DISAPPEARANCE OF CRITICALITY AND IGNITION TIMES OF AN EXOTHERMIC CHEMICAL REACTION IN A REACTOR

BY

ADELEYE, OLABODE EMMANUEL
B.Sc. (Hons) Mathematics, OAU, Ile-Ife, 2003
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ABSTRACT

This study determined the criticality, disappearance of criticality and ignition times in some limiting cases for an unsteady state energy balance equation. It also obtained the critical and transitional values of modified Semenov's number Φ, reduced temperature excess and activation energy parameter for three cases: (I) convective only, (II) radiative only and (III) both convective and radiative heat losses considering Arrhenius, bi-molecular and sensitized kinetics cases. This was with view of incorporating both convective and radiative heat losses in an exothermic chemical reaction with pre-exponential factor.

The transient variation of temperature equation Was Solved under physically reasonable assumptions, employing; Semenov's sufficient and necessary conditions for thermal explosion for case I and the modified El-Sayed definitions were used for cases II and III. Moreover, a parameter a being the ratio of the convective heat transfer coefficient (I), to the radiative hear transfer coefficient Φ_2, was Introduced
into case III to allow for extension of the study to accommodate both convective and radiative heat losses. Subsequently, the ignition times were obtained using a three-term regular perturbation, standard techniques and a numerical procedure. The critical and transitional values of the parameters θ, β and Φ for Arrhenius, bimolecular and sensitized kinetics in case I were investigated.

The results showed that in the special case II, the modified Semenov's number at critical point was obtained, while the dimensionless critical temperature obtained was a polynomial of degree 5. Moreover, a transcendental equation involving; the transitional values of θ, β and the reaction order n, was obtained in the form of a polynomial of degree 4. In the event of case III, the modified Semenov's number at critical point was obtained in terms of the other parameters, while the dimensionless critical temperature was obtained as a transcendental equation relating a, β_c and n in a polynomial of degree 5. A transcendental equation incorporating; a, θ_{tr}, β_{tr} and n in a polynomial of degree 4 was obtained as the point at which transition takes place.

In addition, the ignition time obtained numerically for n = 0, $\beta = 0.012$, $\Phi_1 = 55$ and $\Phi_2 = 70$, was 1.35 X 10-^{13} seconds. This showed that the reaction was very fast. For the first case, (a) Φ_{tr} decreased steadily as n increased provided $n \leq 1$, (b) θ_{tr} decreased as n increased if $n \leq 0$ and increased sharply for $0<n<1$ and (c) β_{tr} was asymptotic as n approaches 1. In the second case, β_{tr} was found as a function of θ_{tr} when n = 0. It was seen in the third aspect that previous results were deduced for the first and second cases when $a \rightarrow 0$ and $a \rightarrow \infty$ respectively. Finally, the ignition time for the system was shown to be monotonically decreasing as the reaction order n, increased.

The study concluded that based on the modified EI-Sayed definitions for combined heat losses, the result obtained had generalized and extended most of the existing; ones in the literature.