

ON EXOTHERMIC EXPLOSIONS IN SYMMETRIC GEOMETRIES*

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Abstract

In this paper, we examined the steady state solutions for the strongly exothermic decomposition of a combustible material uniformly distributed in heated symmetrical geometries under Sensitised, Arrhenius and Bimolecular kinetics, neglecting the consumption of the material. The resulting nonlinear boundary value problems were solved using perturbation method and method of weighted residual. The results were compared and thermal ignition criticality is discussed.

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Key words: symmetric geometries, Sensitised, Arrhenius, and Bimolecular kinetics, perturbation method, method of weighted residual.

1. Introduction

Thermal explosion theory can be described as a phenomenon of spontaneous explosion due to internal heating in combustible materials such as industrial waste fuel, coal hay, wool waste etc.

The main mathematical problem of evaluation of critical regimes thought of as regimes separating the regions of explosive and non-explosive ways of chemical reactions as in (Balakrishnan *et al.*, 1996; Bebernes and Eberly, 1989; Frank Kamenetskii, 1969; Jacobsen and Schmitt, 2002). The classical formulation of this problem was first introduced by (Frank-Kamenetskii, 1969). Neglecting the reactant consumption, the equation for heat balance together with the boundary conditions, under Sensitised, Arrhenius and Bimolecular kinetics, can be written as

$$\frac{1}{r^n} \frac{d}{dr} \left(r^n \frac{dT}{dr} \right) + \frac{QC_0 A}{k} \left(\frac{KT}{vh} \right)^m e^{-\frac{E}{RT}} = 0, \quad (1.1)$$

$$\frac{dT}{dr}(0) = 0, T(a) = T_0, \quad (1.2)$$

where T is the absolute temperature, T_0 the geometry wall temperature, k the thermal conductivity of the material, Q is the heat of reaction, A is the rate constant, E is the activation energy, R is the universal gas constant, C_0 is the initial concentration of the reactant species, h is the Planck's number, K is the Bolt Mann's constant, δ is the vibration frequency, a is the channel width, r is the radial distance measured in the normal direction, m is the numerical exponent such that $m = \{-2, 0, 1/2\}$ corresponding to Sensitised, Arrhenius and Bimolecular Kinetics respectively as in (Odejide and Aregbesola, 2007, Okoya and The Abdussalam International Centre for Theoretical Physics, 2002), and n is the symmetry geometries exponent such that $n = \{0, 1, 2\}$ represent Slab, Cylindrical and Spherical geometries respectively as in (Balakrishnan *et al.*, 1996; Bebernes and Eberly, 1989; Frank Kamenetskii, 1969; Jacobsen and Schmitt, 2002; Makinde, 2006).

Makinde and Osalusi (2005) solve this problem for $m = 0$, corresponding to Arrhenius kinetics. Our objectives are to solve this nonlinear problem for different geometries for $m = \{-2, 0, 1/2\}$ corresponding to Sensitised, Arrhenius and Bimolecular kinetics respectively, using a new numerical scheme-method of weighted residual (MWR) and compare results with perturbation method (PM). Also to examine the thermal ignition criticality conditions for the Sensitised, Arrhenius and Bimolecular kinetics.

Following Frank Kamenetskii (1969), we introduce the following dimensionless variables in equations (1)-(2)

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$$\theta = \frac{E(T - T_0)}{RT_0^2}, \delta = \frac{RT_0}{E}, r = \frac{\bar{r}}{a}, \lambda = \frac{QE A a^2 C_0 e^{\frac{-E}{RT_0}}}{T_0^2 R k} \left(\frac{KT_0}{\nu h} \right)^m, \quad (1.3)$$

we have

$$\frac{1}{r^n} \frac{d}{dr} \left(r^n \frac{d\theta}{dr} \right) + \lambda (1 + \delta\theta)^m e^{\frac{\theta}{(1+\delta\theta)}} = 0 \quad (1.4)$$

$$\frac{d\theta}{dr}(0) = 0, \theta(1) = \theta_0, \quad (1.5)$$

where λ is the Frank-Kamenetskii parameter, θ is the dimensionless temperature variable, δ is the dimensionless combustible variable and r is the dimensionless radial distance variable.

