfrac{RT_a}{E}, & \zeta_1 = \dfrac{RT_1}{E}, \\[2ex] \psi_1 = \dfrac{Y_1 V_1}{\int_{\hat{\Omega}} (Y_1(\hat{r}) + X_1(\hat{r}))d\hat{V}}, & \chi_1 = \dfrac{X_1 V_1}{\int_{\hat{\Omega}} (Y_1(\hat{r}) + X_1(\hat{r}))d\hat{V}}, & \end{array}\right\} \tag{3.31}$$

the non-dimensioned versions of the boundary conditions (3.17) - (3.19) and the initial conditions (3.20) - (3.22) are, respectively,

$$\frac{\partial u}{\partial n} + Bi(u - U) = 0, \quad r \in \partial\Omega, \quad t > 0, \tag{3.32}$$

$$\frac{\partial y}{\partial n} = 0, \quad r \in \partial\Omega, \quad t > 0, \tag{3.33}$$

$$\frac{\partial x}{\partial n} = 0, \quad r \in \partial\Omega, \quad t > 0, \tag{3.34}$$

and

$$u(r, t{=}0) = \zeta_1(r) \geq 0, \quad r \in \bar{\Omega}, \tag{3.35}$$

$$y(r, t{=}0) = \psi_1(r) \geq 0, \quad r \in \bar{\Omega}, \tag{3.36}$$

$$x(r, t{=}0) = \chi_1(r) \geq 0, \quad r \in \bar{\Omega}. \tag{3.37}$$

3.4.2 Dimensionless formulation of the spatially uniform case

By the 'spatially uniform case' we mean the limiting case of the equations (3.17) - (3.26) as $k \to \infty$ and $D \to \infty$. As $k \to \infty$ and $D \to \infty$, equations (3.17) - (3.26) will only be satisfied if $\nabla^2 T \to 0$, $\nabla^2 Y \to 0$ and $\frac{\partial T}{\partial n} \to 0$. So in the limit $k \to \infty$, $D \to \infty$ the state variables T, Y and X will be independent of the space variable $\hat{r}$. Integrating (3.24) across the region $\hat{\Omega}$ and applying Gauss's theorem gives

$$C_s \frac{\partial}{\partial \hat{t}}\left(\int_{\hat{\Omega}} T\, d\hat{V}\right) = Q\rho Z \int_{\hat{\Omega}} \exp\left(\frac{-E}{RT}\right) d\hat{V} + Q_w \rho Z_w \int_{\hat{\Omega}} X \exp\left(\frac{-E_w}{RT}\right) d\hat{V}$$

$$+ L_v \left[Z_c \int_{\hat{\Omega}} Y d\hat{V} - Z_c \int_{\hat{\Omega}} X \exp\left(\frac{-L_v}{RT}\right) d\hat{V} \right] - h \int_{\partial\hat{\Omega}} (T - T_a) d\hat{S}.$$

In the limit $k \to \infty$, $D \to \infty$ we thus obtain

$$V_1 C_s \frac{dT}{d\hat{t}} = Q\rho Z V_1 \exp\left(\frac{-E}{RT}\right) + Q_w \rho Z_w V_1 X \exp\left(\frac{-E_w}{RT}\right)$$

$$+ L_v V_1 \left[Z_c Y - Z_c X \exp\left(\frac{-L_v}{RT}\right)\right] - hS(T - T_a), \quad \hat{t} > 0, \tag{3.38}$$

where $T = T(\hat{t})$, $Y = Y(\hat{t})$ and $X = X(\hat{t})$, and S is the surface area of the region $\hat{\Omega}$.

Similarly for (3.25), (3.26) we obtain

$$\frac{dY}{d\hat{t}} = Z_e X \exp\left(\frac{-L_v}{RT}\right) - Z_c Y, \quad \hat{t} > 0, \tag{3.39}$$

$$\frac{dX}{d\hat{t}} = Z_c Y - Z_e X \exp\left(\frac{-L_v}{RT}\right), \quad \hat{t} > 0. \tag{3.40}$$

The initial conditions (3.20) - (3.22) become

$$T(\hat{t}=0) = T_1, \tag{3.41}$$

$$Y(\hat{t}=0) = Y_1, \tag{3.42}$$

$$X(\hat{t}=0) = X_1. \tag{3.43}$$

As total moisture content is conserved in the system, we can eliminate Y from the above equations (3.38) - (3.43). By adding (3.39), (3.40) we see

$$\frac{d(X+Y)}{d\hat{t}} = 0, \quad \hat{t} > 0,$$

which implies

$$Y(\hat{t}) + X(\hat{t}) = Y_1 + X_1, \quad \text{for all } \hat{t} > 0,$$

that is

$$Y(\hat{t}) = Y_1 + X_1 - X(\hat{t}), \quad \text{for all } \hat{t} > 0.$$

We can then eliminate Y from our equations to give

$$C_s \frac{dT}{d\hat{t}} = Q\rho Z \exp\left(\frac{-E}{RT}\right) + Q_w \rho Z_w X \exp\left(\frac{-E_w}{RT}\right)$$

$$+ L_v \left[Z_c(Y_1+X_1-X) - Z_e X \exp\left(\frac{-L_v}{RT}\right) \right] - \frac{hS}{V_1}(T-T_a), \quad \hat{t} > 0, \tag{3.44}$$

$$\frac{dX}{d\hat{t}} = Z_c(Y_1+X_1-X) - Z_e X \exp\left(\frac{-L_v}{RT}\right), \quad \hat{t} > 0, \tag{3.45}$$

with the initial conditions (3.41), (3.43).

Where applicable, the non-dimensionalization of these equations is similar to that used in (3.27), (3.31) except

$$\left.\begin{aligned} x &= \frac{X}{X_1+Y_1}, \quad \lambda_1 = \frac{X_1+Y_1}{\rho}, \quad L = \frac{hSE}{V_1 R\rho QZ}, \\ \chi_1 &= \frac{X_1}{X_1+Y_1} \end{aligned}\right\} \tag{3.46}$$

This gives the final non-dimensional form of the spatially uniform case as

$$\frac{du}{dt} = \exp\left(\frac{-1}{u}\right) - L(u-U) + \lambda_1 \left\{ h_w\phi_w x \exp\left(\frac{-\alpha_w}{u}\right) - h_c\phi_c x \exp\left(\frac{-\alpha}{u}\right) \right.$$

$$\left. + \; h_c\phi_c(1-x) \right\}, \quad t > 0, \tag{3.47}$$

$$\varepsilon \frac{dx}{dt} = \phi_c(1-x) - \phi_c x \exp\left(\frac{-\alpha}{u}\right), \quad t > 0, \tag{3.48}$$

with the initial conditions

$$u(t=0) = \zeta_1 , \tag{3.49}$$

$$x(t=0) = \chi_1 . \tag{3.50}$$

3.5 The steady state equations for the spatially distributed model

Our conservation of total moisture content assumption also means that at steady state solutions of (3.28) - (3.37), that is where

$$\frac{\partial u}{\partial t} = \frac{\partial y}{\partial t} = \frac{\partial x}{\partial t} = 0,$$

we can eliminate both y and x from the equations to give a single equation in u only.

Adding (3.29), (3.30) and integrating across the region Ω gives

$$\frac{\partial}{\partial t} \int_\Omega (x+y)\, dV = \gamma \int_\Omega \nabla^2 y\, dV$$

$$= \gamma \int_{\partial\Omega} \nabla y \, . \, \underset{\sim}{n}\, dS, \qquad \text{by Gauss's theorem}$$

$$= 0, \qquad \text{as } \frac{\partial y}{\partial n} = 0, \quad r \in \partial\Omega.$$

So

$$\int_\Omega (x+y)\, dV = \int_\Omega (\psi_1+\chi_1)\, dV = V, \quad \text{for all } t > 0, \tag{3.51}$$

where V is the dimensionless volume of the region Ω $(= V_1 / a_0^3)$.

The steady state equations for the spatially distributed model are

$$\nabla^2 u + \eta\left[\exp\left(\frac{-1}{u}\right) + \lambda\left\{h_w\phi_w x \exp\left(\frac{-\alpha_w}{u}\right) - h_c\phi_e x \exp\left(\frac{-\alpha}{u}\right) + h_c\phi_c y\right\}\right] = 0, \quad r \in \Omega,$$

.....(3.52)

$$\gamma\nabla^2 y + \phi_e x \exp\left(\frac{-\alpha}{u}\right) - \phi_c y = 0, \quad r \in \Omega, \tag{3.53}$$

$$\phi_c y - \phi_e x \exp\left(\frac{-\alpha}{u}\right) = 0, \quad r \in \Omega, \tag{3.54}$$

where $\eta = \dfrac{1}{\eta'}$, with the boundary conditions (3.32) - (3.34).

Now adding (3.53), (3.54) shows that the steady state solution for y must satisfy

$$\nabla^2 y = 0, \quad r \in \Omega, \tag{3.55}$$

$$\frac{\partial y}{\partial n} = 0, \quad r \in \partial\Omega,$$

which implies that y must be a constant in Ω at steady state. In fact, using (3.51)

$$y = 1 - \frac{1}{V}\int_\Omega x\, dV,$$

and by (3.54)

$$x = \frac{\phi_c}{\phi_e}\, y \exp\left(\frac{\alpha}{u}\right), \tag{3.56}$$

so

$$y = 1 - \frac{\phi_c}{\phi_e V}\, y \int_\Omega \exp\left(\frac{\alpha}{u}\right) dV,$$

$$\Rightarrow \qquad y = \frac{\phi_e}{\phi_e + \dfrac{\phi_c}{V} \displaystyle\int_\Omega \exp\left(\frac{\alpha}{u}\right) dV} \qquad \text{at steady state.} \tag{3.57}$$

Finally substituting for x and y in (3.52) gives the steady state equation for u as

$$\nabla^2 u + \eta \left[\exp\left(\frac{-1}{u}\right) + \frac{\lambda h_w \phi_w \phi_e}{\phi_e + \dfrac{\phi_c}{V} \displaystyle\int_\Omega \exp\left(\frac{\alpha}{u}\right) dV} \exp\left(\frac{\alpha - \alpha_w}{u}\right) \right] = 0, \quad r \in \Omega, \tag{3.58}$$

with the boundary condition (3.32) i.e.

$$\frac{\partial u}{\partial n} + Bi\,(u - U) = 0, \qquad r \in \partial\Omega.$$

CHAPTER 4

The spatially uniform model

4.1 Introduction

The coupled pair of non-linear ordinary differential equations, i.e. (3.47), (3.48), we will be studying in this Chapter are of the form

$$\frac{du}{dt} = f(u, x, \underset{\sim}{\delta}, \underset{\sim}{\beta}), \quad t > 0, \tag{4.1}$$

$$\frac{dx}{dt} = g(u, x, \underset{\sim}{\delta}, \underset{\sim}{\beta}), \quad t > 0, \tag{4.2}$$

where

$$\underset{\sim}{\delta} = (U, L, \lambda_1),$$

$$\underset{\sim}{\beta} = (\varepsilon, h_w, h_c, \phi_w, \phi_e, \phi_c, \alpha_w, \alpha).$$

We have split the parameters of the system up into two groups, those in $\underset{\sim}{\delta}$ and those in $\underset{\sim}{\beta}$. In a set of experiments to be carried out on a particular self-heating substance, the parameters that can be varied are: T_a the ambient temperature, $\frac{S}{V_1}$ the surface area to volume ratio of the sample, and $X_1 + Y_1$, the total initial moisture content. Thus the vector $\underset{\sim}{\delta}$ contains 'variable' parameters - parameters that can be varied while analysing a particular material. However Q, Q_w, C_s, ρ, Z, Z_w, E, E_w etc. are 'constant' parameters in that they stay fixed for a particular material. We have grouped these 'constant' parameters in the vector $\underset{\sim}{\beta}$. So in effect we are dealing with a two variable, three parameter problem.

To obtain a complete description of all the qualitatively distinct behaviour of the system, we must analyse the full parameter space of each of the components of $\underset{\sim}{\delta}$. To do this we will use the method of degenerate singularity theory which is outlined in detail in Golubitsky and Schaeffer [48]. Degenerate singularity theory provides a means of finding the 'organising centre', or bifurcation of the highest degeneracy possible in the system. Once this point in parameter space has been found we will be able to generate all the possible bifurcation diagrams exhibited by the system in U, L, λ_1 space, and thus obtain all the possible responses, both steady state and oscillatory, to any given U. In particular we will here use the special case of degenerate singularity theory developed by Gray and Roberts [49] to deal with a two variable, three parameter problem. To solve the resulting coupled non-linear equations in parameter space we will use the pseudo-arclength method for the solution of non-linear systems (see e.g. Keller [50]). We will show that the model given by (3.47), (3.48) can exhibit up to five steady state solutions for a particular value of U, as well as limit points, and hysteresis point and quartic fold point degeneracies in U, L, λ_1 space. The introduction of the effects of moisture into the model also leads to the possibility of periodic solutions to the system (the classical Semenov spatially uniform model for self-heating by a single exothermic reaction does not have periodic solutions). We show the model can exhibit Hopf bifurcation points and degenerate Hopf bifurcations of the $H2_1$ and $H3_1$ types (using the notation of Gray and Roberts [49] explained later in this Chapter), as well as double zero eigenvalue degeneracies.

However, we will begin by discussing some general existence, uniqueness and multiplicity results for the solutions of the ordinary differential equations (3.47), (3.48), and for the solution of the associated steady state problem.

4.2 Questions of existence, uniqueness and multiplicity of solutions

The spatially uniform model can be written in the form (4.1), (4.2) where

$$f(u, x, \underset{\sim}{\delta}, \underset{\sim}{\beta}) = \exp\left(\frac{-1}{u}\right) - L(u-U) + \lambda_1 \left\{ h_w \phi_w \, x \exp\left(\frac{-\alpha_w}{u}\right) - h_c \phi_e \, x \exp\left(\frac{-\alpha}{u}\right) \right.$$

$$\left. + h_c \phi_c \, (1-x) \right\}, \qquad (4.3)$$

$$g(u, x, \underset{\sim}{\delta}, \underset{\sim}{\beta}) = \frac{1}{\varepsilon}\left[\phi_c\,(1-x) - \phi_e\, x \exp\left(\frac{-\alpha}{u}\right)\right]. \tag{4.4}$$

Now at steady state f = g = 0, so (4.4) gives

$$x_s = \frac{\phi_c}{\phi_c + \phi_e \exp\left(\dfrac{-\alpha}{u_s}\right)}, \tag{4.5}$$

(where the subscript s denotes steady state), which implies that a priori bounds for x_s are

$$\frac{\phi_c}{\phi_c + \phi_e} \leq x_s \leq 1. \tag{4.6}$$

We can now substitute for x_s into equation (4.3), at steady state, to give the equation satisfied by u_s as

$$\exp\left(\frac{-1}{u_s}\right) + \frac{\lambda_1\, h_w\, \phi_w\, \phi_c \exp\left(\dfrac{-\alpha_w}{u_s}\right)}{\phi_c + \phi_e \exp\left(\dfrac{-\alpha}{u_s}\right)} = L(u_s - U). \tag{4.7}$$

It is then a simple task to show that (4.7) has at least one solution u_s for all $U \geq 0$. Consider the functions

$$G_1(u_s) = \exp\left(\frac{-1}{u_s}\right) + \frac{\lambda_1\, h_w\, \phi_w\, \phi_c \exp\left(\dfrac{-\alpha_w}{u_s}\right)}{\phi_c + \phi_e \exp\left(\dfrac{-\alpha}{u_s}\right)}, \tag{4.8}$$

$$G_2(u_s) = L(u_s - U), \tag{4.9}$$

for any fixed $U \geq 0$, where $G_1(u_s)$ represents the rate of heat release by the various reactions at steady state, and $G_2(u_s)$ the rate of loss of heat due to Newtonian cooling. Now $G_1(0) = 0$, $G_2(0) = -LU$ (so clearly $U = 0$ has the solution $u_s = 0$), $G_1(\infty)$ is positively finite (in fact it equals $1 + (\lambda_1 h_w \phi_w \phi_c / (\phi_e + \phi_c))$, and $G_2(\infty)$ is positively infinite. So by the intermediate value theorem there must be at least one value $u_s = u_s^*$, with $0 \leq u_s^* < \infty$, for which $G_1(u_s) = G_2(u_s)$, for every $U \geq 0$.

In showing that the system can exhibit five steady state solutions for a certain parameter range we will use a similar graphical approach to that of Gray [30]. Figure 4.1 below shows an example set of u_s, $G_1(u_s)$ curves as the dimensionless initial moisture content λ_1 increases (with $\alpha > \alpha_w$).

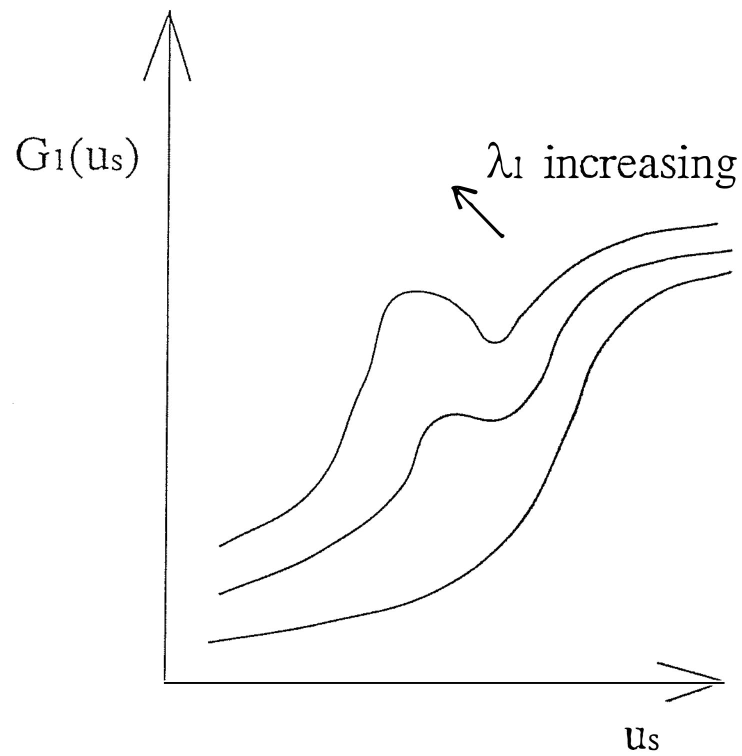

Figure 4.1 Rate of heat release curves as λ_1 increases from zero

We can see that for λ_1 sufficiently large, the heat release rate curve can have a negative slope. Thus, as the function $G_2(u_s)$ is a straight line, for this parameter range (4.7) can have up to five solutions. It is simple to deduce that a necessary condition for this negative slope to appear is that the second term in (4.8) has a maximum. This in turn can occur if $\alpha > \alpha_w$. So $\alpha > \alpha_w$ is a necessary but not sufficient condition for our system to have five steady state solutions. Figure 4.2 below shows some example U, u_s steady state bifurcation diagrams, as λ_1 increases, for the case $\alpha > \alpha_w$.

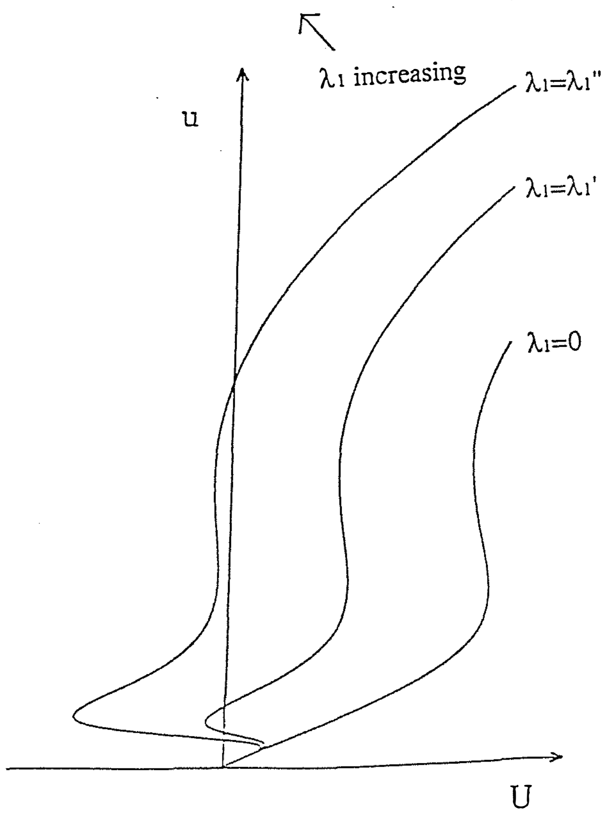

Figure 4.2 Example bifurcation diagrams, as λ_1 increases, for $\alpha > \alpha_w$

We observe that as λ_1 (the dimensionless characterization of the total moisture content in the body) increases the 'traditional' critical ambient temperatures, corresponding to the first limit point on the $\lambda_1 = 0$ curve, decreases. For $\lambda_1 = \lambda_1'$ the diagram has four limit points and an intermediate steady state is reached as U increases past the first limit point. It is interesting to note that for λ_1 sufficiently large, eg $\lambda_1 = \lambda_1''$, the lower right hand limit point is to the right of the higher right hand limit point, so this lower limit point now defines the U_{crit} value for the system. These diagrams show how U_{crit} can be substantially reduced by the inclusion of the effects of moisture content in the model. This may explain the comments in Figure 1.9 of Chapter 1.

A well-known (see e.g. Ray [51]) condition for (4.1), (4.2) to have a unique, stable steady state solution for all $U \geq 0$ is

$$\mathrm{Det}\,(J) > 0, \tag{4.10}$$

$$\mathrm{Tr}\,(J) < 0. \tag{4.11}$$

Here Det (J) is the determinant of the Jacobian matrix of the system (4.1), (4.2) evaluated at the steady state u_s, x_s,

$$J = \begin{pmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{pmatrix} = \left. \begin{pmatrix} \dfrac{\partial f}{\partial u} & \dfrac{\partial f}{\partial x} \\ \dfrac{\partial g}{\partial u} & \dfrac{\partial g}{\partial x} \end{pmatrix} \right|_{\substack{u = u_s \\ x = x_s}}, \tag{4.12}$$

and Tr (J) is the trace of this Jacobian.

So

$$\mathrm{Det}\,(J) = \frac{\partial f}{\partial u}\frac{\partial g}{\partial x} - \frac{\partial f}{\partial x}\frac{\partial g}{\partial u}, \quad \text{evaluated at } u_s,\ x_s, \tag{4.13}$$

and

$$\mathrm{Tr}\,(J) = \frac{\partial f}{\partial u} + \frac{\partial g}{\partial x}, \quad \text{evaluated at } u_s,\ x_s. \tag{4.14}$$

For our system

$$\frac{\partial f}{\partial u} = \frac{\exp\left(\frac{-1}{u}\right)}{u^2} - L + \frac{\lambda_1 x}{u^2}\left\{h_w\, \phi_w\, \alpha_w \exp\left(\frac{-\alpha_w}{u}\right) - h_c\, \phi_e\, \alpha \exp\left(\frac{-\alpha}{u}\right)\right\}, \qquad (4.15)$$

$$\frac{\partial f}{\partial x} = \lambda_1 \left\{h_w\, \phi_w \exp\left(\frac{-\alpha_w}{u}\right) - h_c\, \phi_e \exp\left(\frac{-\alpha}{u}\right) - h_c\, \phi_c \right\}, \qquad (4.16)$$

$$\frac{\partial g}{\partial u} = -\frac{\phi_e\, x\, \alpha}{\varepsilon u^2} \exp\left(\frac{-\alpha}{u}\right), \qquad (4.17)$$

$$\frac{\partial g}{\partial x} = -\frac{1}{\varepsilon}\left(\phi_c + \phi_e \exp\left(\frac{-\alpha}{u}\right)\right). \qquad (4.18)$$

This gives

$$\varepsilon \,\mathrm{Det}\,(J) = L\left(\phi_c + \phi_e \exp\left(\frac{-\alpha}{u}\right)\right) - \frac{\exp\left(\frac{-1}{u}\right)}{u^2}\left(\phi_c + \phi_e \exp\left(\frac{-\alpha}{u}\right)\right)$$

$$- \frac{\lambda_1\, h_w\, \phi_w\, x}{u^2}\left\{\phi_c\, \alpha_w \exp\left(\frac{-\alpha_w}{u}\right) + \phi_e(\alpha_w - \alpha) \exp\left(\frac{-(\alpha+\alpha_w)}{u}\right)\right\}, \qquad (4.19)$$

$$\mathrm{Tr}\,(J) = \frac{\exp\left(\frac{-1}{u}\right)}{u^2} - L + \frac{\lambda_1 x}{u^2}\left\{h_w\, \phi_w\, \alpha_w \exp\left(\frac{-\alpha_w}{u}\right) - h_c\, \phi_e\, \alpha \exp\left(\frac{-\alpha}{u}\right)\right\}$$

$$\frac{-1}{\varepsilon}\left(\phi_c + \phi_e \exp\left(\frac{-\alpha}{u}\right)\right), \qquad (4.20)$$

where u, x are evaluated at u_s, x_s.

We can now give a theorem regarding the unique steady state solution of the spatially uniform system for L sufficiently large.

Theorem 4.1

The system (4.1), (4.2) with f and g defined by (4.3), (4.4) has a unique, stable steady state solution for all $U \geq 0$ if

$$L > \begin{cases} \dfrac{4}{e^2}\left[1 + \dfrac{\phi_e}{\phi_c} + \lambda_1 \dfrac{h_w\,\phi_w}{\alpha_w}\right] & , \quad \alpha > \alpha_w \\[2ex] \dfrac{4}{e^2}\left[1 + \dfrac{\phi_e}{\phi_c} + \lambda_1\, h_w\,\phi_w\left(\dfrac{1}{\alpha_w} + \dfrac{\phi_e(\alpha_w-\alpha)}{\phi_c(\alpha+\alpha_w)^2}\right)\right] & , \quad \alpha_w \geq \alpha. \end{cases}$$

Proof

Using (4.6) and the fact that

$$0 \leq \frac{\exp\left(\dfrac{-k_1}{u}\right)}{u^2} \leq \frac{4}{k_1^2\, e^2}, \qquad (k_1 > 0)\,, \tag{4.21}$$

we see that Tr (J) < 0 certainly if

$$L > \frac{4}{e^2}\left[1 + \lambda_1 \frac{h_w\,\phi_w}{\alpha_w}\right],$$

and Det (J) > 0 certainly if

$$L > \begin{cases} \dfrac{4}{e^2}\left[1 + \dfrac{\phi_e}{\phi_c} + \lambda_1 \dfrac{h_w\,\phi_w}{\alpha_w}\right] & , \quad \alpha > \alpha_w, \\[2ex] \dfrac{4}{e^2}\left[1 + \dfrac{\phi_e}{\phi_c} + \lambda_1\, h_w\,\phi_w\left(\dfrac{1}{\alpha_w} + \dfrac{\phi_e(\alpha_w-\alpha)}{\phi_c(\alpha+\alpha_w)^2}\right)\right] & , \quad \alpha_w > \alpha. \end{cases}$$

This completes the proof.

