ON THE CROSSING OF INTERMEDIATE UNSTABLE STEADY STATE SOLUTIONS FOR THERMAL IGNITION IN A SPHERE

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Abstract

Steady state solutions for spontaneous thermal ignition in a unit sphere are considered. The multiplicity of unstable, intermediate, steady state, temperature profiles is calculated and shown for selected parameter values. The crossing of the temperature profiles corresponding to the unstable, intermediate, steady states is exhibited in a particular case and is proven in general using elementary ideas from analysis. Estimates of the location of crossing points are given.

1. Introduction

Models of spontaneous thermal ignition have a long history, beginning with the Russian literature as listed by Frank-Kamenetskii [7]. A parallel literature in astrophysics has examined many similar problems; for example, Chandrasekhar [5]. In both cases, spherically geometric temperature distributions have been of considerable interest and numerical, as well as analytical, effort has been expended in the cause of obtaining complete solutions.

It was first recognised by Gel'fand [9], Fujita [8] and Steggerda [18] (see also Enig [6], Gray [11], Aris [1, p. 48] and Zeldovich *et al.* [20, p. 159]) that there can be a very large number of solutions for the steady-state, reaction-diffusion equation in spherical geometry with an exponential reaction term or a polynomial reaction term of sufficiently high degree (greater than 5). This was initially regarded as a

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mere mathematical curiosity, but later investigators have wondered if there could be a physical role for the gross multiplicity of steady states, as well as examining the bifurcation in greater detail; for example Ash *et al.* [2], Brindley *et al.* [4], Balakrishnan *et al.* [3], Kapila *et al.* [14], Maddocks [15], Weber *et al.* [19].

In the present paper, we wish to examine the spatial distributions of these multiple steady states. We will demonstrate numerically and then prove rigorously that the existence of multiple unsteady steady states necessitates that their spatial distributions must cross (already suggested diagrammatically, but never formally stated in earlier work as reported by Zeldovich *et al.* [20, p. 160]). Furthermore, we will give estimates for the crossing points and the associated function values.

2. Steady state solutions for spontaneous thermal ignition in a sphere

If we seek a balance between the effect of diffusional fluxes of heat and an exother-mic reaction $f(u)$, then it can be shown (Frank-Kamenetskii [7], Weber, Wake and Balakrishnan [19] and references therein) that the temperature variable u must satisfy

$$\nabla^2 u + f(u) = 0. \tag{1}$$

This equation represents a steady-state and non-dimensionalised statement of the principle of conservation of energy and as such is the starting point for many investi-gations into thermal ignition theory.

In earlier modelling and theoretical work, the reaction function $f(u)$ was taken as being proportional to the exponential function (that is, δe^u). However, more recently, it has been conclusively demonstrated by Gray and Wake [12] that there are tangible benefits (such as a more simple correspondence between the ambient temperature and bifurcation parameters) if the full temperature dependence of the Arrhenius function is retained. Consequently, we shall focus our investigation on (1) with $f(u) = \lambda e^{-1/u}$ (λ is a constant dependent upon the thermo-physical properties of the exothermic material under consideration). Furthermore, Gidas, Ni and Nirenberg [10] have shown that all positive solutions of (1) satisfying Dirichlet boundary conditions are radially symmetric, so we use spherical coordinates and (1) then becomes

$$\frac{d^2 u}{dr^2} + \frac{2}{r}\frac{du}{dr} + \lambda e^{-1/u} = 0. \tag{2}$$

Naturally this equation will need to be solved for the temperature u, as a function of the radial coordinate r and the parameter λ, subject to the appropriate Dirichlet boundary conditions.

In order to keep the subsequent analysis and presentation of results reasonably simple, we shall restrict our study to the case where the exterior is held at a constant
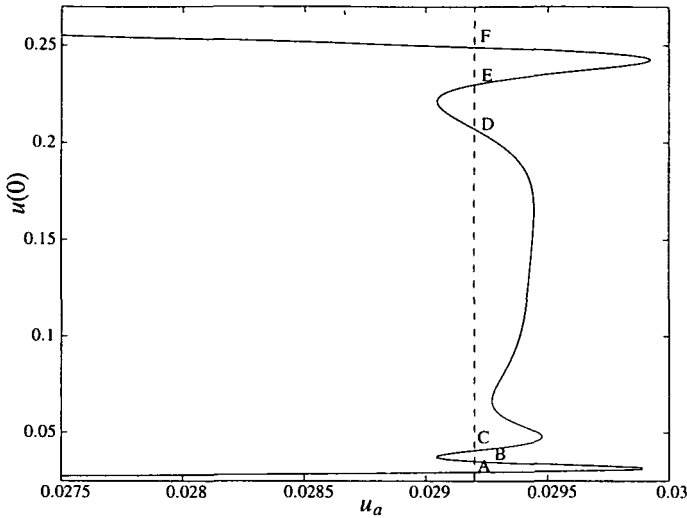
FIGURE 1. Bifurcation diagram showing the central temperature $u(0)$ as a function of ambient temperature u_a for fixed $\lambda = 10^{12}$ for a unit sphere. Unstable, intermediate, steady state profiles are labelled B, C, D, E and F for $u_a = 0.0292$.

