

A Mathematical Study of One-step Models of Polymerization.

R.O. Olayiwola, Ph.D.^{*1}; M.O. Durojaye, Ph.D.²; M.S. Immam, B.Tech.¹;
and S.E. Shuaib, B.Tech.¹

¹Department of Mathematics and Statistics, Federal University of Technology, Minna, Nigeria.

²Department of Mathematics, University of Abuja, Abuja, Nigeria.

E-mail: olayiwolarasaq13@gmail.com*

ABSTRACT

A mathematical model for the free radical polymerization in the presence of the material diffusion is presented. We assume both the temperature of the mixture and the initial monomer concentration depends on the space variable. By actual solutions, we prove the existence and uniqueness of solution of the model. We show that temperature is non-decreasing function of time. We use the parameter-expanding method and seek direct eigenfunctions expansion to obtain analytical solution of the model. The results are presented graphically and discussed. It is discovered that the mixture temperature and monomer concentration are significantly influenced by the Frank-Kamenetskii number, material diffusion coefficient and thermal diffusivity of the mixture.

(Keywords: polymerization, free-radical polymerization, Arrhenius kinetics, polymeric materials, material diffusion, parameter-expanding method)

INTRODUCTION

Polyethylene and polypropylene grades have developed over years as the dominant polymers used in many industries such as, automotive, pipe, cable, and other applications [1]. It is estimated that in the year 2005 about 65 million tons will be produced, which makes up over 55 percent of all plastics.

Polymerization is the formation of long chains of covalently bonded monomer units, and it is commonly subdivided into condensation and chain growth polymerization [2]. The polymerization reactions are exothermic and are modelled with temperature-dependent (Arrhenius) kinetics [3].

Polymers, either synthetic or natural, are present in every aspect of our daily lives. Many modern functional materials, pharmaceutical equipment, electronic devices, automobile parts, etc., have polymeric components. Polymers are replacing traditional materials because of their low cost and special applications. Our lives have been thoroughly changed with the advent of mobile phones, computers, refrigerators, electrical domestic appliances, television, etc.; all of these appliances have parts made of synthetic polymeric materials to a large extent. Polymeric materials are also everywhere in our homes: floor carpeting, glue, pipes, paint, wallpaper, foils, electric insulation and moldings are examples of components based on synthetic polymers. The development of new polymers and the modification and enhancement of the old ones are goals of many researchers in both industry and academia [2].

Polymers can be synthesized via several different methods, such as free radical polymerization, anionic and cationic polymerization, ring-opening polymerization, and coordination polymerization. Of the above mentioned techniques, free radical polymerization is the most widely used industrially. This technique is much simpler than the others and is applicable to a wide variety of monomers [2].

Free-radical polymerization is the process of converting a monomer-initiator mixture into a polymer, which occurs when a thermally unstable initiator is mixed with a monomer. The initiator molecules decompose into radicals that combine with the monomer to form reactive polymer chains (polymer radicals) that continue to grow by incorporating additional molecules of the monomer. The growth may terminate through a reaction with either another reactive polymer chain or an initiator radical. The polymer

molecule becomes inactive following the termination step [3 - 5].

In the more recent literatures, several authors have studied the free-radical polymerization. Among them are Almeida et al. [6] who developed a mathematical model for the free radical polymerization of styrene, to predict the steady-state and dynamic behavior of a continuous process and Cardarelli et al. [3] that used numerical simulation to study the influence of reaction kinetics on one-step frontal polymerization in one dimension. They neglected the material diffusion and showed that the long-time behaviour of systems governed by approximate kinetics significantly differs from the long-time behaviour of systems governed by Arrhenius kinetics.

In this paper, a mathematical study of reaction kinetics model of polymerization in the presence of material diffusion is presented. We assume both the temperature of the mixture and the initial monomer concentration depends on the space variable x . We shift and rescale the temperature so that 0 corresponds to the initial temperature T_0 , which are also taking to be the ignition temperature. Physically relevant solutions must have $0 \leq x \leq L$. So, we consider all solutions in the interval $0 \leq x \leq L$. We prove the existence and uniqueness of solution by actual solutions. We also examine the properties of solution. To simulate the flow, we impose the adiabatic and impenetrability boundary conditions on the temperature and the monomer concentration respectively.