This result has a logical physical interpretation in that it predicts that if the surface area to volume ratio of a body is sufficiently large then criticality will not occur and so spontaneous combustion is very unlikely. That is, if we take any moist self-heating body and store it in, for example, the shape of a sufficiently thin brick, then the body will not spontaneously ignite.

We will now derive some existence and uniqueness results for the solution of the time dependent problem (3.47) - (3.50). Firstly we make a comment on the use of Arrhenius kinetics. The Arrhenius law, given for example for a single exothermic reaction by (1.2) i.e.

$$q(T) = Q\rho Z \exp\left(\frac{-E}{RT}\right),$$

holds only for $T \geq 0$. Since the function $\exp\left(\frac{-E}{RT}\right)$ has a singularity at $T = 0$ there is obviously a problem in extending this theory to the range $T < 0$ (and non-dimensionally to $u < 0$). We will thus assume that, in effect, there is a Heaviside operator in front of each temperature dependent Arrhenius term which 'switches the reaction off' for $T < 0$. This seems realistic physically since it is unlikely that any reaction will still be occurring at 'negative' absolute temperatures. We will not need to look at the range $T < 0$ in general in this thesis, but we do need to consider this range briefly here to derive a priori bounds for the solution of the spatially uniform time dependent problem.

To consider the existence and uniqueness of solutions to the time dependent spatially uniform system (3.47) - (3.50), we will first show that the solutions are bounded for all time.

Theorem 4.2

Suppose u, x is a solution of (3.47) - (3.50) with $\zeta_1 \geq 0$ and $0 \leq \chi_1 \leq 1$. Then, for all $t > 0$,

$$0 \leq x(t) \leq 1,$$

$$0 \leq u(t) \leq \frac{1}{L}[1 + LU + \lambda_1 \{h_w \phi_w + h_c \phi_c\}] + \zeta_1 .$$

Proof

First we will show that x takes values between 0 and 1. Since $\chi_1 \leq 1$, it follows that if x ever became greater than 1 then there exists an interval of time (t_1, t_2) such that $\frac{dx}{dt} > 0$ for $t \in (t_1, t_2)$. But (3.48) gives

$$\frac{dx}{dt} = \frac{1}{\varepsilon}\left\{ \phi_c(1-x) - \phi_e\, x \exp\left(\frac{-\alpha}{u}\right)\right\},$$

$$< 0, \qquad \text{for all } x > 1.$$

So $x(t) \leq 1$ for all $t > 0$.

Similarly it can be shown that $x(t) \geq 0$ for all $t > 0$. Also since $\zeta_1 \geq 0$ it follows that if u ever became less than zero then there exists an interval (t_1, t_2) such that $\frac{du}{dt} < 0$ for $t \in (t_1, t_2)$. However (3.47) gives (remembering our comments above on Arrhenius kinetics for negative u)

$$\frac{du}{dt} = -L(u-U) + h_c\, \phi_c(1-x),$$

$$> 0, \qquad \text{for all } u < 0.$$

So $u(t) \geq 0$ for all $t > 0$.

Finally, since $0 \leq x(t) \leq 1$, we have from (3.47)

$$\frac{du}{dt} \leq 1 - L(u-U) + \lambda_1 \{h_w \phi_w + h_c \phi_c\},$$

$$\Rightarrow \qquad \frac{du}{dt} + Lu \leq 1 + LU + \lambda_1 \{h_w \phi_w + h_c \phi_c\},$$

$$\Rightarrow \qquad \frac{d}{dt}(\exp(Lt)u) \leq \exp(Lt)\,[1 + LU + \lambda_1 \{h_w \phi_w + h_c \phi_c\}],$$

$$\Rightarrow \qquad \exp(Lt)\,u \leq \frac{1}{L}\exp(Lt)\,[1 + LU + \lambda_1 \{h_w \phi_w + h_c \phi_c\}] + C_5,$$

where C_5 is a constant of integration.

Now at $t = 0$, $u = \zeta_1$, so we can choose

$$C_5 = \zeta_1 - \frac{1}{L}[1 + LU + \lambda_1 \{h_w \phi_w + h_c \phi_c\}],$$

which gives

$$u \leq \frac{1}{L}[1 + LU + \lambda_1 \{h_w \phi_w + h_c \phi_c\}] + \zeta_1, \qquad \text{for all } t > 0.$$

This completes the proof.

These a-priori bounds for the solutions of (3.47) - (3.50) can now be used to show that (3.47) - (3.50) has a unique solution if $0 \leq \chi_1 \leq 1$, $\zeta_1 \geq 0$. This follows from classical results on ordinary differential equations given that f and g satisfy Lipschitz conditions on some bounded set in $\mathbb{R}^2$.

4.3 The nature and stability of steady state solutions

The local stability of the steady states of the spatially uniform model can be determined by looking at the stability of the first variation of (3.47), (3.48). Consider a system of the form (4.1), (4.2) i.e.

$$\frac{du}{dt} = f(u, x, \underset{\sim}{\delta}, \underset{\sim}{\beta}),$$

$$\frac{dx}{dt} = g(u, x, \underset{\sim}{\delta}, \underset{\sim}{\beta}).$$

Consider further a particular steady state solution u_s, x_s such that

$$f(u_s, x_s, \underset{\sim}{\delta}, \underset{\sim}{\beta}) = 0, \tag{4.22}$$

$$g(u_s, x_s, \underset{\sim}{\delta}, \underset{\sim}{\beta}) = 0. \tag{4.23}$$

Now perturb u_s, x_s by small amounts Δu, Δx i.e.

$$u = u_s + \Delta u, \tag{4.24}$$

$$x = x_s + \Delta x, \tag{4.25}$$

then Taylor series expansions for f and g about u_s, x_s gives

$$f(u_s + \Delta u, x_s + \Delta x, \underset{\sim}{\delta}, \underset{\sim}{\beta}) = f(u_s, x_s, \underset{\sim}{\delta}, \underset{\sim}{\beta}) + \frac{\partial f}{\partial u}(u_s, x_s, \underset{\sim}{\delta}, \underset{\sim}{\beta})\, \Delta u$$

$$+ \frac{\partial f}{\partial x}(u_s, x_s, \underset{\sim}{\delta}, \underset{\sim}{\beta})\, \Delta x + o((\Delta u), (\Delta x)),$$

$$g(u_s + \Delta u, x_s + \Delta x, \underset{\sim}{\delta}, \underset{\sim}{\beta}) = g(u_s, x_s, \underset{\sim}{\delta}, \underset{\sim}{\beta}) + \frac{\partial g}{\partial u}(u_s, x_s, \underset{\sim}{\delta}, \underset{\sim}{\beta})\, \Delta u$$

$$+ \frac{\partial g}{\partial x}(u_s, x_s, \underset{\sim}{\delta}, \underset{\sim}{\beta})\, \Delta x + o((\Delta u), (\Delta x)).$$

Neglecting terms of $o((\Delta u), (\Delta x))$, using (4.22), (4.23) and substituting into (4.1), (4.2) gives the equations for Δu and Δx to leading order as

$$\frac{\partial(\Delta u)}{\partial t} = \frac{\partial f}{\partial u}(u_s, x_s, \underset{\sim}{\delta}, \underset{\sim}{\beta})\, \Delta u + \frac{\partial f}{\partial x}(u_s, x_s, \underset{\sim}{\delta}, \underset{\sim}{\beta})\, \Delta x, \tag{4.26}$$

$$\frac{\partial(\Delta x)}{\partial t} = \frac{\partial g}{\partial u}(u_s, x_s, \underset{\sim}{\delta}, \underset{\sim}{\beta})\, \Delta u + \frac{\partial g}{\partial x}(u_s, x_s, \underset{\sim}{\delta}, \underset{\sim}{\beta})\, \Delta x, \tag{4.27}$$

which has a solution of the form

$$\Delta u(t) = F_1 \exp(\sigma_1 t) + F_2 \exp(\sigma_2 t), \tag{4.28}$$

$$\Delta x(t) = F_3 \exp(\sigma_1 t) + F_3 \exp(\sigma_2 t), \tag{4.29}$$

where F_1, F_2, F_3, F_4 are real constants and σ_1 and σ_2 are real or imaginary numbers. In fact the values σ_1 and σ_2 are just the eigenvalues of the Jacobian matrix of the system evaluated at the steady state, where the Jacobian is as given in (4.12). These eigenvalues are given by the roots of the characteristic polynomial

$$\sigma^2 - \mathrm{Tr}(J)\sigma + \mathrm{Det}(J) = 0. \tag{4.30}$$

So we can see that the nature and stability of the steady state point u_s, x_s we are considering, depends critically on the form of σ_1 and σ_2, given that σ_1 and σ_2 must either be real or form a complex conjugate pair. In fact there are five possibilities in u, x space if the real parts of σ_1 and σ_2 are non zero

(i) u_s, x_s is a saddle point;

(ii) u_s, x_s is a stable node;

(iii) u_s, x_s is an unstable node;

(iv) u_s, x_s is a stable focus;

(v) u_s, x_s is an unstable focus.

Of course more than one of these 'fixed points' may occur in the same u, x phase space diagram if the system has multiple steady state solutions at those particular parameter values. The dependence of the occurrence of each of these possibilities on σ_1 and σ_2 is summarized below

if Det(J) < 0, then u_s, x_s is a SADDLE POINT,
if Det(J) > 0, Tr(J) < 0, then u_s, x_s is a STABLE STEADY STATE,
if Det(J) > 0, Tr(J) > 0, then u_s, x_s is an UNSTABLE STEADY STATE,

further,

if σ_1, σ_2 are real and < 0, then u_s, x_s is a STABLE NODE,
if σ_1, σ_2 are real and opposite sign, then u_s, x_s is a SADDLE POINT,
if σ_1, σ_2 are real and > 0, then u_s, x_s is an UNSTABLE NODE,
if σ_1, σ_2 are complex with real part < 0, then u_s, x_s is a STABLE FOCUS,
if σ_1, σ_2 are complex with real part > 0, then u_s, x_s is an UNSTABLE FOCUS.

The nature of the u, x phase space diagram close to each of these five possible steady state points is shown in Figures (4.3) - (4.7) below.

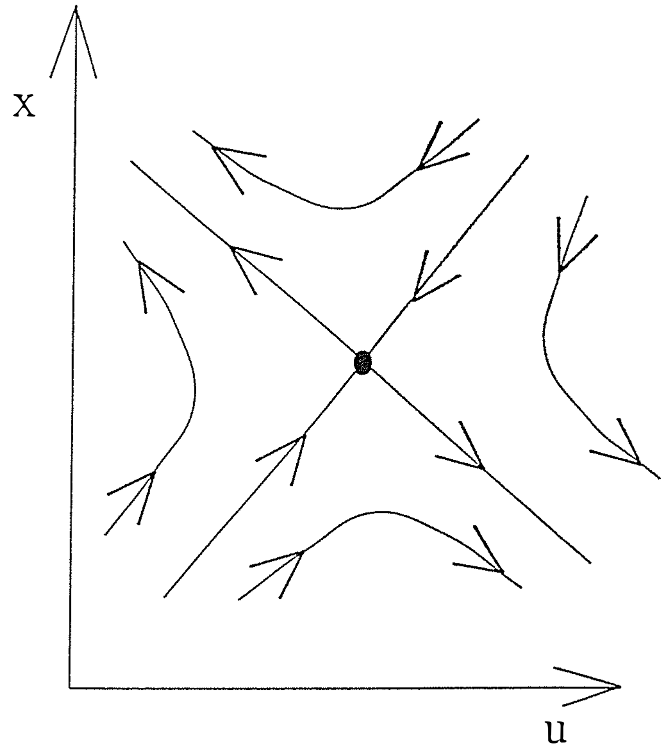

Figure 4.3 Saddle point steady state

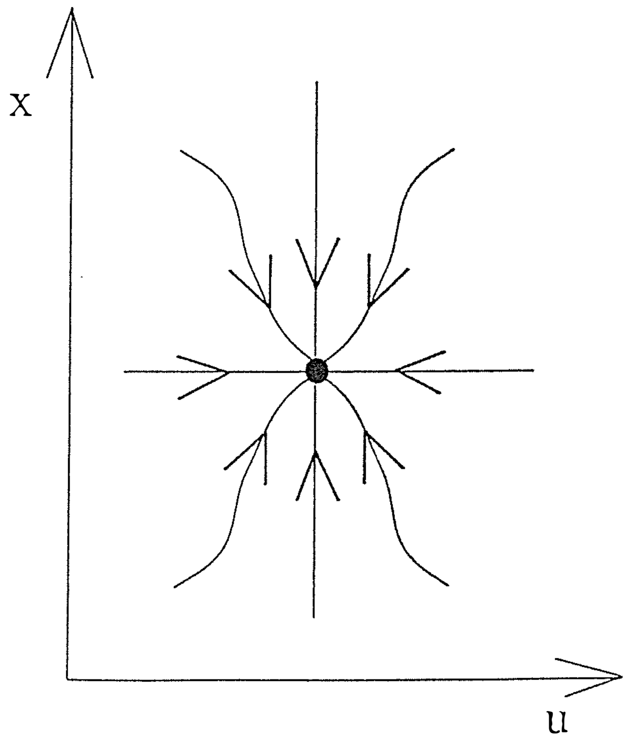

Figure 4.4 Stable node steady state

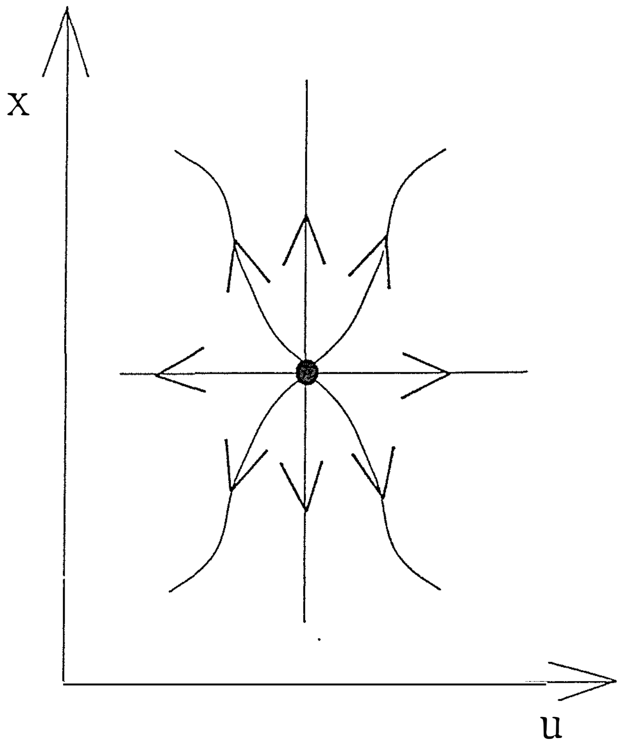

Figure 4.5 Unstable node steady state

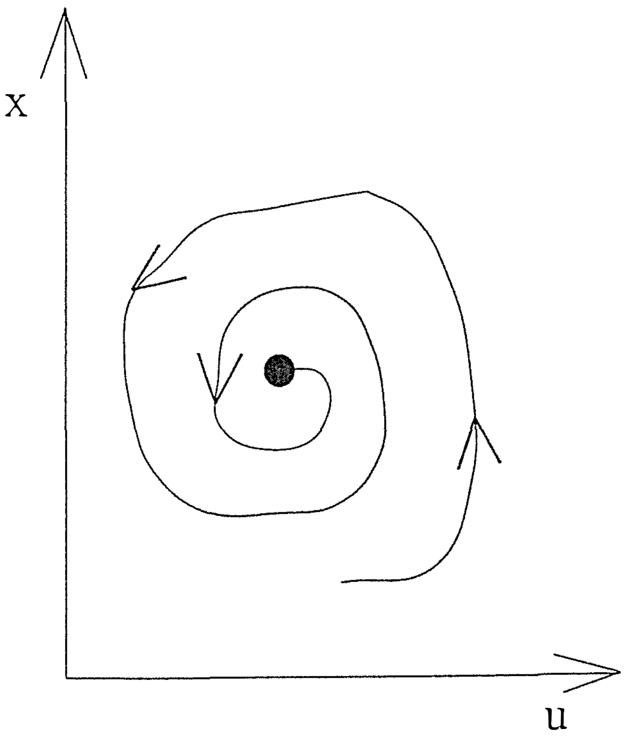

Figure 4.6 Stable focus steady state

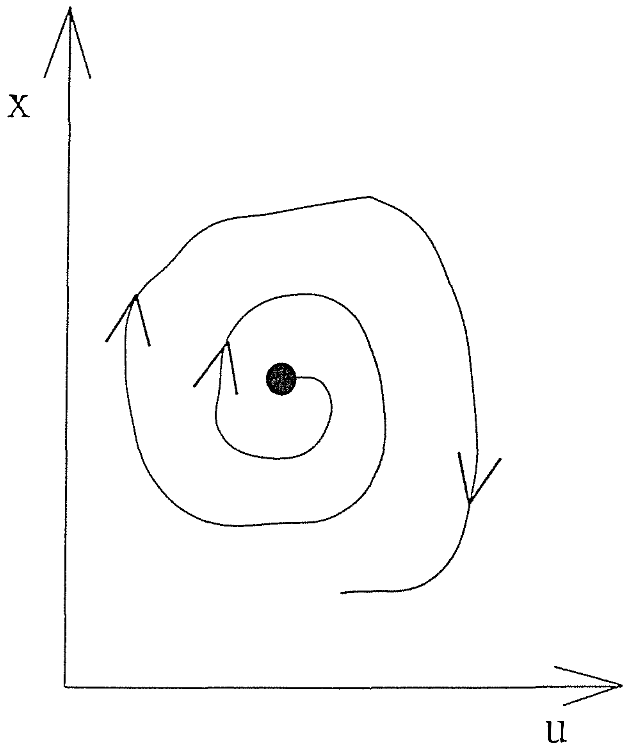

Figure 4.7 Unstable focus steady state

Other possibilities include: Det(J) = 0, this is known as a saddle-node type bifurcation (or in our context a 'limit point') and usually indicates a change in the stability of the steady state solution; Det(J) > 0, Tr(J) = 0, this corresponds to σ_1, σ_2 being complex conjugates with zero real parts and indicates the possibility of periodic solutions, i.e. a Hopf bifurcation point; Det(J) = 0, Tr(J) = 0, this corresponds to σ_1 and σ_2 being identically zero complex numbers, and is known as a double zero eigenvalue degeneracy.

We will discuss periodic solutions and their stability near a Hopf bifurcation point in the next section.

4.4 Hopf bifurcation points and periodic solutions

As we have stated in the last section, the conditions for a steady state solution u_s, x_s to also be a Hopf bifurcation point are

$$\mathrm{Tr}(J) = 0, \tag{4.31}$$

$$\mathrm{Det}(J) > 0. \tag{4.32}$$

Hopf bifurcations are important to locate because (i) they usually represent a point in parameter space where a branch of periodic solutions (limit cycles) emanates from the steady state branch and (ii) they earmark a change in the stability of the steady state solutions. The exception to (i) occurs when the degeneracy condition

$$\frac{d(\mathrm{Tr}(J))}{dU} = 0, \tag{4.33}$$

is satisfied. This corresponds to two Hopf bifurcation points coinciding at the same point on the steady state branch, so there are no emanating periodic branches linking them. The set of conditions (4.31), (4.32), (4.33) is known as the $H2_1$ degeneracy in the notation of Gray and Roberts [49], and we will investigate in detail its occurrence in parameter space.

We can calculate the stability of the limit cycles close to the Hopf bifurcation point by looking at the sign of a parameter we shall refer to as μ_s. The parameter is a function of the first three partial derivatives of f and g evaluated at the Hopf bifurcation point. To calculate μ_s we will follow the formula of Segel [52], which we will now outline.

At a Hopf bifurcation point the Jacobian matrix J given by (4.12) will have purely imaginary conjugate eigenvalues $\pm i\omega_0$. To use the formula of Segel this coefficient matrix must have the canonical form

$$J = \begin{pmatrix} 0 & \omega_0 \\ -\omega_0 & 0 \end{pmatrix}. \tag{4.34}$$

If this is not the case for our original system at the Hopf bifurcation point then new variables

$$\tilde{u} = p_{11}\,u + p_{12}\,x, \tag{4.35}$$

$$\tilde{x} = p_{21}\,u + p_{22}\,x, \tag{4.36}$$

must be introduced so that the modified system

$$\frac{d\tilde{u}}{dt} = \tilde{f}(\tilde{u}, \tilde{x}, \underset{\sim}{\delta}, \underset{\sim}{\beta}), \tag{4.37}$$

$$\frac{d\tilde{x}}{dt} = \tilde{g}(\tilde{u}, \tilde{x}, \underset{\sim}{\delta}, \underset{\sim}{\beta}), \tag{4.38}$$

does have a Jacobian matrix of the desired form.

It is easily verified that

$$\left.\begin{aligned} p_{11} &= 1, \\ p_{12} &= 0, \\ p_{21} &= \frac{J_{11}}{\omega_0}, \\ p_{22} &= \frac{J_{12}}{\omega_0}, \end{aligned}\right\} \tag{4.39}$$

are correct choices for the transformation, where the components of J are evaluated at the Hopf bifurcation point. Now we calculate the following partial derivatives at the Hopf bifurcation point.

$$\left.\begin{aligned}
B_{20} &= \frac{\partial^2 \tilde{f}}{\partial \tilde{u}^2}, & C_{20} &= \frac{\partial^2 \tilde{g}}{\partial \tilde{u}^2}, \\
B_{11} &= \frac{\partial^2 \tilde{f}}{\partial \tilde{u} \partial \tilde{x}}, & C_{11} &= \frac{\partial^2 \tilde{g}}{\partial \tilde{u} \partial \tilde{x}}, \\
B_{02} &= \frac{\partial^2 \tilde{f}}{\partial \tilde{x}^2}, & C_{02} &= \frac{\partial^2 \tilde{g}}{\partial \tilde{x}^2}, \\
B_{30} &= \frac{\partial^3 \tilde{f}}{\partial \tilde{u}^3}, & C_{03} &= \frac{\partial^3 \tilde{g}}{\partial \tilde{x}^3}, \\
B_{12} &= \frac{\partial^3 \tilde{f}}{\partial \tilde{u} \partial \tilde{x}^2}, & C_{21} &= \frac{\partial^3 \tilde{g}}{\partial \tilde{u}^2 \partial \tilde{x}}.
\end{aligned}\right\} \tag{4.40}$$

The scalar quantity μ_s is then given by

$$\mu_s = [B_{30} + B_{12} + C_{21} + C_{03}]/\omega_0$$

$$+ [-B_{11}\,(B_{20}+B_{02}) + C_{11}(C_{20}+C_{02}) + B_{20}C_{20} - B_{02}C_{02}]/(\omega_0)^2. \tag{4.41}$$

The above constitutes Segel's formula. However it is more convenient to write the partial derivatives in (4.40) in terms of the first three partial derivatives of f and g with respect to u and x. We can do this by forming the matrices P and Q where

$$P = \begin{pmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \frac{J_{11}}{\omega_0} & \frac{J_{12}}{\omega_0} \end{pmatrix}, \tag{4.42}$$

$$Q = P^{-1} = \begin{pmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \frac{-J_{11}}{J_{12}} & \frac{\omega_0}{J_{12}} \end{pmatrix}. \tag{4.43}$$