For different values of n and m , we have the following cases subject to the boundary conditions

For Slab:

Case 1; $n = 0, m = -2$ (Sensitised)

$$\frac{d^2\theta}{dr^2} + \lambda (1 + \delta\theta)^{-2} e^{\frac{\theta}{(1+\delta\theta)}} = 0 \quad (1.6)$$

Case 2; $n = 0, m = 0$ (Arrhenius)

$$\frac{d^2\theta}{dr^2} + \lambda e^{\frac{\theta}{(1+\delta\theta)}} = 0 \quad (1.7)$$

Case 3; $n = 0, m = \frac{1}{2}$ (Bimolecular)

$$\frac{d^2\theta}{dr^2} + \lambda (1 + \delta\theta)^{\frac{1}{2}} e^{\frac{\theta}{(1+\delta\theta)}} = 0 \quad (1.8)$$

For Cylinder:

Case 4; $n = 1, m = -2$ (Sensitised)

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{d\theta}{dr} \right) + \lambda (1 + \delta\theta)^{-2} e^{\frac{\theta}{(1+\delta\theta)}} = 0 \quad (1.9)$$

Case 5; $n = 1, m = 0$ (Arrhenius)

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{d\theta}{dr} \right) + \lambda e^{\frac{\theta}{(1+\delta\theta)}} = 0 \quad (1.10)$$

Case 6; $n = 1, m = \frac{1}{2}$ (Bimolecular)

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{d\theta}{dr} \right) + \lambda (1 + \delta\theta)^{\frac{1}{2}} e^{\frac{\theta}{(1+\delta\theta)}} = 0 \quad (1.11)$$

For Sphere:

Case 7; $n = 2, m = -2$ (Sensitised)

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\theta}{dr} \right) + \lambda (1 + \delta\theta)^{-2} e^{\frac{\theta}{(1+\delta\theta)}} = 0 \quad (1.12)$$

Case 8; $n = 2, m = 0$ (Arrhenius)

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\theta}{dr} \right) + \lambda e^{\frac{\theta}{(1+\delta\theta)}} = 0 \quad (1.13)$$

Case 9; $n = 2, m = \frac{1}{2}$ (Bimolecular)

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\theta}{dr} \right) + \lambda (1 + \delta\theta)^{\frac{1}{2}} e^{\frac{\theta}{(1+\delta\theta)}} = 0 \quad (1.14)$$

2. Methods of Solution

Perturbation Method (PM)

To solve equations (1.6)-(1.14) subject to the boundary conditions (1.5), we take a power series expansion in terms of the Frank-Kamenetskii parameter λ in the form

$$\theta = \sum_{i=0}^{\infty} \theta_i \lambda^i \quad (2.1)$$

Substituting equation (2.1) into equations (1.6)-(1.14) and solving the resulting equations, we have

For Case 1:

$$\theta = -\frac{\lambda}{2}(r^2 - 1) + \frac{\lambda^2}{24}(r^2 - 1)(r^5 - 5)(2\delta - 1) - \frac{\lambda^3}{360}(r^2 - 1) \\ (11r^4\delta^2 - 11r^4\delta + 2r^4 - 64r^2\delta^2 + 64r^2\delta - 13r^2 + 221\delta^2 - 221\delta + 47) + 0(\lambda^4) \quad (2.2)$$

For Case 2:

$$\theta = -\frac{\lambda}{2}(r^2 - 1) + \frac{\lambda^2}{24}(r^2 - 1)(r^5 - 5) + \frac{\lambda^3}{360}(r^2 - 1)(3r^4\delta - 2r^4 - 12r^2\delta - 13r^2 - 35\delta - 47) \\ + 0(\lambda^4) \quad (2.3)$$

For Case 3:

$$\theta = -\frac{\lambda}{2}(r^2 - 1) + \frac{\lambda^2}{48}(r^2 - 1)(r^5 - 5)(2 + \delta) + \\ \frac{\lambda^3}{1440}(r^2 - 1)(r^4\delta^2 + 4r^4\delta - 8r^4 + r^2\delta^2 + 4r^2\delta + 52r^2 - 14\delta^2 - 56\delta - 188) + 0(\lambda^4) \quad (2.4)$$

