ON THERMAL STABILITY OF A TWO STEP EXOTHERMIC CHEMICAL REACTION IN A SLAB

DR. PHILIP OLADAPO OLANREWAJU

OVERVIEW

1. Introduction
2. Illustration-Applications
3. Mathematical Model
4. Solution Techniques
   4.1 Semi- discretization finite difference method
   4.2 Perturbation Method
   4.3 Numerical Method
5. Results and Discussion
6. Conclusion and Recommendation
7. Further study

1. INTRODUCTION

- Combustion is defined as a chemical reaction under conditions of progressive self-acceleration which are brought about by accumulation of heat or catalyzing products of reaction in the system: (1) thermal combustion (2) autocatalytic combustion
- Ignition is the process whereby a material capable of reacting exothermically is brought to state of rapid combustion
- Ignition temperature is the temperature to which a fuel must be raised before it begins to burn
- Exothermic reactions release heat as the reactants are consumed, heat is released and the temperature of the reaction increases and the temperature rise may lead to an ignition or explosion
- Two step reactions is the reaction that has only one intermediary between them

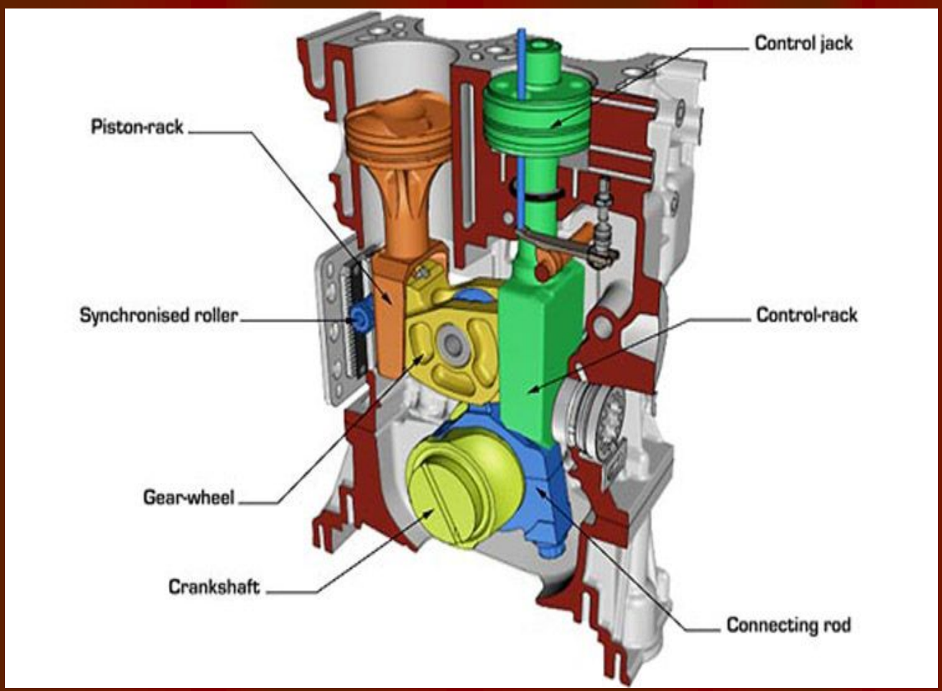
Literature

Frank- Kamenetskii (1969),Williams (1985),Makinde (2004),Olanrewaju (2005), Makinde (2009),

2. Illustration - Applications

Exothermic reaction involved

$$CH_4 + 2O_2 = CO_2 + 2H_2O + Energy$$

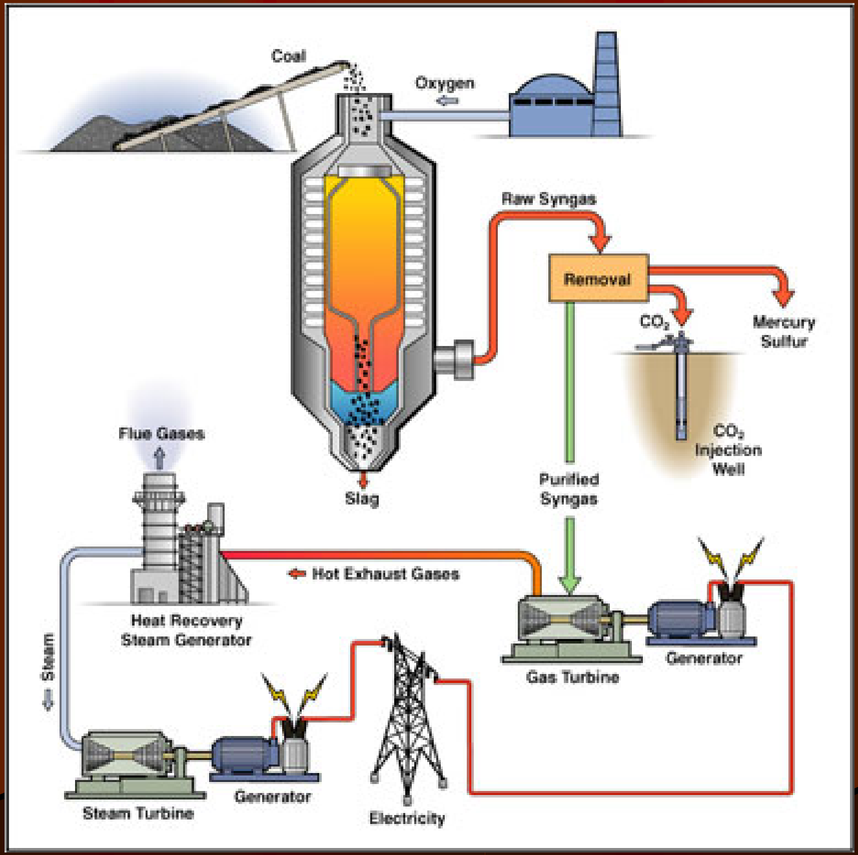


Design Internal Combustion Engine

Application Contd.

Exothermic reaction involved

Burning of Coal + Oxygen to heat water to produce vapor to turn the turbine blade to produce Electricity



Application Contd.