Then

$$\frac{\partial^2 \tilde{f}}{\partial \tilde{u}^2} = \frac{\partial^2 f}{\partial u^2} + 2q_{21}\frac{\partial^2 f}{\partial u \partial x} + q_{21}^2 \frac{\partial^2 f}{\partial x^2}, \tag{4.44}$$

$$\frac{\partial^2 \tilde{f}}{\partial \tilde{x}^2} = q_{22}^2 \frac{\partial^2 f}{\partial x^2}, \tag{4.45}$$

$$\frac{\partial^2 \tilde{f}}{\partial \tilde{u} \partial \tilde{x}} = q_{22}\frac{\partial^2 f}{\partial u \partial x} + q_{21}\, q_{22}\frac{\partial^2 f}{\partial x^2}, \tag{4.46}$$

$$\frac{\partial^2 \tilde{g}}{\partial \tilde{u}^2} = p_{21}\frac{\partial^2 f}{\partial u^2} + 2p_{21}\, q_{21}\frac{\partial^2 f}{\partial u \partial x} + p_{21}\, q_{21}^2 \frac{\partial^2 f}{\partial x^2}$$

$$+ p_{22}\frac{\partial^2 g}{\partial u^2} + 2p_{22}\, q_{21}\frac{\partial^2 g}{\partial u \partial x} + p_{22}\, q_{21}^2 \frac{\partial^2 g}{\partial x^2}, \tag{4.47}$$

$$\frac{\partial^2 \tilde{g}}{\partial \tilde{x}^2} = p_{21}\, q_{22}^2 \frac{\partial^2 f}{\partial x^2} + p_{22}\, q_{22}^2 \frac{\partial^2 g}{\partial x^2}, \tag{4.48}$$

$$\frac{\partial^2 \tilde{g}}{\partial \tilde{u} \partial \tilde{x}} = p_{21}\, q_{22}\frac{\partial^2 f}{\partial u \partial x} + p_{21}\, q_{21}\, q_{22}\frac{\partial^2 f}{\partial x^2} + p_{22}\, q_{22}\frac{\partial^2 g}{\partial u \partial x} + p_{22}\, q_{21}\, q_{22}\frac{\partial^2 g}{\partial x^2}, \tag{4.49}$$

$$\frac{\partial^3 \tilde{f}}{\partial \tilde{u}^3} = \frac{\partial^3 f}{\partial u^3} + 3q_{21}\frac{\partial^3 f}{\partial u^2 \partial x} + 3q_{21}^2 \frac{\partial^3 f}{\partial u \partial x^2} + q_{21}^2 \frac{\partial^3 f}{\partial x^3}, \tag{4.50}$$

$$\frac{\partial^3\tilde{f}}{\partial\tilde{u}\partial\tilde{x}^2} = q_{22}^2\,\frac{\partial^3 f}{\partial u\partial x^2} + q_{22}^2\,q_{21}\,\frac{\partial^3 f}{\partial x^3}\,, \tag{4.51}$$

$$\frac{\partial^3\tilde{g}}{\partial\tilde{x}^3} = p_{21}\,q_{22}^3\,\frac{\partial^3 f}{\partial x^3} + p_{22}\,q_{22}^3\,\frac{\partial^3 g}{\partial x^3}\,, \tag{4.52}$$

$$\frac{\partial^3\tilde{g}}{\partial\tilde{u}^2\partial\tilde{x}} = p_{21}\,q_{22}\,\frac{\partial^3 f}{\partial u^2\partial x} + 2p_{21}\,q_{21}\,q_{22}\,\frac{\partial^3 f}{\partial u\partial x^2} + p_{21}\,q_{21}^2\,q_{22}\,\frac{\partial^3 f}{\partial x^3}$$

$$+\,p_{22}\,q_{22}\,\frac{\partial^3 g}{\partial u^2\partial x} + 2p_{22}\,q_{21}\,q_{22}\,\frac{\partial^3 g}{\partial u\partial x^2} + p_{22}\,q_{21}^2\,q_{22}\,\frac{\partial^3 g}{\partial x^3}\,, \tag{4.53}$$

where for our system

$$\frac{\partial^2 f}{\partial u^2} = \frac{\exp\left(\frac{-1}{u}\right)(1-2u)}{u^4} + \frac{\lambda_1 x}{u^3}\left[-2\left\{ h_w\phi_w\alpha_w \exp\left(\frac{-\alpha_w}{u}\right) - h_c\phi_e\alpha \exp\left(\frac{-\alpha}{u}\right)\right\}\right.$$

$$\left. + \frac{1}{u}\left\{ h_w\phi_w{\alpha_w}^2 \exp\left(\frac{-\alpha_w}{u}\right) - h_c\phi_e\alpha^2 \exp\left(\frac{-\alpha}{u}\right)\right\}\right], \tag{4.54}$$

$$\frac{\partial^2 f}{\partial u\partial x} = \frac{\lambda_1}{u^2}\left\{ h_w\phi_w\alpha_w \exp\left(\frac{-\alpha_w}{u}\right) - h_c\phi_e\alpha \exp\left(\frac{-\alpha}{u}\right)\right\}, \tag{4.55}$$

$$\frac{\partial^2 f}{\partial x^2} = 0, \tag{4.56}$$

$$\frac{\partial^2 g}{\partial u^2} = \frac{\phi_e\,x\,\alpha\,\exp\left(\frac{-\alpha}{u}\right)}{\varepsilon u^3}\left(2 - \frac{\alpha}{u}\right), \tag{4.57}$$

$$\frac{\partial^2 g}{\partial u\partial x} = \frac{-\phi_e\,\alpha\,\exp\left(\frac{-\alpha}{u}\right)}{\varepsilon u^2}, \tag{4.58}$$

$$\frac{\partial^2 g}{\partial x^2} = 0, \tag{4.59}$$

$$\frac{\partial^3 f}{\partial u^3} = \frac{\exp\left(\frac{-1}{u}\right)\{(1-2u)(1-4u) - 2u^2\}}{u^6} - \frac{3\lambda_1 x}{u^4}\left[-2\left\{h_w\phi_w\alpha_w \exp\left(\frac{-\alpha_w}{u}\right) - \right.\right.$$

$$\left.\left. h_c\phi_e\alpha \exp\left(\frac{-\alpha}{u}\right)\right\} + \frac{2}{u}\left\{h_w\phi_w\alpha_w{}^2 \exp\left(\frac{-\alpha_w}{u}\right) - h_c\phi_c\alpha^2 \exp\left(\frac{-\alpha}{u}\right)\right\}\right]$$

$$+\frac{\lambda_1 x}{u^6}\left\{h_w\phi_w\alpha_w{}^3 \exp\left(\frac{-\alpha_w}{u}\right) - h_c\phi_e\alpha^3 \exp\left(\frac{-\alpha}{u}\right)\right\}, \tag{4.60}$$

$$\frac{\partial^3 f}{\partial u^2 \partial x} = \frac{\lambda_1}{u^3}\left[-2\left\{h_w\phi_w\alpha_w \exp\left(\frac{-\alpha_w}{u}\right) - h_c\phi_e\alpha \exp\left(\frac{-\alpha}{u}\right)\right\}\right.$$

$$\left.+\frac{1}{u}\left\{h_w\phi_w\alpha_w{}^2 \exp\left(\frac{-\alpha_w}{u}\right) - h_c\phi_e\alpha^2 \exp\left(\frac{-\alpha}{u}\right)\right\}\right], \tag{4.61}$$

$$\frac{\partial^3 f}{\partial u \partial x^2} = 0, \tag{4.62}$$

$$\frac{\partial^3 f}{\partial x^3} = 0, \tag{4.63}$$

$$\frac{\partial^3 g}{\partial u^2 \partial x} = \frac{\phi_e\alpha \exp\left(\frac{-\alpha}{u}\right)}{\varepsilon u^3}\left(2 - \frac{\alpha}{u}\right), \tag{4.64}$$

$$\frac{\partial^3 g}{\partial u \partial x^2} = 0, \tag{4.65}$$

$$\frac{\partial^3 g}{\partial x^3} = 0. \tag{4.66}$$

These derivatives are to be calculated at u_s, x_s.

If μ_s is negative then the limit cycles emerging from the Hopf bifurcation point will be locally stable, if μ_s is positive then the emerging limit cycles will be unstable.

The condition

$$\mu_s = 0, \tag{4.67}$$

at a Hopf bifurcation point therefore corresponds to a change in stability of the emerging limit cycles, and so represents another important phenomenon in parameter space. The set of conditions (4.31), (4.32), (4.67) is known as the $H3_1$ degeneracy, in the notation of Gray and Roberts [49].

Given the signs of the quantities μ_s and $\frac{d(Tr(J))}{dU}$ at the Hopf bifurcation point, then, the four possibilities for the stability and direction of the loci of emerging limit cycles in the neighbourhood of the Hopf bifurcation point are given schematically below in Figures 4.8 - 4.11. In these diagrams (as in all later U, u bifurcation diagrams) a broken line represents an unstable steady state, an unbroken line represents a stable steady state, an open circle represents an unstable periodic solution and a black circle represents a stable periodic solution.

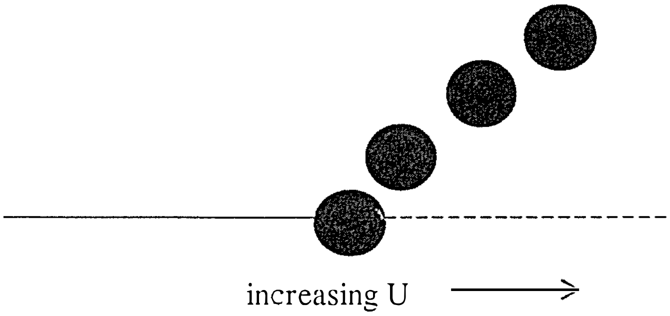

Figure 4.8 Nature of the emerging limit cycles in the neighbourhood of a Hopf bifurcation point for $\mu_s < 0$, $\frac{d(Tr(J))}{dU} > 0$.

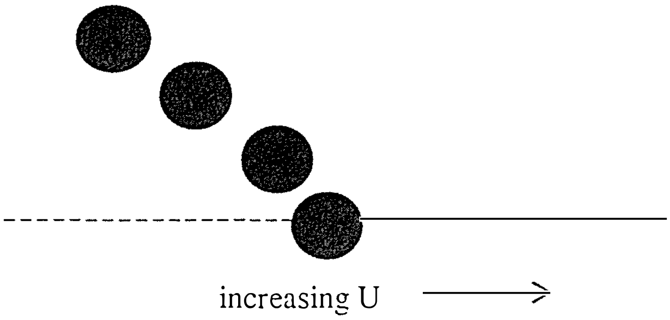

Figure 4.9 Nature of the emerging limit cycles in the neighbourhood of a Hopf bifurcation point for $\mu_s < 0$, $\frac{d(Tr(J))}{dU} < 0$.

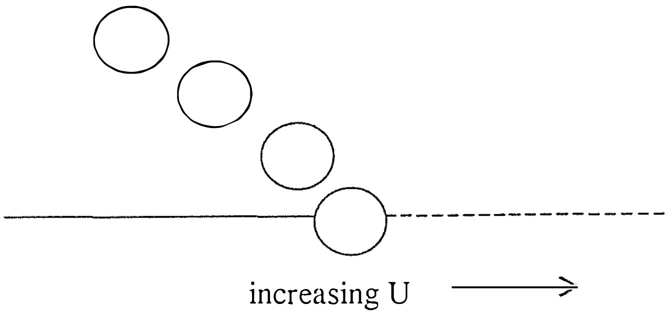

Figure 4.10 Nature of the emerging limit cycles in the neighbourhood of a Hopf bifurcation point for $\mu_s > 0$, $\frac{d(Tr(J))}{dU} > 0$.

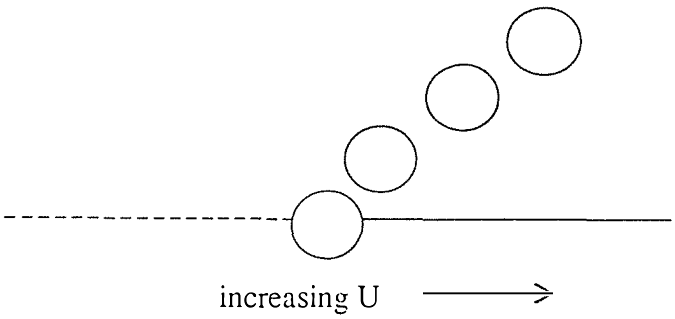

Figure 4.11 Nature of the emerging limit cycles in the neighbourhood of a Hopf bifurcation point for $\mu_s > 0$, $\frac{d(Tr(J))}{dU} < 0$.

There are two possibilities for the ultimate destination of a locus of limit cycles from a Hopf bifurcation point. It can either rejoin a steady state branch at another Hopf bifurcation point, or the locus can abruptly end (or 'evaporate') before reaching another Hopf bifurcation point. This 'evaporation' corresponds to the period of the limit cycle becoming infinite as the amplitude of the limit cycle grows to such an extent that the limit cycle meets the separatrices of a saddle point in phase space. The 'evaporation' of a limit cycle in phase space is illustrated in Figures 4.12 - 4.14.

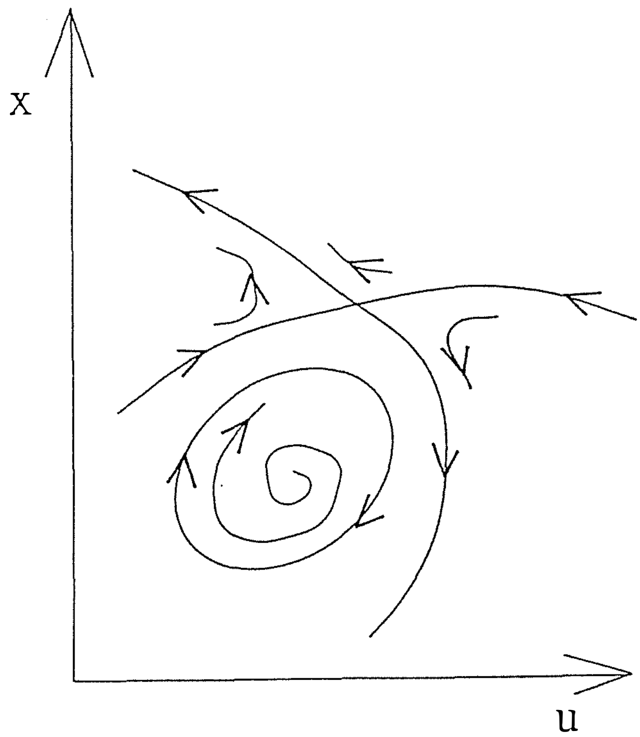

Figure 4.12 Limit cycle in proximity of saddle point.

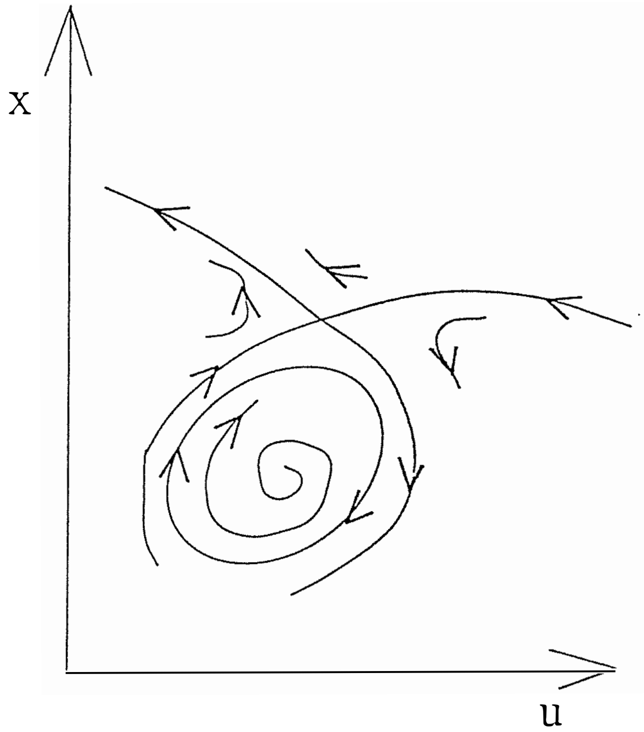

Figure 4.13 Limit cycle 'approaches' saddle point.

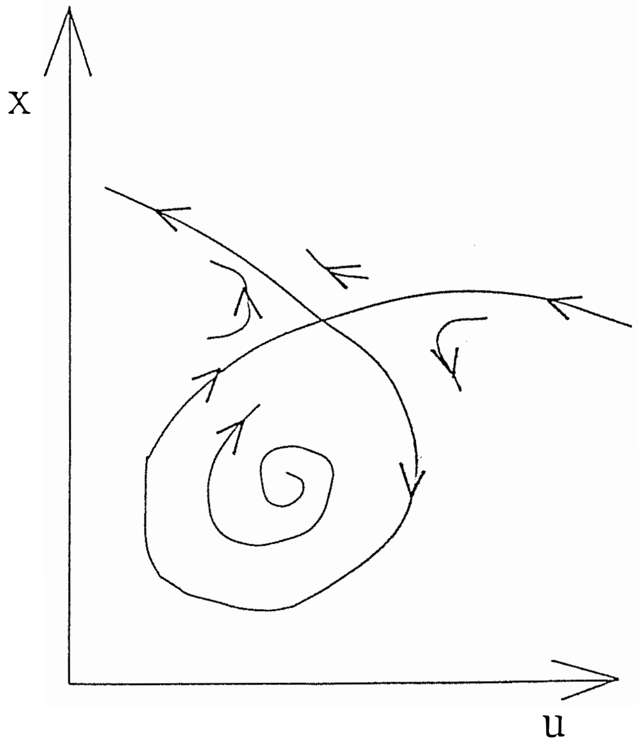

Figure 4.14 Limit cycle merges with separatrices of saddle point.

4.5 Plotting degeneracy and bifurcation curves: the pseudo-arclength method

In order to find each of the possible bifurcation diagrams the model can exhibit for a particular value of the constant parameter vector $\underset{\sim}{\beta}$, we will divide the λ_1, L space up into distinct regions of behaviour by plotting the degeneracy curves. For example $H2_1$ and $H3_1$ degeneracies are both represented by curves in λ_1, L space.

To do this involves solving systems of the form

$$\underset{\sim}{F}(\underset{\sim}{d}, p) = \underset{\sim}{0}, \tag{4.68}$$

where $\underset{\sim}{d}$ is a vector of unknowns and the parameter p is one of the group U, λ_1, L. In general we will use the pseudo-arclength method to solve this system as p varies. The pseudo-arclength method uses the arclength, s, along the solution locus as the continuation parameter. We can see that the arclength is the best choice of continuation parameter by noting, for example, how it is characteristic for steady state bifurcation diagrams in ignition theory to have a discontinuity at $U = U_{crit}$, if U is chosen as the continuation parameter. The steady state locus is, however, continuous with arclength through such points. For a detailed description of the pseudo-arclength method see e.g. Keller [50]. We will outline it briefly below.

Introduce an arclength parameter s and let

$$p = p(s),$$
$$\underset{\sim}{d} = \underset{\sim}{d}(s).$$

Then assuming a solution $\underset{\sim}{d}(s_0)$, $p(s_0)$ is known, a solution at $\underset{\sim}{d}(s_0 + \Delta s)$, $p(s_0 + \Delta s)$ can be generated using a combined Euler predictor/iterated Newton corrector approach.

(a) Euler predictor.

We have

$$\underset{\sim}{F}(\underset{\sim}{d}(s_0),\ p(s_0)) = \underset{\sim}{0}, \tag{4.69}$$

then define

$$(\underset{\sim}{d}_0,\ p_o) \equiv (\underset{\sim}{d}(s_0),\ p(s_0)),$$

and compute

$$(\dot{\underset{\sim}{d}}_0,\ \dot{p}_0), \qquad \text{where } \bullet \equiv \frac{d}{ds},$$

via

$$J_1\, \dot{\underset{\sim}{d}}_0 + \dot{p}_0\, \underset{\sim}{F}_p = 0, \tag{4.70}$$

$$\|\dot{\underset{\sim}{d}}_0\|^2 + |\dot{p}_0|^2 - 1 = 0, \tag{4.71}$$

where J_1 is the Jacobian matrix of (4.68) evaluated at $(\underset{\sim}{d}_0, p_0)$ and $\underset{\sim}{F}_p$ is the gradient vector of $\underset{\sim}{F}$ with respect to p, evaluated at $(\underset{\sim}{d}_0, p_0)$. Equation (4.71) represents the "arclength condition".

Then let

$$\left.\begin{aligned} \underset{\sim}{d}^0(s_0 + \Delta s) &= \underset{\sim}{d}_0 + \Delta s\, \dot{\underset{\sim}{d}}_0 , \\ p^0(s_0 + \Delta s) &= p_0 + \Delta s\, \dot{p}_0 , \end{aligned}\right\} \tag{4.72}$$

(b) Newton iteration

We require the solution at the next point along the solution locus, i.e. at $s = s_0 + \Delta s$, to satisfy

$$\underset{\sim}{F}(\underset{\sim}{d}(s),\ p(s)) = \underset{\sim}{0}, \tag{4.73}$$

$$N(\underset{\sim}{d}(s),\ p(s),\ (s)) = \dot{\underset{\sim}{d}}_0^T(\underset{\sim}{d}(s) - d_0) + \dot{p}_0(p(s) - p_0) - (s - s_0) = 0. \tag{4.74}$$

Here equation (4.74) is the "pseudo-arclength condition". The iterated Newton corrector thus consists of solving

$$\begin{bmatrix} J_1 & \underset{\sim}{F}_p \\ \dot{\underset{\sim}{d}}_0^T & \dot{p}_0 \end{bmatrix} \begin{bmatrix} \delta\underset{\sim}{d}^i \\ \delta p^i \end{bmatrix} = - \begin{bmatrix} \underset{\sim}{F} \\ N \end{bmatrix},$$

for the vector $\delta\underset{\sim}{d}^i$ and the scalar δp^i (where $\underset{\sim}{F}$, N and derivatives are evaluated at $(\underset{\sim}{d}^i(s),\ p^i(s))$). Then we calculate

$$\underset{\sim}{d}^{i+1}(s) = \underset{\sim}{d}^i(s) + \delta\underset{\sim}{d}^i(s)\ ,$$

$$p^{i+1}(s) = p^i(s) + \delta p^i(s),$$

for $i = 1, 2, 3, \ldots$,

and repeat the above process until $\|\delta\underset{\sim}{d}^{i+1}\| + |\delta p^{i+1}|$ is sufficiently small.

4.6 The degeneracy curves in λ_1, L space

The particular value of $\underset{\sim}{\beta}$ we have used to plot the degeneracy curves in this section is

$$\underset{\sim}{\beta} = (1.0, 1.0, 1.0, 1.0, 1.0, 0.01, 0.2, 0.9), \tag{4.75}$$

although a similar procedure could be applied to any $\underset{\sim}{\beta}$ values, and thus to any particular cellulosic material.

4.6.1 The hysteresis and double limit point curves

The hysteresis curve in λ_1, L space corresponds to a curve along which limit points are born on the U, u bifurcation diagram. The equations which must be satisfied by the hysteresis curves are the steady state condition (4.7) as well as

$$\frac{dU}{du_s} = 0, \tag{4.76}$$

and

$$\frac{d^2U}{du_s^2} = 0, \tag{4.77}$$

where

$$\frac{dU}{du_s} = \frac{-\exp\left(\frac{-1}{u_s}\right)}{Lu_s^2} + 1 - \frac{\lambda_1\phi_c\phi_w h_w}{L}\left\{\frac{\alpha_w\phi_c \exp\left(\frac{-\alpha_w}{u_s}\right) + \phi_e(\alpha_w-\alpha)\exp\left(\frac{-(\alpha+\alpha_w)}{u_s}\right)}{u_s^2 K_1^2}\right\}, \tag{4.78}$$

$$\frac{d^2U}{du_s^2} = \frac{-\exp\left(\frac{-1}{u_s}\right)(1-2u_s)}{L\,u_s^4} - \frac{\lambda_1\phi_c\phi_w h_w}{L}\left\{\frac{K_1K_2 - K_3K_4}{u_s^4 K_1^3}\right\}, \tag{4.79}$$

and

$$\left.\begin{aligned}
K_1 &= \phi_c + \phi_e \exp\left(\frac{-\alpha}{u_s}\right),\\
K_2 &= \alpha_w^2\,\phi_c \exp\left(\frac{-\alpha_w}{u_s}\right) + \phi_e\,(\alpha_w-\alpha)(\alpha+\alpha_w)\exp\left(\frac{-(\alpha+\alpha_w)}{u_s}\right),\\
K_3 &= \alpha_w\,\phi_c \exp\left(\frac{-\alpha_w}{u_s}\right) + \phi_e(\alpha_w-\alpha)\exp\left(\frac{-(\alpha+\alpha_w)}{u_s}\right),\\
K_4 &= 2u_s K_1 + 2\alpha\phi_e \exp\left(\frac{-\alpha}{u_s}\right).
\end{aligned}\right\} \tag{4.80}$$

The double limit point (D.L.P.) curve in λ_1, L space corresponds to the curve along which two right hand limit points coincide at the same U value on the U, u bifurcation diagram. This curve has great significance in ignition theory as it is the U value at the right-most of these limit points which will usually (unless branching to periodic solutions has occurred) be the U_{crit} value. Let these two limit points occur at u_{s1} and u_{s2} ($u_{s1} \neq u_{s2}$). Then the conditions that must be satisfied on the D.L.P. curve are that u_{s1} and u_{s2} must both satisfy the limit point condition (4.76) and they must also have the same U value i.e.

$$\frac{-1}{L}\left\{\exp\left(\frac{-1}{u_{s1}}\right)-\exp\left(\frac{-1}{u_{s2}}\right)\right\}+u_{s1}-u_{s2}$$

$$\frac{-\lambda_1\phi_c\phi_w h_w}{L}\left\{\frac{\exp\left(\frac{-\alpha_w}{u_{s1}}\right)}{\phi_c+\phi_c\exp\left(\frac{-\alpha_w}{u_{s1}}\right)}-\frac{\exp\left(\frac{-\alpha_w}{u_{s2}}\right)}{\phi_c+\phi_c'\exp\left(\frac{-\alpha_w}{u_{s2}}\right)}\right\}=0. \qquad (4.81)$$

The hysteresis and D.L.P. curves for the $\underset{\sim}{\beta}$ value given by (4.75) are shown in Figure 4.15 below (D.L.P. curve is labelled separately).

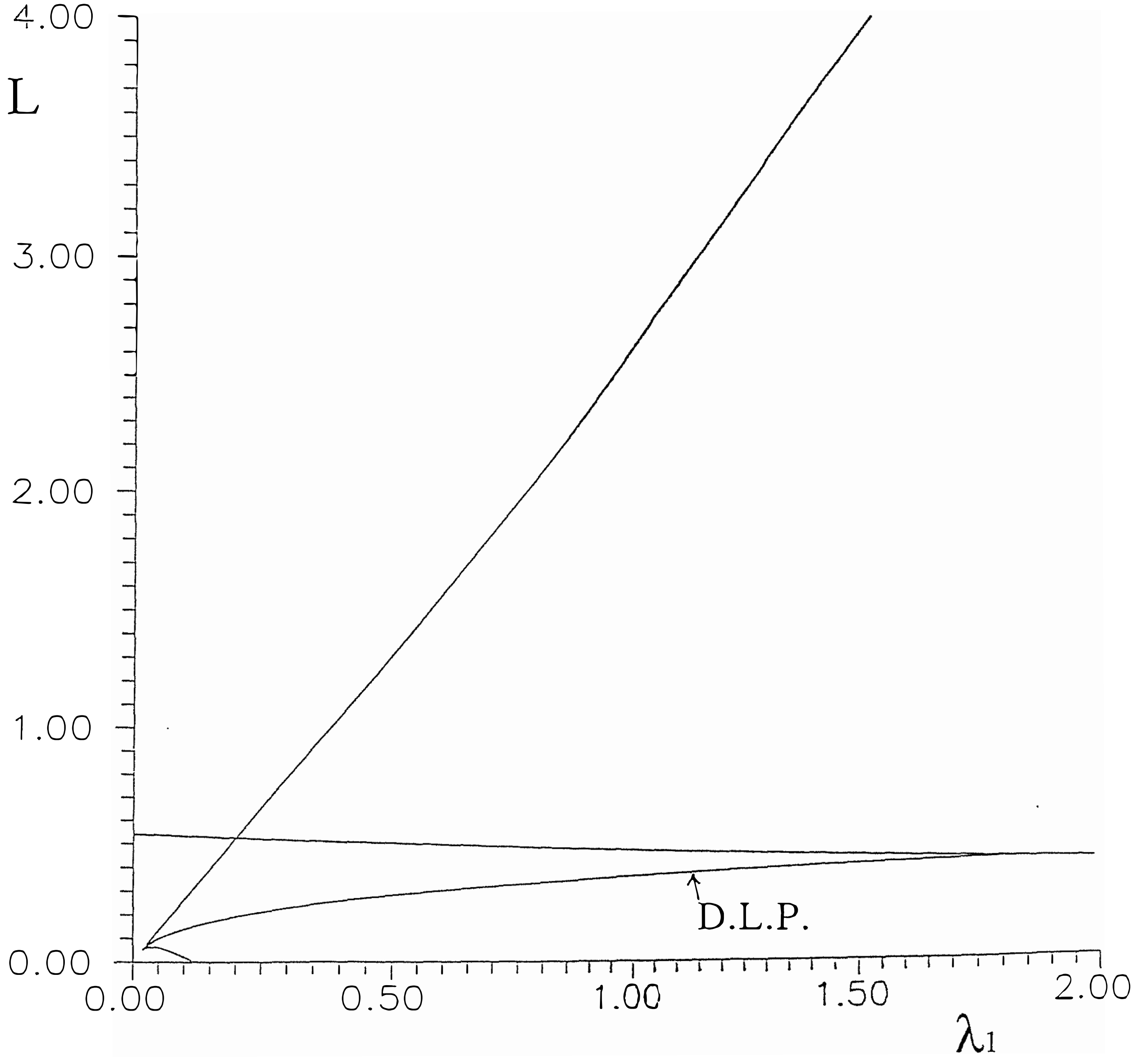

Figure 4.15 Hysteresis and D.L.P. curves

4.6.2 The $H2_1$ degeneracy curves

The conditions for an $H2_1$ degeneracy curve in λ_1, L space (with x_s given in terms of u_s by (4.5)) are (4.7), (4.31), (4.32) and the equation (4.33), i.e.

$$\frac{d(Tr(J))}{dU} = 0,$$

where

$$\frac{d(Tr(J))}{dU} = \frac{d(Tr(J))}{du_s}\frac{du_s}{dU}.$$

Now it is easily seen from (4.78) that $\frac{dU}{du_s}$ is continuous and satisfies

$$\frac{-4}{Le^2}\left(1 + \frac{\lambda_1\phi_w h_w}{\alpha_w}\right) \le \frac{dU}{du_s} \le 1 + \frac{4\lambda_1\phi_w h_w \phi_e}{L\phi_c(\alpha+\alpha_w)^2 e^2}, \qquad \text{for } \alpha > \alpha_w,$$

and

$$\frac{-4}{Le^2}\left(1 + \frac{\lambda_1\phi_w h_w}{\alpha_w} + \frac{\lambda_1\phi_w h_w \phi_e(\alpha_w-\alpha)}{(\alpha+\alpha_w)^2\,\phi_c}\right) \le \frac{dU}{du_s} \le 1, \qquad \text{for } \alpha_w > \alpha.$$

So in either case $\frac{dU}{du_s}$ is bounded above and below, hence $\frac{du_s}{dU} \neq 0$.