MATHEMATICAL MODEL

Consider a test tube containing the monomer-initiator mixture. Let $M(x, t)$ be the monomer concentration and $T(x, t)$ the temperature of the mixture at the point x , $0 \leq x \leq L$ and the time t , $t > 0$. Then the process of free-radical polymerization in the presence of material diffusion can be described by what is known as a single-step, effective kinetics model of monomer-to-polymer conversion:

$$\frac{\partial M}{\partial t} = D \frac{\partial^2 M}{\partial x^2} - AM^n \exp\left(\frac{E}{R_g T_0} \left(1 - \frac{T_0}{T}\right)\right) \quad (1)$$

$$\frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} + AM^n q \exp\left(\frac{E}{R_g T_0} \left(1 - \frac{T_0}{T}\right)\right) \quad (2)$$

The initial and boundary conditions were formulated as follows:

Initial condition:

At $t = 0$ and $\forall x$, $0 \leq x \leq L$

$$T = \frac{R_g T_0^2}{E} \left(1 - \frac{x}{L}\right) + T_0, \quad M = M_0 \left(1 - \frac{x}{L}\right) \quad (3)$$

Boundary conditions:

$$\left. \begin{aligned} M_x(0, t) = 0, \quad T_x(0, t) = 0, \quad t \geq 0 \\ M_x(L, t) = 0, \quad T_x(L, t) = 0, \quad t \geq 0 \end{aligned} \right\}, \quad (4)$$

where n is the order of reaction, D is the material diffusion coefficient, A is the Arrhenius constant, E is the activation energy, k is the thermal diffusivity of the mixture / final product, and R_g is the gas constant, T_0 and M_0 are the initial temperature and concentration, respectively. The constant parameter q is $\frac{\Delta H}{\rho c}$,

where ΔH is the reaction enthalpy; c and ρ are the specific heat and the mixture density, respectively.

METHOD OF SOLUTION

Non-Dimensionalization

To non-dimensionalized the problem (1) – (4), we introduce following dimensionless variables:

$$\theta = \frac{E}{R_g T_0^2} (T - T_0), \quad M' = \frac{M}{M_0}, \quad x' = \frac{x}{L},$$

$$t' = \frac{t}{t_0}, \quad \epsilon = \frac{R_g T_0}{E}, \quad (5)$$

where t_0 is the time for ignition.

Using (5), we obtain, after dropping the prime,

$$\frac{\partial M}{\partial t} = D_1 \frac{\partial^2 M}{\partial x^2} - \sigma M^n \exp\left(\frac{\theta}{1 + \epsilon \theta}\right) \quad (6)$$

$$\frac{\partial \theta}{\partial t} = k_1 \frac{\partial^2 \theta}{\partial x^2} + \delta M^n \exp\left(\frac{\theta}{1 + \epsilon \theta}\right) \quad (7)$$

together with initial and boundary conditions:

$$\left. \begin{aligned} M(x, 0) = 1 - x, \quad \theta(x, 0) = 1 - x \\ M_x(0, t) = 0, \quad M_x(1, t) = 0, \quad t \geq 0 \\ \theta_x(0, t) = 0, \quad \theta_x(1, t) = 0, \quad t \geq 0 \end{aligned} \right\}, \quad (8)$$

where

$$\sigma = At_0 M_0^{n-1} e^{-\frac{E}{RT_0}}, \quad k_1 = \frac{kt_0}{L^2}, \quad D_1 = \frac{Dt_0}{L^2},$$

$$\delta = \frac{At_0 M_0^n q e^{-\frac{E}{RT_0}}}{\epsilon T_0}$$

Existence and Uniqueness of Solution

Theorem 1 Let $D_1 = k_1$, $\sigma = \delta$. Then there exists a unique solution of problem (6) and (7) satisfy (8).