Exothermic reaction involved (Air bag)

For safety in auto-collision

$$NaN_3 \rightarrow Na + N_2$$

$$Na + KNO_3 \rightarrow K_2O + Na_2O + N_2$$

$$K_2O + Na_2O + SiO_2 \rightarrow alkaline\,Solicate(glass)$$

Application Contd.

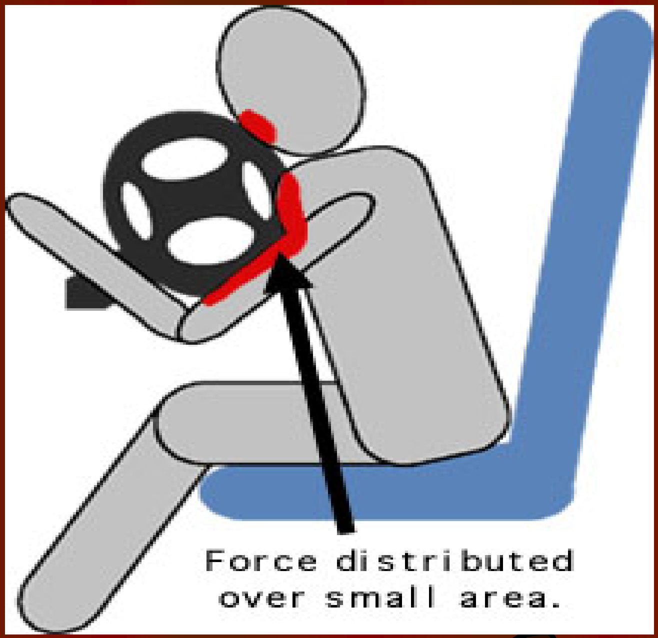
Exothermic reaction involved

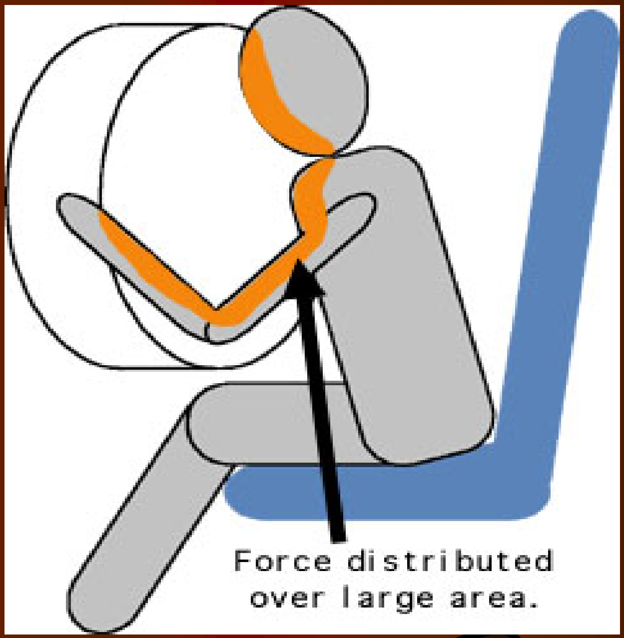
Safety- Using of Air bags in Cars

$$NaN_3 \rightarrow Na + N_2$$

$$Na + KNO_3 \rightarrow K_2O + Na_2O + N_2$$

$$K_2O + Na_2O + SiO_2 \rightarrow alkaline\,Solicate(glass)$$



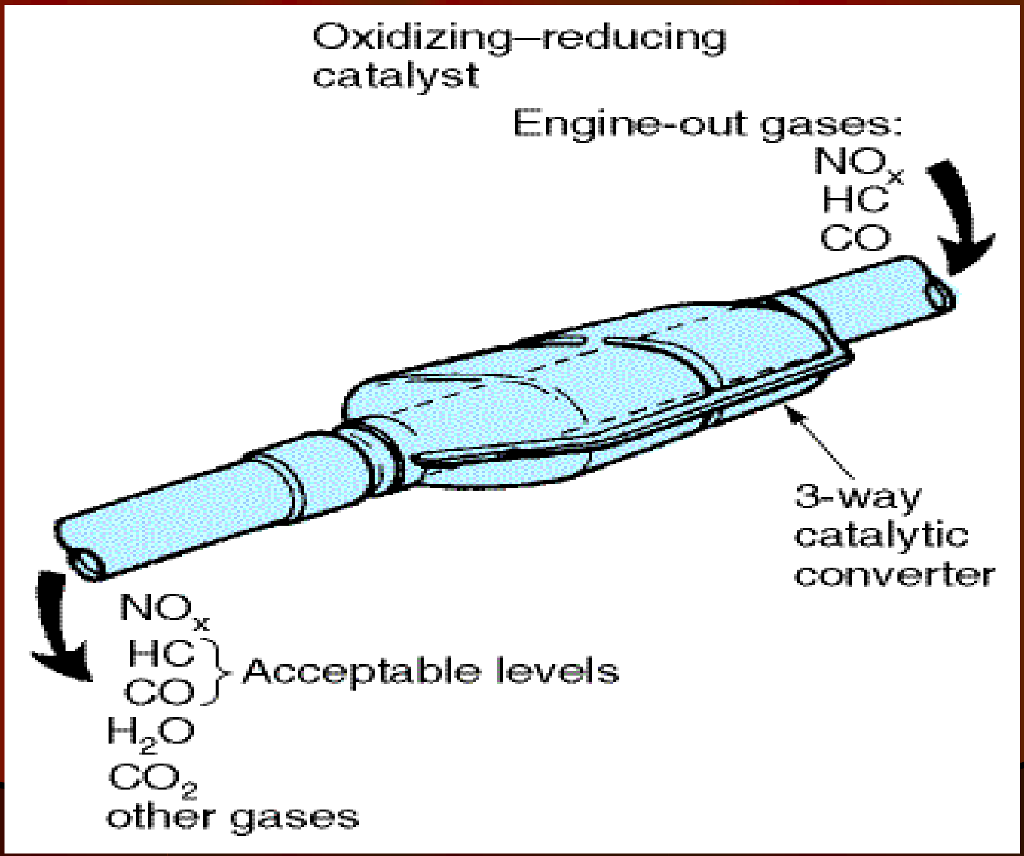


Application Contd.