Therefore (4.33) can occur if and only if

$$\frac{d(Tr(J))}{du_s} = 0,$$

that is (equivalently),

$$\exp\left(\frac{-1}{u_s}\right)(1-2u_s) + \frac{\lambda_1\phi_c u_s}{\phi_c + \phi_e \exp\left(\frac{-\alpha}{u_s}\right)}\left\{ -\left(2 + \frac{\alpha\phi_e \exp\left(\frac{-\alpha}{u_s}\right)}{u_s\left(\phi_c + \phi_e \exp\left(\frac{-\alpha}{u_s}\right)\right)}\right)\right.$$

$$\left(h_w\phi_w\alpha_w \exp\left(\frac{-\alpha_w}{u_s}\right) - h_c\phi_e\alpha \exp\left(\frac{-\alpha}{u_s}\right)\right) + \frac{1}{u_s}\left(h_w\phi_w\alpha_w^{\,2} \exp\left(\frac{-\alpha_w}{u_s}\right)\right.$$

$$\left.\left. - h_c\phi_e\alpha^2 \exp\left(\frac{-\alpha}{u_s}\right)\right)\right\} - \frac{\phi_e\alpha \exp\left(\frac{-\alpha}{u_s}\right)u_s^{\,2}}{\varepsilon} = 0. \qquad (4.82)$$

The $H2_1$ degeneracy curves for the given $\underset{\sim}{\beta}$ value are shown below in Figure 4.16. The dashed line corresponds to a portion of a curve along which Det(J) < 0 and is included only for completeness.

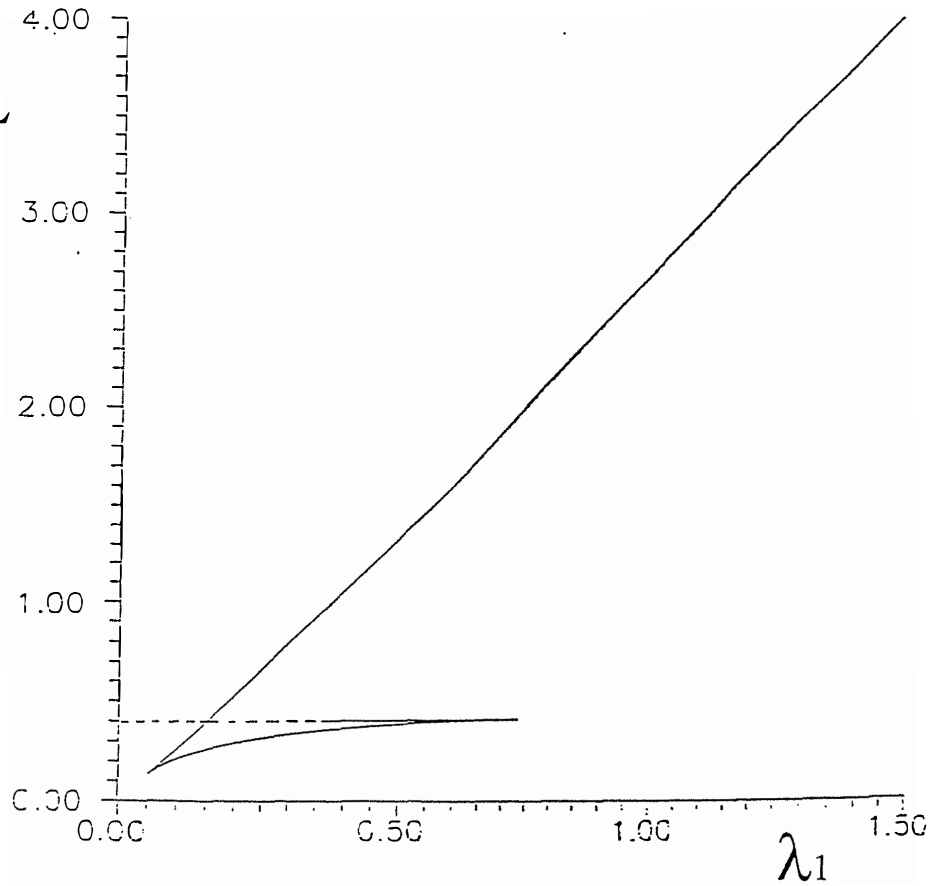

Figure 4.16 $H2_1$ degeneracy curves

4.6.3 The $H3_1$ degeneracy curves

The equations defining $H3_1$ degeneracy curves in λ_1, L space are (4.7), (4.31), (4.32) and (4.67), with x_s given in terms of u_s by (4.5). Figure 4.17 below shows the $H3_1$ degeneracy curves for the chosen value of $\underset{\sim}{\beta}$.

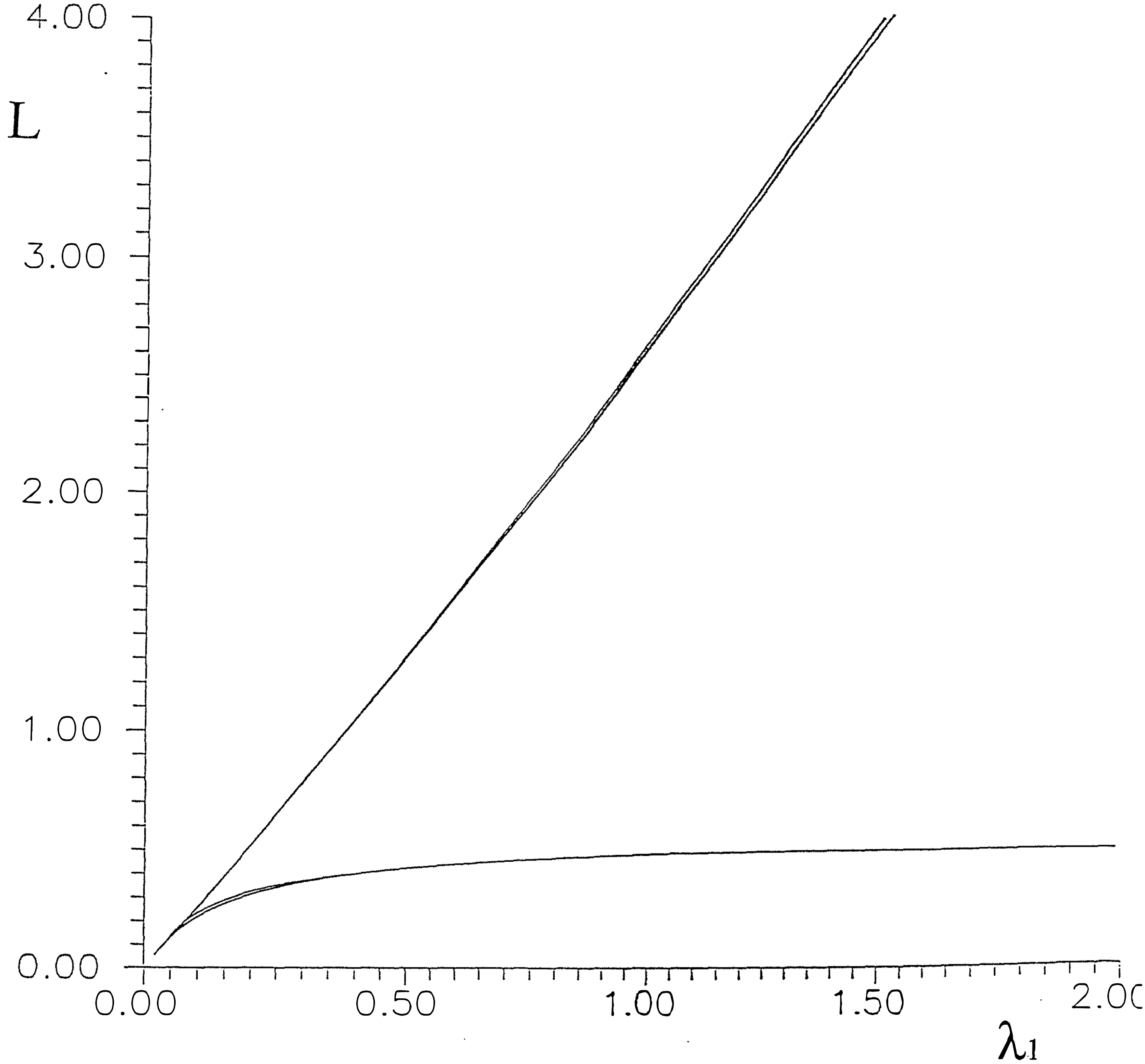

Figure 4.17 The $H3_1$ degeneracy curves

4.6.4 The double zero eigenvalue curves

A double zero eigenvalue (D.Z.E.) point in λ_1, L space usually corresponds to the abrupt appearance (or disappearance) of a Hopf bifurcation point on the U, u bifurcation diagram. The equations the D.Z.E. curve must satisfy are (4.7), (4.31) and

$$\mathrm{Det}(J) = 0, \tag{4.83}$$

where Det(J) is given by (4.19), (with x_s given in terms of u_s by (4.5)). The D.Z.E. curves for our value of $\underset{\sim}{\beta}$ are given below in Figure 4.18.

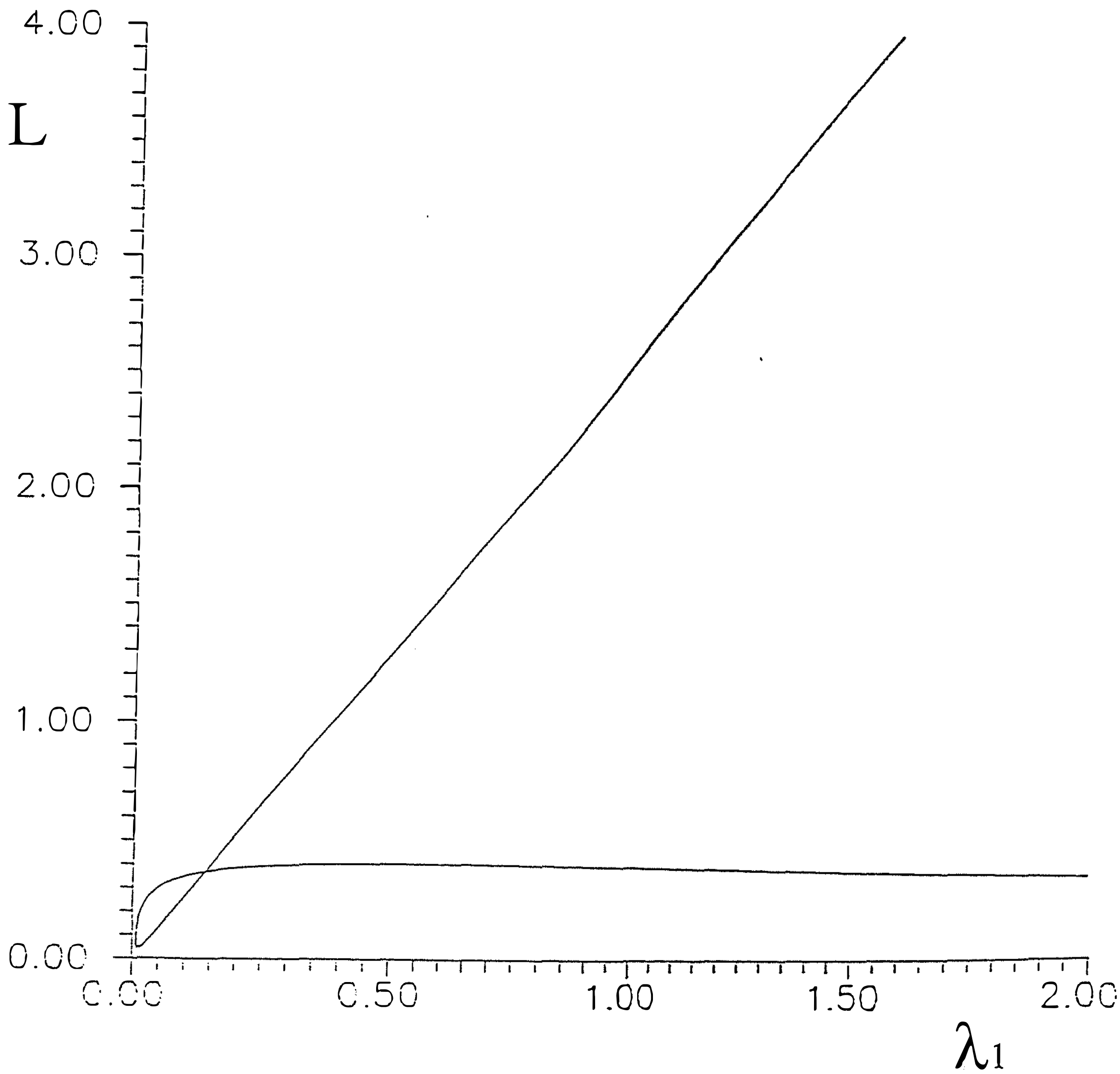

Figure 4.18 The D.Z.E. curves

Note Since by (4.79), $\frac{d^2U}{du_s^2} \to 0$ as $u_s \to 0$ and $u_s \to \infty$, and $\frac{d^2U}{du_s^2}$ is continuous in u_s, we have $\frac{d^2U}{du_s^2} \neq \infty, \forall\ u_s > 0$. Therefore, using the condition of Gray and Roberts [49] p 367, the system has no isolas or transcritical bifurcations.

4.7 The distinct bifurcation diagrams

Our aim in this section is to find all the distinct U, u bifurcation diagrams the model can exhibit for the value of $\underset{\sim}{\beta}$ given by (4.75), and thus all the possible steady state and periodic behaviour of the model as the group of parameters $\underset{\sim}{\delta}$ varies. We can do this by simply superimposing all the curves plotted in the previous section on the same λ_1, L diagram. Each closed region on this new diagram will correspond to a set of λ_1, L values which give a distinct bifurcation diagram in U, u space.

The superimposed degeneracy curves are given below in Figure 4.19. Figure 4.20 shows a blow up of the part of Figure 4.19 with $\lambda_1 \in [0, 0.5]$, $L \in [0. 0.6]$. The distinct regions are given labels 1, ..., 25.

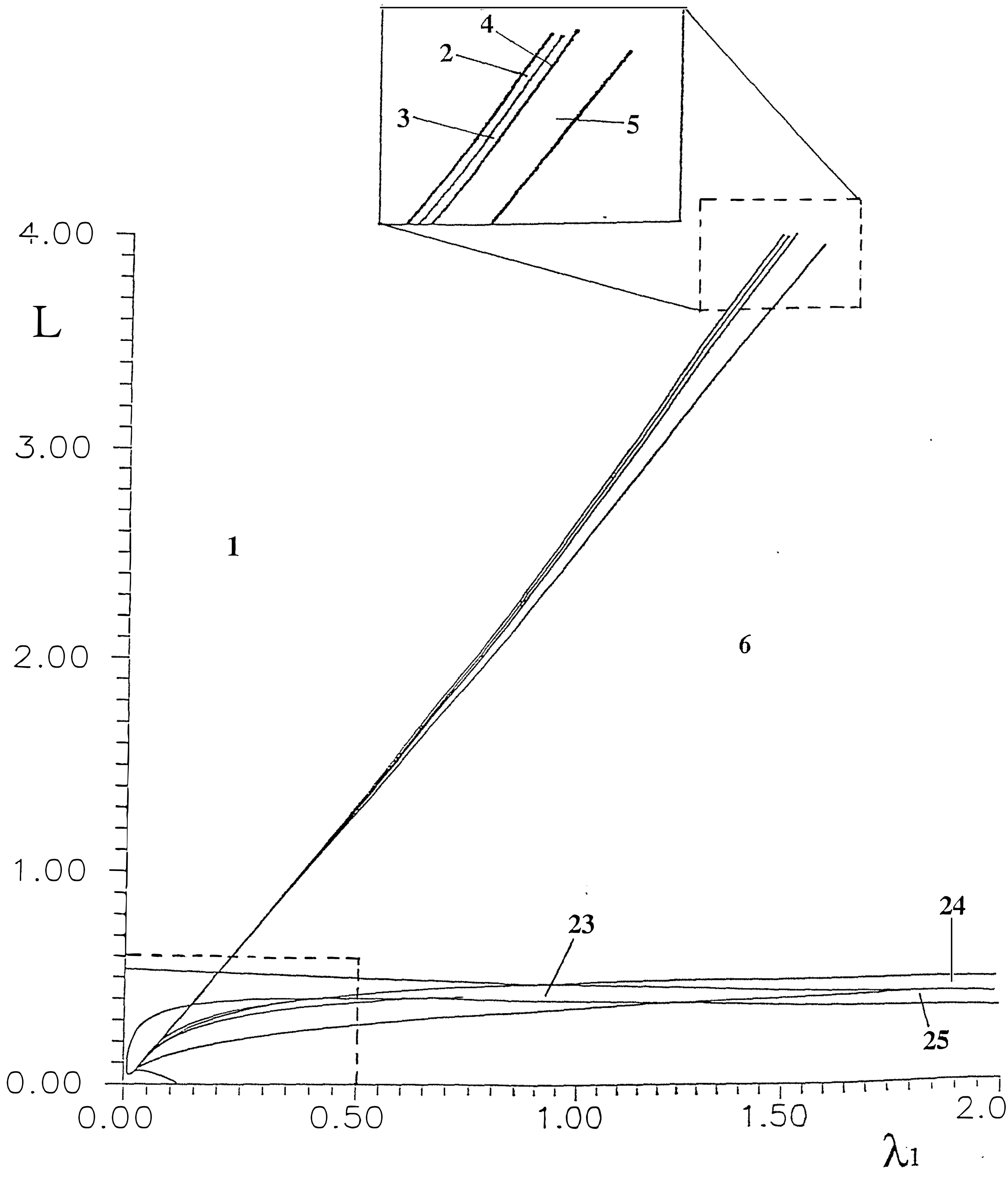

Figure 4.19 Superimposed degeneracy curves

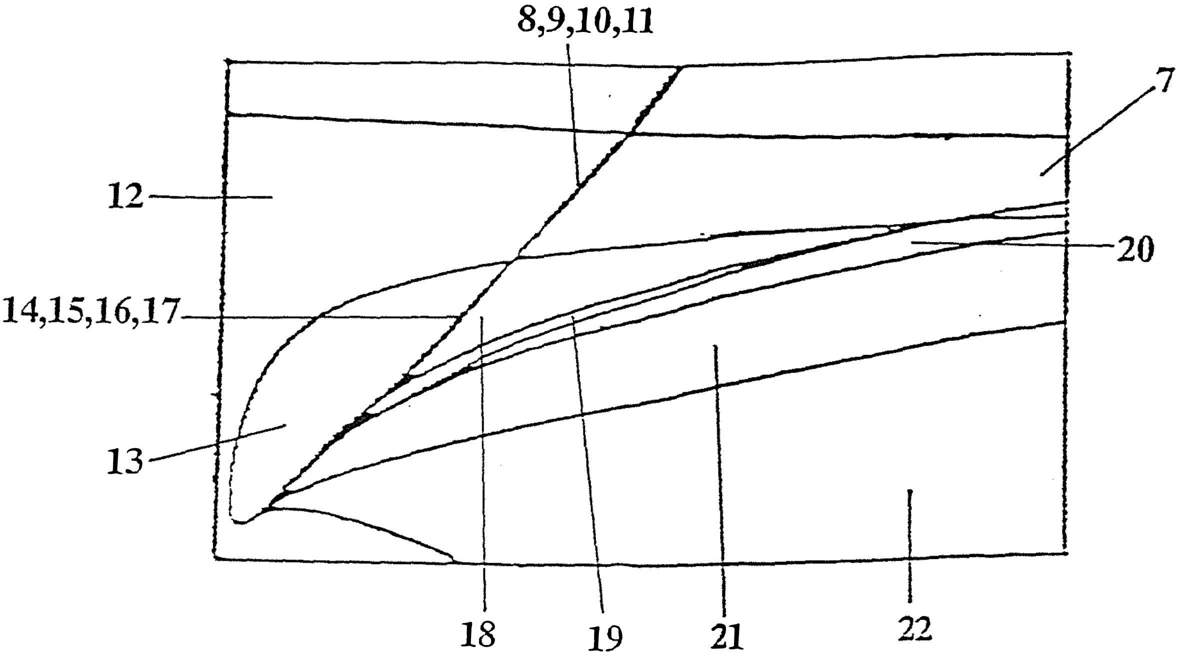

Figure 4.20 Blow-up of region near origin

Figures 4.21 - 4.45 below show schematically the twenty-five distinct U, u bifurcation diagrams possible for the given value of $\underset{\sim}{\beta}$.