Proof: Let $D_1 = k_1$, $\sigma = \delta$ and $\phi = (\theta + M)$

Then (6) - (8) become:

$$\frac{\partial \phi}{\partial t} = k_1 \frac{\partial^2 \phi}{\partial x^2} \quad (9)$$

$$\phi(x, 0) = 2(1 - x), \quad \phi_x(0, t) = 0, \quad \phi_x(1, t) = 0 \quad (10)$$

Using variable separation method, we obtain the solution of problem (9) and (10) as:

$$\phi(x, t) = \left(\begin{aligned} & 2 + \\ & \sum_{n=1}^{\infty} \frac{8}{(2n-1)^2 \pi^2} \cdot \\ & \exp\left(-k_1 \left(\frac{2n}{-1}\right)^2 \pi^2 t\right) \cos\left(\frac{2n}{-1}\right) \pi x \end{aligned} \right) \quad (11)$$

Then, we obtain:

$$\theta(x, t) = (\phi(x, t) - M(x, t)) \quad (12)$$

$$M(x, t) = (\phi(x, t) - \theta(x, t)) \quad (13)$$

Hence, there exists a unique solution of problem (6) - (8). This completes the proof.

However, using (13), we can write equation (6) and (7) as:

$$\frac{\partial M}{\partial t} = D_1 \frac{\partial^2 M}{\partial x^2} - \sigma (\phi - \theta)^n \exp\left(\frac{\theta}{1 + \epsilon \theta}\right) \quad (14)$$

$$\frac{\partial \theta}{\partial t} = k_1 \frac{\partial^2 \theta}{\partial x^2} + \delta (\phi - \theta)^n \exp\left(\frac{\theta}{1 + \epsilon \theta}\right) \quad (15)$$

Properties of Solution

Theorem 2 Let $\epsilon > 0$, $k_1 = 1$ and $n = 1$ in

$$(15). \text{ Then } \frac{\partial \theta}{\partial t} \geq 0.$$

In the proof, we shall make use of following Lemma of Kolodner and Pederson [7].

Lemma (Kolodner and Pederson [7]) Let

$u(x, t) = 0 \left(e^{\alpha|x|^2} \right)$ be a solution on $R^n \times [0, t)$ of the differential inequality:

$$\frac{\partial u}{\partial t} - \Delta u + K(x, t)u \geq 0$$

where K is bounded from below. If $u(x,0) \geq 0$, then $u(x,t) \geq 0$ for all $(x,t) \in R^n \times [0,t_0)$.

Proof of Theorem 2: Let $\epsilon > 0$, $k_1 = 1$ and $n = 1$ in (15). We obtain:

$$\frac{\partial \theta}{\partial t} - \frac{\partial^2 \theta}{\partial x^2} - \delta(\phi - \theta)e^{\frac{\theta}{1+\epsilon\theta}} = 0$$

Differentiating with respect to t , we have:

$$\begin{aligned} & \frac{\partial}{\partial t} \left(\frac{\partial \theta}{\partial t} \right) - \frac{\partial^2}{\partial x^2} \left(\frac{\partial \theta}{\partial t} \right) + \\ & \delta \left(1 - (\phi - \theta) \left(\frac{1}{1 + \epsilon \theta} \right)^2 \right) e^{\frac{\theta}{1 + \epsilon \theta}} \frac{\partial \theta}{\partial t} = \\ & \delta e^{\frac{\theta}{1 + \epsilon \theta}} \frac{\partial \phi}{\partial t} \end{aligned}$$

Let,

$$u = \frac{\partial \theta}{\partial t}$$

Then,

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} + \delta \left(1 - (\phi - \theta) \left(\frac{1}{1 + \epsilon \theta} \right)^2 \right) e^{\frac{\theta}{1 + \epsilon \theta}} u \geq 0$$

$$\text{since } \delta e^{\frac{\theta}{1 + \epsilon \theta}} \frac{\partial \phi}{\partial t} \geq 0$$

This can be written as:

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} + K(x,t)u \geq 0,$$

where

$$K(x,t) = \delta \left(1 - (\phi - \theta) \left(\frac{1}{1 + \epsilon \theta} \right)^2 \right) e^{\frac{\theta}{1 + \epsilon \theta}}$$

Clearly, K is bounded from below. Hence by Kolodner and Pederson's lemma $u(x,t) \geq 0$

i.e., $\frac{\partial \theta}{\partial t} \geq 0$. This completes the proof.

