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CRITERIA FOR UNIQUE SOLUTION OF A RADIAL POROUS MEDIUM COMBUSTION

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ABSTRACT

The problem of finding conditions for a unique solution is considered. New criteria for a unique and global existence are found. These are achieved through numerical method.

1. INTRODUCTION

Semi-linear parabolic equation of the form

$$u_t = \ u + f(u) \qquad (1)$$

are known to be capable of exhibiting blow-up for functions f which grow sufficiently fast with u. If we considered the initial boundary problem which is (1) in some open bounded region Ω in $\Re^n$, $t > 0$ with the (linear) boundary condition

$$Bu \equiv \alpha u_n + (1 - \alpha)u = 0, \text{ on } \ , t > 0 \qquad (2)$$

where we assume $\partial\Omega$ is smooth, $0 \leq \ (x) \leq 1$, u_n is the outer normal derivative on $\partial\Omega$, and the initial method condition is

$$u(x, 0) = \phi(x) \text{ in } \overline{\Omega} \text{ at } t = 0$$

Lacey et. al. [8] claimed that the solution u(x, t) is unbounded above as $t \to t^* < \infty$, t^* is called blow-up time.

In this paper, we consider (1) as modelling and exothermic chemical reaction, with u representing temperature and f being essentially the temperature-dependent reaction rate. The representation by a single equation, so that reactant depletion is neglected is valid provided that u does not get too large.

In this case the reaction rate which is more accurately modelled by the Arrherius law

$$f(u) = \frac{\lambda_1 e^{\frac{u}{1+\epsilon u}}}{\lambda_2 e^{\frac{u}{1+\epsilon u}} + 1} \qquad (3)$$

can be approximated by an exponential function (the Frank-Kamenetskii's approximation) see Boddington et al [2]

$$f(u) = \lambda e^{u} \text{ for some } \lambda > 0 \text{ (see Boddington et. al.[2])}.$$

Also when

$$f(u) = \lambda e^{(u/1+\epsilon u)}$$

has been studied (see Lacey et. al. [8]).
For such problems, where f(s), f'(s), and f''(s) are all positive for $s \geq 0$ and

$$\int_0^\infty \frac{ds}{f(s)} < \infty \tag{4}$$

It has been shown that for region Ω, λ, or α sufficiently large that there is no steady state solution of (1), (2) (see Keller and Cohen [6], Lacey [8], Bellout [3]).

In this case there is ignition for physical system being modelled. As the temperature u becomes large thermal runaway occurs (see Ayeni [1]).
In many applications, the region and boundary conditions are such that the steady-states are possible, but given sufficiently large initial data, the system still blows up.

In this paper, we are considering the practical application due to Koriko [6]. Consider a non-reacting flow through a porous cylindrical shell with inner and outer radii r_1 and r_2. At these surfaces the pressures are known to be p_1 and p_2 respectively.

From the flow of a fluid through a porous medium the equations continuity and motion may be replaced by the modified equation of continuity

$$\epsilon_1 \frac{\partial p}{\partial t} = -\nabla \rho V_{or} \tag{5}$$

Darcy's law

$$V_{or} = -\frac{\phi(\nabla p - \rho g)}{\mu} \tag{6}$$

The velocity V_{or} in these equations is the superficial velocity (volume rate of flow through a unit cross-sectional area of the solid plus fluid averaged over a small region of space) small with respect to macroscopic dimensions in the flow system but large with respect to the size.

The quantities ρ and p are density and pressure respectively averaged over a region available to flow that is large with respect to the pore size.

Equation (5) and (6) can be combined to give

$$\epsilon_1 \frac{\partial p}{\partial t} = -\frac{\phi}{\mu}\nabla.[\rho(\nabla p - \rho g)] \qquad (7)$$

In this case gravity is zero and when ρ is constant (in-compressible fluid) Therefore

$$\nabla^2 p = 0 \qquad (8)$$

Hence

$$V_{or} = \left\{-\frac{\phi}{\mu}\frac{(p_2 - p_1)}{\ln r_2 | r_1}\right\}\frac{1}{r} \qquad (9)$$

$$= -\frac{\delta_1}{r}$$

where

$$\delta_1 = -\frac{\phi}{\mu}\frac{(p_2 - p_1)}{\ln r_2 | r_1} \qquad (10)$$

The general mathematical formulation for planar case are due to Norbury and Lawson [9].