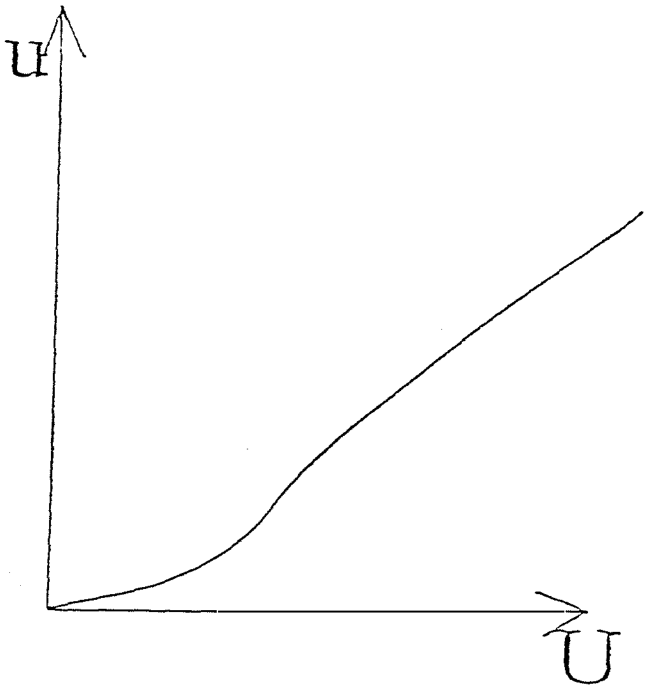

Figure 4.21 Bifurcation diagram for region 1

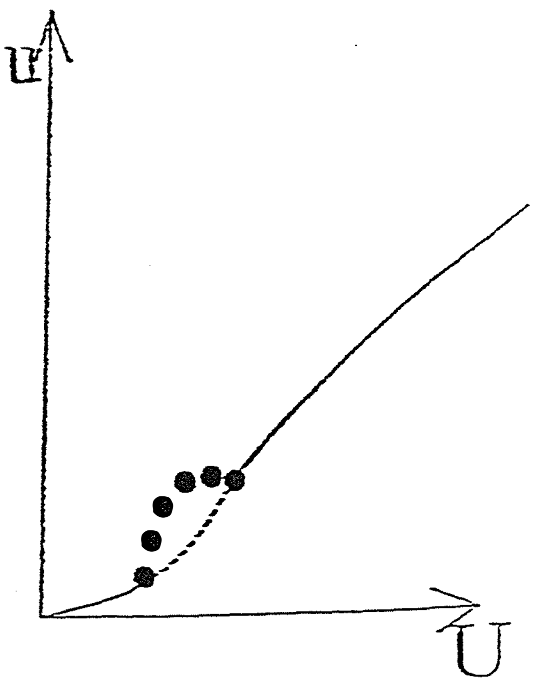

Figure 4.22 Bifurcation diagram for region 2

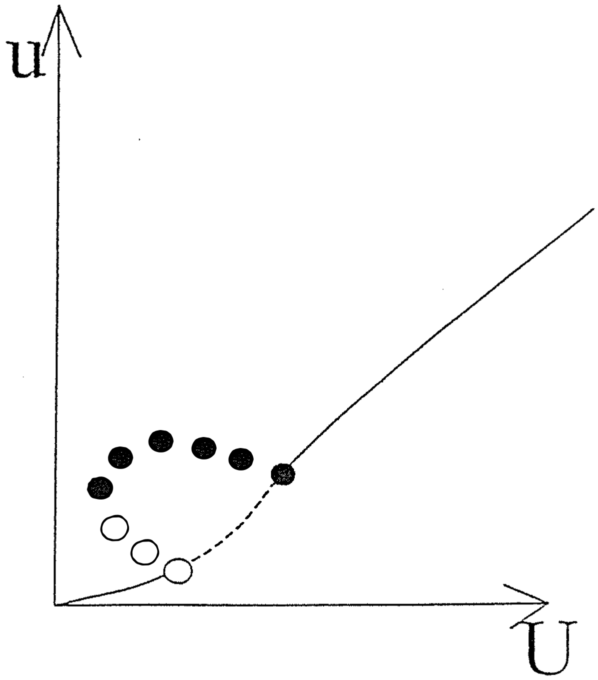

Figure 4.23 Bifurcation diagram for region 3

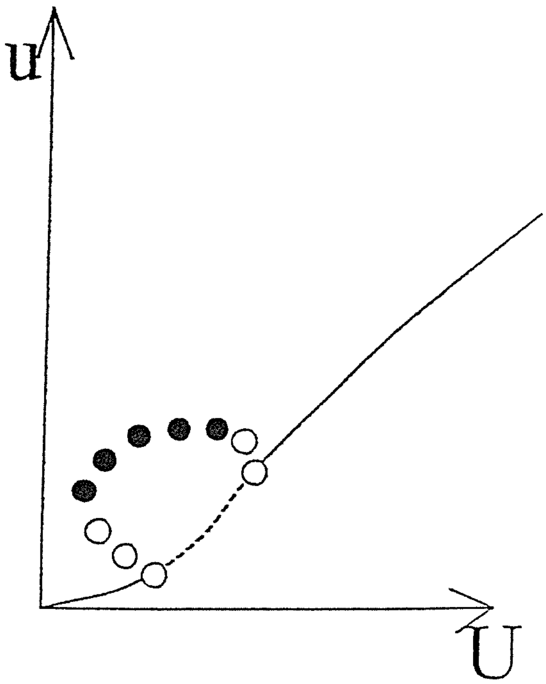

Figure 4.24 Bifurcation diagram for region 4

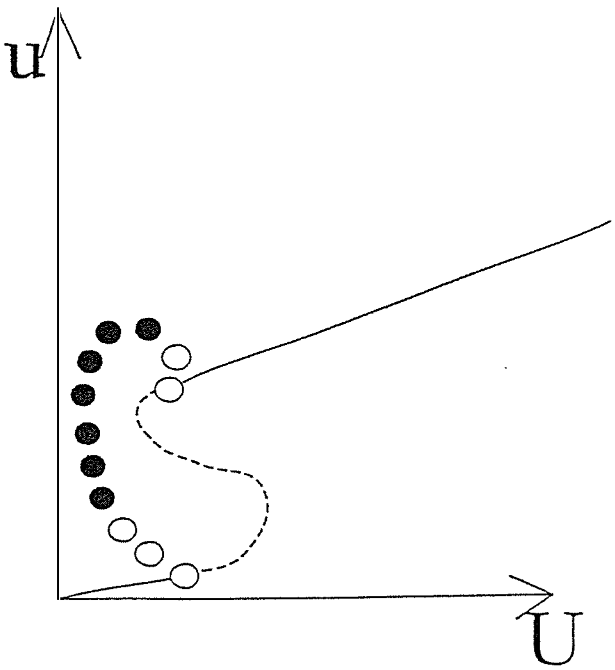

Figure 4.25 Bifurcation diagram for region 5

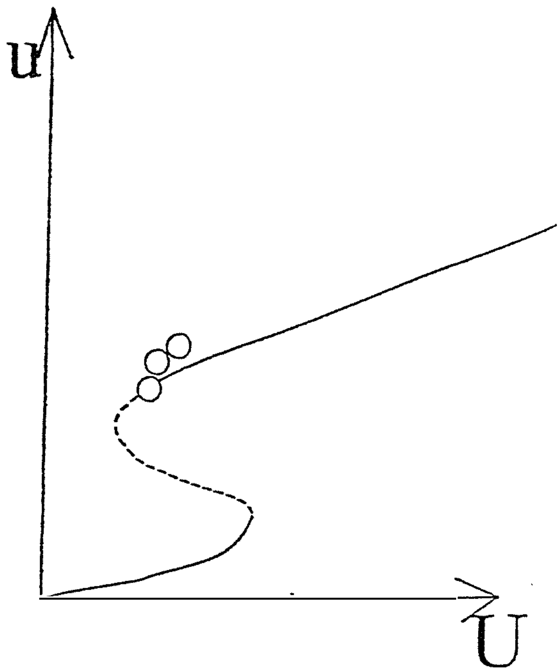

Figure 4.26 Bifurcation diagram for region 6

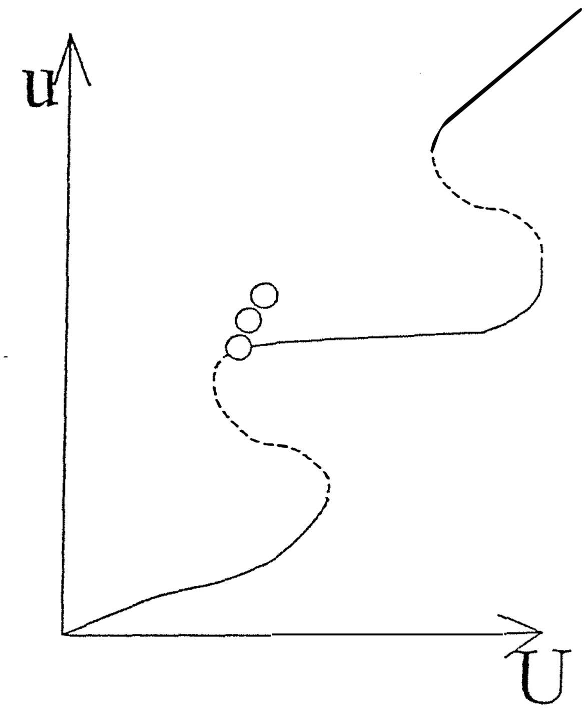

Figure 4.27 Bifurcation diagram for region 7

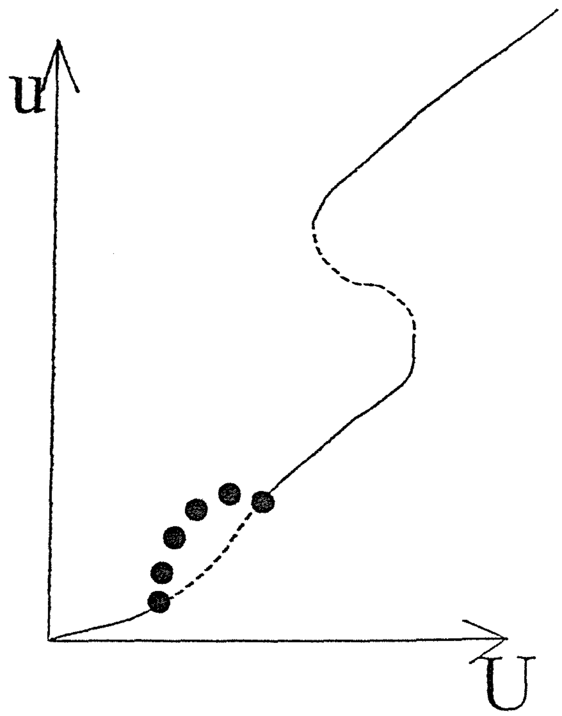

Figure 4.28 Bifurcation diagram for region 8

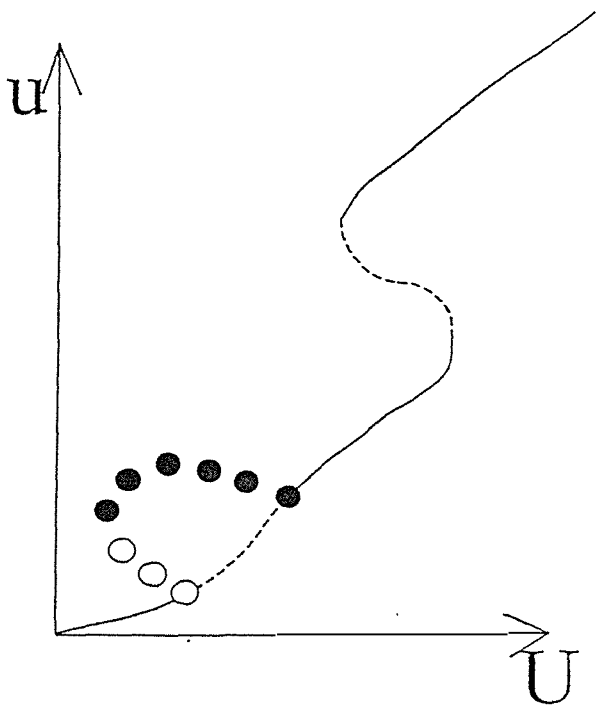

Figure 4.29 Bifurcation diagram for region 9

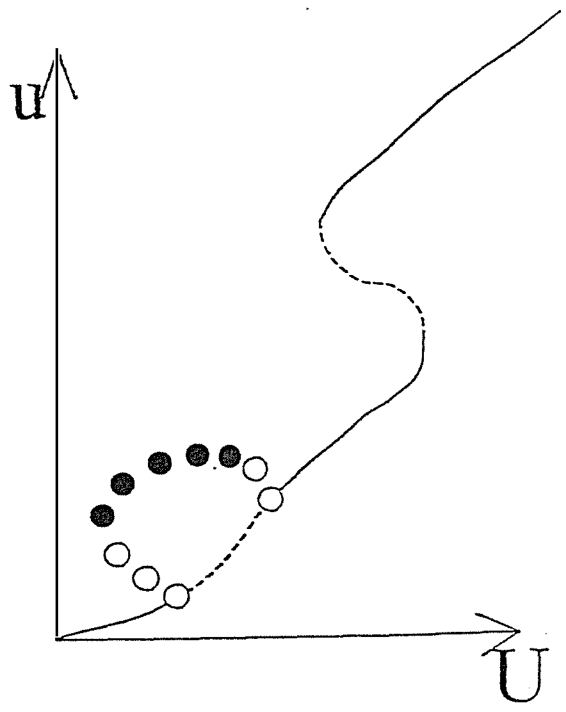

Figure 4.30 Bifurcation diagram for region 10

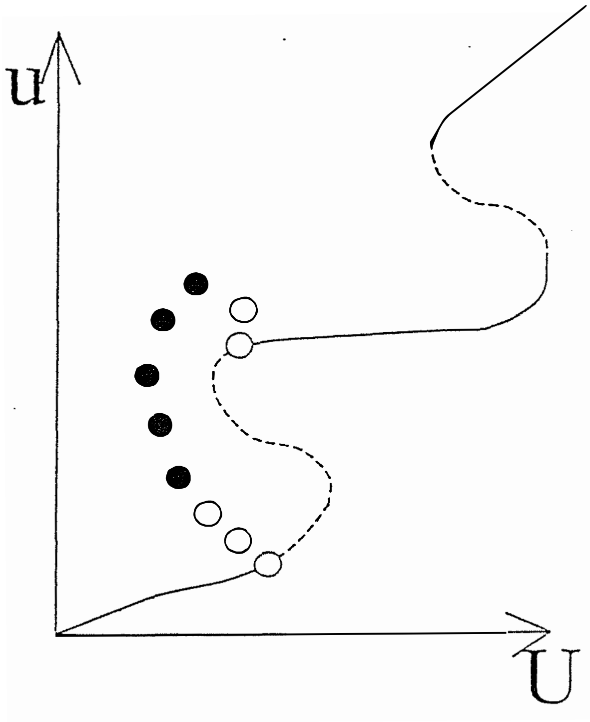

Figure 4.31 Bifurcation diagram

for region 11

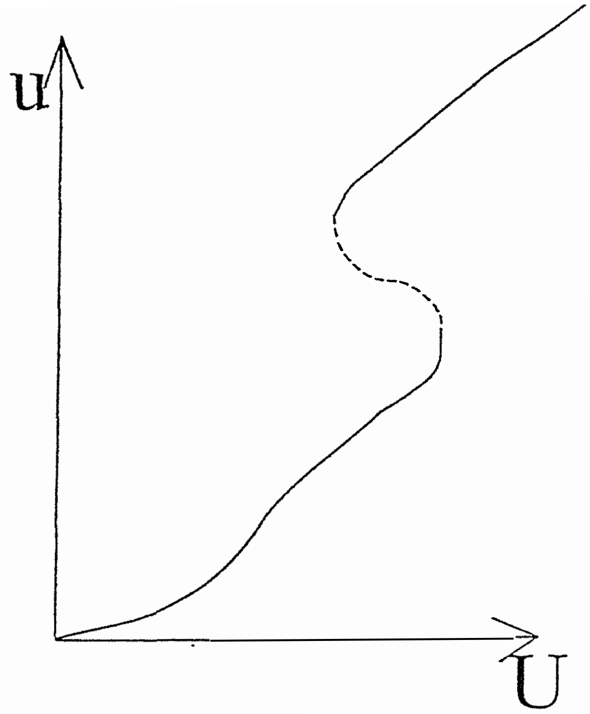

Figure 4.32 Bifurcation diagram

for region 12

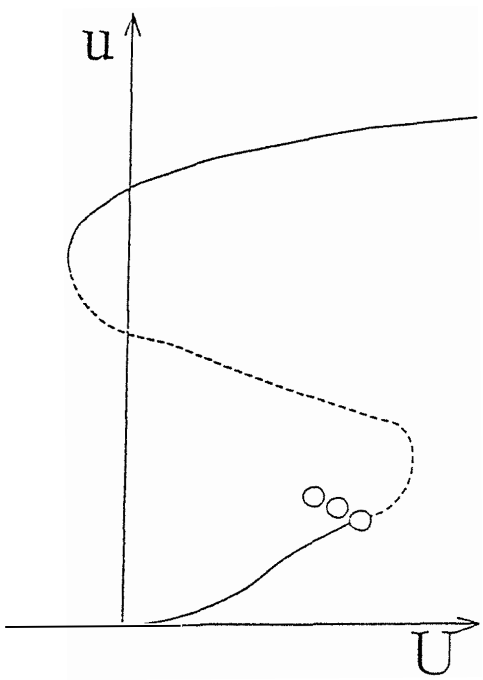

Figure 4.33 Bifurcation diagram

for region 13

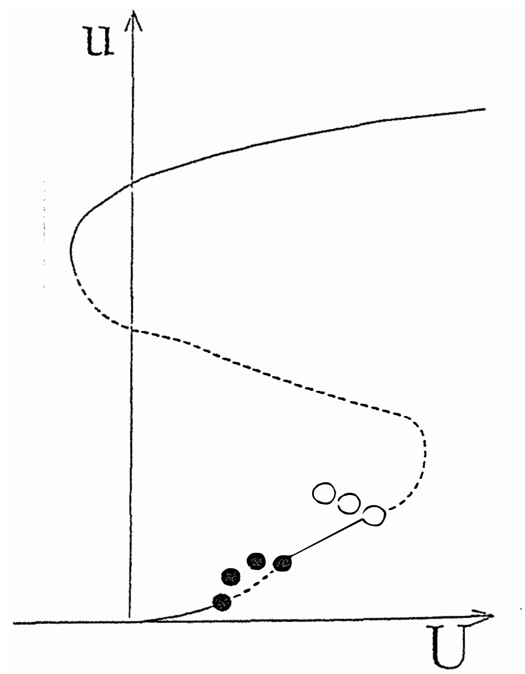

Figure 4.34 Bifurcation diagram

for region 14

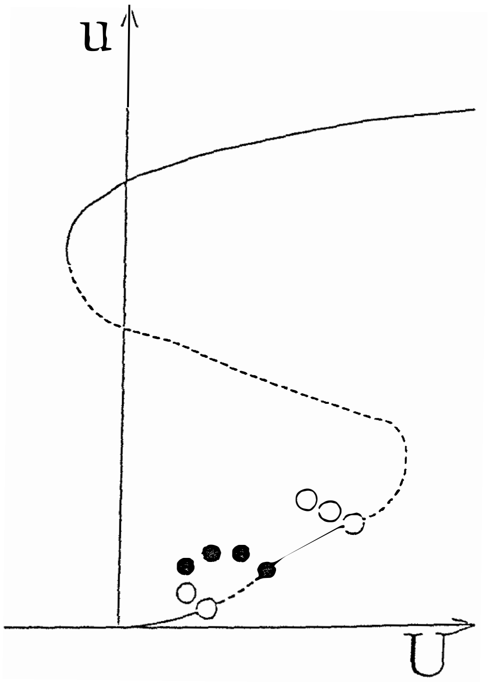

Figure 4.35 Bifurcation diagram

for region 15

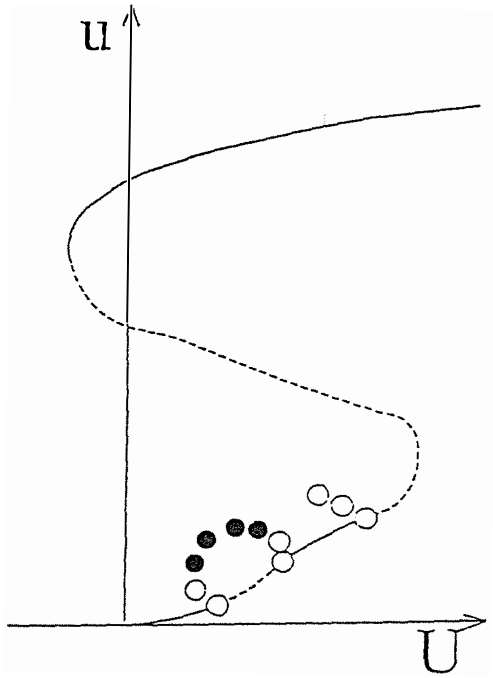

Figure 4.36 Bifurcation diagram

for region 16

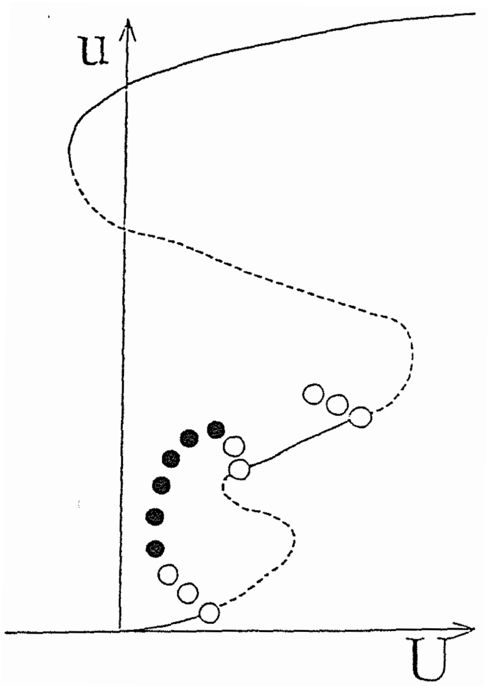

Figure 4.37 Bifurcation diagram

for region 17

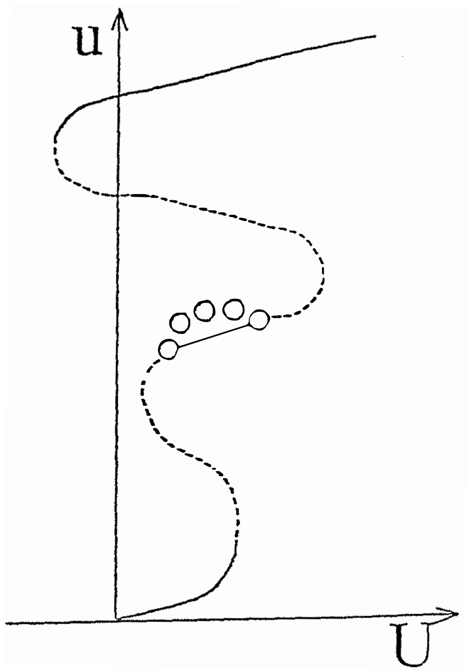

Figure 4.38 Bifurcation diagram

for region 18

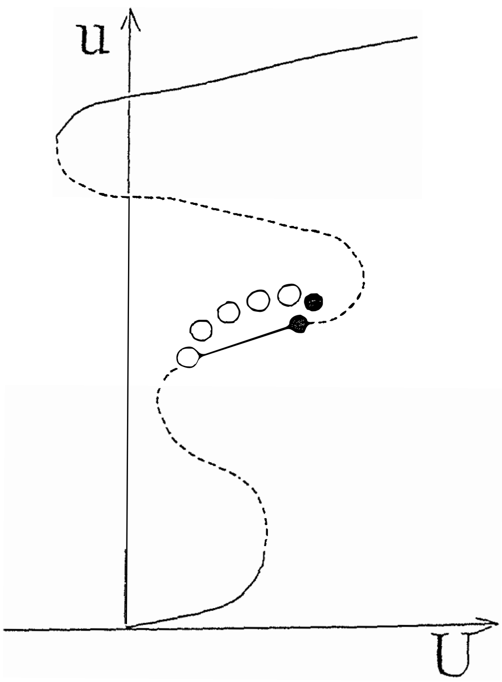

Figure 4.39 Bifurcation diagram for region 19

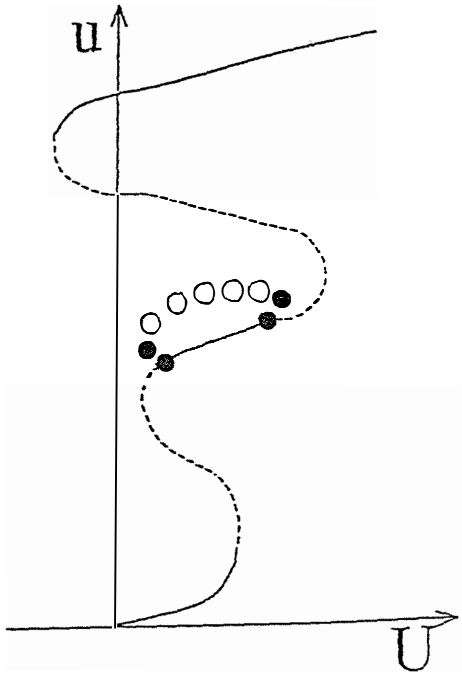

Figure 4.40 Bifurcation diagram for region 20

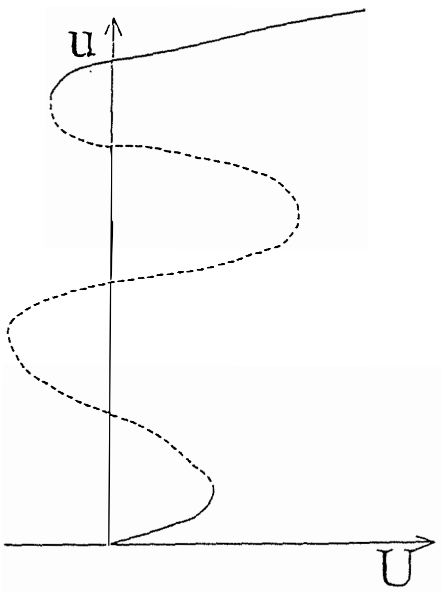

Figure 4.41 Bifurcation diagram for region 21

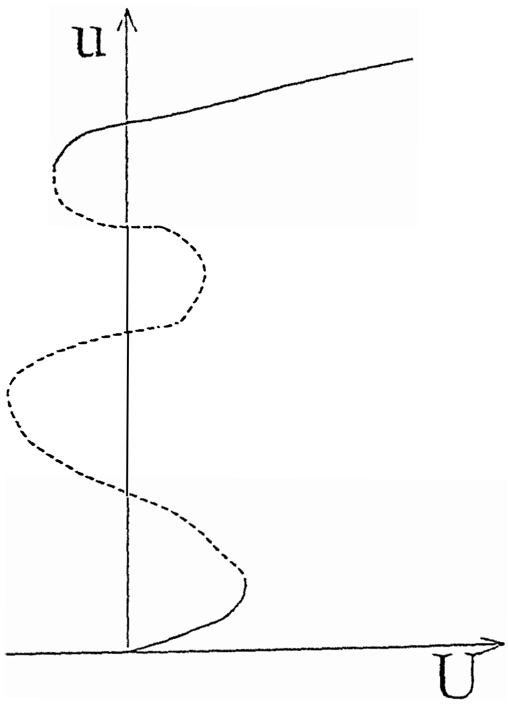

Figure 4.42 Bifurcation diagram for region 22

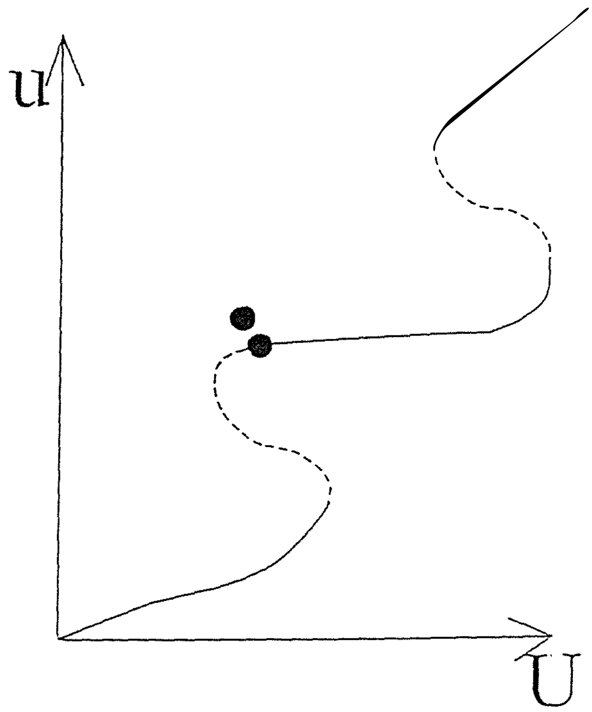

Figure 4.43 Bifurcation diagram

for region 23

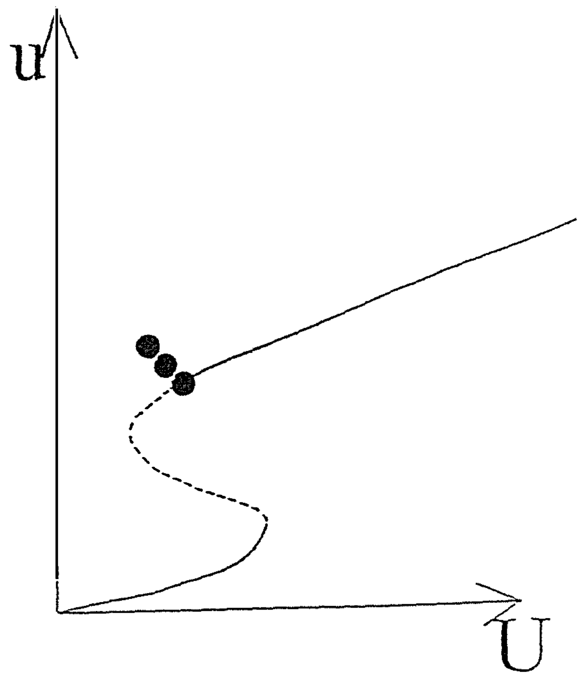

Figure 4.44 Bifurcation diagram

for region 24

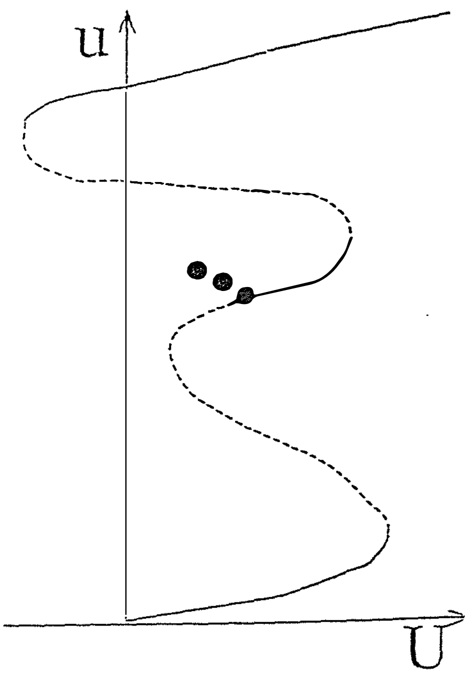

Figure 4.45 Bifurcation diagram

for region 25

As we can see from the diagrams above the spatially uniform model including the effects of moisture exhibits a very wide range of behaviour when compared to the model which ignores the moisture content (i.e. $\lambda_1 = 0$). In fact the 'dry' model can show only two distinct bifurcation diagrams (namely those corresponding to regions 1 and 12).

An important point to note about this particular formulation of the variables (i.e. that of Burnell et al [12]) is that the steady state and periodic loci can move into the negative U section of the bifurcation diagram. Since the body will not be stored at or below absolute zero the solutions in this section are irrelevant physically, although we are interested in following them to see where (and if) they re-enter the positive U section of the diagram. This phenomenon does not lead to any computational difficulties in the spatially uniform case (as we can see from the diagrams, $u_s \geq 0$ always), but it will certainly lead to difficulties if steady state profiles are to be calculated for the spatially distributed model (as there will always be a portion of the profile with $u_s < 0$). We will not consider this phenomenon further in this thesis, but the solution will obviously involve using a Heaviside operator in front of all Arrhenius terms, as discussed in section 4.2.

CHAPTER 5

Existence, uniqueness and multiplicity results for the spatially distributed steady state model.