Theorem 3 Let $\epsilon > 0$, $k_1 = 1$ and $n = 1$ in (15). Then $\theta(x,t) \geq 0$ for $(x,t) \in (0,\infty) \times (0,t_0)$, $t_0 > 0$.

Proof: Let $\epsilon > 0$, $k_1 = 1$ and $n = 1$ in (15). We obtain:

$$\frac{\partial \theta}{\partial t} - \frac{\partial^2 \theta}{\partial x^2} + \delta e^{\frac{\theta}{1 + \epsilon \theta}} \theta = \delta \phi e^{\frac{\theta}{1 + \epsilon \theta}}$$

That is:

$$\frac{\partial \theta}{\partial t} - \frac{\partial^2 \theta}{\partial x^2} + \delta e^{\frac{\theta}{1 + \epsilon \theta}} \theta \geq 0 \quad \text{since } \delta \phi e^{\frac{\theta}{1 + \epsilon \theta}} \geq 0$$

This can be written as:

$$\frac{\partial \theta}{\partial t} - \frac{\partial^2 \theta}{\partial x^2} + k(x,t)\theta \geq 0,$$

where

$$k(x,t) = \delta e^{\frac{\theta}{1 + \epsilon \theta}}$$

Hence, by Kolodner and Pederson's lemma $\theta(x,t) \geq 0$. This completes the proof.

Solution by Parameter-expanding Method

Here, we consider equations (14) and (15) when $k_1 = D_1$ and $n = 1$. Ayeni [8] has shown that

$\exp\left(\frac{\theta}{1 + \epsilon \theta}\right)$ can be approximated as $1 + (e - 2)\theta + \theta^2$. In this paper we are going to take an approximation of the form,

$$\exp\left(\frac{\theta}{1 + \epsilon \theta}\right) \approx 1 + (e - 2)\theta \tag{16}$$

Suppose the solutions $M(x, t)$, $\theta(x, t)$ and the constant δ in equations (14) and (15) can be expressed as:

$$\theta = \theta_0 + \epsilon \theta_1 + \epsilon^2 \theta_2 + h.o.t. \quad (17)$$

$$M = M_0 + \epsilon M_1 + \epsilon^2 M_2 + h.o.t. \quad (18)$$

$$\delta = \epsilon \delta_0 + \epsilon^2 \delta_1 + h.o.t., \quad (19)$$

where *h.o.t.* read "higher order terms in ϵ ". In our analysis we are interested only in the first two terms.

Substituting (16) – (19) into (14) and (15), and processing, we obtain:

$$\frac{\partial \theta_0}{\partial t} = k_1 \frac{\partial^2 \theta_0}{\partial x^2} \quad (20)$$

$$\theta_0(x, 0) = 1 - x, \theta_{0x}(0, t) = 0, \theta_{0x}(1, t) = 0, t \geq 0$$

$$\frac{\partial M_0}{\partial t} = D_1 \frac{\partial^2 M_0}{\partial x^2} - \sigma(\phi - \theta_0)(1 + (e - 2)\theta_0) \quad (21)$$

$$M_0(x, 0) = 1 - x, M_{0x}(0, t) = 0, M_{0x}(1, t) = 0, t \geq 0$$

$$\frac{\partial \theta_1}{\partial t} = k_1 \frac{\partial^2 \theta_1}{\partial x^2} + \delta_0(\phi - \theta_0)(1 + (e - 2)\theta_0) \quad (22)$$

$$\theta_1(x, 0) = 0, \theta_{1x}(0, t) = 0, \theta_{1x}(1, t) = 0, t \geq 0$$

$$\frac{\partial M_1}{\partial t} = D_1 \frac{\partial^2 M_1}{\partial x^2} + \sigma(1 + (e - 2)\theta_0)\theta_1 - \quad (23)$$

$$\sigma(\phi - \theta_0)(e - 2)\theta_1$$

$$M_1(x, 0) = 0, M_{1x}(0, t) = 0, M_{1x}(1, t) = 0, t \geq 0$$

Seeking direct eigen functions expansion, we obtain:

$$\theta_0(x, t) = 1 + \sum_{n=1}^{\infty} \frac{4}{(2n-1)^2 \pi^2} e^{-k_1(2n-1)^2 \pi^2 t} \cos(2n-1)\pi x \quad (24)$$

$$M_0(x, t) = 1 + \sum_{n=1}^{\infty} \frac{4}{(2n-1)^2 \pi^2} e^{-D_1(2n-1)^2 \pi^2 t} \cos(2n-1)\pi x - 2\sigma(1 + (e - 2))t + \quad (25)$$

$$\sum_{n=1}^{\infty} \frac{4\sigma}{(2n-1)^2 \pi^2} \left(\sum_{n=1}^{\infty} \frac{4(e-2)(e^{-2k_1(2n-1)^2 \pi^2 t} - 1)}{2k_1(2n-1)^4 \pi^4} \right)$$

$$\theta_1(x, t) = 2\delta_0(1 + (e - 2))t -$$

$$\sum_{n=1}^{\infty} \frac{4\delta_0}{(2n-1)^2 \pi^2} \left(\sum_{n=1}^{\infty} \frac{4(e-2)(e^{-2k_1(2n-1)^2 \pi^2 t} - 1)}{2k_1(2n-1)^4 \pi^4} \right) \quad (26)$$

$$M_1(x, t) = 2\sigma(1 + 2(e - 2)).$$

$$\left(\delta_0(1 + (e - 2))t^2 + \frac{4\delta_0}{(2n-1)^2 \pi^2} \sum_{n=1}^{\infty} \left(\sum_{n=1}^{\infty} \frac{4(e-2) \left(2k_1(2n-1)^2 \pi^2 t + \left(\frac{-1 + e^{-2k_1(2n-1)^2 \pi^2 t}}{e^{-2k_1(2n-1)^2 \pi^2 t}} \right) \right)}{4k_1^2(2n-1)^6 \pi^6} \right) \right) \quad (27)$$

The computations were done using computer symbolic algebraic package MAPLE.

RESULTS AND DISCUSSION

The existence and uniqueness of solution of the Problem is proved by actual solutions. Also, under certain condition, we have shown that $\theta(x, t)$ is non-decreasing function of time. Analytical solutions of equations (20) - (23) are computed for the values of $\sigma = 0.5$, $\epsilon = 0.01$, $e = 2.718$. The monomer concentration and mixture temperature values are depicted graphically in Figures 1 - 12.

The mixture temperature distribution behavior is shown in Figures 1 - 3. Figure 1 depicts the graph of $\theta(x, t)$ against x and t for different values of δ . It is observed that the temperature of the mixture increases as Frank-Kamenetskii number increases. Figure 2 depicts the graph of

$\theta(x, t)$ against x for different values of δ . It is observed that the temperature of the mixture increases along the spatial direction as Frank-Kamenetskii number increases. Figure 3 depicts the graph of $\theta(x, t)$ against t for different values of δ . It is observed that the temperature of the mixture increases along the time direction as Frank-Kamenetskii number increases.

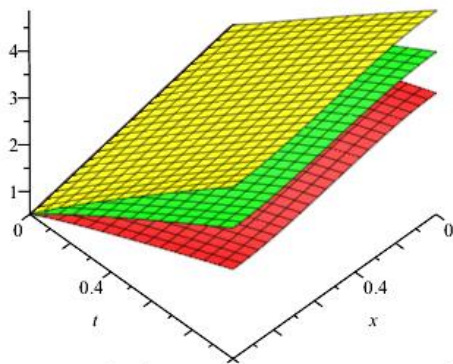


Figure 1: Plots of $\theta(x, t)$ against x and t for different values of δ and $k_1 = 0.02, D_1 = 0.02, \sigma = 0.5, \epsilon = 0.01, e = 2.718$