Exothermic reaction involved (Pollution reduction of carbon mono-oxide)

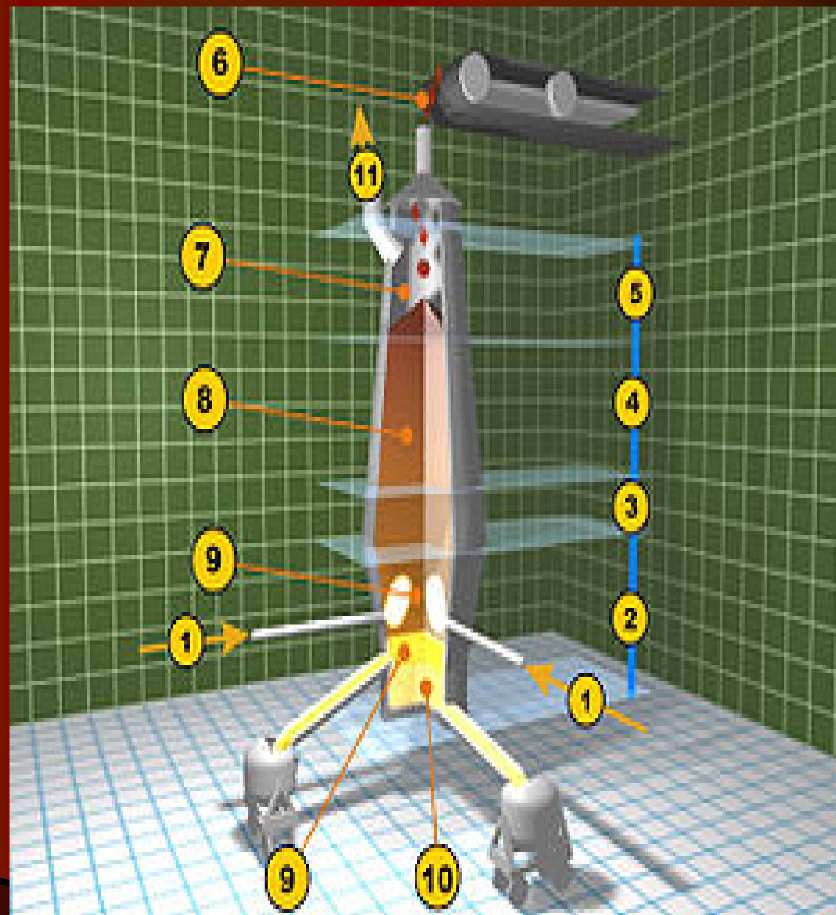
$2NO \Rightarrow N_2 + O_2 \; (\text{Re}\,duction\;\; process)$

$2CO + O_2 \Rightarrow 2CO_2 \; (Oxidation\;\; process)$



Application Contd.

Production of Engineering Materials
i.e Iron, steel,… through direct heating
(Blast furnace)



Application Contd.

Household and Industrial Heating

Solar heater- Utilizing the sun thermal energy

Application Contds.

Fire out brake or explosion

Application Contd.

Exothermic reaction involve(Quenching fire or explosion)

Chemical reactions is been taken place and water is been released to expand the volume of the fire then quench the flame

3. AIMS AND OBJECTIVES

- To stimulate certain combustion processes
- To develop predictive capability for combustion systems under various operating conditions
- To guide the design of combustion experiments
- To determine the effect of individual parameters in combustion processes by conducting parametric studies
- To burn fuel efficiently
- To avoid knocking of engines
- To determine thermal stability of combustion problems
- To enhance safety under Emergency situations
- To reduce pollution of combustion products

$\bar{y}$

4. MATHEMATICAL MODEL

We consider a two step exothermic chemical reaction of combustible materials in a slab, taking into account the diffusion of the reactant and the temperature dependent variable pre-exponential factor (see Fig. 1).

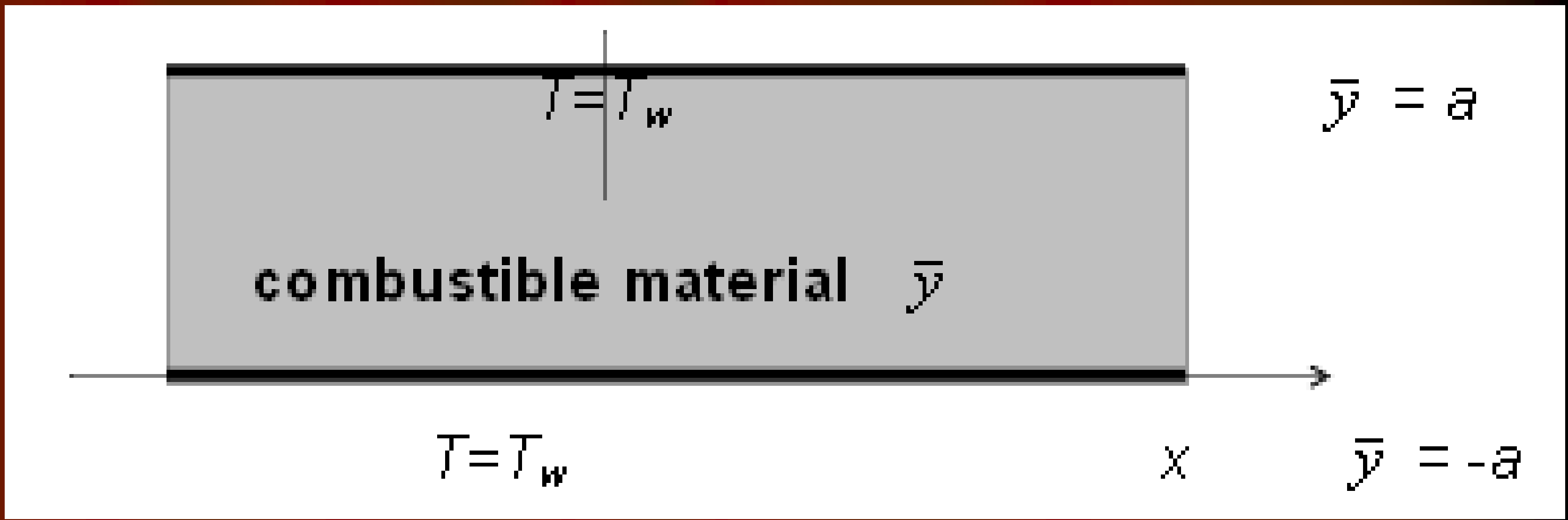


Fig. 1. Sketch of the physical model.