temperature; called the ambient temperature and denoted u_a. Due to the use of dimensionless parameters, we can assume, without loss of generality, that the sphere has unit radius. Hence our boundary conditions can be written as

$$\frac{du}{dr}\bigg|_{r=0} = 0, \tag{3a}$$

$$u(1) = u_a. \tag{3b}$$

The first of these is merely a statement requiring bounded solutions at the centre of our spherically symmetric domain. Additionally, it should be noted that our choice of reasonably simple boundary conditions is not essential for the surprisingly complex solutions which we will display. It does, however, make our task of presenting, explaining and analysing the results somewhat easier and (hopefully) less confusing.

Solutions of (2) subject to boundary conditions (3) need to be constructed numerically (with the possible exception of a series approach for the simple exponential reaction as detailed in Frank-Kamenetskii [7]). Certainly there has been considerable effort in this direction and a consistent picture of the results has emerged. For sufficiently large λ and for some $0 < u_a < 1/4$, there is found to exist one low temperature solution, stable to temporal perturbations, and one high temperature solution, also stable to temporal perturbations. In addition, there exists a large number of intermediate solutions, all of which are unstable to temporal perturbations. This
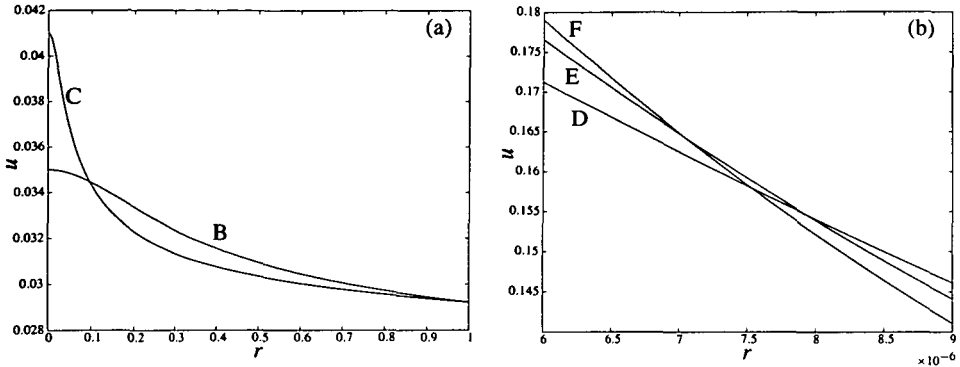
FIGURE 2. Unstable, intermediate, steady state profiles corresponding to points in Figure 1 (that is, $u_a = 0.0292$). Note the different scales in (a) and (b) required in order to clearly display these profiles.

is best displayed and understood with a bifurcation diagram, plotting the maximal steady state temperature $u(0)$ as a function of a bifurcation parameter; for example u_a, and holding the other parameter, λ, constant. In Figure 1, the result for $\lambda = 10^{12}$, a realistic value for milk powder (see Weber *et al.* [19]), is shown and it can be clearly seen that for certain values of u_a, there exist five intermediate steady states; all of which turn out to be unstable if analysed by a linear, temporal, stability analysis or if analysed numerically. Note that due to scaling difficulties, the high temperature branch is not shown on Figure 1.

The bifurcation diagram was obtained using MATLAB™. The results were checked by using the path following software AUTO97.

3. Spatial profiles of steady state solutions

Spatial profiles of the steady state temperature were also obtained numerically by a shooting method; integrating from the already known central temperature out to the temperature at the exterior of the sphere (u_a).