The equations governing the concentration of the solid and the gas species are simply mass conservation laws. Since the solid is stationery, the chemical reaction is the only effect of any importance to equations (11) follows.

The presence of mass transport effect means that the conservation of mass for each of the gas components gives rise to the continuity equation as shown in equation (12), Q_k and q_k are reaction terms.

The dominant heat processes in the gas are the convection and the heat transfer from the solid. There is no heat source term from the combustion because the reaction sites are in the porous material and so the heat energy generated by the reaction can only enter the gas by being transferred from the solid. Thus equation (16) follows. The solid heat energy balance must include terms to represent the heat generated by the reaction heat transfer between the solid and the gas and conduction, radiation and heat storage. Thus equation (13) follows. The effect of heat transfer modelled by a linear exchange term and the effect of radiation and conduction are combined to form a single non-linear diffusion term. We take the radiation coefficients of the form $\beta_1 T^3_s$ (β_1 is a constant, the product of emissivity of the solid, its radiation length and Stefan

Boltzman number). Since the usual radiation term is proportional to T^4_s occurs between elements of the solid in the porous medium that are near to each other and are separated by only small temperature differences.

The heat capacity T_s depends on the composition of the solid phase and $D'\lambda$ represents the heat source due to chemical reaction. Therefore λ is the heat of the reaction. Since the air passing through the porous medium is a mixture of ideal gases, we take the ideal gas law together with Darcy's law as the relevant constraints to determine the pressure variations and the movement of the gas.

The porosities of the medium are typically greater than 0.5, so that over 50 percent of the medium is occupied by gas. The resultant driving pressure variations are small and negligible compared with temperature variations. Thus we approximate the ideal gas law by Charles' law;
The governing equations are given below

$$\frac{\partial \gamma_k}{\partial t} = M_k Q_k \qquad k = 1, 2 \tag{11}$$

$$\frac{\partial \gamma_k}{\partial t} + \frac{\partial (v_r \alpha_k)}{\partial r} = M_k q s_k \qquad k = 1, 2, 3 \tag{12}$$

$$\sigma_s \frac{\partial T_s}{\partial t} = \frac{1}{r}\left\{\frac{\partial}{\partial r}\left[r\left(\beta_1 T^3_s + \beta_2\right)\frac{\partial T_s}{\partial r}\right]\right\} + h_c(T_g - T_s) + D'\lambda \tag{13}$$

$$\lambda = \frac{kb\,[\gamma]\,[\alpha]}{k\,[\gamma] + b} \tag{14}$$

$$k = Ae^{-E/RTS} \tag{15}$$

k the Arrhennos reaction rate, where A and E depends upon the materials involved in the combustion reaction).

$$\sigma_g \frac{\partial T_g}{\partial t} + V_r \frac{\partial T_g}{\partial r} = f(T_s - T_g) \tag{16}$$

The medium has porosity function ϕ so that the unit volume of space is occupied by $(1 - \phi)$ units of solid and ϕ units of gas. The function ϕ depends on the concentrations of unburnt material and ash.

$$T_g \rho_g = T_g \left(\sum_{k=1}^{3} \alpha_k\right) \Big/ \phi = \text{constant on air parcels} \tag{17}$$

In all these equations

M_k and m_k are the molecular weights of the solid and gas species respectively .