For Case 4:

$$\theta = -\frac{\lambda}{4}(r^2 - 1) + \frac{\lambda^2}{64}(r^2 - 1)(r^2 - 3)(1 - 2\delta) - \frac{\lambda^3}{2304}(r^2 - 1) \\ (16r^4\delta^2 - 4r^4\delta + 3r^4 - 74r^2\delta^2 + 74r^2\delta - 15r^2 + 142\delta^2 - 142\delta + 30) + 0(\lambda^4) \quad (2.5)$$

For Case 5:

$$\theta = -\frac{\lambda}{4}(r^2 - 1) + \frac{\lambda^2}{64}(r^2 - 1)(r^3 - 3) + \frac{\lambda^3}{2304}(r^2 - 1)(4r^4\delta - 3r^4 - 14r^2\delta + 15r^2 + 22\delta - 30) \\ + 0(\lambda^4) \quad (2.6)$$

For Case 6:

$$\theta = -\frac{\lambda}{4}(r^2 - 1) + \frac{\lambda^2}{128}(r^2 - 1)(r^2 - 3)(2 + \delta) + \frac{\lambda^3}{9216}(r^2 - 1) \\ (r^4\delta^2 + 4r^4\delta - 12r^4 + r^2\delta^2 + 4r^2\delta + 60r^2 - 8\delta^2 - 32\delta - 120) + 0(\lambda^4) \quad (2.7)$$

For Case 7:

$$\theta = -\frac{\lambda}{6}(r^2 - 1) + \frac{\lambda^2}{360}(r^2 - 1)(3r^2 - 7)(1 - 2\delta) - \frac{\lambda^3}{7560}(r^2 - 1) \\ (21r^4\delta^2 - 21r^4\delta + r^4 - 84r^2\delta^2 + 84r^2\delta - 17r^2 + 119\delta^2 - 119\delta + 25) \quad (2.8)$$

For Case 8:

$$\theta = -\frac{\lambda}{6}(r^2 - 1) + \frac{\lambda^2}{360}(r^2 - 1)(3r^2 - 7) + \frac{\lambda^3}{15120}(r^2 - 1)(10r^4\delta - 3r^4 - 32r^2\delta + 18r^2 + 38\delta - 31) \\ + 0(\lambda^4) \quad (2.9)$$

For Case 9:

$$\theta = -\frac{\lambda}{6}(r^2 - 1) + \frac{\lambda^2}{720}(r^2 - 1)(3r^2 - 7)(2 + \delta) + \frac{\lambda^3}{30240}(r^2 - 1) \\ (r^4\delta^2 + 4r^4\delta - 16r^4 + r^2\delta^2 + 4r^2\delta + 68r^2 - 6\delta^2 - 24\delta - 100) + 0(\lambda^4) \quad (2.10)$$

Method of Weighted Residual (MWR)

The idea of MWR is to approximate the solution with a polynomial involving a set of parameters.

A polynomial of the form

$$R(r) = (r-a)^N \sum_{k=0}^{N-1} B_k (r-b)^k + (r-b)^N \sum_{k=0}^{N-1} A_k (r-a)^k \quad (2.11)$$

where A_k and B_k are constants to be determined which satisfies the given boundary conditions is assumed to be the solution of (1.6)-(1.14). The function $\theta(r)$ is then used as an approximation to the exact solution in the equations (1.6)-(1.14) to give $R(r)$.

The function $R(r)$ is the residual error. The idea is to make $R(r)$ as small as possible. $R(r)$ is set to zero at some points in the interval $[a, b]$. The system of these equations is then solved to determine the parameters A_k and B_k . $\theta(r)$ is then considered as the approximate solution. For detail of this method see (Aregbesola, 1996; Aregbesola, 2003; Aregbesola and Odejide, 2005; Makinde and Osalusi, 2005; Odejide and Aregbesola, 2006; Odejide and Aregbesola, 2007).