As an example we display in Figures 2 (a) and 2 (b) the results for the points labelled B, C, D, E and F in Figure 1. It is apparent that these five points all have the same values for the parameters λ and u_a, yet they correspond to different, unstable, intermediate, temperature profiles. Furthermore, it can be clearly seen that these profiles cross each other so that the one with the highest value for $u(0)$ ends up below all of the others near the exterior of the sphere. To see this, it is necessary to note that different scales were required on the axes so that the distributions could be clearly displayed. We also note the natural ordering of the crossing points, as indicated schematically in Figure 3. Namely, if $u_i(0) < u_j(0) < u_k(0)$ for intermediate steady states, then the coordinate values where crossing occurs is given by $r_{jk} < r_{ik} < r_{ij}$. Part of this will be rigorously
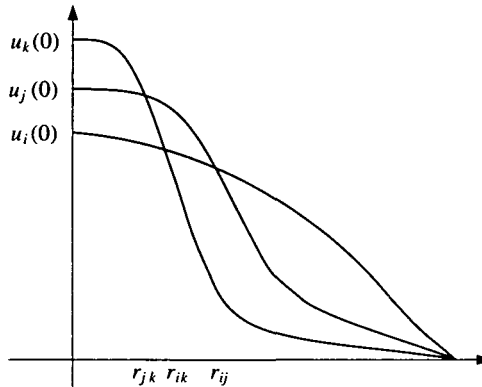
FIGURE 3. Schematic of the unstable, intermediate, steady state profiles showing the ordering of the crossing points.

proven in Section 5.

4. Crossing as a natural requirement of the evolution of initial conditions

Having noted from the numerical results that the spatial distributions of the unstable intermediate steady states cross, we naturally wonder if this is a general requirement, or if we are considering a special case. Prior to proving that this is indeed a general requirement (in the next section) we shall consider reasons for this which follow from ideas on the evolution of initial conditions applied to the semi-linear parabolic equation

$$u_t = u_{rr} + \frac{2}{r} u_r + \lambda e^{-1/u}. \tag{4}$$

Assume that there exist two, unstable, intermediate, steady state profiles as solutions to (4) with boundary conditions (3), that their profiles do not cross on $r \in [0, 1]$ and that there is no stable steady state profile in between these two. Then, as an initial condition begin with the average of these two, unstable, intermediate, steady state profiles. Clearly the evolution of this initial profile will be constrained to lie between the unstable profiles (for such equations, extremum principles, for example, Protter and Weinberger [17], prove that profiles everywhere below cannot cross at some later time). At the same time, the initial profile cannot find a steady state to evolve towards, so it would seem that it must be ever changing in time. Norbury and Wake [16] have proven that evolving solutions to partial differential equations such as (4) cannot oscillate with a fixed frequency. Consequently the only fate for such an initial profile

would be to evolve randomly in time while being constrained to lie in between the two unstable, intermediate, steady state profiles. This is a most unlikely scenario and we are led to conclude that our supposition that the profiles do not cross is incorrect. Hence we expect the crossing of unstable, intermediate, steady state profiles to be required.

5. Crossing proof and estimates for crossing points

Multiply (2) by r^2 and integrate from 0 to r, obtaining

$$r^2 u'(r) = - \int_0^r s^2 f(u(s)) \, ds < 0, \tag{5}$$

so that every solution $u(r)$ of (2) and (3) is monotone decreasing on [0,1]. Define $g(u, u_i) = (f(u) - f(u_i))/(u - u_i)$ (where u_i is some solution to be defined later) and differentiate with respect to u yielding

$$\frac{\partial g}{\partial u} = \frac{f(u)}{u^2(u - u_i)^2} \left[u - u_i + u^2 \left(\frac{f(u_i)}{f(u)} - 1 \right) \right] = \frac{f(u)}{u^2(u - u_i)^2} G(u) \tag{6}$$

with $G(u)$ defined to be the contents of the square bracket. Then $G(u_i) = 0$ and $G'(u) = (2u - 1)(f(u_i)/f(u) - 1) > 0$, for $u_i < u < 0.5$, so $G(u)$ is positive and $g(u, u_i)$ is strictly increasing in $u_i < u < 0.5$. Denote the low temperature stable solution by $u_{\min}(r)$, then any other solution $u(r)$ must satisfy $u_{\min}(r) \leq u(r)$ at every point in the domain $0 \leq r \leq 1$.

THEOREM 1. *Let $u_1(r)$ and $u_2(r)$ be two intermediate solutions of (2) and (3), with $u_{\min}(0) < u_1(0) < u_2(0) < 0.5$. Then there is at least one value $0 < r_{12} < 1$ such that $u_1(r_{12}) = u_2(r_{12})$.*

PROOF. Assume that $u_2 > u_1$ on [0, 1) and define $v_i = u_i - u_{\min}$, $i = 1, 2$, so that $v_2 > v_1 > 0$ in [0, 1) and $v_1(1) = v_2(1) = 0$. By Green's theorem

$$\int_{|r|<1} (v_1 \nabla^2 v_2 - v_2 \nabla^2 v_1) \, dV = \int_{|r|=1} (v_1(v_2)_n - v_2(v_1)_n) \, dS = 0. \tag{7}$$

However, $\nabla^2 v_i = \nabla^2 u_i - \nabla^2 u_{\min} = f(u_{\min}) - f(u_i)$, so that (7) becomes

$$0 = \int_{|r|<1} (v_1 v_2 [g(u_1, u_{\min}) - g(u_2, u_{\min})]) \, dV < 0, \tag{8}$$

which is a contradiction, since $g(u_1(r), u_{\min}(r)) < g(u_2(r), u_{\min}(r))$ as g is strictly increasing.

