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OF THE EXISTENCE AND UNIQUENESS OF MATHEMATICAL MODEL OF CHAIN-BRANCHING AND CHAIN- BREAKING KINETICS

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Abstract

In this paper we consider Mathematical Model of Chain-Branching and Chain-Breaking Kinetics in which we use the lower and upper methods of solution to establish the existence and uniqueness of the solution. The behavior of solutions for certain second order nonlinear differential equation is considered. By employing properties of solution to establish sufficient conditions that guarantee existence and uniqueness solution.

***Keywords*:** Gronwall inequality, integro-differential equations, Banach fixed point, Galerkin approximation, lower and upper solutions, Existence and Uniqueness.

1.0 Introduction

Many scientists have contributed to knowledge in the area of Flames with Chain-breaking and Chain- branching kinetics and their outstanding contributions have led to series of inventions.

The existence and uniqueness of the solution to certain fractional differential equation was employed using Banach fixed point theorem under Lipschits and linear growth condition. It established existence theorem for the solution of an uncertain fractional differential equation by Schander fixed point theorem under continuity condition [1]. The solution of third order non-linear differential equation with multiple deviating arguments is considered. It employed Lyapunov's second method, a complete Lyapunov functional is constructed and used to establish sufficient condition that guarantee existence of unique solutions that are periodic, uniformly asymptotically stable, and uniformly ultimately bounded [2].

The existence and uniqueness of solution for one and two dimensional non-linear fractional order partial integro-differential equations by employed Banach fixed point theorem in which the sufficient conditions are presented in order to ensure the existence and uniqueness of a unique fixed point related to the integro-differential equation in operator form [3].

The existence, uniqueness and stability of solution to second order non-linear differential equations with non-instantaneous impulses was investigated, they employed strongly continuous cosine Family of linear operators and Banach fixed point method to study the existence and uniqueness of the solution of the non-instantaneous impulsive system and the existence and uniqueness was proved and established [4].

The existence and uniqueness of fractional differential equations with boundary value conditions. Gronwall inequality is used to obtained the existence and uniqueness results of solution of fractional calculus fixed point method under some week conditions [5]. The existence, uniqueness and asymptotic behavior of the solution for a non-classical diffusion were obtained using delay forcing term [6].The existence and uniqueness of solution were proved by the use of Galerkin approximation and energy method. The regularity property of solution to Fokker-Planck type equation was studied. H^K-regularity property of solution to a class of Fokker-Planck type of equation with sobolev coefficients and L^2 initial condition were used and the existence and uniqueness of weak L^H solutions for Fokker – Planck types equations with L^P initial values were obtained [7]. The solutions of two-step reactions with variable thermal conductivity were examined and the existence and uniqueness were established [9]. He considered not only the generalized temperature dependences of reaction rate, but he also proposed suitable approximation of the kinetics reactions in the limit of large/small activation energy.

2.0 MATHEMATICAL FORMULATIONS

The mathematical equations describing the flames with Chain-breaking and Chain –branching Kinetics is given by [8].
Combustion Equation for Flames Kinetics IS giving by

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$$\rho c_p \frac{\partial T}{\partial t} = K\frac{\partial^2 T}{\partial x^2} + \frac{(T-T_0)^n QAe^{\frac{-E}{RT}}}{a+be^{\frac{-E_1}{RT}}} \quad (2.1)$$

As initial and boundary conditions, we take

$T(x, 0) = T_0$ $\quad T(0, t) = T_0$, $T(L, t) = T_0$

Where,

T is the temperature of the medium

T_0 is the initial temperature of the medium

K is the thermal conductivity

Q is the heat of reaction

ρ is the density

A is the pre-exponential factor

E_1 is the activation energy of the first stage

E is the activation energy of the second reaction

a, b, are permeability constants

n is the order of the reactions

c_p is the specific heat at constant pressure

3.0 METHOD OF SOLUTION

We make the variable dimensionless by introducing

$$\theta = \frac{E}{RT_O^2}(T-T_0), \quad x^1 = \frac{x}{L} \quad \text{and} \quad \varepsilon = \frac{RT_0}{E}, \quad (3.1)$$

and we assume that,

$$E_1 = E + \varepsilon E \quad (3.2)$$

$$\theta = \frac{1}{\varepsilon T_0}(T-T_0) \quad (3.3)$$

After non-dimensionalisation we obtain

$$\frac{\partial \theta}{\partial t} = K\frac{\partial^2 \theta}{\partial x^2} + \frac{\lambda_1 \theta^n e^{\frac{\theta}{1+\varepsilon\theta}}}{1+\lambda_2 e^{\frac{\theta-1}{1+\varepsilon\theta}}} \quad (3.4)$$