Throughout this Chapter we shall assume the region Ω satisfies the interior sphere property of Sperb [32], and further is convex (although the convexity condition can be relaxed in a number of the results). In addition we will assume all the constants η, λ, h_w, ϕ_w, ϕ_c, ϕ_e are non-negative. This is a valid assumption on physical grounds (see Chapter 3). We will also make further use of the function w, first mentioned in (2.4), i.e.

$$\nabla^2 w + 1 = 0, \qquad r \in \Omega, \tag{5.1}$$

$$\frac{\partial w}{\partial n} + \mathrm{Bi}\, w = 0, \qquad r \in \partial\Omega, \tag{5.2}$$

5.1 Existence results

In this section we will consider the existence of solutions to the steady state problem (3.58), (3.32) i.e.

$$\nabla^2 u + \eta\left[\exp\left(\frac{-1}{u}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{u}\right) dV} \exp\left(\frac{\alpha - \alpha_w}{u}\right)\right] = 0, \qquad r \in \Omega,$$

$$\frac{\partial u}{\partial n} + \mathrm{Bi}\,(u - U) = 0, \qquad r \in \partial\Omega.$$

Due to the nature of the term $\exp\left(\frac{\alpha-\alpha_w}{u}\right)$, we will consider the cases $\alpha_w \geq \alpha > 0$ and $\alpha > \alpha_w > 0$ separately. In particular we will show that a solution exists for all $U \geq 0$ when $\alpha_w \geq \alpha > 0$, and a solution exists for all $U > 0$ when $\alpha > \alpha_w > 0$. We first give some preliminary results.

Theorem 5.1

If u is any solution of (3.58), (3.32) with $U \geq 0$, then $u \geq U$ in $\bar{\Omega}$.

Proof

Consider the function $u - U$, $r \in \Omega$.

Now

$$\nabla^2(u-U) = -\eta\left[\exp\left(\frac{-1}{u}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{u}\right)dV}\exp\left(\frac{\alpha-\alpha_w}{u}\right)\right]$$

$$\leq 0, \quad r \in \Omega,$$

and

$$\frac{\partial}{\partial n}(u-U) + Bi\,(u-U) = \frac{\partial u}{\partial n} + Bi\,(u-U) = 0, \quad r \in \partial\Omega.$$

So by the maximum principle $\boxed{B}$, $u - U \geq 0$, $r \in \bar{\Omega}$, i.e. $u \geq U$, $r \in \bar{\Omega}$.

■

Theorem 5.2

If $\alpha_w \geq \alpha > 0$, $U \geq 0$, then

$$\beta = U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\right] w \text{ is an upper solution of (3.58), (3.32).}$$

Proof

The function β satisfies

$$\nabla^2\beta + \eta\left[\exp\left(\frac{-1}{\beta}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\beta}\right) dV}\exp\left(\frac{\alpha-\alpha_w}{\beta}\right)\right]$$

$$= -\eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\right] + \eta\left[\exp\left(\frac{-1}{\beta}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\beta}\right) dV}\exp\left(\frac{\alpha-\alpha_w}{\beta}\right)\right],$$

$$\leq 0, \quad r \in \Omega,$$

and

$$\frac{\partial\beta}{\partial n} + \mathrm{Bi}\,\beta = \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\right]\frac{\partial\beta}{\partial n} + \mathrm{Bi}\left(U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c}\right] w\right),$$

$$= \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\right]\left(\frac{\partial w}{\partial n} + \mathrm{Bi}\,w\right) + \mathrm{Bi}\,U,$$

$$= \mathrm{Bi}\,U, \quad r \in \partial\Omega.$$

So, by Definition 2.1.6, β is an upper solution of (3.58), (3.22).

■

Theorem 5.3

If $\alpha_w \geq \alpha > 0$, $U \geq 0$, then

$$\psi = U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)}\exp\left(\frac{\alpha-\alpha_w}{U}\right)\right] w$$

is a lower solution of (3.58), (3.32).

Proof

The function ψ satisfies

$$\nabla^2\psi + \eta\left[\exp\left(\frac{-1}{\psi}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\psi}\right) dV} \exp\left(\frac{\alpha - \alpha_w}{\psi}\right)\right]$$

$$= -\eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha - \alpha_w}{U}\right)\right]$$

$$+ \eta\left[\exp\left(\frac{-1}{\psi}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\psi}\right) dV} \exp\left(\frac{\alpha - \alpha_w}{\psi}\right)\right],$$

$$\geq 0, \quad r \in \Omega \qquad \text{(by Theorem 5.1)},$$

and

$$\frac{\partial\psi}{\partial n} + \text{Bi}\,\psi = \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha - \alpha_w}{U}\right)\right] \frac{\partial w}{\partial n}$$

$$+ \text{Bi}\left(U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha - \alpha_w}{U}\right)\right] w\right),$$

$$= \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha - \alpha_w}{U}\right)\right]\left(\frac{\partial w}{\partial n} + \text{Bi}\,w\right) + \text{Bi}\,U,$$

$$= \text{Bi}\,U, \quad r \in \partial\Omega.$$

So, by Definition 2.1.6, ψ is a lower solution of (3.58), (3.32).

■

We can now give an existence result for the case $\alpha_w \geq \alpha > 0$, $U \geq 0$.

Theorem 5.4

If $\alpha_w \geq \alpha > 0$, $U \geq 0$ there exists a solution u to (3.58), (3.32) with

$$U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha - \alpha_w}{U}\right)\right] w \leq u \leq U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c}\right] w, \qquad r \in \Omega.$$

Proof

For this proof we will use Theorem 2.1.7. Now $w(r) > 0$, $r \in \Omega$ (by Theorem 2.1.8) so

$$U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\right] w \geq U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha - \alpha_w}{U}\right)\right] w, \qquad r \in \Omega.$$

It is easily shown that J(u)(h), defined in Theorem 2.1.7, for (3.58), (3.32) satisfies

$$J(u)(h) = \eta\left[\left\{\frac{\exp\left(\frac{-1}{u}\right)}{u^2} + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{u}\right) dV}\left(\frac{\alpha_w - \alpha}{u^2}\right)\exp\left(\frac{\alpha - \alpha_w}{u}\right)\right\} h\right.$$

$$\left. + \frac{\lambda h_w \phi_w \phi_c^2 \alpha}{V\left(\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{u}\right) dV\right)^2} \exp\left(\frac{\alpha - \alpha_w}{u}\right) \int_\Omega \frac{\exp\left(\frac{\alpha}{u}\right)}{u^2} h \, dV\right], \qquad (5.3)$$

$$\geq 0, \quad \text{if } \alpha_w \geq \alpha > 0, \quad r \in \Omega.$$

Therefore, by Theorem 2.1.7, there exists a solution u with

$$U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)}\exp\left(\frac{\alpha-\alpha_w}{U}\right)\right] w \le u \le U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\right] w, \qquad r \in \Omega.$$

Further to these results, we can show that any solution of (3.58), (3.32) must lie between these upper and lower solutions. We do this using Theorems 5.5 and 5.6 below.

Theorem 5.5

If $\alpha_w \ge \alpha > 0$, $U \ge 0$ and u is any solution of (3.58), (3.32), then

$$u \le U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\right] w, \qquad r \in \bar{\Omega}.$$

Proof

Consider the function $u - \left\{U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\right] w\right\}, r \in \Omega.$

Now

$$\nabla^2\left(u - \left\{U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\right] w\right\}\right) = -\eta\left[\exp\left(\frac{-1}{u}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{u}\right) dV}\exp\left(\frac{\alpha-\alpha_w}{u}\right)\right]$$

$$+\eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\right],$$

$$\ge 0, \qquad r \in \Omega,$$

and

$$\frac{\partial}{\partial n}\left(u-\left\{U+\eta\left[1+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c}\right]w\right\}\right)+\mathrm{Bi}\left(u-\left\{U+\eta\left[1+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c}\right]w\right\}\right)$$

$$=\frac{\partial u}{\partial n}+\mathrm{Bi}(u-U)-\eta\left[1+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c}\right]\left(\frac{\partial w}{\partial n}+\mathrm{Bi}\,w\right),$$

$$=0,\qquad r\in\partial\Omega.$$

So by the maximum principle $\boxed{A}$, $u-\left\{U+\eta\left[1+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c}\right]w\right\}\leq 0,\qquad r\in\bar{\Omega},$

i.e.
$$u\leq U+\eta\left[1+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c}\right]w,\qquad r\in\bar{\Omega}.$$

■

Theorem 5.6

If $\alpha_w\geq\alpha>0$, $U\geq 0$ and u is any solution of (3.58), (3.32), then

$$u\geq U+\eta\left[\exp\left(\frac{-1}{U}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c\exp\left(\frac{\alpha}{U}\right)}\exp\left(\frac{\alpha-\alpha_w}{U}\right)\right]w,\qquad r\in\bar{\Omega}.$$

Proof

Consider the function $u-\left\{U+\eta\left[\exp\left(\frac{-1}{U}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c\exp\left(\frac{\alpha}{U}\right)}\exp\left(\frac{\alpha-\alpha_w}{U}\right)\right]w\right\},\qquad r\in\Omega.$

Now

$$\nabla^2\left(u-\left\{U+\eta\left[\exp\left(\frac{-1}{U}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c\exp\left(\dfrac{\alpha}{U}\right)}\exp\left(\frac{\alpha-\alpha_w}{U}\right)\right]w\right\}\right)$$

$$=-\eta\left[\exp\left(\frac{-1}{u}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\dfrac{\phi_c}{V}\displaystyle\int_\Omega\exp\left(\frac{\alpha}{u}\right)dV}\exp\left(\frac{\alpha-\alpha_w}{u}\right)\right]$$

$$+\eta\left[\exp\left(\frac{-1}{U}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c\exp\left(\dfrac{\alpha}{U}\right)}\exp\left(\frac{\alpha-\alpha_w}{U}\right)\right],$$

$$\leq 0, \quad r\in\Omega,$$

and

$$\frac{\partial}{\partial n}\left(u-\left\{U+\eta\left[\exp\left(\frac{-1}{U}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c\exp\left(\dfrac{\alpha}{U}\right)}\exp\left(\frac{\alpha-\alpha_w}{U}\right)\right]w\right\}\right)$$

$$+\,Bi\left(u-\left\{U+\eta\left[\exp\left(\frac{-1}{U}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c\exp\left(\dfrac{\alpha}{U}\right)}\exp\left(\frac{\alpha-\alpha_w}{U}\right)\right]w\right\}\right)$$

$$=\frac{\partial u}{\partial n}+Bi\,(u-U)+\eta\left[\exp\left(\frac{-1}{U}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c\exp\left(\dfrac{\alpha}{U}\right)}\exp\left(\frac{\alpha-\alpha_w}{U}\right)\right]\left(\frac{\partial w}{\partial n}+Bi\,w\right)$$

$$=0, \quad r\in\Omega.$$

So, by the maximum principle $\boxed{B}$,

$$u-\left\{U+\eta\left[\exp\left(\frac{-1}{U}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c\exp\left(\frac{\alpha}{U}\right)}\exp\left(\frac{\alpha-\alpha_w}{U}\right)\right]w\right\}\geq 0,\qquad r\in\bar{\Omega},$$

i.e.
$$u\geq U+\eta\left[\exp\left(\frac{-1}{U}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c\exp\left(\frac{\alpha}{U}\right)}\exp\left(\frac{\alpha-\alpha_w}{U}\right)\right]w,\qquad r\in\bar{\Omega}.$$

■

We now derive corresponding results for the case $\alpha>\alpha_w>0$.

Theorem 5.7

If $\alpha>\alpha_w>0$, $U\geq 0$ then

$$\psi=U+\eta\left[\exp\left(\frac{-1}{U}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c\exp\left(\frac{\alpha}{U}\right)}\right]w,\qquad r\in\Omega,$$

is a lower solution of (3.58), (3.32).

Proof

The function ψ satisfies

$$\nabla^2\psi+\eta\left[\exp\left(\frac{-1}{\psi}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\frac{\phi_c}{V}\int_\Omega\exp\left(\frac{\alpha}{\psi}\right)dV}\exp\left(\frac{\alpha-\alpha_w}{\psi}\right)\right]$$

$$=-\eta\left[\exp\left(\frac{-1}{U}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c\exp\left(\frac{\alpha}{U}\right)}\right]+\eta\left[\exp\left(\frac{-1}{\psi}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\frac{\phi_c}{V}\int_\Omega\exp\left(\frac{\alpha}{\psi}\right)dV}\exp\left(\frac{\alpha-\alpha_w}{\psi}\right)\right],$$

$$\geq 0,\qquad r\in\Omega,$$

and

$$\frac{\partial\psi}{\partial n} + \mathrm{Bi}\,\psi = \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)}\right]\left(\frac{\partial w}{\partial n} + \mathrm{Bi}\,w\right) + \mathrm{Bi}\,U,$$

$$= \mathrm{Bi}\,U, \qquad r \in \partial\Omega.$$

So by Definition 2.1.6, ψ is a lower solution of (3.58), (3.32)

■

Theorem 5.8

If $\alpha > \alpha_w > 0$, $U > 0$ then

$$\beta = U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\exp\left(\frac{\alpha - \alpha_w}{U}\right)\right] w, \qquad r \in \Omega,$$

is an upper solution of (3.58), (3.32).

Proof

The function β satisfies

$$\nabla^2\beta + \eta\left[\exp\left(\frac{-1}{\beta}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\beta}\right)dV}\exp\left(\frac{\alpha - \alpha_w}{\beta}\right)\right]$$

$$= -\eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\exp\left(\frac{\alpha - \alpha_w}{U}\right)\right] + \eta\left[\exp\left(\frac{-1}{\beta}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\beta}\right)dV}\exp\left(\frac{\alpha - \alpha_w}{\beta}\right)\right],$$

$$\leq 0, \qquad r \in \Omega,$$

and

$$\frac{\partial \beta}{\partial n} + \text{Bi}\,\beta = \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\exp\left(\frac{\alpha - \alpha_w}{U}\right)\right]\left(\frac{\partial w}{\partial n} + \text{Bi}\,w\right) + \text{Bi}\,U,$$

$$= \text{Bi}\,U, \qquad r \in \partial\Omega.$$

So, by Definition 2.1.6, β is an upper solution of (3.58), (3.32).

■

Note: Clearly the above upper solution becomes infinite at $U = 0$, indeed we have been unable to find an upper solution that holds for $\alpha > \alpha_w > 0$, $U = 0$. It should be noted again, however, that in physical situations an absolute zero ambient storage temperature is unlikely to arise.

Theorem 5.9

If $\alpha_w > \alpha > 0$, $U > 0$ there exists a solution u to (3.58), (3.32) with

$$U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)}\right] w \le u \le U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\exp\left(\frac{\alpha - \alpha_w}{U}\right)\right] w, \qquad r \in \Omega.$$

Proof

We will again use Theorem 2.1.7.

It is easily shown that

$$U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\exp\left(\frac{\alpha - \alpha_w}{U}\right)\right] w \ge U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)}\right] w, \qquad r \in \Omega.$$

Also from (5.3) we have

$$J(u)(h) \geq \frac{\eta\, \lambda h_w \phi_w \phi_c}{\phi_c + \phi_c}\left(\frac{\alpha_w - \alpha}{U^2}\right)\exp\left(\frac{\alpha - \alpha_w}{U}\right)h.$$

So the positive constant Θ we must choose in this case to satisfy the conditions of Theorem 2.1.7 is

$$\Theta = \frac{\eta\, \lambda h_w \phi_w \phi_c}{\phi_c + \phi_c}\left(\frac{\alpha - \alpha_w}{U^2}\right)\exp\left(\frac{\alpha - \alpha_w}{U}\right).$$

Then, by Theorem 2.1.7, there exists a solution u with

$$U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c \exp\left(\frac{\alpha}{U}\right)}\right] w \leq u \leq U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c}\exp\left(\frac{\alpha - \alpha_w}{U}\right)\right] w, \qquad r \in \Omega.$$

■

Theorem 5.10

If $\alpha > \alpha_w > 0$, $U \geq 0$ and u is any solution of (3.58), (3.32) then

$$u \geq U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c \exp\left(\frac{\alpha}{U}\right)}\right] w, \qquad r \in \bar{\Omega}.$$

Proof

Consider the function $u - \left\{U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c \exp\left(\frac{\alpha}{U}\right)}\right] w\right\}, \qquad r \in \Omega.$

Now

$$\nabla^2\left(u-\left\{U+\eta\left[\exp\left(\frac{-1}{U}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c\exp\left(\frac{\alpha}{U}\right)}\right]w\right\}\right)$$

$$=-\eta\left[\exp\left(\frac{-1}{u}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\frac{\phi_c}{V}\int_\Omega\exp\left(\frac{\alpha}{u}\right)dV}\exp\left(\frac{\alpha-\alpha_w}{u}\right)\right]$$

$$+\eta\left[\exp\left(\frac{-1}{U}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c\exp\left(\frac{\alpha}{U}\right)}\right]$$

$$\leq 0, \quad r\in\Omega,$$

and

$$\frac{\partial}{\partial n}\left(u-\left\{U+\eta\left[\exp\left(\frac{-1}{U}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c\exp\left(\frac{\alpha}{U}\right)}\right]w\right\}\right)$$

$$+\mathrm{Bi}\left(u-\left\{U+\eta\left[\exp\left(\frac{-1}{U}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c\exp\left(\frac{\alpha}{U}\right)}\right]w\right\}\right)$$

$$=\frac{\partial u}{\partial n}+\mathrm{Bi}\,(u-U)+\eta\left[\exp\left(\frac{-1}{U}\right)+\frac{\lambda h_w\phi_w\phi_c}{\phi_e+\phi_c\exp\left(\frac{\alpha}{U}\right)}\exp\left(\frac{\alpha-\alpha_w}{U}\right)\right]\left(\frac{\partial w}{\partial n}+\mathrm{Bi}\,w\right),$$

$$=0, \quad r\in\partial\Omega.$$

So, by the maximum principle $\boxed{B}$,

$$u \geq U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)}\right] w, \quad r \in \bar{\Omega}.$$

■

The following Corollary to Theorem 5.10 will enable us to produce an improved (i.e. smaller) upper solution for $\alpha > \alpha_w > 0$ and U small and positive.

Corollary 5.11

By Corollary 2.1.11, if Ω is convex there exists a $\delta > 0$ such that $w \geq \delta > 0$, $r \in \Omega$. So we can say that if $\alpha > \alpha_w > 0$, $U \geq 0$ and u is any solution of (3.58), (3.32) then

$$u \geq U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c \exp\left(\frac{\alpha}{U}\right)}\right] \delta, \quad r \in \bar{\Omega}.$$

■

This gives,

Theorem 5.12

If $\alpha > \alpha_w > 0$, $U > 0$ and u is any solution of (3.58), (3.32) then

$$u \leq U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c} \exp\left(\frac{\alpha - \alpha_w}{G}\right)\right] w, \quad r \in \bar{\Omega},$$

where

$$G = U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)}\right] \delta.$$

Proof

Consider the function $u - \left\{ U + \eta \left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c} \exp\left(\frac{\alpha - \alpha_w}{G} \right) \right] w \right\}, \quad r \in \Omega.$

Now

$$\nabla^2 \left(u - \left\{ U + \eta \left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c} \exp\left(\frac{\alpha - \alpha_w}{G} \right) \right] w \right\} \right)$$

$$= -\eta \left[\exp\left(\frac{-1}{u} \right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \frac{\phi_c}{V} \int_\Omega \exp\left(\frac{\alpha}{u} \right) dV} \exp\left(\frac{\alpha - \alpha_w}{u} \right) \right]$$

$$+ \eta \left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c} \exp\left(\frac{\alpha - \alpha_w}{G} \right) \right],$$

$$\geq 0, \quad r \in \Omega \ \text{(since by Corollary 5.11, } u \geq G, \ r \in \bar{\Omega}\text{)},$$

and

$$\frac{\partial}{\partial n} \left(u - \left\{ U + \eta \left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c} \exp\left(\frac{\alpha - \alpha_w}{G} \right) \right] w \right\} \right) + \mathrm{Bi} \left(u - \left\{ U + \eta \left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c} \exp\left(\frac{\alpha - \alpha_w}{G} \right) \right] w \right\} \right)$$

$$= \frac{\partial u}{\partial n} + \mathrm{Bi}(u - U) - \eta \left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c} \exp\left(\frac{\alpha - \alpha_w}{G} \right) \right] \left(\frac{\partial w}{\partial n} + \mathrm{Bi}\, w \right),$$

$$= 0, \quad r \in \partial\Omega.$$

So, by the maximum principle $\boxed{A}$,

$$u \leq U + \eta \left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c} \exp\left(\frac{\alpha - \alpha_w}{G} \right) \right] w, \quad r \in \bar{\Omega}.$$

∎

We can now combine the results for $\alpha > \alpha_w > 0$ to provide the following improved result regarding existence.

Theorem 5.13

If $\alpha > \alpha_w > 0$, $U > 0$ then there exists a solution u to (3.58), (3.32) with

$$U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c \exp\left(\frac{\alpha}{U}\right)}\right] w \le u \le U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c}\exp\left(\frac{\alpha - \alpha_w}{G}\right)\right] w, \quad r \in \Omega,$$

where G is as defined in Theorem 5.12. Further any solution of (3.58), (3.32) must lie in this range.

Proof

Simple consequence of Theorems 5.7 - 5.12.

■

We give a final result regarding existence,

Theorem 5.14

The problem (3.58), (3.32) has a minimal solution and a maximal solution if $\alpha_w \ge \alpha > 0$, $U \ge 0$, or $\alpha > \alpha_w > 0$, $U > 0$.

Proof

We have shown that

$$U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c \exp\left(\frac{\alpha}{U}\right)}\exp\left(\frac{\alpha - \alpha_w}{U}\right)\right] w$$

is a lower solution and

$$U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\right] w$$

is an upper solution of (3.58), (3.32) if $\alpha \geq \alpha_w > 0$, $U \geq 0$. Therefore (3.58), (3.32) has a minimal and a maximal solution between these upper and lower solutions. The result now follows since every solution lies between these bounds. A similar approach holds for $\alpha > \alpha_w > 0$, $U > 0$.

$\blacksquare$

Note: In the limiting case $Bi \to \infty$, the boundary condition (3.32) becomes

$$u = U, \quad r \in \partial\Omega. \tag{5.4}$$

If we now use the function w which satisfies (5.1) with

$$w = 0, \quad r \in \partial\Omega, \tag{5.5}$$

then the existence results given by Theorems 5.4 and 5.9 for the cases $\alpha_w \geq \alpha > 0$, $U \geq 0$ and $\alpha > \alpha_w > 0$, $U > 0$ respectively, still hold for this limiting case. However, we cannot now prove the existence of the $\delta > 0$ required by Corollary 5.11, hence Theorems 5.12, 5.13 no longer hold. Further the convexity condition on Ω can be relaxed for all results in this section except Theorems 5.12, 5.13.

5.2 Uniqueness results

In this section we will consider the range of η, U values for which the steady state problem given by (3.58), (3.32) has a unique solution. The basic procedure we follow is similar to that of Dancer [53] and Wake et al [13]. However, due to the functional form of the equation we are dealing with, we need to define a different norm to that used in the references mentioned above. In particular we will show that if U is sufficiently large and η is either sufficiently large or sufficiently small, then (3.58), (3.32) has a unique solution.

We first conduct some preliminary analysis from which all the uniqueness results will stem.

5.2.1 Preliminary analysis

Let u_1, u_2 be the minimal and maximal solutions of (3.58), (3.32), so that $\psi = u_2 - u_1$ is non-negative in $\bar{\Omega}$. By the mean value theorem and our construction of the Frèchet derivative J(u)(h) for the system, ψ satisfies

$$\nabla^2\psi + \eta\left[\left\{\frac{\exp\left(\frac{-1}{\zeta}\right)}{\zeta^2} + \frac{\lambda h_w\phi_w\phi_c}{\phi_c + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\zeta}\right)dV}\left(\frac{\alpha_w-\alpha}{\zeta^2}\right)\exp\left(\frac{\alpha-\alpha_w}{\zeta}\right)\right\}\psi\right.$$

$$\left. + \frac{\lambda h_w\phi_w\phi_c^2\,\alpha}{V\left(\phi_c + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\zeta}\right)dV\right)^2}\exp\left(\frac{\alpha-\alpha_w}{\zeta}\right)\int_\Omega \frac{\exp\left(\frac{\alpha}{\zeta}\right)}{\zeta^2}\psi\, dV\right] = 0, \qquad r \in \Omega,$$

$$\frac{\partial\psi}{\partial n} + \mathrm{Bi}\,\psi = 0, \qquad r \in \partial\Omega,$$

where ζ is a function satisfying $u_1 \le \zeta \le u_2$. Consider the Banach space $C_w(\Omega)$ defined by

$$C_w(\Omega) = \left\{ u \in C(\Omega) : \|u\|_w = \frac{\sup_{r \in \Omega} |u(r)|}{\inf_{r \in \Omega} |w(r)|} < \infty \right\}.$$

Note: again we use Corollary 2.1.11 to show that there exists a $\delta > 0$ such that $w \ge \delta > 0$ in $\bar{\Omega}$.

Let g denote the symmetric Green's function for $-\nabla^2$ with the boundary condition $\frac{\partial u}{\partial n} + \mathrm{Bi}\, u = 0$. Then the integral operator G_1 given by

$$(G_1 u)(r) = \int_\Omega g(r,\zeta)\, u(\zeta)\, d\zeta, \qquad r \in \Omega, \tag{5.6}$$

is a compact map $L_q(\Omega) \to W_{2,q}(\Omega)$. Also if $q > 3$ it is easily verified (see e.g. Friedman [54]) that $W_{2,q}(\Omega)$ can be continuously imbedded in $C^1(\Omega)$, and $C^1(\Omega)$ can be continuously imbedded in $C_w(\Omega)$. So G_1 is a compact map from $L_q(\Omega)$ into $C_w(\Omega)$ if $q > 3$.