Mechanisms of two steps reaction

$$A + B \rightarrow C + D \rightarrow E$$

$2NO \Rightarrow N_2 + O_2$ or $2NO_2 \Rightarrow N_2 + 2O_2$ (Reduction process)

$2CO + O_2 \Rightarrow 2CO_2$ (Oxidation process)

$$CH_4 + 1.5\left(O_2 + 3.76N_2\right) = CO + 2H_2O + 5.6N_2$$

$$CO + 0.5\left(O_2 + 3.76N_2\right) = CO_2 + 1.88N_2.$$

5. PROBLEMS TO BE SOLVED

$$\frac{\partial\theta}{\partial t}=\frac{\partial^2\theta}{\partial y^2}+\lambda(1+\varepsilon\theta)^m\left[e^{\left(\frac{\theta}{1+\varepsilon\theta}\right)}+\beta e^{\left(\frac{r\theta}{1+\varepsilon\theta}\right)}\right], \quad (1)$$

$$\theta(y,0)=b\,, \quad (2)$$

$$\frac{\partial\theta}{\partial y}(0,t)=0,\theta(1,t)=0,\ \text{for}\quad t>0 \quad (3)$$

where *λ, ε, β, r, b* represent the Frank-Kamenetskii parameter, activation energy parameter, two step exothermic reaction parameter, activation energy ratio parameter and the initial temperature parameter respectively. In the following section, Eqs. (1)-(3) are solved numerically using a semi-discretization finite difference method.

SEMI-DISCRETIZATION FINITE DIFFERENCE METHOD

$$\frac{d\theta_i}{dt}=\frac{1}{(\Delta y)^2}\left(\theta_{i+1}-2\theta_i+\theta_{i-1}\right)+\lambda\left(1+\varepsilon\theta_i\right)^m\left[e^{\left(\frac{\theta_i}{1+\varepsilon\theta_i}\right)}+\beta e^{\left(\frac{\gamma\theta_i}{1+\varepsilon\theta_i}\right)}\right], \qquad (8)$$

with initial conditions

$$\theta_i(0)=b\,, \quad 1\le i\le N+1\ . \qquad (9)$$

PERTURBATION METHOD

$$
\begin{aligned}
\theta(y) = &-\frac{\lambda}{2}(y^2-1)(1+\beta)+\frac{\lambda^2}{24}(y^2-1)(y^2-5)(1+\beta)(\beta r\\
&+m\,\varepsilon\,\beta+m\,\varepsilon+1)-\frac{\lambda^3}{720}(y^2-1)(1+\beta)\big(94+12\,m\,\varepsilon^2\,y^2\,\beta^2\\
&+2\,\beta\,r\,y^4+8\,\beta\,r\,m\,\varepsilon\,y^4+33\,r^2\,\beta+122\,\beta\,r-6\,r\,\varepsilon\,y^4\,\beta\\
&+24\,\varepsilon\,y^2\,\beta+8\,m\,\varepsilon\,y^4\,\beta-66\,r\,\varepsilon\,\beta^2+4\,r^2\,y^4\,\beta^2-6\,m\,\varepsilon^2\,y^4\,\beta\\
&-28\,\beta\,r\,y^2-26\,r^2\,y^2\,\beta^2+3\,r^2\,y^4\,\beta+94\,m^2\,\varepsilon^2\,\beta^2-66\,\varepsilon\\
&+188\,m\,\varepsilon\,\beta-3\,m\,\varepsilon^2\,y^4+4\,m^2\,\varepsilon^2\,y^4-52\,m\,\varepsilon\,y^2+4\,m^2\,\varepsilon^2\,y^4\,\beta^2\\
&+188\,m\,\varepsilon+24\,m\,\varepsilon^2\,y^2\,\beta+188\,m^2\,\varepsilon^2\,\beta-12\,r^2\,y^2\,\beta+94\,r^2\,\beta^2\\
&-26\,m^2\,\varepsilon^2\,y^2\,\beta^2-6\,\varepsilon\,y^4\,\beta-52\,\beta^2\,r\,m\,\varepsilon\,y^2-66\,\varepsilon\,\beta\\
&-52\,m^2\,\varepsilon^2\,y^2\,\beta-66\,m\,\varepsilon^2\,\beta-52\,\beta\,r\,m\,\varepsilon\,y^2+188\,\beta^2\,r\,m\,\varepsilon\\
&+24\,r\,\varepsilon\,y^2\,\beta^2-3\,m\,\varepsilon^2\,y^4\,\beta^2-52\,m\,\varepsilon\,y^2\,\beta+24\,r\,\varepsilon\,y^2\,\beta\\
&+188\,\beta\,r\,m\,\varepsilon-6\,r\,\varepsilon\,y^4\,\beta^2+8\,m^2\,\varepsilon^2\,y^4\,\beta+4\,y^4+33\,\beta+24\,\varepsilon\,y^2\\
&+94\,m^2\,\varepsilon^2-12\,y^2\,\beta-6\,\varepsilon\,y^4+8\,\beta^2\,r\,m\,\varepsilon\,y^4+3\,y^4\,\beta\\
&-26\,m^2\,\varepsilon^2\,y^2-66\,r\,\varepsilon\,\beta+12\,m\,\varepsilon^2\,y^2-33\,m\,\varepsilon^2\,\beta^2-26\,y^2\\
&+8\,m\,\varepsilon\,y^4-33\,m\,\varepsilon^2\big)+O(\lambda^4)
\end{aligned}
$$

6. RESULTS AND DISCUSSION

Table 1: Computations Showing the Procedure Rapid Convergence for ε =0; r = 0.1

d	N	θ_{max}	$\lambda_c\ (\beta = 0)$	θ_{max}	$\lambda_c\ (\beta = 0.1)$
2	4	1.1870100201	0.878460424	1.227844400	0.8439468937
3	8	1.1868421611	0.878457674	1.227679765	0.8439465740
4	13	1.1868421686	0.878457679	1.227679636	0.8439465691
5	19	1.1868421686	0.878457679	1.227679636	0.8439465682