With initial, and boundary conditions

$$\theta(x,o) = 0 \;, \theta(o,t) = 0 \;, \theta\,(1,t) = 0 \quad (3.5)$$

Where

$K = \frac{k}{\rho c_p}$ is the scaled thermal conductivity

$\lambda_1 = \frac{(\varepsilon T_0)^n AQe^{\frac{-E}{RT_0}}}{\rho c_p \varepsilon T_0 a}$ is the Frank – kamenentskii parameter

$\lambda_2 = \frac{b}{a}e^{\frac{-E_1}{RT_0}}$ is the dimensionless permeability parameter.

Therefore we have

$$\frac{\partial \theta}{\partial t} = K\frac{\partial^2 \theta}{\partial x^2} + \frac{\lambda_1 \theta^n e^{\frac{\theta}{1+\varepsilon\theta}}}{1+\lambda_2 e^{\frac{\theta+1}{1+\varepsilon\theta}}}$$

With initial, and boundary conditions

$$\theta(x,0) = 0 \;, \theta(0,t) = 0 \;, \theta(1,t) = 0$$

4.0. Existence and Uniqueness of Solution of Unsteady state

Definition 1: A smooth function $\overline{U}$ is said to be an upper solution of the problem

$\overline{LU} = F(y,t,u)$

Where

L $\equiv \frac{\partial}{\partial t} - (a,(y,t)\frac{\partial}{\partial t} + b(y,t)\frac{\partial^2}{\partial y^2} + c(y,t)$ (4.1)

if $\bar{u}$ satisfies

$\overline{LU} \geq F(y,t,u)$

$\bar{u}(y,0) \geq F(y), u(0,t) \geq h(y), u(\infty,t)h(y)$

Definition 2: A solution function $\underline{V}$ is said to be a lower solution of the problem

$\underline{LV} = F(y,t,v)$

L $\equiv \frac{\partial}{\partial t} - (a,(y,t)\frac{\partial}{\partial t} + b(y,t)\frac{\partial^2}{\partial y^2} + c(y,t)$

Where

If $\underline{v}$ satisfies LV $\leq F(y,t,v)$

$\underline{v}(y,0) \leq F(y), u(0,t) \leq h(y), v(\infty,t)h(y)$

Theorem 1: Let k > 0, $\lambda_1 > 0$, $\lambda_2 > 0, \in > 0, n = 0$. Then the equation (3.4) with the boundary and initial condition (3.5) has a solution for all $t \geq 0$.

Proof: Equation (3.4) can be written as

L $\theta = f(x,t,\theta)$

Where

$L\theta = \frac{\partial \theta}{\partial t} = K\frac{\partial^2 \theta}{\partial x^2}$

$f(x,t,\theta) = \frac{\lambda_1 e^{\frac{\theta}{1+\varepsilon\theta}}}{1+\lambda_2 e\frac{\theta-1}{1+\varepsilon\theta}}$

$\underline{\theta}$ (x, t) = 0

we shall show that $\underline{\theta}$ (x, t) = 0 is a lower solution.

Clearly,

$\underline{\theta}$ (x ,t) =0, $\underline{\theta}$ (0,t) = $\underline{\theta}$ (1,t) = 0

Now,

$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial x^2}$ = 0

This implies

$L\theta = \frac{\partial \theta}{\partial t} = K\frac{\partial^2 \theta}{\partial x^2}$ = 0 – 0 = 0

$f(x,t,\theta) = \frac{\lambda_1}{1+\lambda_2 e^{-1}}$

Hence,

$L\theta \leq f(x,t,\theta)$

By definition 1, $\underline{\theta}$ (x, t) =0 is a lower solution.