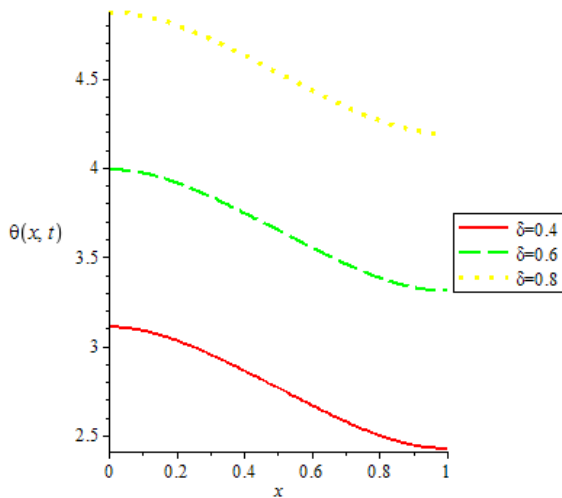


Figure 2: Plots of $\theta(x, t)$ against x for different values of δ and $k_1 = 0.02, D_1 = 0.02, \sigma = 0.5, \epsilon = 0.01, e = 2.718, t = 1$

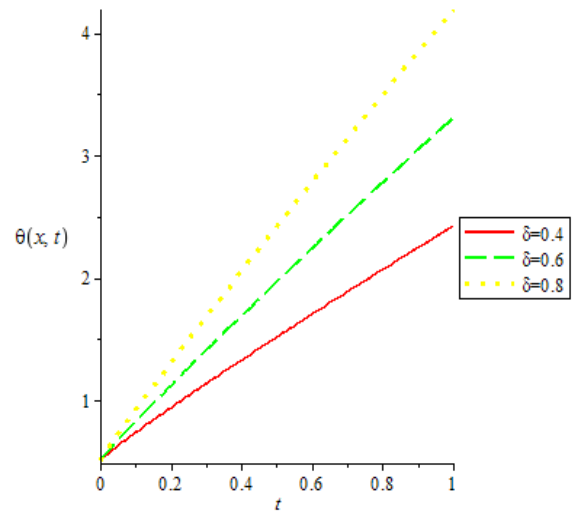


Figure 3: Plots of $\theta(x, t)$ against t for different values of δ and $k_1 = 0.02, D_1 = 0.02, \sigma = 0.5, \epsilon = 0.01, e = 2.718, x = 1$

The monomer concentration distribution behavior is shown in Figure 4 - 6. Figure 4 depicts the graph of $M(x, t)$ against x and t for different values of δ . It is observed that the monomer concentration increases as Frank-Kamenetskii number increases.

Figure 5 depicts the graph of $M(x, t)$ against x for different values of δ . It is observed that the monomer concentration increases along the spatial direction as Frank-Kamenetskii number increases.

Figure 6 depicts the graph of $M(x, t)$ against t for different values of δ . It is observed that the monomer concentration increases along the time direction as Frank-Kamenetskii number increases.

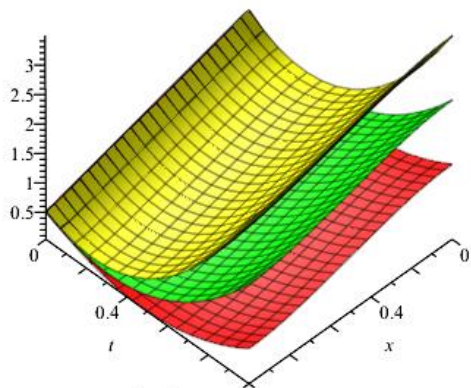


Figure 4: Plots of $M(x, t)$ against x and t for different values of δ and $k_1 = 0.02, D_1 = 0.02, \sigma = 0.5, \epsilon = 0.01, e = 2.718$