RESULTS AND DISCUSSION

Table 2: Computations Showing Criticality for Sensitized, Arrhenius and Bimolecular Reaction

β	M	r	ε	θ_{max}	λ_c
0.0	0.5	0.1	0.1	1.4202438751	0.932216072
0.1	0.5	0.1	0.1	1.4764743462	0.897649656
0.2	0.5	0.1	0.1	1.5294654400	0.866522770
0.1	0.0	0.1	0.1	1.5858990493	0.953645221
0.1	-2.0	0.1	0.1	2.3207781381	1.282091040
0.1	0.5	0.5	0.1	1.4679267465	0.880606329
0.1	0.5	1.0	0.1	1.4202438751	0.847469156
0.1	0.5	0.1	0.2	1.9052742346	0.968086041
0.1	0.5	0.1	0.3	3.0468419324	1.074421454

RESULTS AND DISCUSSION

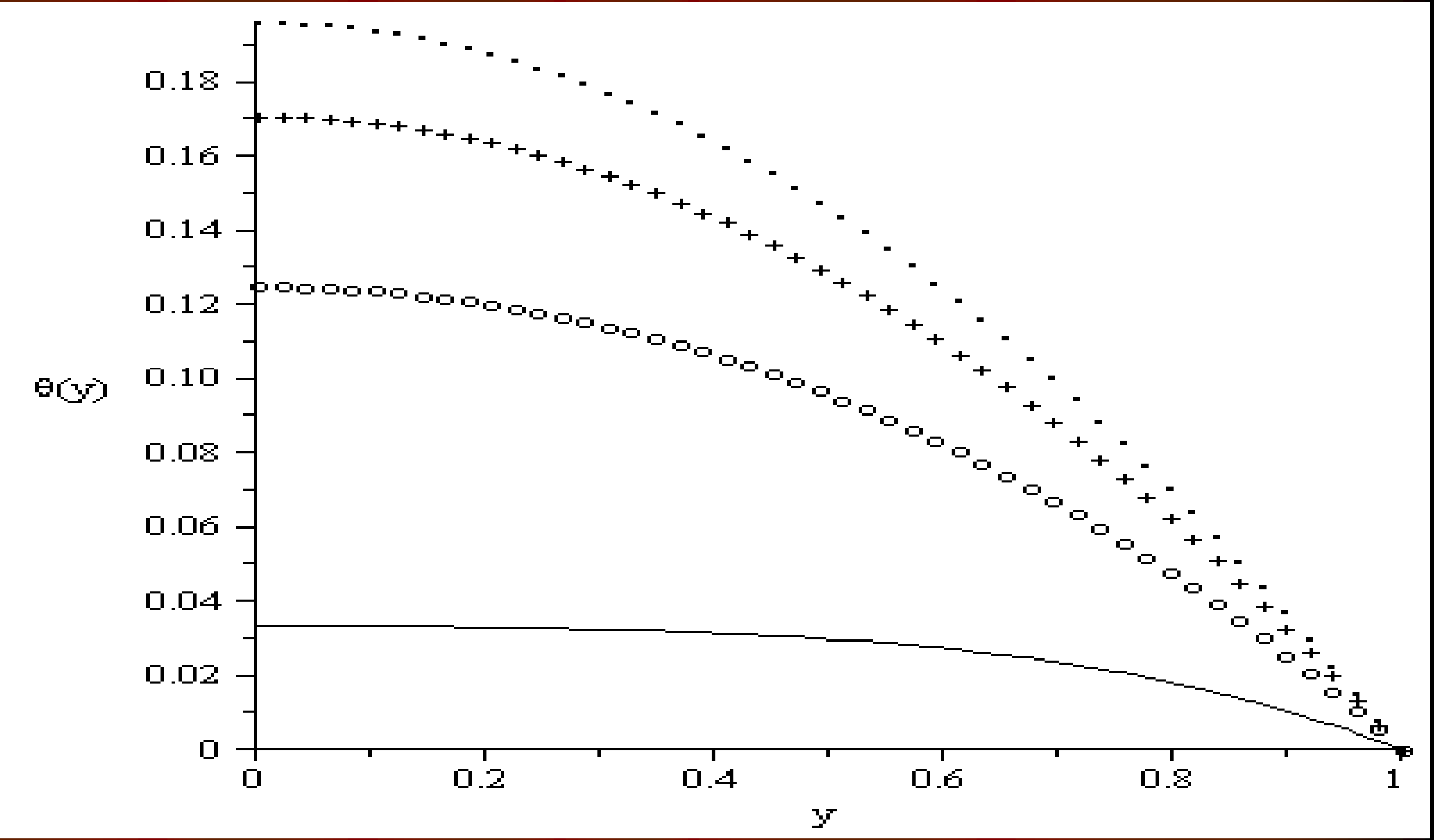


Fig.2: Temperature profiles: b=0; λ =0.3; ε =0.4; β = 0.1; m=0.5; r = 0.1; _______ t = 0.1; ooooo t = 0.5; ++++ t = 1; ……t = 5.

