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THE EFFECT OF A SPATIAL VARIABLE ON THE CRITICALITY OF A BOUNDARY VALUE PROBLEM

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Abstract. The aim of this work is to investigate the effect of the function, $f(x) > 0$ on the boundary value problem

$$\frac{d^2\theta}{dx^2} + \frac{j}{x}\frac{d\theta}{dx} + \delta f(x)\exp(\theta) = 0$$

$$\frac{d\theta}{dx}(x = s) \ = \ 0 \qquad \theta(1) \ = \ 0$$

for some $f(x) > 0$. We established that there exist a $\delta_{cr} > 0$, such that if $0 \leq \delta \leq \delta_{cr}$, a steady state solution for the boundary value problem exist, while for $\delta > \delta_{cr}$, no solution exist. Analytical solutions were obtained for some $f(x) > 0$ and geometry, while a numerical method is applied to others where analytical method fails. In particular, the variational method was implemented using the Mathematica software package. These solutions have thus given us the choice of comparing the behaviour of the solutions for the special cases of slab and cylinder. Our results have not only confirmed previous, it has has facilitated a better understanding of the problem not previously considered.

1. INTRODUCTION

The concept of criticality or non-existence of steady state solutions in boundary value problems has been established several decades ago. This may not be unconnected with the physical applications of the study, especially in science and technological applications. This paper is concerned with the class of solutions for the boundary value problem,

$$\frac{d^2\theta}{dx^2} + \frac{j}{x}\frac{d\theta}{dx} + \delta f(x)\exp(\theta) = 0 \tag{1}$$

$$\frac{d\theta}{dx}(x = s) = 0 \qquad \theta(1) = 0, \tag{2}$$

where j is the geometry factor ($j = 0, 1$, for slab and cylinder respectively), δ is the Frank-Kamenetskii parameter which determines non-existence of the steady state solutions (criticality), θ is the temperature and x is the spatial coordinate. The task here is to examine how some function ($f(x) > 0$) would affect the solutions of (1) and (2). The function $f(x) > 0$ takes a variety of forms depending on the nature of the problem. Stolin et al. [8] obtained an analytical expressions for the critical conditions under which hydrodynamic thermal explosion in power law fluids may be expected in flat($j = 0$) or cylindrical rotary viscosimeter ($j = 1$) under various thermal conditions at the walls for $s = -1$ and $f(x) = 1$. Subcritical conditions for steady temperature and velocity fields are determined. Hill and Marchant [6] has also studied the critical conditions for thermal explosion for the problem where $f(x) = 1$ and $s = 0$ for the slab and the cylinder, using a numerical method. They also carried out a stability analysis of the solutions and their results is good in agreement with the well known exact solution in literature. Instead of the interval $0 < s < 1$ considered by Hill and Marchant [6], Novozhilov et al [12], studied the thermal explosion of same problem in the interval $0 \le a < s < b \le 1$ and the criticality formulation in the three regions is investigated. Here the critical parameter δ_{cr} which is the requirement for criticality (or thermal explosion), now depends on a and b. This problem is solved by a numerical method and the effect of stirring on the criticality or thermal explosion of the system is shown.

In the modelling of Microwave, Hill and Pincombe [7] considered the spatial dependence,

$$f(x) \;=\; \exp(-\beta x), \qquad \beta > 0, \tag{3}$$

as an approximation of the electric field intensity which decays exponentially. Similarly, Coleman [3] proposed a polynomial decay,

$$f(x) \;=\; \alpha_1 x^{-\beta}, \qquad \beta > 0 \tag{4}$$

which may be seen as the Taylor's series expansion of (3) about the origin, where α_1 is a constant.

Okoya [9] obtained new exact solutions for a variation of (1) and (2) with source term which decreases spatially and increases with temperature. These solutions are derived for the infinite slab, infinite cylinder and sphere through a simple Mathematical procedure. Recently Okoya and Ajadi [10] also studied a variation of (1) and (2), where the thermal conductivity is a function of temperature and the source term decreasing spatially. They ascertain the way in which thermal explosion is affected by different boundary conditions for $\beta > 0$. In combustion modelling, $f(x)$ is known to be an approximation of the concentration of the reactants, where $\beta > 0$ is the order of the reactants. Specifically, Choi [2] studied (1) and (2) for the slab ($j = 0$) for $f(x) \in C^1(0,1]$ for isothermal boundary conditions. They showed using some qualitative argument, that there exist a δ_{cr} such that for $0 \leq \delta \leq \delta_{cr}$, a solution is in $C^1(0,1] \cap C^2(0,1]$. In general, the proposed functions $f(x)$ may satisfy the following properties;

(i) $f(x)$ is in $C^1(0,1]$

(ii) $f(x) > 0$ and can be singular at $x = 0$ (origin).