For example, for $N=4$, the trial function is of the form

$$\theta = b_0 r^4 + b_1 r^4 (r-1) + b_2 r^4 (r-1)^2 + b_3 r^4 (r-1)^3 + a_0 (r-1)^4 + a_1 r (r-1)^4 + a_2 r^2 (r-1)^4 + a_3 r^3 (r-1)^4 \quad (2.12)$$

Applying boundary conditions (5) to equation (2.12), we have $b_0 = 0$, $a_1 = 4a_0$.

Therefore, θ becomes

$$\theta = b_1 r^4 (r-1) + b_2 r^4 (r-1)^2 + b_3 r^4 (r-1)^3 + a_0 (r-1)^4 + 4a_0 r (r-1)^4 + a_2 r^2 (r-1)^4 + a_3 r^3 (r-1)^4 \quad (2.13)$$

We now use equation (2.13) to solve equations (1.6)-(1.14) subject to equation (1.5), we have the following:

For Slab:

Case 1; $n=0, m=-2$ (Sensitised), $\lambda = 1.313926$

$$a_0 = 2.219833393, a_2 = 19.49293379, a_3 = 33.57215434,$$

$$b_1 = -3.678793963, b_2 = 14.06141164, b_3 = -33.50966856 \text{ and}$$

$$\theta = -3.678793963r^4(r-1) + 14.06141164r^4(r-1)^2 - 33.50966856r^4(r-1)^3 + 2.219833393(r-1)^4 + 8.879333572r(r-1)^4 + 19.49293379r^2(r-1)^4 + 33.57215434r^3(r-1)^4 \quad (2.14)$$

Case 2; $n=0, m=0$ (Arrhenius), $\lambda = 0.988326$

$$a_0 = 23.05206590, a_2 = 13.38346806, a_3 = 23.05206590,$$

$$b_1 = -2.541042968, b_2 = 9.673775656, b_3 = -23.00883296 \text{ and}$$

$$\theta = -2.541042968r^4(r-1) + 9.673775656r^4(r-1)^2 - 23.00883296r^4(r-1)^3 + 1.523487172(r-1)^4 + 6.093948688r(r-1)^4 + 13.38346806r^2(r-1)^4 + 23.05206590r^3(r-1)^4 \quad (2.15)$$

Case 3; $n=0, m=\frac{1}{2}$ (Bimolecular), $\lambda = 0.932340$

$$a_0 = 21.48556480, a_2 = 12.47394706, a_3 = 21.48556480,$$

$$b_1 = -2.370300085, b_2 = 9.018725374, b_3 = -21.44537512 \text{ and}$$

$$\theta = -2.370300085r^4(r-1) + 9.018725374r^4(r-1)^2 - 21.44537512r^4(r-1)^3 + 1.419879194(r-1)^4 + 5.679516776r(r-1)^4 + 12.47394706r^2(r-1)^4 + 21.48556480r^3(r-1)^4 \quad (2.16)$$

For Cylinder:

Case 4; $n=1, m=-2$ (Sensitised), $\lambda = 3.016464$

$$a_0 = 2.652911007, a_2 = 22.70788908, a_3 = 37.68282286,$$

$$b_1 = -3.690739530, b_2 = 15.13481833, b_3 = -37.45372383 \text{ and}$$

$$\theta = -3.690739530r^4(r-1) + 15.13481833r^4(r-1)^2 - 37.45372383r^4(r-1)^3 + 2.652911007(r-1)^4 + 10.61164403r(r-1)^4 + 22.70788908r^2(r-1)^4 + 37.68282286r^3(r-1)^4 \quad (2.17)$$

Case 5; $n=1, m=0$ (Arrhenius), $\lambda = 2.261551$

$$a_0 = 1.801712403, a_2 = 15.43044163, a_3 = 25.57190134, \\ b_1 = -2.541695072, b_2 = 10.334008236, b_3 = -25.45714065 \text{ and} \\ \theta = -2.541695072r^2(r-1) + 10.334008236r^3(r-1)^2 - 25.45714065r^4(r-1)^3 + 1.801712403r^5(r-1)^4 + 7.206849612r(r-1)^4 + 15.43044163r^2(r-1)^4 + 25.57190134r^3(r-1)^4 \quad (2.18)$$