RESULTS AND DISCUSSION

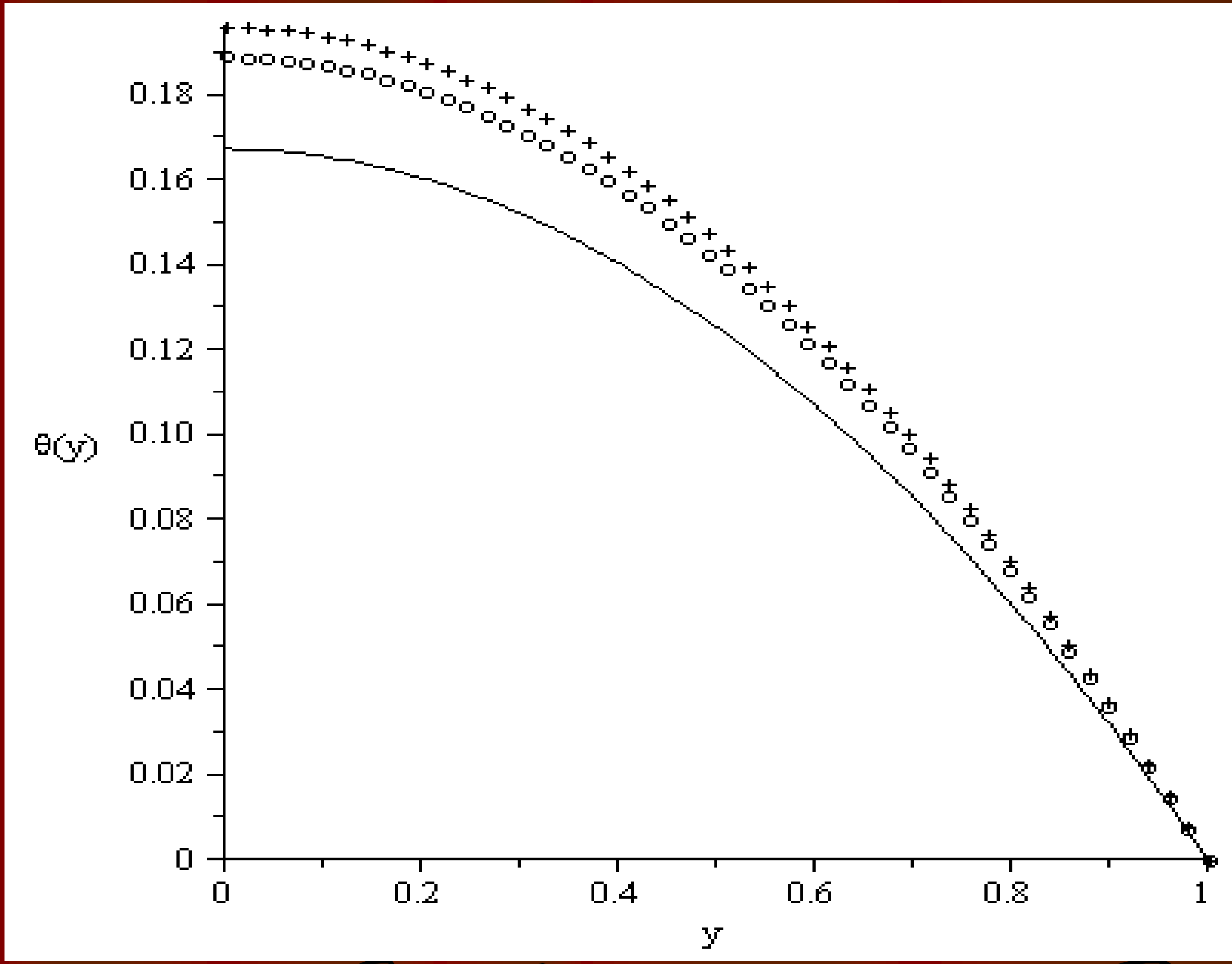


Fig.3: Temperature profiles: b=0; λ =0.3; ε =0.4; β = 0.1; t=5; r = 0.1; ______ *m* = -2; ooooo *m* = 0; ++++ *m* = 0.5