Since closed form (or exact) solutions are not always easy to come-by, approximate methods are usually employed. Boddington et al. [1] studied problems (1) and (2) for a pair of simultaneous exothermic reactions using a quadrature method earlier proposed for plane geometry (slab). A more flexible method, the variational method, is capable of handling all the geometries. Graham-Eagle et al. [4] extends the investigation of Boddington et al. [1] to the other two geometries of the infinite cylinder and sphere. There results are presented numerically in tabular form.

In our considerations, we have investigated criticality for the Slab and cylindrical geometries for a class of functions

$$f(x) \in \left\{1, x^{-\beta}, \exp(-\beta x)\right\}.$$

We presented in tabular form the variation of δ_{cr} with $s \in (0,1)$, where analytical solution is possible, while a tabular presentation variation of δ_{cr} with β was carried out where the variational method is used. This is so because the variational method has been developed for $s = 0$. However, the variational result for some fixed β at $s = 0$ is compared with that obtained by exact solution and there is a close agreement.

2. MATHEMATICAL FORMULATION

We study the non-existence of steady state solutions of the boundary value problem (1) and (2) for the slab and cylinder for the spatial functions; $f(x) = 1$, $f(x) = x^{-\beta}$ and $f(x) = \exp(-\beta x)$ using the analytical and the variational methods.

3. ANALYTICAL SOLUTIONS

3.1. THE PLANAR GEOMETRY (SLAB)

$\underline{f(x) \;=\; 1}$

In this consideration, equation (1) reduces to

$$\frac{d^2\theta}{dx^2} + \delta \exp(\theta) = 0, \tag{3}$$

which has a well known closed - form solution (see Stolin et al [8], Hill and Marchant [6] and Okoya [9]).

$$\exp(\theta) = \frac{A}{\cosh^2\left(\sqrt{\frac{A\delta}{2}}\ln x - B\right)}, \tag{4}$$

where A and B are constant of integration. Using the boundary conditions (2), we obtain

$$\sqrt{\frac{\delta}{2}} = \frac{B}{\ln s \cosh B}$$

and the expression for criticality is $\frac{d\delta}{dB} = 0$. Thus,

$$B \tanh B - 1 \ = \ 0, \quad \text{and } B_{cr} \ = \ 1.2$$

s	.1	.2	.3	.4	.5	.6	.7	.8	.9
δ_{cr}	.165687	.339135	.6060	1.046	1.828	3.3665	6.9050	17.64	79.13

Table 1. δ_{cr} against s.

From Table 1. δ is a monotonically increasing function of s.

$f(x) \ = \exp(-\beta x)$

Here equation (1) reduces to

$$\frac{d^2\theta}{dx^2} + \delta \exp(-\beta x) \exp(\theta) = 0. \tag{5}$$

By using the transformation $V = \theta - \beta x$, equation (5) reduces to

$$\frac{d^2V}{dx^2} + \delta \exp(\theta), \tag{6}$$

which is similar to (3). Hence the solution is

$$\exp(\theta) = \frac{A \exp(\beta x)}{\cosh^2\left(\sqrt{\frac{A\delta}{2}} \ln x - B\right)}. \tag{7}$$

By using the boundary condition (2), we obtain

$$A = \exp(-\beta) \cosh^2(B) \quad \text{and} \quad \sqrt{\frac{\delta}{2}} \ = \ \frac{\beta s \coth[\sqrt{\frac{A\delta}{2}} \ln(s) - B]}{2\sqrt{A}}. \tag{8}$$

Combining these equations, we obtain

$$\sqrt{\frac{\delta}{2}} = \frac{\beta s}{2} \frac{[\sqrt{\frac{\delta}{2}} \ln(s) \cosh B - B]}{\exp(\frac{-\beta}{2}) \cosh B}. \tag{9}$$

Thus the Mathematical expression for criticality i.e $\frac{d\delta}{dB} \ = \ 0$ and we obtain

$$2\left(1 - \sqrt{\frac{\delta}{2}} \sinh B \ln s\right) \coth(B) - \sinh\left[2(\sqrt{\frac{\delta}{2}} \ln(s) \cosh B - B)\right] = 0. \tag{10}$$

s	.1	.2	.3	.4	.5	.6	.7	.8
θ_{cr}	1.474	1.586	.883	1.642	1.617	1.568	1.498	1.4113
δ	0.442	0.793	0.1265	2.291	4.122	8.045	17.92	50.67

Table 2. δ_{cr} against s for $\beta = 2$.