Case 6; $n=1, m=\frac{1}{2}$ (Bimolecular), $\lambda = 2.132465$

$$a_0 = 1.677673547, a_2 = 14.36882048, a_3 = 23.80695424, \\ b_1 = -2.370915438, b_2 = 9.628456746, b_3 = -23.70602557 \text{ and} \\ \theta = -2.370915438r^2(r-1) + 9.628456746r^3(r-1)^2 - 23.70602557r^4(r-1)^3 + 1.677673547r^5(r-1)^4 + 6.710694188r(r-1)^4 + 14.36882048r^2(r-1)^4 + 23.80695424r^3(r-1)^4 \quad (2.19)$$

For Sphere:

Case 7; $n=2, m=-2$ (Sensitised), $\lambda = 5.051249$

$$a_0 = 3.153179091, a_2 = 26.23418906, a_3 = 41.44177323, \\ b_1 = -3.696878549, b_2 = 16.09380410, b_3 = -41.06464592 \text{ and} \\ \theta = -3.696878549r^4(r-1) + 16.09380410r^4(r-1)^2 - 41.06464592r^4(r-1)^3 + 3.153179091(r-1)^4 + 12.61271636r(r-1)^4 + 26.23418906r^2(r-1)^4 + 41.44177323r^3(r-1)^4 \quad (2.20)$$

Case 8; $n=2, m=0$ (Arrhenius), $\lambda = 3.769999$

$$a_0 = 1.988383311, a_2 = 16.62506308, a_3 = 26.38190729, \\ b_1 = -2.446476685, b_2 = 10.41498600, b_3 = -26.31428343 \text{ and} \\ \theta = -2.446476685r^2(r-1) + 10.41498600r^3(r-1)^2 - 26.31428343r^4(r-1)^3 + 1.988383311r^5(r-1)^4 + 7.953533244r(r-1)^4 + 16.62506308r^2(r-1)^4 + 26.38190729r^3(r-1)^4 \quad (2.21)$$

Case 9; $n=2, m=-$ (Bimolecular), $\lambda = 3.557901$

$$a_0 = 1.967631544, a_2 = 16.36997045, a_3 = 25.68335025, \\ b_1 = -2.368043439, b_2 = 10.13050248, b_3 = -25.69872997 \text{ and} \\ \theta = -2.368043439r^2(r-1) + 10.13050248r^3(r-1)^2 - 25.69872997r^4(r-1)^3 + 1.967631544r^5(r-1)^4 + 7.870526176r(r-1)^4 + 16.36997045r^2(r-1)^4 + 25.68335025r^3(r-1)^4 \quad (2.22)$$

Table 1: Computation showing the maximum temperature and thermal criticality for different methods with $\delta = 0.0$:

Shape	Critical λ_c			Critical θ_c		
	Analytical	PM	MWR	Analytical	PM	MWR
Slab	0.88	0.8784576797	0.878700	1.19	1.186842168	1.186544994
Cylinder	2.0	2.0	2.0	1.39	1.386294361	1.361294468
Sphere	3.32	3.3219921183	3.322311	1.60	1.607456775	1.605400926

Table 2: Computation showing the maximum temperature and thermal criticality using MWR with $\delta = 0.0$:

Shape	m	Critical λ_c	Critical θ_c
Slab	-2	1.313926	2.219833393
	0	0.988326	1.523487172
	0.5	0.932340	1.419879194
Cylinder	-2	3.016464	2.652911007
	0	2.261551	1.801712403
	0.5	2.132465	1.677673547
Sphere	-2	5.051249	3.153179091
	0	3.769999	1.988383311
	0.5	3.557901	1.967631544

3. Discussion and Conclusion

We have used two methods to solve this problem: the perturbation method (PM) and the method of weighted residual (MWR). The results in Table 1 show the maximum temperature \dot{e}_c and thermal criticality \ddot{e}_c for different methods with $\ddot{a} = 0.0$ corresponding to Sensitised, Arrhenius and Bimolecular kinetics $\{m = -2.0, 0.0, 1/2\}$. We observed that the results were in close agreement in all the methods. We also observed that with MWR the critical values of \dot{e}_c were smaller than that obtained using PM.