RESULTS AND DISCUSSION

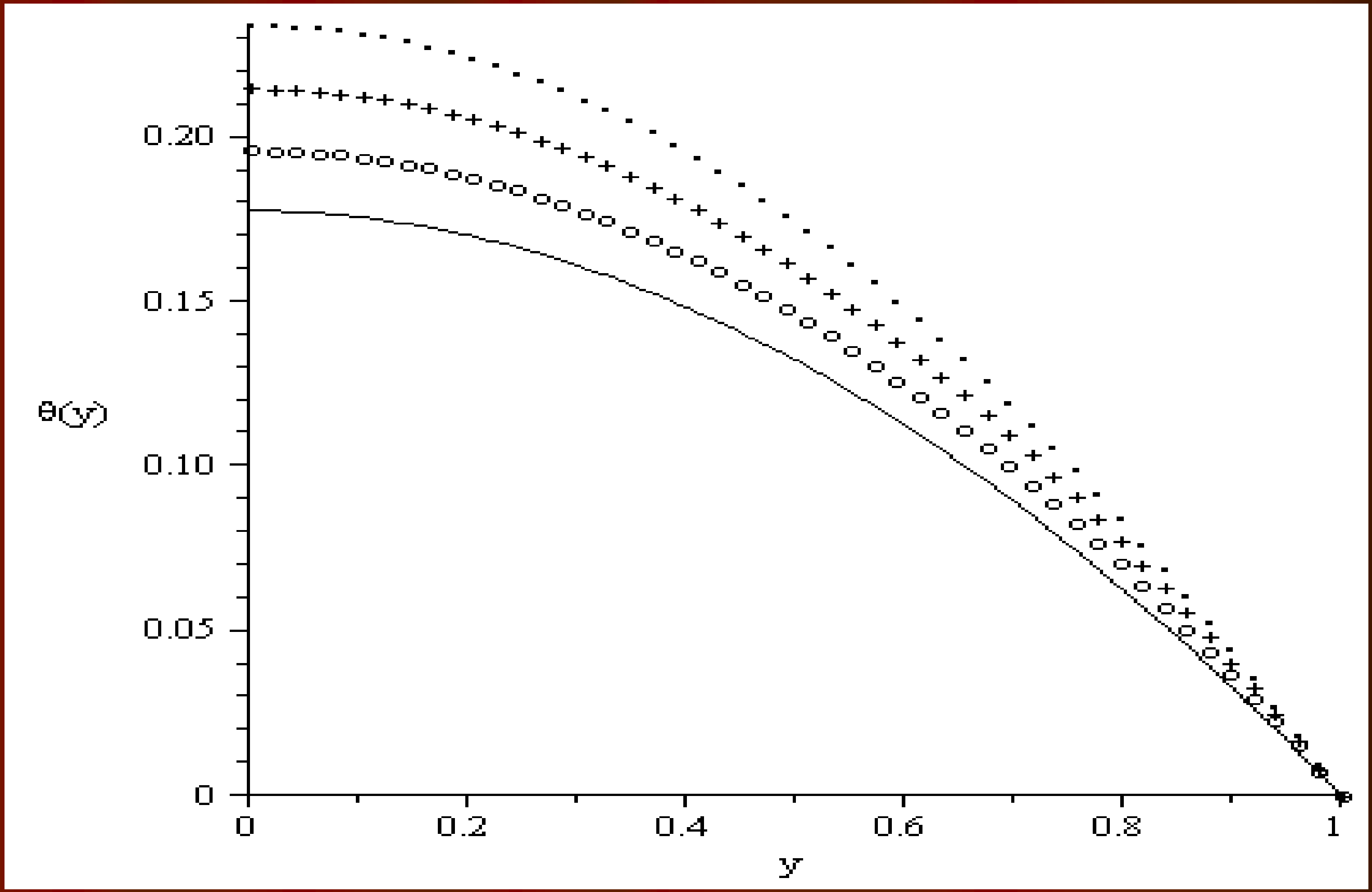


Fig.4: Temperature profiles: b=0; λ =0.3; ε =0.4; t = 5; m=0.5; r = 0.1; ______β = 0; oooooβ = 0.1; ++++ β = 0.2; ......β = 0.3

RESULTS AND DISCUSSION

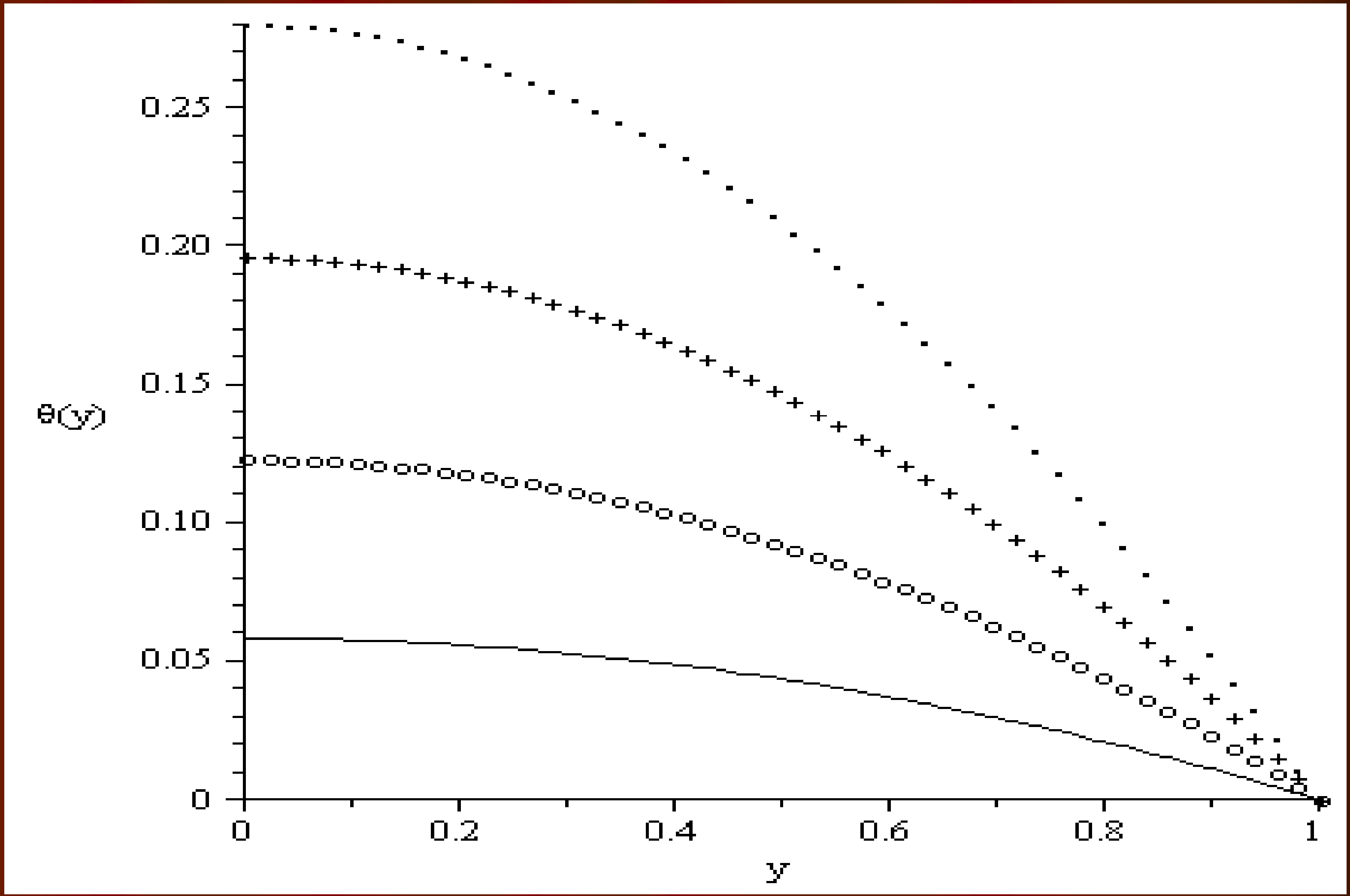


Fig.5: Temperature profiles: b=0; β =0.1; ε =0.4; t = 5; m=0.5; r = 0.1; ______λ = 0.1; oooooλ = 0.2; ++++ λ= 0.3; ……λ= 0.4