From Table 2., we also observe that δ is monotonically increasing function of s. The case of $f(x) = x^{-\beta}$ cannot be solved analytically(see Sachdev [12]).

3.2. THE CYLINDRICAL GEOMETRY

$f(x) \;=\; 1$

The well known closed form solution for

$$\frac{d^2\theta}{dx^2} + \frac{1}{x}\frac{d\theta}{dx} + \delta \exp(\theta) = 0, \tag{11}$$

is

$$\theta(x) = B - 2\ln\left[1 + \frac{\delta \exp(B) x^2}{8}\right],$$

which becomes

$$\delta = 8\exp(-B)(\exp(\frac{B}{2}) - 1),$$

when the boundary conditions (2) for $s = 0$ is applied (see Hill and Marchant [6]). Similarly, the expression for criticality is

$$\frac{d\delta}{dB} = 0, \quad \text{which implies that} \quad \exp(-B_{cr})\left(\frac{-1}{2}\exp(\frac{B_{cr}}{2}) + 1\right) = 0. \tag{12}$$

Hence, $B_{cr} = 2\ln 2$ and $\delta_{cr} = 2$. The profiles of the solution in $0 < s < 1$ is not feasible.

$f(x) \;=\; x^{-\beta}$

In this case (1) reduces to

$$\frac{d^2\theta}{dx^2} + \frac{1}{x}\frac{d\theta}{dx} + \delta x^{-\beta} \exp(\theta) = 0. \tag{13}$$

To obtain a closed form solution, we invoke the transforamtion $x = \exp(z)$, then (13) is transformed to

$$\frac{d^2\theta}{dx^2} + \delta \exp(\theta) = 0, \tag{14}$$

for $\beta = 2$. Hence the solution is of the form (4), thus

$$\exp(\theta) = \frac{A}{\cosh^2\left(\sqrt{\frac{A\delta}{2}} \ln\ln x - B\right)}. \tag{15}$$

If we also subject (15) to the boundary conditions (2), we obtain

$$B = \sqrt{\frac{A\delta}{2}} \ln\ln(s+\epsilon) \;\; and \;\; A = \cosh^2\left[\sqrt{\frac{A\delta}{2}} \ln\ln(1+\epsilon) - B\right], \tag{16}$$

where $\epsilon > 0$, a very small number has been introduced to take care of the singularity at $s = 0$. The combination of equations (16) gives

$$\sqrt{\frac{\delta}{2}} = \frac{B}{\cosh\left[\frac{\ln\ln(1+\epsilon)}{\ln\ln(s+\epsilon)} - 1\right] B},$$

and the expression for criticality $\frac{d\delta}{dB} = 0$ gives

$$\left[\frac{\ln\ln(1+\epsilon)}{\ln\ln(s+\epsilon)} - 1\right] B_{cr} \times \tanh\left[\frac{\ln\ln(1+\epsilon)}{\ln\ln(s+\epsilon)} - 1\right] B_{cr} = 1. \tag{17}$$

It is necessary to seek for $|B|$ in (17) to order to obtain a real value. Using Newton's iterative scheme in the Mathematica software, we obtain the roots of the equation, $|B_{cr}|$ and the corresponding values δ_{cr} for $0 < s < 1$.

s	.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
θ_{cr}	.179	.415	.911	.922	.94	.97	1.015	.21	.247
δ_{cr}	0.0304	0.139	0.2933	0.297	0.301	.306	.31	0.34	0.355

Table 3. δ_{cr} against s for $\beta = 2$.

In Table 3. δ_{cr} is a monotonically increasing function of s, which indicates the disappearance of criticality as s increases.

The case of $f(x) = \exp(-\beta x)$ for $j = 1$ is also not amenable to analytical solution, hence would be treated numerically.

4. THE VARIATIONAL METHOD

This method has been used extensively in [4] and [5]. In this section, the boundary value problem (1) and (2) uses a fixed functional

$$H_\delta(\theta) \;=\; \int_D \left(\frac{1}{2}|\nabla\theta|^2 - \delta G(\theta)\right) dV, \tag{18}$$

where G is a primitive of F. In particular, this method would be used for the source terms,

$$F(\theta) = x^{-\beta}\exp(\theta) \quad \text{and} \quad \exp(-\beta x)\exp(\theta), \tag{19}$$

for the slab and cylinder respectively. Hence (18) becomes

$$H_\delta(\theta) \;=\; \int_0^1 \left(x^j(\frac{d\theta}{dx})^2\right) dx - \delta \int_{0^1} \left(x^j G(\theta)dx\right). \tag{20}$$