The results in Table 2 show the maximum temperature \dot{e}_c and thermal criticality \ddot{e}_c using MWR with $\ddot{a} = 0.0$ for Sensitised, Arrhenius and Bimolecular kinetics $\{m = -2.0, 0.0, 1/2\}$ respectively. This is an extension of the work of Makinde and Osalusi (2005). We observed that the critical value of \dot{e}_c varies with geometries. The highest were observed for Sensitised kinetics $m = -2.0$ and the least for the case of Bimolecular kinetics $m = 1/2$. Also we have the highest thermal criticality for Slab and least for Sphere under Sensitised, Arrhenius and Bimolecular kinetics $\{m = -2.0, 0.0, 1/2\}$ respectively.

From our analysis, we observed that with the new numerical scheme-MWR thermal criticality are quickly attained than using PM. Also, more terms are required for convergence of the results using PM [10] whereas we need just few terms to obtain the desired results using MWR. This shows that the new scheme can be used to solve any nonlinear boundary value problems. We believe that the PM is excellent tools for solving initial and boundary value problems BVP's. However, for this type of BVP's the MWR works better than PM.

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REFERENCES

- Aregbesola, Y.A.S., 1996. *Two-Point Taylor Series for the Numerical Solution of Two-Point Boundary Value Problems*, Analele Stintifice AleUniversit ă tii "AL.I.CUZA"IASI Tomul XLII S.I.a. Matematică,71-77.
- Aregbesola, Y.A.S., 2003. *Numerical Solution of Bratu problem using the Method of Weighted Residual*, Electronic Journal of Southern African Mathematical Sciences Association, 3(1), 1-7.
- Aregbesola, Y.A.S. and Odejide, S.A., 2005. *A Note on the Bratu Problem*, Mathematical Sciences Research Journal, 9(9), 236-243.
- Balakrishnan, E., Swift, A. and Wake, G.C., 1996. *Critical values for some non-class A geometries in thermal ignition theory*, *Mathl. Comput. Modelling*, 8, 1-10.
- Bebernes, J. and Eberly, D., 1989. *Mathematical problems from Combustion theory*, Springer-Verlag, New York.
- Frank Kamenetskii, D.A., 1969. *Diffusion and Heat Transfer in Chemical Kinetics*, Plenum Press, New York.
- Jacobsen, J. and Schmitt, K., 2002. *The Liouville-Bratu-gelfand Problem for radial Operators*, *J. Diff. Equations*, 184, 283-298.
- Makinde, O.D., 2006. *Thermal Ignition in a Reactive Viscous Flow Through a Channel Filled With a Porous Medium*. Journal of Heat Transfer (Technical Brief) Vol. 128.
- Makinde, O.D., 2005. *Strong Exothermic Explosions in a Cylindrical Pipe: A Case Study of Series Summation Technique*, *Mech. Res. Commun.* 32, 191-195.
- Makinde, O.D. and Osalusi, E. 2005. *Exothermic Explosions in Symmetric Geometries: An Exploitation of Perturbation Technique*, *Rom. Journ. Phys.*, 50(5-6), 621-625.
- Odejide, S.A. and Aregbesola, Y.A.S., 2006. *A Note on Two Dimensional Bratu Problem*, *Kragujevac Journal of Mathematics*, 29, 49-56.
- Odejide, S.A. and Aregbesola, Y.A.S., 2007. *On Exothermic Explosion in a Reactive Viscous Flow through a Channel Filled with a Porous Medium*, *Mathematical Sciences Research Journal*, 11(6), 454-468.
- Okoya, S.S. and the Abdus Salam International Centre for Theoretical Physics, Trieste, Italy, 2002. *Thermal Stability for a Reactive Viscous Flow in a Slab*. The Abdus Salam International Centre for Theoretical Physics, MIRAMARE-TRIESTE, 1-13.