D^1	:	the heat of reaction is a positive constant since the reaction is exothermic
δ_s	:	Heat capacity of solid
δ_g	:	Heat capacity of gas
hc	:	Heat transfer between solid and the gas
E	:	Activation energy
$\in$	:	$\frac{RT_o}{E}$
γ_1	:	The mass of unburnt material (carbon)
γ_2	:	The mass of ash per unit volume of space
α_1	:	Mass of carbondioxide per unit volume of space
α_2	:	Mass of oxygen per unit volume of space
α_3	:	Mass of Nitrogen per unit volume of space

$u = \frac{T_s - T_0}{\in T_0}$ ... dimensionless solid temperature

$v = \frac{T_g - T_0}{\in T_0}$ ... dimensionless gas temperature

The heat capacities of the solid and the gas species are defined as follows (see Norbury and Stuart [10])

$$\sigma_s = \sum_{k=1}^{2} C_{sk}\,\gamma_k \tag{18}$$

$$\sigma_g = \sum_{k=1}^{2} C_{gk}\,\gamma_k \tag{19}$$

Where C_{sk} and C_{gk} are the specific heats of the individual solid and the gas components. The source terms Q_k and q_k are all proportional to the reaction rate λ. Specifically

$$Q_1 = \lambda \qquad Q_2 = -\lambda$$
$$q_1 = \lambda \qquad q_2 = -\lambda \tag{20}$$
$$q_3 = 0$$

Baker [3] has demonstrated experimentally that b is given by

$$b = \eta(\phi) / \sqrt{V_{r\,mean}}\, Tog \qquad (21)$$

where η is a constant proportional to Φ and m ≈ 2.5
Introducing non-dimensional variables into equations (13) and (16), we arrive at t the following equation.

$$\frac{\partial T_s}{\partial t} = \frac{A}{r}\frac{\partial}{\partial r}\, r\,(T_s^3 + w)\frac{\partial T_s}{\partial r} + h\,(T_g - T_s + D^* \lambda \qquad (22)$$

$$\frac{\partial T_g}{\partial t} + \frac{e}{r}\frac{\partial T_g}{\partial r} = f(T_s - T_g) \qquad (23)$$

where

$$A = k,\, R_o\, d_1$$

$$W = \frac{d_2}{R_o d_1}$$

$$D^* = \frac{D'\theta}{\sigma_s}$$

$$f = \frac{ct_o}{\Sigma_g \sigma_g}$$

$$e = \frac{V_o}{\Sigma_g \sigma_g}$$

Let $$\lambda = \frac{D_1\, e^{-E/RTs}}{D_2\, e^{-E/RTs}} + b \qquad (24)$$

Suppose

$$D_1 = \lambda_1 e^{E/RTo}$$

$$D_2 = \lambda_2 e^{E/RT}$$

we take the expansion of the temperature as follows

$$T_s = T_o(1 + \in u)$$

$$T_g = T_o(1 + \in v) \qquad (26)$$

substituting for λ, D_1, D_2, T_s and T_g in (22) and (23), we obtain

$$\frac{\partial u}{\partial t} = \frac{A}{r}\frac{\partial}{\partial_r}\left\{(r\,T_o^3(1 + \in_u)^3 + w)\frac{\partial u}{\partial r}\right\} + h(v - u) + \frac{\lambda_1 e^{u/(1 + \in u)}}{\lambda_2 e^{u/(1 + \in u)}} + b \qquad (27)$$

$$\frac{\partial v}{\partial t} + \frac{e}{r}\frac{\partial v}{\partial r} = f(u - v) \qquad (28)$$

Boundary conditions

$$u(i, t) = u(l, t) = 0$$
$$v(i, t) = 0 \qquad (29)$$

For $f \longrightarrow \infty$

$$T_s = T_g = u \qquad (30)$$

Now considering steady state with

$\in = 0$ and $w = 0$, (27) becomes

$$\frac{d^2u}{dr^2} + \left(1 + \frac{\delta}{A}\right)\frac{1}{r}\frac{du}{dr} + \frac{\lambda_1 e^u}{\lambda_1 e^u + b} = 0$$

$$u(1) = u(L) = 0 \qquad (31)$$

The principal aim of this paper is to establish that for some values of λ_1 and λ_2 there is no blow up.

That is we want to examine the uniqueness of solution of (31). Hence give the practical implications. This fact is achieved through numerical methods.