Since the domain of H_δ is restricted to those functions satisfying (2) for $s = 0$, an example is $\theta(x) = A\cos(\frac{\pi x}{2}) + B\cos(\frac{3\pi x}{2})$. Hence the variational principle suggests that A, B be determined as the solutions of the systems

$$\frac{\partial H_\delta}{\partial A} = 0 \;\text{ and }\; \frac{\partial H_\delta}{\partial B} = 0, \tag{21}$$

which gives an approximate solution of θ corresponding to the chosen δ. The condition determining the criticality is according to the implicit function theorem, i.e

$$\text{Det}\begin{pmatrix} \frac{\partial^2 H_\delta}{\partial A^2} & \frac{\partial^2 H_\delta}{\partial A \partial B} \\ \frac{\partial^2 H_\delta}{\partial A \partial B} & \frac{\partial^2 H_\delta}{\partial B^2} \end{pmatrix} = 0. \tag{22}$$

Hence from equations (20), (21) and (22), we obtain the simultaneous equations,

$$\frac{1}{4}\pi^2(uA + 3vB) - \delta\int_0^1 x^j \frac{dG}{dA}(\theta)dx = 0 \tag{23}$$

$$\frac{3}{4}\pi^2(vA + 3wB) - \delta\int_0^1 x^j \frac{dG}{dB}(\theta)dx = 0 \tag{24}$$

$$\left\{\frac{\pi^2 u}{4} - \delta\int_0^1 x^j \frac{d^2}{dA^2}G(\theta)\right\} \times \left\{\frac{9\pi^2 w}{4} - \delta\int_0^1 x^j \frac{d^2}{dB^2}G(\theta)dx\right\} = \left\{\frac{3\pi^2 v}{4} - \delta\int_0^1 x^j \frac{d^2}{dAdB}G(\theta)\right\}^2 \tag{25}$$

which are to be solved simultaneously for A, B and δ.

The constants u, v, w are obtained from

$$\begin{aligned} u &= \int_0^1 x^j \sin^2(\frac{\pi x}{2})dx = \begin{cases} \frac{1}{2}, & j=0, \\ \frac{1}{2(j+1)} + \frac{1}{\pi^2}, & j=1 \end{cases} \\ v &= \int_0^1 x^j \sin^2(\frac{\pi x}{2})\sin^2(\frac{3\pi x}{2})dx = \begin{cases} 0, & j=0, \\ \frac{-1}{\pi^2}, & j=1 \end{cases} \\ w &= \int_0^1 x^j \sin^2(\frac{3\pi x}{2})dx = \begin{cases} \frac{1}{2}, & j=0, \\ \frac{1}{2(j+1)} + \frac{1}{9\pi^2}, & j=1 \end{cases} \end{aligned}$$

Since these equations are difficult to handle by simple numerical calculations, a short numerical code implemented in the Mathematica software package is used. This code uses the Simpson's method to evaluate the integral.

Slab($j=0$) and $f(x) \ = \ x^{-\beta}$

Here, equation (1) reduces to

$$\frac{d^2\theta}{dx^2} + \delta x^{-\beta}\exp(\theta) = 0 \tag{26}$$

$$\frac{d\theta}{dx}(x=0) \ = \ 0 \qquad \theta(1) \ = \ 0. \tag{27}$$

By using the code, we obtain the result tabulated in Table 4.

β	0	.5	1.0	1.5	2.0	2.5	3.0
θ_{cr}	1.167	1.146	1.1286	1.1142	1.1026	1.0933	1.0857
δ_{cr}	0.878355	1.01663	1.16259	1.31525	1.4737	1.637	1.80466

Table 4. δ_{cr} against β for $s=0$.

Cylinder ($j=1$) and $f(x) \ = \ \exp(-\beta x)$

The resulting equations are

$$\frac{d^2\theta}{dx^2} + \delta\exp(-\beta x)\exp(\theta) \tag{28}$$

$$\frac{d\theta}{dx}(x=0) \; = \; 0 \qquad \theta(1) \; = \; 0. \tag{29}$$

Using the same numerical code,

β	0	.5	1.0	1.5	2.0
θ_{cr}	1.3553	1.3085	1.208	1.0257	1.0000
δ_{cr}	0.878355	1.01663	1.16259	1.31525	1.4737

Table 5. δ_{cr} against β for $s = 0$.

As a check, at the point $s = 0$, we observe from Tables 4 and 5 that the values of θ_{cr} and δ_{cr} are in full agreement with the exact result values in literature (see [1] and [4] and [3]). In addition, the results has provided us with the opportunity of being able to compare results and choose a suitable model.

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