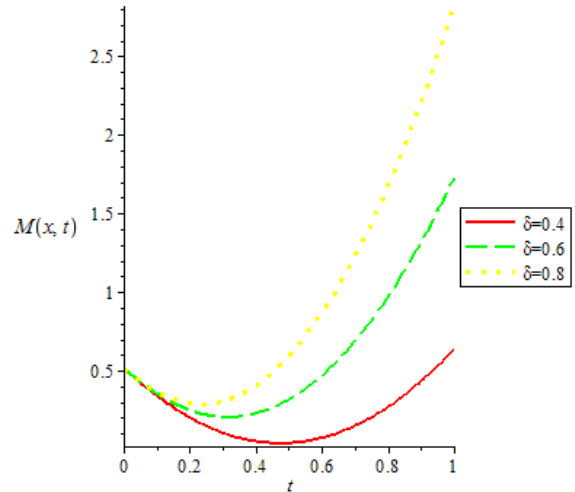


Figure 6: Plots of $M(x, t)$ against t for different values of δ and $k_1 = 0.02, D_1 = 0.02, \sigma = 0.5, \epsilon = 0.01, e = 2.718, x = 1$

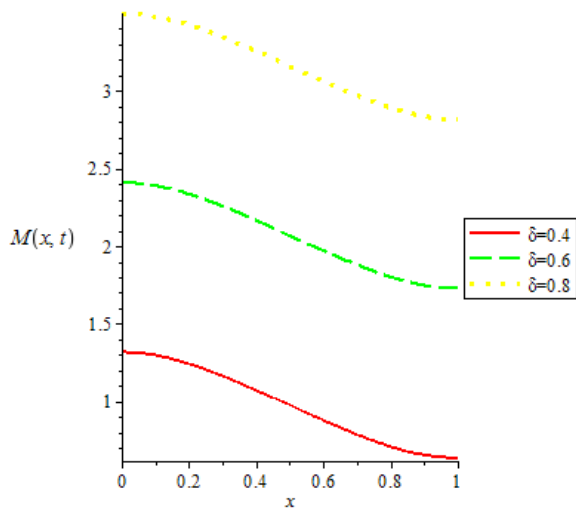


Figure 5: Plots of $M(x, t)$ against x for different values of δ and $k_1 = 0.02, D_1 = 0.02, \sigma = 0.5, \epsilon = 0.01, e = 2.718, t = 1$

The mixture temperature distribution behavior is shown in Figures 7 - 9. Figure 7 depicts the graph of $\theta(x, t)$ against x and t for different values of k_1 . It is observed that the temperature of the mixture increases along time and decreases along space as thermal diffusivity of the mixture increases.

Figure 8 depicts the graph of $\theta(x, t)$ against x for different values of k_1 . It is observed that the temperature of the mixture decreases along the spatial direction as thermal diffusivity of the mixture increases.

Figure 9 depicts the graph of $\theta(x, t)$ against t for different values of k_1 . It is observed that the temperature of the mixture increases along the time direction as thermal diffusivity of the mixture increases.

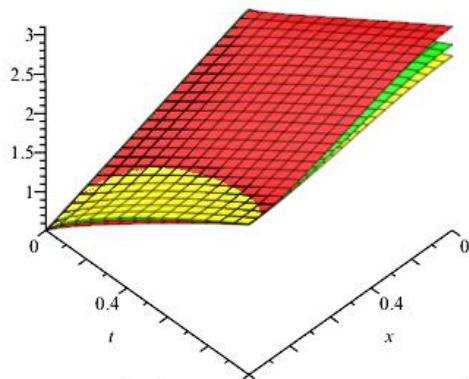


Figure 7: Plots of $\theta(x, t)$ against x and t for different values of k_1 and $\delta = 0.4, \sigma = 0.5, \epsilon = 0.01, e = 2.718$

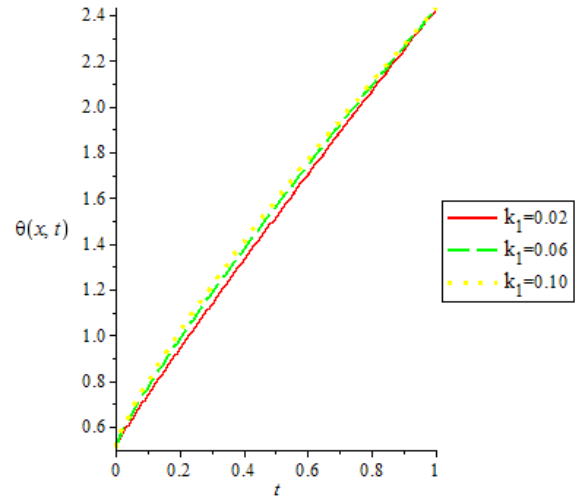


Figure 9: Plots of $\theta(x, t)$ against t for different values of k_1 and $\delta = 0.4, \sigma = 0.5, \epsilon = 0.01, e = 2.718, x = 1$