THEOREM 2. *Let u_1, u_2, and u_3 be three intermediate solutions of* (2) *and* (3), *with* $u_{min}(0) < u_1(0) < u_2(0) < u_3(0) < 0.5$. *Then* $r_{23} < r_{13}$ *and* $r_{23} < r_{12}$.

PROOF. The functions $z = u_3 - u_1$ and $w = u_2 - u_1$ satisfy the boundary value problems

$$
\begin{aligned}
(r^2 z')' + r^2 g(u_1, u_3)z = 0, &\qquad z'(0) = z(1) = 0, \\
(r^2 w')' + r^2 g(u_1, u_2)w = 0, &\qquad w'(0) = w(1) = 0.
\end{aligned}
\tag{9}
$$

Assume $r_{23} \geq r_{12}$, so that $u_3 > u_2 > u_1$ and $g(u_1, u_2) > g(u_1, u_2)$ on $|r| < r_{12}$. Multiply the first equation in (9) by w and the second by z and subtract:

$$
(r^2 w')' - (r^2 w')'z + r^2[g(u_1, u_3) - g(u_1, u_2)]zw = 0.
$$

Integrating over $(0, r_{12})$ yields

$$
\begin{aligned}
0 &< \int_0^{r_{12}} r^2[g(u_1, u_3) - g(u_1, u_2)]zw \, dr = - \int_0^{r_{12}} [(r^2 z')'w - (r^2 w')'z] \, dr \\
&= [(r^2 w')z - (r^2 z')w]_0^{r_{12}} = r_{12}^2 z(r_{12})w'(r_{12}) < 0
\end{aligned}
$$

which is impossible. Hence $r_{23} < r_{12}$ and by continuity it follows that $r_{23} < r_{13}$.

We have not been able to prove that $r_{13} < r_{12}$ although the numerical profiles suggest this is true. The proofs of Theorems 1 and 2 can be generalized to n-dimensional space.

THEOREM 3. *Let u_1 and u_2 be two intermediate solutions of* (2) *and* (3), *with* $u_{min}(0) < u_1(0) < u_2(0) < 0.5$. *Then, if ρ is the last value in* $(0, 1)$ *at which* $u_1(\rho) = u_2(\rho)$,

$$
4 < \frac{4}{(1 - \rho)^2} \leq f'(u_1(\rho)) < f'(u_1(0)).
\tag{10}
$$

PROOF. Let $w = u_2 - u_1$ satisfy (9). Then $y = rw$ is a nontrivial solution of the boundary value problem in region $(\rho, 1)$:

$$
y'' + g(u_1, u_2)y = 0 \quad \text{in} \quad (\rho, 1), \ y(\rho) = y(1) = 0.
\tag{11}
$$

By Lyapunov's theorem (see for example Hartman [13, p. 346]), since y has at least two zeros in $[\rho, 1]$,

$$
\frac{4}{1 - \rho} < \int_\rho^1 g(u_1(r), u_2(r)) \, dr \leq g(u_2(\rho), u_2(\rho))(1 - \rho) = f'(u_1(\rho))(1 - \rho).
$$

REMARK. Since $f'(u)$ is monotone increasing in $0 < u < 0.5$, it is useful to determine where $f'(u_0) = 4$. For example this occurs when $\lambda = 10^{12}$ at approximately $u_0 = 0.0300724586$. Consequently all pairs of intermediate solutions must have their last crossover above u_0. This is certainly the case in Figure 2. Further, the initial values of the intermediate solutions must exceed u_0, suggesting that u_0 determines the rightmost limit point in Figure 1.

6. Conclusion

The evolution of certain initial conditions is clearly influenced by the crossing of the infinity of unstable steady states. We have proven and demonstrated interesting properties of the spatially distributed unstable steady states, in particular the crossing over of the distributions which is a necessary consequence of well known properties of the ordinary differential equation, as well as the instability of the intermediate steady states. The consequences for the crossing with the inclusion of fuel consumption is currently under investigation.

Acknowledgements

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