On the Induction Period for One-Step and a Two-Step Arrhenius Reaction

P.O. Olanrewaju
Department of Pure and Applied Mathematics,
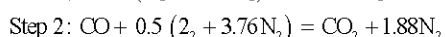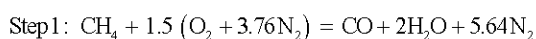Ladoke Akintola University of Technology, Ogbomoso, Nigeria

Abstract: In thisstudy, we investigate the induction period for one-step and a two step Arrhenius reaction to give further insight into the theory of combustion under reasonable and physical conditions. We compare the ignition time for one step and a two step reaction under the same necessary and sufficient conditions of explosion. Numerical solution was constructed for the resulting problem using finite difference scheme.

Key words: Induction period, one step reaction and two-step reactions

INTRODUCTION

In some cases the one step reaction is sufficient to explain some reaction processes even when there are intermediary steps.

However, in the cases of cool flames, Williams one step reaction has been found to be insufficient to explain all the features observed in the cool flames phenomenon, one therefore needs at least two steps. Also a cigarette like burning requires more than one step according to koriko and Ayeni (1978) Similarly, combustion taking place within k-fluid (Olanrewaju, 2005) is treated as a two-step irreversible chemical reaction of methane oxidation as follows:

$$Step 1: \; CH_4 + 1.5 \left(O_2 + 3.76 N_2 \right) = CO + 2H_2O + 5.64 N_2$$
$$Step 2: \; CO + 0.5 \left(2_2 + 3.76 N_2 \right) = CO_2 + 1.88 N_2$$

The pioneer researches of several renown scientists in the past and recent years are relevant in this research work.

Ayeni (1978) investigated problem concerning one-dimensional mixing and simultaneous reaction of a fuel and oxidizer. Of particular interest is the so-called ignition time, before which temporal changes are given as a function of activation energy, which can vary over all positive value. He showed that thermal runaway occur, at a finite time in the limit of large activation and a lower bound is derived for that time by mean of a comparison theorem.

Ayeni (1981, 1982) traced the time history of a spatially homogeneous model of a non-isothermal branched-chain reaction through asymptotic expansion of state variable. The former developed a subcritical solution (fizzle), where the state variable change by small amount and a supercritical solution (explosion) where extremely rapid transients occur with the assumptions that the activation energy is large and the sole recombination process occurs at the wall.

The latter (Ayeni, 1982) assumed a three body collision for the termination step and provided an upper bound for the explosion time as a function of the activation energy; which can vary over all positive values. Variable pre-exponential factor of the chain branching step was also assumed besides others.

In (Ayeni, 1981) the two afore-mentioned recombination steps as well as large activation energy for the chain- branching step were assumed and the analysis uncovered the critical for explosion and the relationship between the induction period and the amount of sensitizer in the medium. In all of the above reported works small concentration of the chain carrier was assumed present in the starting mixture.

Nunziato *et al.* (1977) investigated the thermal ignition time for homogeneous explosion involving two parallel reactions. An expression was derived for the thermal ignition time of a homogeneous explosion which is exothermically decomposing by two parallel Arrhenius reactions under the assumption of constant thermophysical properties and Frank-Kamenetskii approximation of the Arrhenius term. The results involved the thermal ignition time of each reaction alone and expressed in terms of hyper geometric function.

In Okoya (1999) he derived an analytical expression for the thermal ignition time of a reactive system. He employed effective activation energy approach which allows the elimination of previous difficulties arising in the estimation of the ignition time. The results of this novel technique is compared with numerical results as well as those obtained previously and there is good agreement.

Olanrewaju (2005) examined solutions of two step reactions with variable thermal conductivity. Numerical investigations were carried out on the explosion and ignition processes with two step mechanisms as well as the effect of variation thermophysical properties. The method of high activation energy asymptotic is used in the analysis.

Trevino (1991) examined ignition phenomena in H_2-O_2 mixtures and varatharajan and Williams (2000) investigated ignition times in the theory of branched chain thermal explosions.

In this research, we extract from the work of Olanrewaju (2005).

MATERIALS AND METHODS

The unsteady state energy equation that represents a two-step Arrhenius reaction is of the form

$$\rho c_p \left(\frac{dT}{dt} + u \frac{dT}{dx} \right) = k \frac{d^2 T}{dx^2} + A_1 Q_1 X^a T^n e^{-E_1/RT} \qquad (1)$$
$$+ A_2 Q_2 Y^b T^m e^{-E_2/RT}$$

Where

k	=	Thermal conductivity
R	=	Universal gas constant
T	=	Temperature
ρ	=	Density
c_p	=	Specific heat at constant pressure
A_i	=	Pre-exponential factors, i = 1,2
X	=	Mass fraction of species A
Y	=	Mass fraction of species B
a	=	Reaction order of species A
b	=	Reaction order of species B
Q_i	=	Heat release/unit mass i= 1, 2
t	=	Time
x	=	Space variable
m, n	=	Numerical exponents

Method of solution: Suitable dimensionless variables are:

$$\beta = \frac{RT_0}{E_1}, \quad \theta = \frac{T - T_0}{\beta T_0}, \quad u' = \frac{u}{v_0} \text{ and } r = \frac{E_2}{E_1} \qquad (2)$$