RESULTS AND DISCUSSION

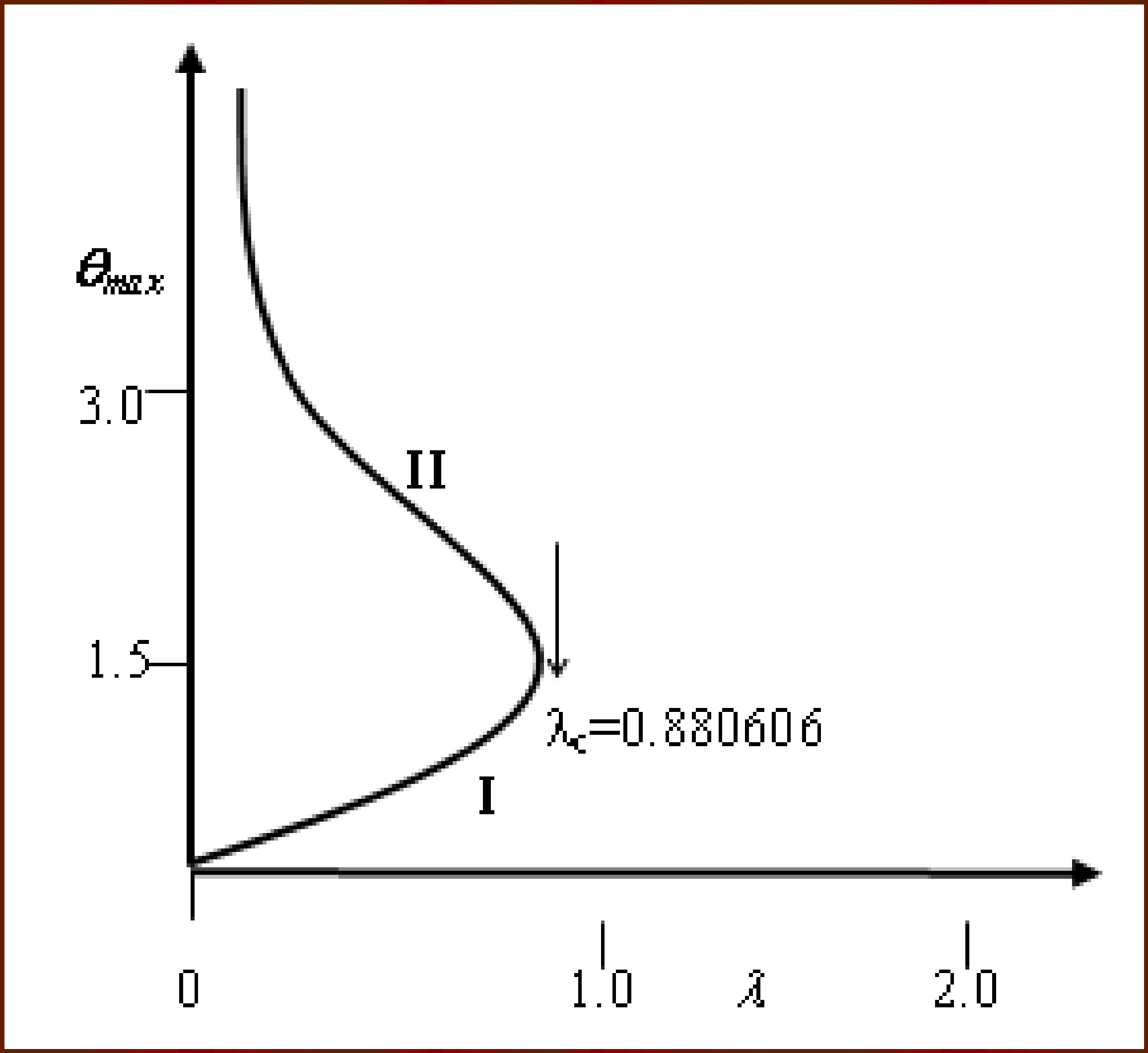


Fig. 6. A slice of approximate bifurcation diagram in the (λ , θmax (β = 0.1, m = 0.5, r = 0.5, ε = 0.1)) plane

7. CONCLUSION AND RECOMMENDATION

- Thermal criticality conditions and the solution branches were accurately obtained (Fig. 6)
- Influence of parameters coming into the model were accurately Determined (Tables 1, 2)
- Steady state solution was accurately obtained (Figs. 2-5)
- Overheating avoided – knocking of engines prevented (Figs. 2-5)
- Reduction of pollution of combustion products obtained (Combustion Mechanism)
- Two steps reaction enhances explosion or thermal runaway (Tables 1-2)

8. FURTHER STUDY

- The problem can be studied in a cylindrical pipe
- The problem can be studied in the presence of heat loss
- More steps may also be involved

References

- [1] J. Bebernes, D. Eberly, Mathematical problems from combustion theory. Springer-Verlag, New York, (1989).
- [2] E. Balakrishnan, A. Swift, G.C. Wake, Critical values for some non-class A geometries in thermal ignition theory, Math. Comput. Modell. 24, l–10, (1996).
- [3] D. A. Frank Kamenetskii. Diffusion and heat transfer in chemical kinetics. Plenum Press, New York, (1969).
- [4] G.I. Barenblatt, J.B. Bell, W.Y. Crutchfield, The thermal explosion revisited, Proc. Natl. Acad. Sci. USA 95, 13384–13386, (1998).
- [5] P.L. Chambré, On the solution of the Poisson–Boltzmann equation with application to the theory of thermal explosions, J. Chem. Phys. 20, 1795–1797, (1952).
- [6] T. Dumont, S. Génieys, M. Massot, V.A. Volpert, Interaction of thermal explosion and natural convection: Critical conditions and new oscillating regimes, SIAM J. Appl. Math. 63, 351–372, (2002).
- [7] O. D. Makinde, Exothermic explosions in a slab: A case study of series summation technique. International Communications in Heat and Mass Transfer, Vol. 31, No.8, 1227-1231, (2004).

References (Cont')

- [8] F. S. Dainton, Chain Reaction: An introduction Wiley, New York. (1960
- [9] Z. G. Szabo, Advances in kinetics of homogeneous gas reactions, Methusen and Co. Ltd, Great Britain (1964).
- [10] O. D. Makinde, Thermal stability of a reactive viscous flow through a porous-saturated channel with convective boundary conditions. Applied Thermal Engineering, Vol. 29, 1773-1777, (2009)
- [11] F. A. Williams, Combustion theory. Second Edition, Benjamin & Cuminy publishing Inc. Menlo Park, Califonia. (1985).
- [12] D. L. Hunter, G. A. Baker, Methods of series analysis III: Integral approximant methods. Phys. Rev. B 19, 3808-3821, (1979).
- [13]M. M. Vainberg, V. A. Trenogin, Theory of branching of solutions of nonlinear equations. Noordoff, Leyden, USA (1974).

THANK YOU FOR YOUR TIME