Also consider

$\bar{\theta}$ (x, t) = $(\frac{\lambda_1 e^{\frac{1}{\varepsilon}}}{1+\lambda_2 e^{\frac{1}{\varepsilon}}})t$ (4.2)

We shall show that $\bar{\theta}$ (x, t) as defined previously is an upper solution

Clearly,

$\overline{\theta}(x, 0) = 0$, $\overline{\theta}(0, t) = \dfrac{\lambda_1 e^{\frac{1}{\varepsilon}} t}{1+\lambda_2 e^{\frac{1}{\varepsilon}}}$, $\overline{\theta}(1, t) = \dfrac{\lambda_1 e^{\frac{1}{\varepsilon}} t}{1+\lambda_2 e^{\frac{1}{\varepsilon}}}$ (4.3)

Now,

$$\frac{\partial\theta}{\partial t} = \frac{\lambda_1 e^{\frac{1}{\varepsilon}}}{1+\lambda_2 e^{\frac{1}{\varepsilon}}}$$

This implies

$$L\overline{\theta} = \frac{\partial\overline{\theta}}{\partial t} - k\frac{\partial^2\overline{\theta}}{\partial x^2} = 1+\lambda_2 e^{\frac{1}{\varepsilon}} \quad (4.4)$$

$$f(x,t,\overline{\theta}) = \frac{\lambda_1 e^{\frac{\theta}{1+\varepsilon\theta}}}{1+\lambda_2 e\frac{\theta-1}{1+\varepsilon\theta}} \le \frac{\lambda_1 e^{\frac{1}{\varepsilon}}}{1+\lambda_2 e^{\frac{1}{\varepsilon}}} \quad (4.5)$$

Hence,

$L\overline{\theta} \ge (x, t, \overline{\theta})$

By definition 2, $\overline{\theta}(x, t) = \dfrac{\lambda_1 e^{\frac{1}{\varepsilon}}}{1+\lambda_2 e^{\frac{1}{\varepsilon}}}$ is an upper solution

Hence, there exists a solution of problem (3.5). This completes the proof.

5.0 Properties of Solution of Unsteady State

Theorem 2 : Let $\varepsilon>0$ and $n= 0$.

$$\frac{\partial\theta}{\partial t} = k\frac{\partial^2\theta}{\partial x^2} + \frac{\lambda_1 \theta^n e^{\frac{\theta}{1+\varepsilon\theta}}}{1+\lambda_2 \; e^{\frac{\theta-1}{1+\varepsilon\theta}}}$$

then

$$\frac{d\theta}{dt} \ge 0 \quad (5.1)$$

We have

$$\frac{\partial\theta}{\partial t} = k\frac{\partial^2\theta}{\partial x^2} + \frac{\lambda e^{\frac{\theta}{1+\varepsilon\theta}}}{1+\lambda_2 e^{\frac{\theta-1}{1+\varepsilon\theta}}}$$

$$\theta(0,t) = \theta(1,t) = 0 = \theta(x,0) \quad (5.2)$$

Then

$$\frac{\partial\theta}{\partial t} \ge 0$$

In the proof, we shall make use of the following lemma of Kolodner and Pederson (1966) Lemma [10].

Let $u(x,t) = 0(e^{a/x/^2})$ be a solution on $R^n \times [0, t_0)$ of differential inequality

$$\frac{\partial u}{\partial t} - \Delta u + k(x,t)u \ge 0 \quad (5.3)$$

Where k is bounded from below. If $u(x,0) \ge 0$ then $u(x,t) \ge 0$ for all

Proof of the Theorem 1: Given let n=0

Then (3.4) becomes

$$\frac{\partial\theta}{\partial t} = k\frac{\partial^2\theta}{\partial x^2} + \frac{\lambda e^{\frac{\theta}{1+\varepsilon\theta}}}{1+\lambda_2 e^{\frac{\theta-1}{1+\varepsilon\theta}}}$$

Differentiating with respect to t, we have

$$\frac{\partial^2\theta}{\partial t^2}=\frac{\partial}{\partial t}\left(k\frac{\partial^2\theta}{\partial x^2}\right)+\frac{\partial}{\partial t}\left[\frac{\lambda_1 e^{\frac{\theta}{1+\varepsilon\theta}}}{1+\lambda_2 e^{\frac{\theta-1}{1+\varepsilon\theta}}}\right]$$

$$\frac{\partial^2\theta}{\partial t^2}=k\frac{\partial^2\theta}{\partial x^2}\left(\frac{\partial\theta}{\partial t}\right)+\frac{\partial}{\partial t}\left[\frac{\lambda_1 e^{\frac{\theta}{1+\varepsilon\theta}}}{1+\lambda_2 e^{\frac{\theta-1}{1+\varepsilon\theta}}}\right]\frac{\partial\theta}{\partial t} \quad (5.4)$$