2. NUMERICAL METHOD OF SOLUTION

Now consider equation (31) with $\frac{\delta}{A} = 0$ using the transformation r = ax

$$\frac{d^2u}{dx^2} + \frac{1}{x}\frac{du}{dx} + \frac{a^2\lambda_1 e^u}{\lambda_2 e^u + 1} = 0 \qquad (32)$$

using the fact that

$$u(1) = u(L) = 0$$

Suppose the solution u(x) of (32) attains its maximum at $x = \left(\frac{L+1}{2}\right)$

We now consider the transformation

$$x = \frac{1+L}{2} + \frac{L-1}{2}y \qquad (33)$$

when

$$x = \left(\frac{L+1}{2}\right)$$
$$y = 0$$

when

$$x = L$$
$$y = 1$$

we now wish to replace the boundary conditions at x = L by

$$u_x\left(\frac{L+1}{2}\right) = 0$$

Hence we have a modified boundary value problem

$$\frac{d^2u}{dx^2} + \frac{1}{x}\frac{du}{dx} + \frac{\lambda_1 e^u}{\lambda_1 e^u + b} = 0$$
$$u_x(0) = 0$$
$$u(1) = 0$$

However, we shall run unto problem of singularity with the middle term

$$\frac{1}{x}\frac{du}{dx}$$

In order to avoid this problem, we adapt the methods of Hicks and Weisz [11] as follows:

Expand du/dx in a Taylor series about x = 0

$$\frac{du}{dx} = \left(\frac{du}{dx}\right)_{x=0} + x\left(\frac{d^2u}{dx^2}\right)_{x=0} + \frac{x^2}{2!}\left(\frac{d^3u}{dx^3}\right)_{x=0} + \ldots$$

since odd derivatives are zero because of symmetry, we have

$$\frac{du}{dx} = x\left(\frac{d^2u}{dx^2}\right)_{x=0} + \frac{x^3}{3!}\left(\frac{d^4u}{dx^4}\right)_{x=0} + \ldots$$

Since $\left[\frac{du}{dx}\right] = x\left[\frac{d^3u}{dx^3}\right]_{x=0} = \left[\frac{d^5u}{dx^5}\right]_{x=0} = 0$

$$\frac{1}{x}\left[\frac{du}{dx}\right] = \frac{1}{2}\left[\frac{d^2u}{dx^2}\right]_{x=0}$$

(Neglecting terms higher than order 2)
Therefore

$$\underset{x\to 0}{\text{limit}}\ \frac{1}{x}\frac{du}{dx} = \frac{1}{2}\left(\frac{d^2u}{dx^2}\right)_{x=0}$$

and

$$\left(\frac{d^2u}{dx^2}\right)_{x=0} = \frac{-\frac{1}{2}a^2\lambda_1 e^{u_0}}{\lambda_2 e^{u_0} + 1} \tag{34}$$

Now to solve (32) we shall make use of (34) as follows

Consider

$$\left(u_x\right)_{0.01} = \left(u_x\right)_{x=0} + 0.01\left(u_{xx}\right)_{x=0} + \frac{0.001^2}{2}\left(u_{xxx}\right)_{x=0} + \ldots$$

Neglecting terms than order two, we have

$$\left(u_x\right)(0.001) = u_x(0.00) - \frac{0.01a^2\lambda_1 e^{u_0}}{2\lambda_2 e^{u_0}+1}\left(u_{xx}\right)_{x=0}$$

Hence our boundary value problem (32) can be solved with shooting method that uses Runge-Kutta fourth method as its integrator with the following boundary conditions.

$$u(1) = 0$$

$$\left(u_x\right)(0.01) = \frac{0.01a^2\lambda_1 e^{u_0}}{2\lambda_2 e^{u_0}+1}$$

DISCUSSION OF RESULTS

We were able to show that the solution is unique when $\lambda_1 > 0$ and $\lambda_2 > 1$. Also we found that there exists a critical value λ_1^{cr} when $\lambda_2 > 0$ for which any $0 < \lambda_1 < \lambda_1^{cr}$ there are multiple solutions. When λ_2 is zero, a fortiori there are multiple solutions for any $0 < \lambda_1 < \lambda_1^{cr}$ see Kapila [5].