Now $\psi \in C_w(\Omega)$, hence from the definition of G_1

$$\psi = G_1\left(\eta\left[\left\{\frac{\exp\left(\frac{-1}{\zeta}\right)}{\zeta^2} + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\zeta}\right) dV}\left(\frac{\alpha_w - \alpha}{\zeta^2}\right)\exp\left(\frac{\alpha - \alpha_w}{\zeta}\right)\right\}\psi\right.\right.$$

$$\left.\left. + \frac{\lambda h_w \phi_w \phi_c^2 \alpha}{V\left(\phi_c + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\zeta}\right) dV\right)^2}\exp\left(\frac{\alpha - \alpha_w}{\zeta}\right)\int_\Omega \frac{\exp\left(\frac{\alpha}{\zeta}\right)}{\zeta^2}\psi\, dV\right]\right).$$

So if q > 3.

$$\|\psi\|_w = \left\| G_1\left(\eta\left[\left\{\frac{\exp\left(\frac{-1}{\zeta}\right)}{\zeta^2} + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\zeta}\right) dV}\left(\frac{\alpha_w - \alpha}{\zeta}\right)\exp\left(\frac{\alpha - \alpha_w}{\zeta}\right)\right\}\psi\right.\right.\right.$$

$$\left.\left.\left. + \frac{\lambda h_w \phi_w \phi_c^2 \alpha}{V\left(\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\zeta}\right) dV\right)^2}\exp\left(\frac{\alpha - \alpha_w}{\zeta}\right)\int_\Omega \frac{\exp\left(\frac{\alpha}{\zeta}\right)}{\zeta^2}\psi\, dV\right]\right)\right\|_w,$$

$$\leq \|G_1\|_{w,q}\left\| \eta\left[\left\{\frac{\exp\left(\frac{-1}{\zeta}\right)}{\zeta^2} + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\zeta}\right) dV}\left(\frac{\alpha_w - \alpha}{\zeta^2}\right)\exp\left(\frac{\alpha - \alpha_w}{\zeta}\right)\right\}\psi\right.\right.$$

$$\left.\left. + \frac{\lambda h_w \phi_w \phi_c^2 \alpha}{V\left(\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\zeta}\right) dV\right)^2}\exp\left(\frac{\alpha - \alpha_w}{\zeta}\right)\int_\Omega \frac{\exp\left(\frac{\alpha}{\zeta}\right)}{\zeta^2}\psi\, dV\right]\right\|_{q,\Omega},$$

(where $\|G_1\|_{w,q}$ is the operator norm of the operator in equation (5.6) and $\|\bullet\|_{q,\Omega}$ is the norm given in Definition 2.1.4),

$$\leq \|G_1\|_{w,q}\left\{\left\| \eta\, \frac{\exp\left(\frac{-1}{\zeta}\right)}{\zeta^2}\psi \right\|_{q,\Omega}\right.$$

$$+\left\|\left|\frac{\eta\lambda h_w\phi_w\phi_c}{\phi_e+\frac{\phi_c}{V}\int_\Omega\ \exp\left(\frac{\alpha}{\zeta}\right)dV}\left(\frac{\alpha_w-\alpha}{\zeta^2}\right)\exp\left(\frac{\alpha-\alpha_w}{\zeta}\right)\psi\right|\right\|_{q,\Omega}$$

$$\left.+\left\|\left|\frac{\eta\lambda h_w\phi_w\phi_c^2\alpha}{V\left(\phi_e+\frac{\phi_c}{V}\int_\Omega\ \exp\left(\frac{\alpha}{\zeta}\right)dV\right)^2}\exp\left(\frac{\alpha-\alpha_w}{\zeta}\right)\int_\Omega\ \frac{\exp\left(\frac{\alpha}{\zeta}\right)}{\zeta^2}\psi\, dV\right|\right\|_{q,\Omega}\right\},$$

$$\leq \|G_1\|_{w,q}\ \left\{\left\|\left|\left\{\eta\,\frac{\exp\left(-\frac{1}{2}\right)}{\zeta^2}\,w\right\}\frac{\sup_{r\in\Omega}|\psi|}{w}\right|\right\|_{q,\Omega}\right.$$

$$+\left\|\left|\left\{\frac{\eta\lambda h_w\phi_w\phi_c}{\phi_e+\frac{\phi_c}{V}\int_\Omega\ \exp\left(\frac{\alpha}{\zeta}\right)dV}\left(\frac{\alpha_w-\alpha}{\zeta^2}\right)\exp\left(\frac{\alpha-\alpha_w}{\zeta}\right)w\right\}\frac{\sup_{r\in\Omega}|\psi|}{w}\right|\right\|_{q,\Omega}$$

$$\left.+\left\|\left|\left\{\frac{\eta\lambda h_w\phi_w\phi_c^2\alpha}{V\left(\phi_e+\frac{\phi_c}{V}\int_\Omega\ \exp\left(\frac{\alpha}{\zeta}\right)dV\right)^2}\exp\left(\frac{\alpha-\alpha_w}{\zeta}\right)\int_\Omega\ \frac{\exp\left(\frac{\alpha}{\zeta}\right)}{\zeta^2}dV\ w\right\}\frac{\sup_{r\in\Omega}|\psi|}{w}\right|\right\|_{q,\Omega}\right\}.$$

So this gives

$$\|\psi\|_w \leq \|G_1\|_{w,q}\ \|\psi\|_w\ \left\{\left\|\left|\eta\,\frac{\exp\left(-\frac{1}{\zeta}\right)}{\zeta^2}\,w\right|\right\|_{q,\Omega}\right.$$

$$+ \left\| \frac{\eta\lambda h_w\phi_w\phi_c}{\phi_c + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\zeta}\right) dV} \left(\frac{\alpha_w-\alpha}{\zeta^2}\right) \exp\left(\frac{\alpha-\alpha_w}{\zeta}\right) w \right\|_{q,\Omega}$$

$$\left. + \left\| \frac{\eta\lambda h_w\phi_w\phi_c^2\alpha}{V\left(\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\zeta}\right) dV\right)^2} \exp\left(\frac{\alpha-\alpha_w}{\zeta}\right) \int_\Omega \frac{\exp\left(\frac{\alpha}{\zeta}\right)}{\zeta^2} dV\, w \right\|_{q,\Omega} \right\} . \tag{5.7}$$

From here we will consider the cases $\alpha_w \geq \alpha > 0$, $\alpha > \alpha_w > 0$ separately.

5.2.2 The case $\alpha_w \geq \alpha > 0$

For $\alpha_w \geq \alpha > 0$, $U \geq 0$ the bounds derived in section 5.1 gave us

$$U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w\phi_w\phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha-\alpha_w}{U}\right)\right] w \leq \zeta \leq U + \eta\left[1 + \frac{\lambda h_w\phi_w\phi_c}{\phi_e + \phi_c}\right] w, \quad r \in \bar{\Omega}.$$

So

$$\int_\Omega \frac{\exp\left(\frac{\alpha}{\zeta}\right)}{\zeta^2} dV \leq \frac{\exp\left(\frac{\alpha}{U}\right) V}{\left(U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w\phi_w\phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha-\alpha_w}{U}\right)\right]\delta\right)^2},$$

where δ is as defined in Corollary 2.1.11.

Therefore

$$\|\psi\|_w \le \|G_1\|_{w,q}\,\|\psi\|_w \left\{ \left\| \frac{\eta}{\zeta^2} w \right\|_{q,\Omega} + \left\| \frac{C_1 \eta}{\zeta^2} w \right\|_{q,\Omega} + \left\| \frac{C_2\, \eta \exp\left(\frac{\alpha}{U}\right) w}{\left(U + \eta \left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha - \alpha_w}{U}\right) \right] \delta \right)^2} \right\|_{q,\Omega} \right\}, \tag{5.8}$$

where

$$C_1 = \frac{\lambda h_w \phi_w \phi_c (\alpha_w - \alpha)}{\phi_e + \phi_c}, \qquad C_2 = \frac{\lambda h_w \phi_w \phi_c^2 \alpha}{(\phi_e + \phi_c)^2}.$$

We now define the integrals I_1, I_2, I_3 where

$$I_1 = \left(\left\| \frac{\eta}{\zeta^2} w \right\|_{q,\Omega} \right)^q = \int_\Omega \left(\frac{\eta}{\zeta^2} w \right)^q dV, \tag{5.9}$$

$$I_2 = \left(\left\| \frac{C_1 \eta}{\zeta^2} w \right\|_{q,\Omega} \right)^q = \int_\Omega \left(\frac{C_1 \eta}{\zeta^2} w \right)^q dV, \tag{5.10}$$

$$I_3 = \left(\left\| \frac{C_2\, \eta \exp\left(\frac{\alpha}{U}\right) w}{\left(U + \eta \left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right) \exp\left(\frac{\alpha - \alpha_w}{U}\right)} \right] \delta \right)^2} \right\|_{q,\Omega} \right)^q,$$

$$= \int_\Omega \left(\frac{C_2 \eta \exp\left(\frac{\alpha}{U}\right) w}{\left(U + \eta \left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha - \alpha_w}{U}\right) \right] \delta \right)^2} \right)^q dV. \qquad (5.11)$$

We can now give:

Theorem 5.15

If $\alpha_w \geq \alpha > 0$, then for every $U_0 > 0$ there exists a η_0 so that (3.58), (3.32) has a unique solution whenever $U \geq U_0$ and $\eta \geq \eta_0$.

Proof

We first show that the integrals I_1, I_2, I_3 defined by (5.9), (5.10), (5.11) all tend to zero as $\eta \to \infty$.

(i) Consider I_1.

Since ζ satisfies $\eta w \leq (\zeta - U) \left\{ \exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha - \alpha_w}{U}\right) \right\}^{-1}$,

if we fix $U_0 > 0$, then for $U \geq U_0$

$$I_1 \leq \int_\Omega \left(\left(\frac{\zeta - U_0}{\zeta^2}\right) \left\{ \exp\left(\frac{-1}{U_0}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U_0}\right)} \right\}^{-1} \right)^q dV.$$

Also $\zeta \geq U_0 + \eta \left[\exp\left(\frac{-1}{U_0}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U_o}\right)} \exp\left(\frac{\alpha - \alpha_w}{U_0}\right) \right] w, \qquad r \in \Omega,$

so $\quad \zeta \to \infty$ and $\left(\left(\frac{\zeta - U}{\zeta^2}\right)\left\{\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha - \alpha_w}{U}\right)\right\}^{-1}\right)^q \to 0$

uniformly for $U \geq U_0$, as $\eta \to \infty$. Further as $\zeta \geq U_0$ we have

$$\left(\left(\frac{\zeta - U_0}{\zeta^2}\right)\left\{\exp\left(\frac{-1}{U_0}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U_0}\right)} \exp\left(\frac{\alpha - \alpha_w}{U_0}\right)\right\}^{-1}\right)^q$$

$$\leq \left(\frac{1}{4U_0}\left\{\exp\left(\frac{-1}{U_0}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U_0}\right)} \exp\left(\frac{\alpha - \alpha_w}{U_0}\right)\right\}^{-1}\right)^q \quad \text{in } \Omega.$$

So, by the dominated convergence theorem, we have

$$\int_\Omega \left(\left(\frac{\zeta - U}{\zeta^2}\right)\left\{\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha - \alpha_w}{U}\right)\right\}^{-1}\right)^q dV \to 0$$

uniformly for $U \geq U_0$, as $\eta \to \infty$.

(ii) Consider I_2.

A similar process to that outlined above shows that for $U \geq U_0$

$$I_2 \leq \int_\Omega \left(C_1\left(\frac{\zeta - U_0}{\zeta^2}\right)\left\{\exp\left(\frac{-1}{U_0}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U_0}\right)} \exp\left(\frac{\alpha - \alpha_w}{U_0}\right)\right\}^{-1}\right)^q dV,$$

and

$$\int_\Omega \left(C_1 \left(\frac{\zeta - U}{\zeta^2}\right) \left\{ \exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha - \alpha_w}{U}\right) \right\}^{-1} \right)^q dV \to 0$$

uniformly for $U \geq U_0$ as $\eta \to \infty$.

(iii) Consider I_3.

If we again fix $U_0 > 0$, then for $U \geq U_0$

$$I_3 \leq \int_\Omega \left(\frac{C_2\, \eta \exp\left(\frac{\alpha}{U_0}\right) \|w\|_0}{\left(U_0 + \eta \left[\exp\left(\frac{-1}{U_0}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U_0}\right)} \exp\left(\frac{\alpha - \alpha_w}{U_0}\right) \right] \delta \right)^2} \right)^q dV$$

Note: It can be shown, using a method similar to that used in the proof of Theorem 2.1.10 (but with an escribed sphere) that $\|w\|_0$ is finite.

We then observe that

$$V \left(\frac{C_2\, \eta \exp\left(\frac{\alpha}{U}\right) \|w\|_0}{\left(U + \eta \left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha - \alpha_w}{U}\right) \right] \delta \right)^2} \right)^q \to 0$$

uniformly for $U \geq U_0$ as $\eta \to \infty$.

Finally we note that there is a $\eta_0 > 0$, so that whenever $\eta \geq \eta_0$ and $U \geq U_0$,

$$I_1 + I_2 + I_3 \leq \int_\Omega \left(\left(\frac{\zeta-U}{\zeta^2}\right) \left\{ \exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha-\alpha_w}{U}\right) \right\}^{-1} \right)^q dV$$

$$+ \int_\Omega \left(C_1 \left(\frac{\zeta-U}{\zeta^2}\right) \left\{ \exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha-\alpha_w}{U}\right) \right\}^{-1} \right)^q dV$$

$$+ V \left(\frac{C_2\, \eta \exp\left(\frac{\alpha}{U_0}\right) \|w\|_0}{\left(U + \eta \left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha-\alpha_w}{U}\right) \right] \delta \right)^2} \right)^q$$

$$< \frac{1}{\|G_1\|_{w,q}^q}.$$

So for $U \geq U_0$, $\eta \geq \eta_0$ this inequality and (5.8) gives

$$\|\psi\|_w \leq D_3 \, \|\psi\|_w \, ,$$

where D_3 is a constant less than one. Clearly only $\psi = 0$ can satisfy this inequality and thus our theorem is proved.

■

We can also give:

Theorem 5.16

If $\alpha_w \geq \alpha > 0$, then for every $U_0 > 0$ there exists a η_0 so that (3.58), (3.32) has a unique solution whenever $U \geq U_0$ and $\eta \leq \eta_0$.

Proof

Returning to equation (5.7) and observing

$$\frac{\exp\left(\frac{-k_1}{u}\right)}{u^2} \leq \frac{4}{k_1^2 e^2} \qquad (k_1 > 0),$$

we have (fixing $U_0 > 0$ and $U \geq U_0$)

$$\|\psi\|_w \leq \|G_1\|_{w,q} \|\psi\|_w \left\{ \left\| \frac{4\eta}{e^2} \|w\|_0 \right\|_{q,\Omega} + \left\| \frac{4C_1\eta}{(\alpha-\alpha_w)^2 e^2} \|w\|_0 \right\|_{q,\Omega} \right.$$

$$\left. + \left\| \frac{C_2\eta \exp\left(\frac{\alpha}{U_0}\right) \|w\|_0}{\left(U_0 + \eta\left[\exp\left(\frac{-1}{U_0}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c \exp\left(\frac{\alpha}{U_0}\right)} \exp\left(\frac{\alpha-\alpha_w}{U_0}\right)\right]\delta\right)^2} \right\|_{q,\Omega} \right\},$$

$$= \|G_1\|_{w,q} \|\psi\|_w V^{1/q} \|w\|_0 \left\{ \frac{4\eta}{e^2} + \frac{4C_1\eta}{(\alpha-\alpha_w)^2 e^2} \right.$$

$$\left. + \frac{C_2\eta \exp\left(\frac{\alpha}{U_0}\right)}{\left(U_0 + \eta\left[\exp\left(\frac{-1}{U_0}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c \exp\left(\frac{\alpha}{U_0}\right)} \exp\left(\frac{\alpha-\alpha_w}{U_0}\right)\right]\delta\right)^2} \right\}.$$

Now

$$\left\{ \frac{4\eta}{e^2} + \frac{4C_1\eta}{(\alpha-\alpha_w)^2\, e^2} + \frac{C_2\eta \exp\left(\frac{\alpha}{U}\right)}{\left(U + \eta \left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha-\alpha_w}{U}\right) \right] \delta \right)^2} \right\} \to 0$$

uniformly for $U \geq U_0$ as $\eta \to 0$, so in particular there is a $\eta_0 > 0$ so that whenever $\eta \leq \eta_0$ and $U \geq U_0$

$$V^{1/q}\, \|w\|_0 \left\{ \frac{4\eta}{e^2} + \frac{4C_1\eta}{(\alpha-\alpha_w)^2\, e^2} + \frac{C_2\eta \exp\left(\frac{\alpha}{U}\right)}{\left(U + \eta \left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha-\alpha_w}{U}\right) \right] \delta \right)^2} \right\}$$

$$< \frac{1}{\|G_1\|_{w,q}}.$$

So for $U \geq U_0$ and $\eta \leq \eta_0$ this inequality and (5.8) gives

$$\|\psi\|_w \leq D_4 \|\psi\|_w ,$$

where D_4 is a constant less than one. Again $\psi = 0$ is the only function that can satisfy this inequality, and so we have a unique solution as desired.

■

5.2.3 The case $\alpha > \alpha_w > 0$

The results in this section are similar to those derived in section 5.2.2 except we have

$$U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)}\right] w \le \zeta \le U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\exp\left(\frac{\alpha - \alpha_w}{U}\right)\right] w, \quad r \in \bar{\Omega}.$$

Of course we must also account for the change in monotonicity of the function $\exp\left(\frac{\alpha-\alpha_w}{u}\right)$.

Theorem 5.17

If $\alpha > \alpha_w > 0$, then for every $U_0 > 0$ there exists a η_0 so that (3.58), (3.32) has a unique solution whenever $U \ge U_0$ and $\eta \ge \eta_0$.

Proof

Similar to the proof of Theorem 5.15, except we must choose

$$I_2' = \left(\left\|\frac{C_1\eta}{\zeta^2}\exp\left(\frac{\alpha-\alpha_w}{U}\right) w\right\|_{q,\Omega}\right)^q = \int_\Omega \left|\frac{C_1\eta}{\zeta^2}\exp\left(\frac{\alpha-\alpha_w}{U}\right) w\right|^q dV,$$

$$I_3' = \left(\left\|\frac{C_2\eta\exp\left(\frac{\alpha-\alpha_w}{U}\right)\exp\left(\frac{\alpha}{U}\right) w}{\left(U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w\phi_w\phi_c}{\phi_e + \phi_c\exp\left(\frac{\alpha}{U}\right)}\right]\delta\right)^2}\right\|_{q,\Omega}\right)^q,$$

$$= \int_\Omega \left(\frac{C_2\eta\exp\left(\frac{2\alpha-\alpha_w}{U}\right) w}{\left(U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w\phi_w\phi_c}{\phi_e + \phi_c\exp\left(\frac{\alpha}{U}\right)}\right]\delta\right)^2}\right)^q dV,$$

and use the inequality $\eta w \leq (\zeta - U)\left\{\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)}\right\}^{-1}$.

■

Theorem 5.18

If $\alpha > \alpha_w > 0$, then for every $U_0 > 0$ there exists a η_0 so that (3.58), (3.32) has a unique solution whenever $U \geq U_0$ and $\eta \leq \eta_0$.

Proof

Similar to that proof of Theorem 5.16 except we must use the initial inequality

$$\|\psi\|_w \leq \|G_1\|_{w,q} \|\psi\|_w \left\{ \left\| \left| \frac{4\eta}{e^2} \|w\|_0 \right| \right\|_{q,\Omega} + \left\| \left| \frac{C_1\eta}{U_0^2} \exp\left(\frac{\alpha - \alpha_w}{U_0}\right) \|w\|_0 \right| \right\|_{q,\Omega} \right.$$

$$\left. + \left\| \left| \frac{C_2\eta \exp\left(\frac{\alpha-\alpha_w}{U_0}\right) \exp\left(\frac{\alpha}{U_0}\right) \|w\|_0}{\left(U_0 + \eta\left[\exp\left(\frac{-1}{U_0}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U_0}\right)}\right]\delta\right)^2} \right| \right\|_{q,\Omega} \right\}.$$

■

5.2.4 Comments

Concerning uniqueness for small η, we would liked to have obtained the following result: if η is sufficiently small then there exists a unique solution of (3.58), (3.32) for all $U \geq 0$. We have been unable to obtain this best possible result. We would, however, be able to obtain this result for the case $\alpha_w \geq \alpha > 0$ if we could show that the function (in equation (5.7))

$$\frac{\displaystyle\int_\Omega \frac{\alpha \exp\left(\frac{\alpha}{\zeta}\right)}{\zeta^2}\,dV}{\left(\phi_e + \frac{\phi_c}{V}\displaystyle\int_\Omega \exp\left(\frac{\alpha}{\zeta}\right)dV\right)^2},$$

is bounded above by a value which does not tend to infinity as U becomes small (at least for the range of ζ under consideration). We strongly suspect that this function is indeed bounded above by a function independent of U, but we have been unable to prove this. We should also mention that none of the above uniqueness results hold for the limiting case $Bi \to \infty$ (i.e. the case corresponding to the boundary condition (5.4)), as we cannot verify the existence of the $\delta > 0$ necessary for the proofs.

5.3 Results on the multiplicity of solutions

In this section we construct further upper and lower solutions for the case $\alpha_w \geq \alpha > 0$, and hence show the system (3.58), (3.32) can have at least two solutions. We finally apply a result of Amann [54] to show that the system can have at least three solutions for $\alpha_w \geq \alpha > 0$.

Theorem 5.18

If $\alpha_w \geq \alpha > 0$, $U \geq 0$ and U is sufficiently small, in particular

$$\eta\ \|w\|_0 \leq \left\{\exp\left(\frac{-1}{2U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha - \alpha_w}{2U}\right)}\right\}^{-1} U,$$

then

$$\beta = U + \eta\left[\exp\left(\frac{-1}{2U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{2U}\right)} \exp\left(\frac{\alpha - \alpha_w}{2U}\right)\right] w$$

is an upper solution of (3.58), (3.32).

Proof

The function β satisfies

$$\nabla^2\beta + \eta\left[\exp\left(\frac{-1}{\beta}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\beta}\right) dV} \exp\left(\frac{\alpha-\alpha_w}{\beta}\right)\right]$$

$$= -\eta\left[\exp\left(\frac{-1}{2U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{2U}\right)} \exp\left(\frac{\alpha-\alpha_w}{2U}\right)\right]$$

$$+ \eta\left[\exp\left(\frac{-1}{\beta}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\beta}\right) dV} \exp\left(\frac{\alpha-\alpha_w}{\beta}\right)\right].$$

Now if U is sufficiently small so that

$$\eta\ \|w\|_0 \le \left\{\exp\left(\frac{-1}{2U}\right) + \frac{\lambda h_w \phi_c \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{2U}\right)} \exp\left(\frac{\alpha-\alpha_w}{2U}\right)\right\}^{-1} U,$$

then

$$\beta = U + \eta\left[\exp\left(\frac{-1}{2U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{2U}\right)} \exp\left(\frac{\alpha-\alpha_w}{2U}\right)\right] w \le U + U = 2U.$$

So for these U values β satisfies

$$\nabla^2\beta + \eta\left[\exp\left(\frac{-1}{\beta}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\beta}\right) dV} \exp\left(\frac{\alpha-\alpha_w}{\beta}\right)\right]$$

$$\leq -\eta\left[\exp\left(\frac{-1}{2U}\right)+\frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c \exp\left(\frac{\alpha}{2U}\right)}\exp\left(\frac{\alpha-\alpha_w}{2U}\right)\right]$$

$$+\ \eta\left[\exp\left(\frac{-1}{2U}\right)+\frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c \exp\left(\frac{\alpha}{2U}\right)}\exp\left(\frac{\alpha-\alpha_w}{2U}\right)\right]$$

$$= 0, \quad r \in \Omega,$$

and

$$\frac{\partial \beta}{\partial n} + \mathrm{Bi}\,\beta = \eta\left[\exp\left(\frac{-1}{2U}\right)+\frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c \exp\left(\frac{\alpha}{2U}\right)}\exp\left(\frac{\alpha-\alpha_w}{2U}\right)\right]\left(\frac{\partial w}{\partial n} + \mathrm{Bi}\, w\right) + \mathrm{Bi}\, U,$$

$$= \mathrm{Bi}\, U, \quad r \in \Omega.$$

So by Definition 2.1.6, β is an upper solution of (3.58), (3.32).

■

We can combine this result with Theorem 5.3 to give:

Theorem 5.19

If $\alpha_w \geq \alpha > 0$, $U \geq 0$ and U is sufficiently small then (3.58), (3.32) has a solution u satisfying

$$U + \eta\left[\exp\left(\frac{-1}{U}\right)+\frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c \exp\left(\frac{\alpha}{U}\right)}\exp\left(\frac{\alpha-\alpha_w}{U}\right)\right] w \leq u$$

$$\leq U + \eta\left[\exp\left(\frac{-1}{2U}\right)+\frac{\lambda h_w \phi_w \phi_c}{\phi_c + \phi_c \exp\left(\frac{\alpha}{2U}\right)}\exp\left(\frac{\alpha-\alpha_w}{2U}\right)\right] w, \quad r \in \Omega.$$

Proof

We showed in Theorem 5.3 that

$$U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)}\right] w$$

is a lower solution for all $U \geq 0$, and in Theorem 5.18 that

$$U + \eta\left[\exp\left(\frac{-1}{2U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{2U}\right)} \exp\left(\frac{\alpha - \alpha_w}{2U}\right)\right] w$$

is an upper solution for U sufficiently small. The result follows using the inequality

$$U + \eta\left[\exp\left(\frac{-1}{U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{U}\right)} \exp\left(\frac{\alpha - \alpha_w}{U}\right)\right] w$$

$$\leq U + \eta\left[\exp\left(\frac{-1}{2U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{2U}\right)} \exp\left(\frac{\alpha - \alpha_w}{2U}\right)\right] w,$$

and Theorem 2.1.7.

∎

We now construct another lower solution. The lower solution in the following result was first used by Wake et al [13] for the limiting case $Bi \to \infty$ (and the 'dry' reaction only i.e. $\lambda = 0$).

Theorem 5.20

If $\alpha_w \geq \alpha > 0$, $U \geq 0$ and η is sufficiently large, then

$$\psi = U + \exp(Aw\ \ell n\eta) - 1, \quad \text{where} \quad A = \frac{1}{2\|w\|_0},$$

is a lower solution of (3.58), (3.32).

Proof

The function ψ satisfies

$$\nabla^2\psi + \eta\left[\exp\left(\frac{-1}{\psi}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\psi}\right) dV} \exp\left(\frac{\alpha - \alpha_w}{\psi}\right)\right]$$

$$= [(A\ \ell n\eta)^2 |\nabla w|^2 + A\ \ell n\eta\ \nabla^2 w] \exp(Aw\ \ell n\eta)$$

$$+ \eta\left[\exp\left(\frac{-1}{\psi}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\psi}\right) dV} \exp\left(\frac{\alpha - \alpha_w}{\psi}\right)\right]$$

$$\geq [(A\ \ell n\eta)^2 |\nabla w|^2 - A\ \ell n\eta] \exp(Aw\ \ell n\eta)$$

$$+ \eta \exp\left(\frac{-1}{\exp(Aw\ \ell n\eta) - 1}\right), \quad r \in \Omega.$$

Now, by Theorem 2.1.8, $w(r) > 0$, $r \in \Omega$ and $\frac{\partial w}{\partial n}(r) < 0$, $r \in \partial\Omega$. Therefore Ω can be expressed as the disjoint union

$$\Omega = \Omega_{k_4} \cup \bar{\Omega}_{\ell_4},$$

where Ω_{k_4}, Ω_{ℓ_4} are open sets with

$$|\nabla w|^2 \geq k_4 > 0, \qquad \text{in } \Omega_{k_4},$$

$$w \geq \ell_4 > 0, \qquad \text{in } \bar{\Omega}_{\ell_4}$$

for some constants k_4, ℓ_4. Given that $Aw \leq \frac{1}{2}$, ψ then satisfies

$$\nabla^2\psi + \eta\left[\exp\left(\frac{-1}{\psi}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_c + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\psi}\right) dV} \exp\left(\frac{\alpha - \alpha_w}{\psi}\right)\right]$$

$$\geq A\,\ell n\eta\,(Ak_4\,\ell n\eta - 1)\exp(Aw\,\ell n\eta), \qquad r \in \Omega_{k_4},$$

$$\geq -A\,\ell n\eta\,\exp\left(\frac{\ell n\eta}{2}\right) + \eta\exp\left(\frac{-1}{\exp(A\ell_4\,\ell n\eta) - 1}\right), \qquad r \in \bar{\Omega}_{\ell_4}.$$

We now choose η so large that

$$\ell n\eta \geq \frac{1}{Ak_4},$$

and

$$\eta\exp\left(\frac{-1}{\exp(A\ell_4\,\ell n\eta) - 1}\right) > A\sqrt{\eta}\,\ell n\eta, \tag{5.12}$$

(e.g. if η satisfies $\exp(A\ell_4\,\ell n\eta) > 2$ then $\eta\exp\left(\frac{-1}{\exp(A\ell_4\,\ell n\eta) - 1}\right) > \eta\,e^{-1}$, so (5.12) is satisfied if $\sqrt{\eta} > Ae\,\ell n\eta$).