We obtained

$$\frac{\partial}{\partial t}\left(\frac{\partial\theta}{\partial t}\right)-k\frac{\partial^2}{\partial x^2}\left(\frac{\partial\theta}{\partial t}\right)-\left[\frac{\lambda_1\frac{e^{\frac{\theta}{1+\varepsilon\theta}}}{(1+\varepsilon\theta)^2}}{\left(1+\lambda_2 e^{\frac{\theta-1}{1+\varepsilon\theta}}\right)^2}\right]U\geq 0 \quad (5.5)$$

Equation (5.5) can be written as

$$\frac{\partial U}{\partial t}=k\frac{\partial^2 U}{\partial x^2}-V(x,t)U\geq 0$$

Where

$$V(x,t)=-\frac{\lambda_1\frac{e^{\frac{\theta}{1+\varepsilon\theta}}}{(1+\varepsilon\theta)^2}}{\left(1+\lambda_2 e^{\frac{\theta-1}{1+\varepsilon\theta}}\right)^2} \quad (5.6)$$

Clearly V is bounded from below. Hence by [10]

$$U(x,t)\geq 0 \qquad i.e\ \frac{\partial\theta}{\partial t}\geq 0$$

$$V(x,t)=-\frac{\lambda_1 e^{\frac{\theta}{1+\varepsilon\theta}}(1+\varepsilon\theta)^2}{\left(1+\lambda_2 e^{\frac{\theta-1}{1+\varepsilon\theta}}\right)^2} \quad (5.7)$$

V(x,t) is bounded

$$-\frac{\lambda_1}{1+\lambda_2}\leq V(x,t)\leq 0 \quad (5.8)$$

By Theorem 2, the problem has a solution and the solution is unique.

6.0 Existence and Uniqueness of Solution for the Steady Model

$$k\frac{d^2\theta}{dx^2}+\frac{\lambda_1\theta^n e^{\frac{\theta}{1+\varepsilon\theta}}}{1+\lambda_2 e^{\frac{\theta+1}{1+\varepsilon\theta}}}=0 \quad (6.1)$$

$$\theta(o)=0$$

$\theta^1(o)=\beta,$ guessed value (6.2)

Theorem 3: For $n=0,\varepsilon>0,\lambda_1>0,\lambda_2>0,0<\lambda<1$ the steady state problem (6.1) which satisfies the condition (6.2) has a unique solution.

<u>Proof</u>

To show that equation (6.1) has a unique solution Re-write (6.2) as a system of first order differential equation.

$$\begin{bmatrix}x_1\\x_2\\x_3\end{bmatrix}=\begin{bmatrix}x\\\theta\\\theta^1\end{bmatrix}$$

Then

$$\begin{bmatrix} x_1^1 \\ x_2^1 \\ x_3^1 \end{bmatrix} = \begin{bmatrix} 1 \\ \theta^1 \\ \theta^{11} \end{bmatrix} = \begin{bmatrix} 1 \\ \lambda_3 \\ \dfrac{-\lambda_1 e^{\frac{\lambda_2}{1+\varepsilon\lambda_2}}}{k\left(1+\lambda_2 e^{\frac{\lambda_2+1}{1+\varepsilon\lambda_2}}\right)} \end{bmatrix} \tag{6.3}$$

Together with initial conditions

$$\begin{bmatrix} x_1(0) \\ x_2(0) \\ x_3(0) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \beta \end{bmatrix}$$

Where β is guessed such that the boundary condition is satisfied

$$\left|\frac{\partial F_i}{\partial x_i}\right| i,\ j = 1,2,3$$

are bounded and Lipchitz continuous.
Thus there exists a unique solution of the problem.

7.0 Conclusion

We examine the properties of solution in the mathematical model of the chain-breaking and chain-branching kinetics. The lower and upper solutions method was used to proof the existence and uniqueness of solution. Also we make use of approach of [10] to establish the properties of solutions. The result revealed that partial differential equations considered have existence and unique solutions. It is very interesting to extend these results for higher dimensional problems.

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