In figure 1, $\in = 0.1, \lambda_1 = 0.01$, we can see that there exist a λ_1^{cr} such that the equation under investigation has multiple solutions for $0.25 < \lambda_1 < \lambda_1^{cr}$ =1.09.

The solution as displaced on this diagram is a graph of the maximum value of u against λ_1. As can be seen λ_1 passes through a minimum and finally grows without bound as u tends towards infinity.

Also figure 2 shows the case $\in = 0.1, \lambda_2 = 0.01$, in our equation. λ_1 shows a maximum value at a finite value of u. Beyond this value λ_1 grows steadily as u increases Also this curve shows that there exists a critical value of λ_1 below which there are multiple solutions for the problem and above this the solution does not exist.

Figure 3 is the case $\in = 0.1, \lambda_2 = 0.1$. The figure shows that the solution of the equation exists and unique for all value of λ_2

The further shows that for $\in = 0 < \lambda_2 < 0.1$, there are multiple solutions for the equation but for $\lambda_2 \geq 0.1$ the equation has a unique solution for all λ_1.

4 PHYSICAL IMPLICATIONS OF THE RESULT

Figure 1 is said to be s – shaped and the minimum corresponds to ignition while the maximum corresponds to extinction. The ability to determine the ignition and extinction time are of special interest to combustion engineers most especially those in explosives. The reason being that it is necessary for them to know whether a reaction will explode or not and if it does, how long is the safe period.

The multiple solutions obtained raises a lot of questions as regards the stability of the problem. The number of solutions is very important because in the case of multiple solutions some of solutions may not be stable. Apart from this, a system designed with a solution in mind may not give optimal performance when there are two or more solutions, since the system may eventually prefer the solution which was not envisaged.

One of the major accomplishment of this work is the ability to find suitable conditions for uniqueness of solution. The response diagram in figure 4, shows that the solution exists and unique for all Frank-Kamenetskii parameter λ_1.