Then ψ satisfies

$$\nabla^2\psi + \eta\left[\exp\left(\frac{-1}{\psi}\right) + \frac{\lambda h_w\phi_w\phi_c}{\phi_e + \frac{\phi_c}{V}\int_\Omega \exp\left(\frac{\alpha}{\psi}\right)dV}\exp\left(\frac{\alpha-\alpha_w}{\psi}\right)\right]$$

$$\geq 0, \quad r \in \Omega_{k_4}$$

$$\geq 0, \quad r \in \bar{\Omega}_{\ell_4}$$

for these values of η.

Also

$$\frac{\partial\psi}{\partial n} + \mathrm{Bi}\,\psi = A\,\ell n\eta\,\exp(Aw\,\ell n\eta)\frac{\partial w}{\partial n} + \mathrm{Bi}\,(U + \exp(Aw\,\ell n\eta) - 1),$$

$$= -\mathrm{Bi}\,wA\,\ell n\eta\,\exp(Aw\,\ell n\eta) + \mathrm{Bi}\,(U + \exp(Aw\,\ell n\eta) - 1),$$

$$\leq \mathrm{Bi}\,\{\exp(Aw\,\ell n\eta)\,(1 - A\delta\,\ell n\eta) - 1\} + \mathrm{Bi}\,U, \quad r \in \partial\Omega,$$

where δ is again as defined in Corollary 2.1.11. Now if η is also sufficiently large so that $\ell n\eta > \dfrac{1}{A\delta}$, then

$$\frac{\partial\psi}{\partial n} + \mathrm{Bi}\,\psi \leq \mathrm{Bi}\,U, \quad r \in \partial\Omega.$$

So, for these η values, ψ is a lower solution of (3.58), (3.32).

Note: For the limiting case $Bi \to \infty$, we will be dealing with the boundary condition (5.4), and the function w that satisfies the boundary condition (5.5). In this case the boundary inequality becomes

$$\begin{aligned}\psi &= U + \exp(Aw\, \ell n\eta) - 1,\\ &= U, \quad r \in \partial\Omega,\end{aligned}$$

hence ψ is also a lower solution in this limiting case.

■

We can combine this result with Theorem 5.2 to give:

Theorem 5.21

If $\alpha_w \geq \alpha > 0$, $U \geq 0$ and η is sufficiently large, then (3.58), (3.32) has a solution u satisfying

$$U + \exp(Aw\, \ell n\eta) - 1 \leq u \leq U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\right]w, \quad r \in \Omega.$$

Proof

We have previously shown that the lower bound is a lower solution for η sufficiently large, and the upper bound is an upper solution for all $U \geq 0$. Then using Theorem 2.1.7 we must simply show

$$U + \exp(Aw\, \ell n\eta) - 1 < U + \eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\right]w. \tag{5.13}$$

Now

$$\frac{\exp(Aw\,\ell n\eta) - 1}{w} \le \frac{\exp(A\,\|w\|_0\,\ell n\eta) - 1}{\|w\|_0} = \frac{\exp\left(\frac{\ell n\eta}{2}\right) - 1}{\|w\|_0} = \frac{\sqrt{\eta} - 1}{\|w\|_0}.$$

So if η is sufficiently large so that

$$\eta\left[1 + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c}\right] > \frac{\sqrt{\eta} - 1}{\|w\|_0},$$

then (5.13) is satisfied.

■

We can now combine Theorems 5.19 and 5.21 to give:

Theorem 5.22

If $\alpha_w \ge \alpha > 0$, U is sufficiently small and η is sufficiently large, then (3.58), (3.32) has at least two solutions.

Proof

We have constructed two pairs of upper and lower solutions. To prove the result we must show that the hypotheses of Theorems 5.19, 5.21 hold and in addition

$$U + \eta\left[\exp\left(\frac{-1}{2U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{2U}\right)} \exp\left(\frac{\alpha - \alpha_w}{2U}\right)\right] w < U + \exp(Aw\,\ell n\eta) - 1,$$

for U sufficiently small and η sufficiently large. If η_1 is such that Theorem 5.21 holds for all $\eta \ge \eta_1$, then fix $\eta_2 > \eta_1$. Then for $\eta \in [\eta_1, \eta_2]$, Theorem 5.19 holds when U satisfies

$$\eta\,\|w\|_0 < \left[\exp\left(\frac{-1}{2U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{2U}\right)}\right]^{-1} U.$$

If in particular U_1 satisfies

$$\eta_2 \; \|w\|_0 < \left[\exp\left(\frac{-1}{2U_1}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{2U_1}\right)} \exp\left(\frac{\alpha - \alpha_w}{2U_1}\right) \right]^{-1} U_1,$$

then Theorem 5.19 holds $\forall\; U \in [0, U_1]$ and $\eta \in [\eta_1, \eta_2]$.

If U_1 is also required to satisfy

$$\exp\left(\frac{-1}{2U_1}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{2U_1}\right)} \exp\left(\frac{\alpha - \alpha_w}{2U_1}\right) < \min\left(\frac{\ell n \eta_1}{2\eta_1 \; \|w\|_0}, \frac{\ell n \eta_2}{2\eta_2 \; \|w\|_0}\right),$$

then for $U \in [0, U_1]$, $\eta \in [\eta_1, \eta_2]$

$$\exp\left(\frac{-1}{2U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{2U}\right)} \exp\left(\frac{\alpha - \alpha_w}{2U}\right) < \frac{\ell n \eta}{2\eta \; \|w\|_0} \le \frac{\exp(Aw \; \ell n \eta) - 1}{\eta \; w}.$$

So

$$U + \eta \left[\exp\left(\frac{-1}{2U}\right) + \frac{\lambda h_w \phi_w \phi_c}{\phi_e + \phi_c \exp\left(\frac{\alpha}{2U}\right)} \exp\left(\frac{\alpha - \alpha_w}{2U}\right) \right] w < U + \exp(Aw \; \ell n \eta) - 1,$$

as required

■

In fact, using the two solutions (u_{01}, u_{02} say) derived above and a result of Amann [54] we can say:

Theorem 5.23

If $\alpha_w \geq \alpha > 0$, U is sufficiently small and η is sufficiently large, then (3.58), (3.32) has at least three solutions.

Proof

The result of Amann [54] can easily be extended to include the functional form we are considering here. Amann's result states that if the problem

$$\left.\begin{aligned} \nabla^2 u + j(u) = 0\,, \quad & r \in \Omega, \\ Bu = 0\,, \quad & r \in \partial\Omega\,, \end{aligned}\right\} \tag{5.14}$$

(where B is a boundary operator of the form given in Definition 2.1.6), has two solutions u_1, u_2, then it also has at least one further solution u_3 satisfying $u_1 < u_3 < u_2$, provided the linearized problems

$$\left.\begin{aligned} \nabla^2 \chi + j'(u_i)\,\chi = 0\,, \quad & r \in \Omega\,, \\ B\chi = 0\,, \quad & r \in \partial\Omega, \end{aligned}\right\} \tag{5.15}$$

$i = 1, 2$, have only the trivial solution (where $j'(u_i)$ is the Frèchet derivative of j evaluated at u_i). We extend this result to include the case we are studying here by first making the transformation $v = u - U$ to achieve a modified system with homogeneous boundary conditions. Equations (3.58), (3.32) are then of the form

$$\left.\begin{aligned} \nabla^2 v + f\left(v + U, \int_\Omega g(v+U)\, dV\right) = 0\ , \qquad r \in \Omega\ , \\ Bv = 0\ , \quad r \in \partial\Omega\ , \end{aligned}\right\} \tag{5.16}$$

the linearized form of which is

$$\left.\begin{aligned} \nabla^2 \zeta + J(v+U)\,(\zeta) = 0\ , \qquad r \in \Omega\ , \\ B\zeta = 0\ , \quad r \in \partial\Omega\ , \end{aligned}\right\} \tag{5.17}$$

where $J(v+U)\,(\zeta)$ is the Frèchet derivative whose form is given in (5.3).

If we note that the solution of (5.16) can be written in the form

$$v = \int_\Omega G_2(r, \tau)\, f\left(v(\tau) + U, \int_\Omega g(v+U)\, dV\right) dV_\tau,$$

where dV_τ is a volume element with respect to the dummy variable τ and G_2 is the Green's function for $-\nabla^2$ with the boundary operator B, then it is easy to show that the main result of Amann also holds for our functional case.

■

Note: The above results also hold in the limiting case $Bi \to \infty$, with the boundary conditions for u and w given by (5.4) and (5.5) respectively. We have been unable to derive corresponding multiplicity results for the case $\alpha > \alpha_w > 0$, due to the difficulty of constructing an upper solution which does not get large as $U \to 0$. All the results in this section still hold if the convexity condition on Ω is relaxed.

CHAPTER 6

Existence and uniqueness results for the time dependent problem.

In this final chapter we show that the time dependent problem defined by (3.28) - (3.30), (3.32) - (3.37) has a unique solution on the region $\Omega_T = \Omega \times (0, T]$, $\partial\Omega_T = \partial\Omega \times (0, T]$, where $T < \infty$, but can be arbitrarily large. Firstly we rewrite the equations (3.28) - (3.30), (3.32) - (3.34) in the following form

$$\frac{\partial u}{\partial t} - \eta' \nabla^2 u = \exp\left(\frac{-1}{u}\right) + \lambda\left\{h_w\phi_w \, x \exp\left(\frac{-\alpha_w}{u}\right) - h_c\phi_e \, x \exp\left(\frac{-\alpha}{u}\right) + h_c\phi_c \, y\right\}$$

$$= f_1 (u, y, x), \quad \text{in } \Omega_T, \quad (6.1)$$

$$\frac{dy}{dt} - \frac{\gamma}{\varepsilon}\nabla^2 y = \frac{1}{\varepsilon}\left\{\phi_c \, x \exp\left(\frac{-\alpha}{u}\right) - \phi_c y\right\} = f_2 (u, y, x), \quad \text{in } \Omega_T, \quad (6.2)$$

$$\frac{\partial x}{\partial t} = \frac{1}{\varepsilon}\left\{\phi_c y - \phi_e \, x \exp\left(\frac{-\alpha}{u}\right)\right\} = f_3 (u, y, x), \quad \text{in } \Omega_T, \quad (6.3)$$

$$\frac{\partial u}{\partial n} + Bi\, u = Bi\, U, \quad \text{on } \partial\Omega_T, \quad (6.4)$$

$$\frac{\partial y}{\partial n} = 0, \quad \text{on } \partial\Omega_T, \quad (6.5)$$

$$\frac{\partial x}{\partial n} = 0, \quad \text{on } \partial\Omega_T. \quad (6.6)$$

The form of the initial conditions remains unchanged.

The most interesting aspect of this system is the fact that the function f_1 (u, y, x) is not necessarily monotone in the x variable. To obtain the desired existence/uniqueness theorems we will therefore use the results of McNabb. In his 1961 paper, McNabb [55] gave existence/uniqueness results for parabolic systems with source functions that satisfy a monotone property, these have been extended to systems with more general boundary conditions, see e.g. Ladde et al [56]. These results were later (1986) further extended (McNabb [57]) to include non-monotone functions. These results involve imbedding the non-monotone system in another system of twice the order. The following Theorem represents the application of the main result contained in McNabb [57] to our system:

Theorem 6.1

Suppose the functions f_1, f_2, f_3 defined in (6.1) - (6.3) are Hölder continuous and satisfy a Lipschitz condition in Ω_T. Suppose further that there exist continuous functions $\bar{u}$, $\underline{u}$, $\bar{y}$, $\underline{y}$, $\bar{x}$, $\underline{x}$ (with $\bar{u} \geq \underline{u}$, $\bar{y} \geq \underline{y}$, $\bar{x} \geq \underline{x}$) that satisfy the following inequalities

$$\frac{\partial \bar{u}}{\partial t} - \eta' \nabla^2 \bar{u} \geq \bar{F}_1 (\bar{u}, \underline{u}, \bar{y}, \underline{y}, \bar{x}, \underline{x}), \quad \text{in } \Omega_T, \tag{6.7}$$

$$\frac{\partial \bar{y}}{\partial t} - \frac{\gamma}{\varepsilon} \nabla^2 \bar{y} \geq \bar{F}_2 (\bar{u}, \underline{u}, \bar{y}, \underline{y}, \bar{x}, \underline{x}), \quad \text{in } \Omega_T, \tag{6.8}$$

$$\frac{\partial \bar{x}}{\partial t} \geq \bar{F}_3 (\bar{u}, \underline{u}, \bar{y}, \underline{y}, \bar{x}, \underline{x}), \quad \text{in } \Omega_T, \tag{6.9}$$

$$\frac{\partial \underline{u}}{\partial t} - \eta' \nabla^2 \underline{u} \leq \underline{F}_1 (\bar{u}, \underline{u}, \bar{y}, \underline{y}, \bar{x}, \underline{x}), \quad \text{in } \Omega_T, \tag{6.10}$$

$$\frac{\partial \underline{y}}{\partial t} - \frac{\gamma}{\varepsilon} \nabla^2 \underline{y} \leq \underline{F}_2 (\bar{u}, \underline{u}, \bar{y}, \underline{y}, \bar{x}, \underline{x}), \quad \text{in } \Omega_T, \tag{6.11}$$

$$\frac{\partial \underline{x}}{\partial t} \leq \underline{F}_3 (\bar{u}, \underline{u}, \bar{y}, \underline{y}, \bar{x}, \underline{x}), \quad \text{in } \Omega_T, \tag{6.12}$$

$$\frac{\partial \bar{u}}{\partial n} + Bi\,\bar{u} \geq Bi\,U \geq \frac{\partial \underline{u}}{\partial n} + Bi\,\underline{u}, \quad \text{on } \partial\Omega_T, \tag{6.13}$$

$$\frac{\partial \bar{y}}{\partial n} \geq 0 \geq \frac{\partial \underline{y}}{\partial n}, \quad \text{on } \partial\Omega_T, \tag{6.14}$$

$$\frac{\partial \bar{x}}{\partial n} \geq 0 \geq \frac{\partial \underline{x}}{\partial n}, \quad \text{on } \partial\Omega_T, \tag{6.15}$$

$$\bar{u}\,(r,0) \geq \zeta_1(r) \geq \underline{u}\,(r,0), \quad \text{on } \bar{\Omega}, \tag{6.16}$$

$$\bar{y}\,(r,0) \geq \psi_1(r) \geq \underline{y}\,(r,0), \quad \text{on } \bar{\Omega}, \tag{6.17}$$

$$\bar{x}\,(r,0) \geq \chi_1(r) \geq \underline{x}\,(r,0), \quad \text{on } \bar{\Omega}, \tag{6.18}$$

where

$$\bar{F}_1\,(\bar{u},\ \underline{u},\ \bar{y}, \underline{y},\ \bar{x},\ \underline{x}) = \sup_{\substack{\underline{y} \leq \theta_2 \leq \bar{y} \\ \underline{x} \leq \theta_3 \leq \bar{x}}} f_1\,(\bar{u}, \theta_2, \theta_3),$$

$$\bar{F}_2\,(\bar{u},\ \underline{u},\ \bar{y}, \underline{y},\ \bar{x},\ \underline{x}) = \sup_{\substack{\underline{u} \leq \theta_1 \leq \bar{u} \\ \underline{x} \leq \theta_3 \leq \bar{x}}} f_2\,(\theta_1, \bar{y}, \theta_3),$$

$$\bar{F}_3\,(\bar{u},\ \underline{u},\ \bar{y}, \underline{y},\ \bar{x},\ \underline{x}) = \sup_{\substack{\underline{u} \leq \theta_1 \leq \bar{u} \\ \underline{y} \leq \theta_2 \leq \bar{y}}} f_3\,(\theta_1, \theta_2, \bar{x}),$$

$$\underline{F}_1\,(\bar{u},\ \underline{u},\ \bar{y}, \underline{y},\ \bar{x},\ \underline{x}) = \inf_{\substack{\underline{y} \leq \theta_2 \leq \bar{y} \\ \underline{x} \leq \theta_3 \leq \bar{x}}} f_1\,(\underline{u}, \theta_2, \theta_3),$$

$$\underline{F}_2\,(\bar{u},\ \underline{u},\ \bar{y}, \underline{y},\ \bar{x},\ \underline{x}) = \inf_{\substack{\underline{u} \leq \theta_1 \leq \bar{u} \\ \underline{x} \leq \theta_3 \leq \bar{x}}} f_2\,(\theta_1, \underline{y}, \theta_3),$$

$$\underline{F}_3(\overline{u}, \underline{u}, \overline{y}, \underline{y}, \overline{x}, \underline{x}) = \inf_{\substack{\underline{u} \le \theta_1 \le \overline{u} \\ \underline{y} \le \theta_2 \le \overline{y}}} f_3(\theta_1, \theta_2, \underline{x}).$$

Then there exists a unique solution u, y, x of (6.1) - (6.6), (3.35) - (3.37) with

$$\underline{u} \le u \le \overline{u}, \;\; \underline{y} \le y \le \overline{y}, \;\; \underline{x} \le x \le \overline{x}, \quad \text{in } \Omega_T.$$

Proof

See McNabb [55], [57],

■

Using the above Theorem leads to the main result of this chapter:

Theorem 6.2

The system (6.1) - (6.6), (3.35) - (3.37) has a unique solution u, y, x satisfying

$$0 \le u \le \|\zeta_1\| + U + \frac{C_1 + D_1 \exp(\mu_2 t)}{\eta'} w,$$

$$0 \le y \le A_1 \exp(\mu_1 t) + B_1 \exp(\mu_2 t),$$

$$0 \le x \le \frac{A_1}{\phi_c} \varepsilon\mu_1 \exp(\mu_1 t) + \frac{B_1}{\phi_c} \varepsilon\mu_2 \exp(\mu_2 t),$$

where

w is the solution of (5.1), (5.2),

$$\mu_1 = -\sqrt{\frac{\phi_e \phi_c}{\varepsilon^2}}, \tag{6.19}$$

$$\mu_2 = \sqrt{\frac{\phi_e \phi_c}{\varepsilon^2}}\,, \tag{6.20}$$

$$B_1 = \frac{\phi_e \, \|\chi_1\|_0 - \|\psi_1\|_0 \, \varepsilon\mu_1}{\varepsilon\,(\mu_2 - \mu_1)}\,, \tag{6.21}$$

$$A_1 = \|\psi_1\|_0 - B_1\,, \tag{6.22}$$

$$C_1 = 1 + \lambda\,|A_1| \left\{\frac{h_w\phi_w\,\varepsilon\,|\mu_1|}{\phi_e} + h_c\,\phi_c\right\}, \tag{6.23}$$

$$D_1 = \lambda\; B_1 \left\{\frac{h_w\phi_w\,\varepsilon\,\mu_2}{\phi_e} + h_c\phi_c\right\}. \tag{6.24}$$

Proof

It is easy to show that the f_i, $i = 1, 2, 3$ satisfy the desired Hölder and Lipschitz conditions, since the partial derivatives of the f_i with respect to u, y, x are bounded on any bounded region ($u \geq 0$), (for $u = 0$ we replace $\exp\left(\frac{-\alpha}{u}\right)$ etc. by zero). So we must simply find functions $\bar{u}$, $\underline{u}$, $\bar{y}$, $\underline{y}$, $\bar{x}$, $\underline{x}$ that satisfy the inequalities (6.7) - (6.18). Now reinforcing inequalities (6.7) - (6.12) gives

$$\frac{\partial\bar{u}}{\partial t} - \eta'\,\nabla^2\bar{u} \geq 1 + \lambda\,\{h_w\,\phi_w\,\bar{x} + h_c\,\phi_c\,\bar{y}\}\,, \tag{6.25}$$

$$\frac{\partial\bar{y}}{\partial t} - \frac{\gamma}{\varepsilon}\nabla^2\bar{y} \geq \frac{1}{\varepsilon}\,\{\phi_e\,\bar{x} - \phi_c\,\bar{y}\}\,, \tag{6.26}$$

$$\frac{\partial\bar{x}}{\partial t} \geq \frac{1}{\varepsilon}\,\phi_c\,\bar{y}\,, \tag{6.27}$$

$$\frac{\partial \underline{u}}{\partial t} - \eta' \nabla^2 \underline{u} \le \lambda \left\{ -h_c \, \phi_e \, \overline{x} \exp\left(\frac{-\alpha}{\underline{u}}\right) + h_c \, \phi_c \, \underline{y} \right\}, \tag{6.28}$$

$$\frac{\partial \underline{y}}{\partial t} - \frac{\gamma}{\varepsilon} \nabla^2 \underline{y} \le -\frac{1}{\varepsilon} \phi_c \, \underline{y}, \tag{6.29}$$

$$\frac{\partial \underline{x}}{\partial t} \le -\frac{1}{\varepsilon} \phi_e \, \underline{x}. \tag{6.30}$$

Clearly $\underline{u} = \underline{y} = \underline{x} \equiv 0$ satisfy the inequalities (6.28) - (6.29) and the right-hand inequalities of (6.13) - (6.18). Now consider the functions $\overline{x}_1$, $\overline{y}_1$ that satisfy the coupled ordinary differential equations

$$\frac{d\overline{y}_1}{dt} = \frac{1}{\varepsilon} \phi_e \, \overline{x}_1 , \qquad t > 0,$$

$$\frac{d\overline{x}_1}{dt} = \frac{1}{\varepsilon} \phi_c \, \overline{y}_1 , \qquad t > 0,$$

$$\overline{y}_1 \, (t = 0) = \|\psi_1\|_0 , \qquad \overline{x}_1 \, (t = 0) = \|\chi_1\|_0 .$$

This system has the simple analytic solution

$$\overline{y}_1 = A_1 \exp(\mu_1 \, t) + B_1 \exp(\mu_2 \, t),$$

$$\overline{x}_1 = \frac{A_1}{\phi_e} \varepsilon \, \mu_1 \exp(\mu_1 \, t) + \frac{B_1}{\phi_e} \varepsilon \, \mu_2 \exp(\mu_2 \, t),$$

where μ_1, μ_2, B_1, A_1 are as defined in (6.19) - (6.22). It is easy to show that $B_1 > 0$ and A_1 can be positive or negative depending on the initial conditions. Further, $\overline{y}_1 \ge \|\psi_1\|_0$ for all $t > 0$ and $\overline{x}_1 \ge \|\chi_1\|_0$ for all $t > 0$. Clearly $\overline{y} \equiv \overline{y}_1$ and $\overline{x} \equiv \overline{x}_1$ satisfy the inequalities

(6.26), (6.27) and the left-hand inequalities of (6.14), (6.15), (6.17), (6.18). Next, reinforcing inequality (6.25) gives

$$\frac{\partial \bar{u}}{\partial t} - \eta' \nabla^2 \bar{u} \geq C_1 + D_1 \exp(\mu_2 t) , \qquad (6.31)$$

where C_1, D_1 are as defined in (6.23), (6.24).

Now consider the function

$$\bar{u}_1 = \|\zeta_1\|_0 + U + \frac{C_1 + D_1 \exp(\mu_2 t)}{\eta'} w ,$$

this function satisfies

$$\frac{\partial \bar{u}}{\partial t} - \eta' \nabla^2 \bar{u}_1 = \frac{\mu_2 D_1 \exp(\mu_2 t)}{\eta'} w + C_1 + D_1 \exp(\mu_2 t),$$

$$\geq C_1 + D_1 \exp(\mu_2 t) , \quad \text{in } \Omega_T.$$

So clearly $\bar{u} \equiv \bar{u}_1$ satisfies (6.31), as well as the left-hand inequality of (6.16). Finally this choice of $\bar{u}$ satisfies

$$\frac{\partial \bar{u}}{\partial n} + Bi\, \bar{u} = \frac{C_1 + D_1 \exp(\mu_2 t)}{\eta'} \frac{\partial w}{\partial n} + Bi \left(\|\zeta_1\|_0 + U + \frac{C_1 + D_1 \exp(\mu_2 t)}{\eta'} w \right),$$

$$= \frac{C_1 + D_1 \exp(\mu_2 t)}{\eta'} \left(\frac{\partial w}{\partial n} + Bi\, w \right) + Bi\, (\|\zeta_1\|_0 + U),$$

$$= Bi\, (\|\zeta_1\|_0 + U),$$

$$\geq \ \text{Bi}\, U, \qquad \text{on } \partial\Omega_T,$$

so the left-hand inequality of (6.13) is satisfied also.

This completes the proof.

■

Note: The above results also hold in the limiting case Bi $\rightarrow \infty$, with the boundary conditions for u and w given by (5.4) and (5.5) respectively, and a modified boundary inequality (6.13) of the form

$$\bar{u} \geq U \geq \underline{u}\,, \qquad \text{on } \partial\Omega_T.$$

Concluding comments

One of the most interesting aspects of this work has been the wide range of behaviour which can be introduced into the model by the addition of the effects of moisture. In fact the use of degenerate singularity theory demonstrated the existence of at least twenty-five distinct bifurcation diagrams for the spatially uniform model (i.e. in the limiting case as the thermal conductivity and diffusivity of the body become large). Also, as indicated in Figure 4.2, the model predicts that the body can be substantially more prone to spontaneous ignition when the effects of moisture are included. Results for the spatially distributed model were obviously more difficult to obtain. The existence, uniqueness and multiplicity results achieved for the steady state profiles give a good insight into the behaviour of the model equations, but further results will still be required before the full steady state behaviour can be predicted. These results include: (i) a better upper solution for the case $\alpha>\alpha_w$ (i.e. one that does not get large as U gets small), (ii) a uniqueness result for all positive U with η sufficiently small, and (iii) a result on multiple solutions for the case $\alpha>\alpha_w$ (indeed the author conjectures that there can also be at least five solutions for finite thermal conductivity and diffusivity).

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