We take the advantages of the suitable dimensionable variable Eq. 2 in 1 with the assumption that $\beta \rightarrow 0$, m, n = 0. Then we have

$$\frac{\partial \theta}{\partial t} + \alpha_1 \frac{\partial \theta}{\partial x} = \alpha_2 \frac{\partial^2 \theta}{\partial x^2} + \delta_1 e^{\theta} + \delta_2 e^{r\theta} \qquad (3)$$

under the conditions

$$\left. \begin{array}{rcl} \theta(x,0) &=& 0 \\ \theta(-1,t) &=& 0 \ , \ t>0 \\ \theta(1,t) &=& 0 \ , \ t>0 \end{array} \right\} \qquad (4)$$

take k = 0.005, h = 0.1
Where

$$\alpha_1 = u' v_0 \beta T_0$$

$$\alpha_2 = \frac{k \beta T_0^2}{\rho c_p}$$

$$\delta_1 = \frac{Q_1 A_1 x^a e^{-E_1/ET_0}}{\rho c_p} \qquad (5)$$

$$\delta_2 = \frac{Q_2 A_2 Y^b e^{-rE_1/ET_0}}{\rho c_p}$$

$$r = \frac{E_2}{E_1}$$

RESULTS AND DICUSSION

The results of Eq. 3 satisfying Eq. 4 were used to plot the following graphs:

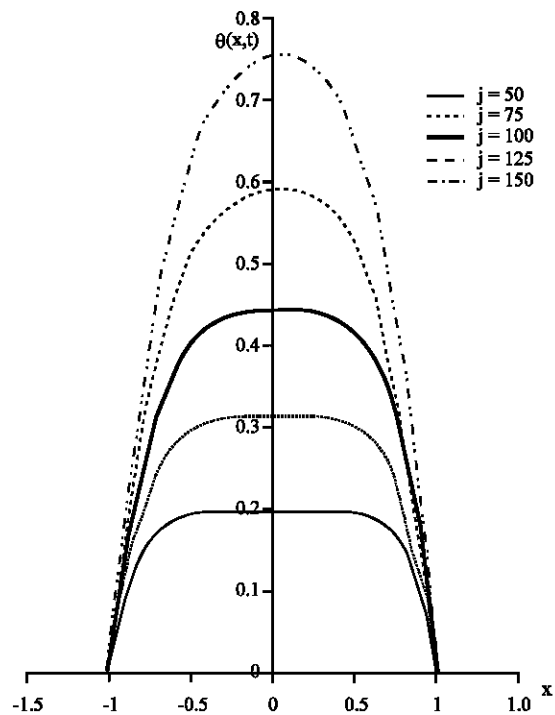Figure 1 represents the graph of temperature against position x for various values time t when

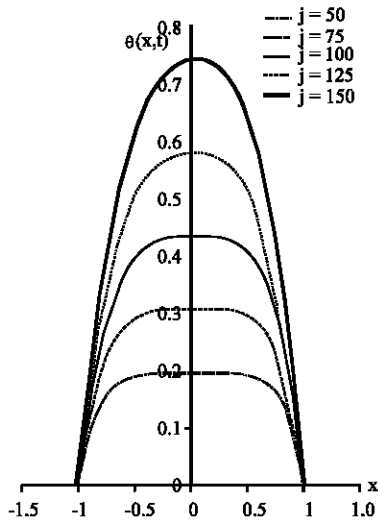Fig. 1: The graph of θ (x,t) against x for various time at $\delta_2 = 0.01$ and dl = 0.71

Fig. 2: The graph of θ (x,t) against x for δ_1 = 0.71 and Svatious time at δ_2 = 0
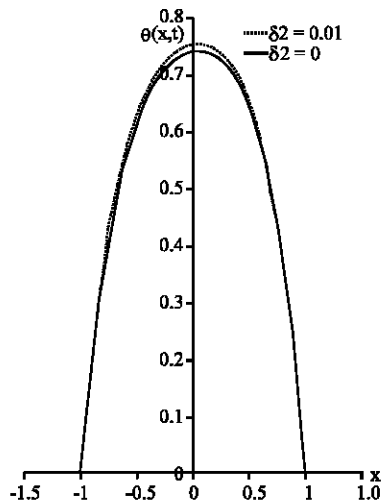

Fig. 3: The graph of θ (x,t) agaiunst x for variousδ_2 when j = 150

δ_1 = 0.71, δ_2 = 0.01. We observe that an increase in time t leads to an increase in temperature of the system (two-step reaction).

Figure 2 represents the curve of temperature against position x for various values of time t when δ_1 = 0.71, δ_2 = 0. It shows that increase in time t leads to an increase in temperature (one-step reaction)

Figure 3 shows the graph of temperature against position x for δ_2 = 0.01, δ_2 = 0.00. When j = 150.

REFERENCES

Ayeni, R.O., 1978. Thermal runaway. Ph.D. Thesis, Cornell University, Ithaca. New York.

Ayeni, R.O., 1981. Critical for branched chain explosion. Nig. J. Nat. Sci., 3: 45-30.

Ayeni, R.O., 1982. On the explosion of chain-thermal reactions. J. Aus. Maths. Soc. Series B, 21: 194-202.

Nunziato, J.W., J.E. Kennedy and D.E. Amos, 1977. The thermal ignition time for homogeneous explosion involving two parallel reaction. Combust. Flame, 29: 265-268.

Okoya, S.S., 1999. On the thermal ignition time for a spatially homogenous reaction. Direction Mathe., pp: 169-176.

Olanrewaju, P.O., 2005. Solutions of two step reactions with variable thermal conductivity. Ph.D thesis, Lautech, Ogbomoso, Nigeria.

Trevino, C., 1991. Ignition phenomena in H_2-O_2 mixtures, progress in Astronautics and Acrobatics, AIAA, 131: 19-43.

Varatharajan, B. and F.A. Williams, 2000. Ignition times in the theory of branched chain thermal explosions. Combust. flame, 121: 551-554.