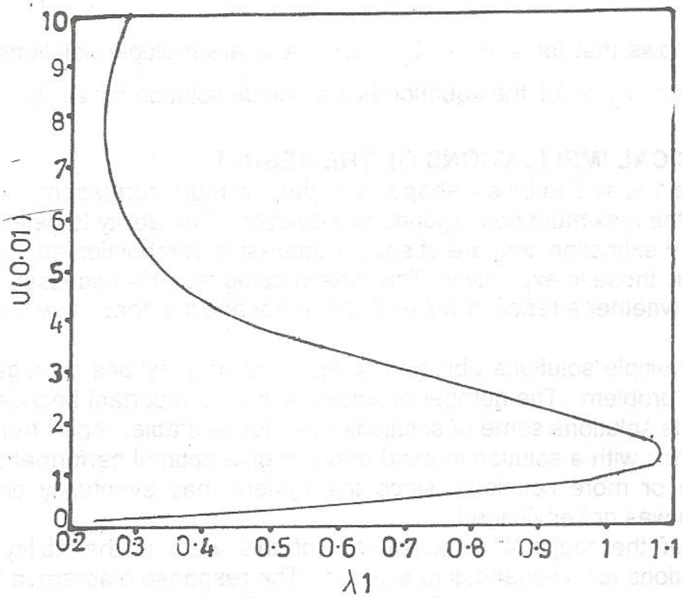

Fig 1: Curve of U(0·01) against $\lambda 1$ when $\lambda 1$=0·01
ε = 0·1

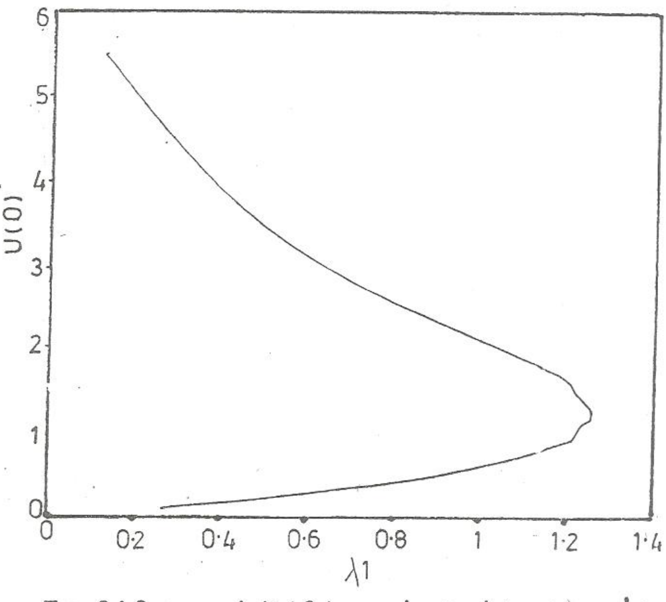

Fig 2: Curve of U(0) against $\lambda 1$ when $\lambda 2$=0·01
ε = 0·1

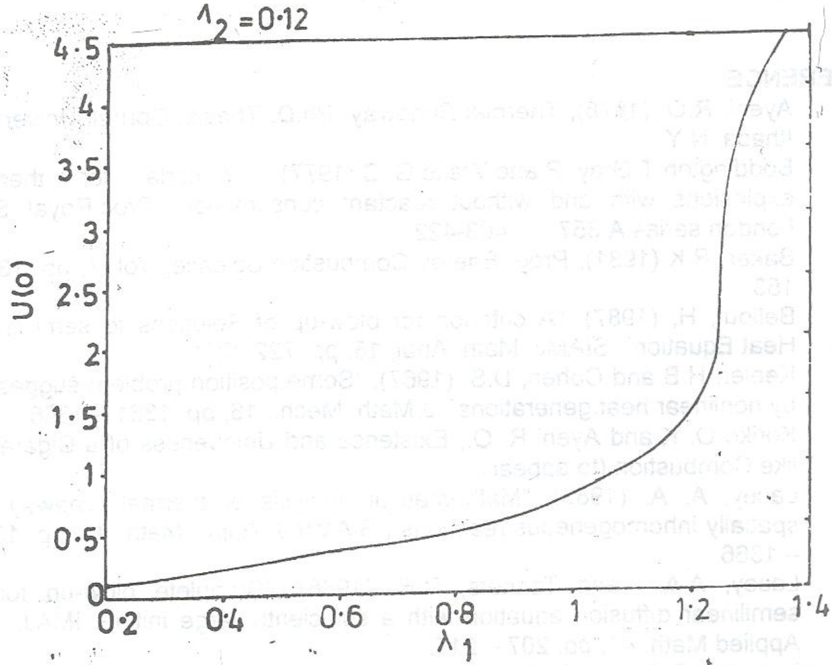

Fig 3 : Curve of U(0·1) against λ1 when λ2=0·12 ε=0·1

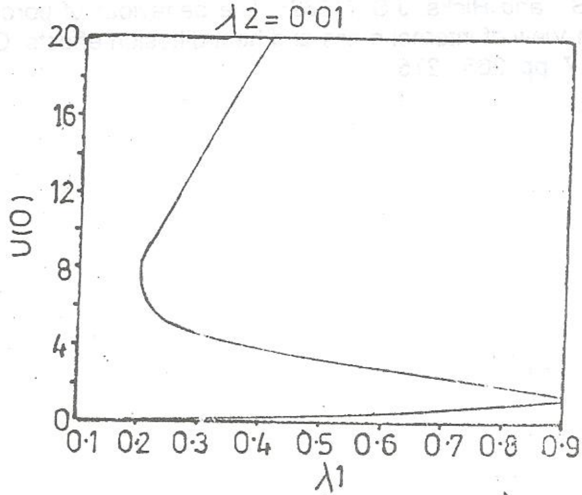

Fig 4 : Curve of U(O) against λ1 when $\lambda_2 = 0.01$ $\epsilon = 0.1$

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