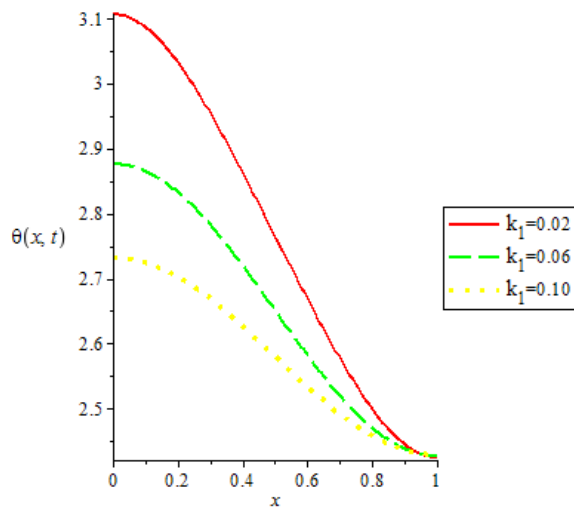


Figure 8: Plots of $\theta(x, t)$ against x for different values of k_1 and $\delta = 0.4, \sigma = 0.5, \epsilon = 0.01, e = 2.718, t = 1$

The monomer concentration distribution behavior is shown in Figure 10 - 12. Figure 10 depicts the graph of $M(x, t)$ against x and t for different values of D_1 . It is observed that the monomer concentration increases as material diffusion coefficient increases.

Figure 11 depicts the graph of $M(x, t)$ against x for different values of D_1 . It is observed that the monomer concentration decreases and later increases along the spatial direction as material diffusion coefficient increases.

Figure 12 depicts the graph of $M(x, t)$ against t for different values of D_1 . It is observed that the monomer concentration increases along the time direction as material diffusion coefficient increases.

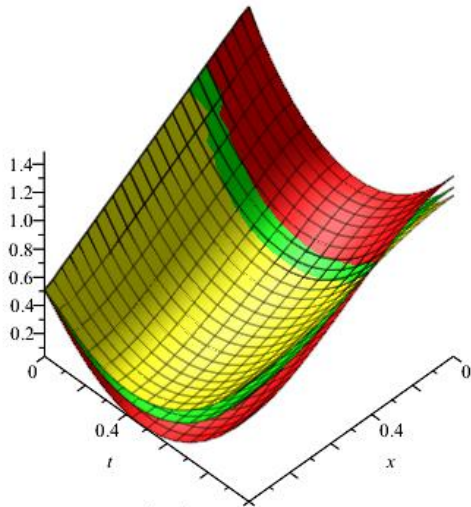


Figure 10: Plots of $M(x, t)$ against x and t for different values of D_1 and $\delta = 0.4, \sigma = 0.5, \epsilon = 0.01, e = 2.718$

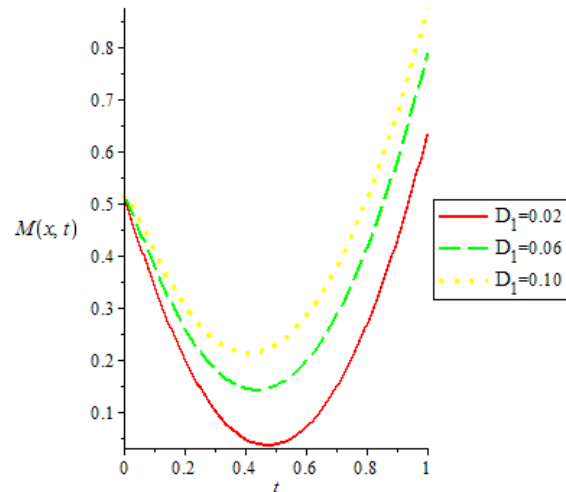


Figure 12: Plots of $M(x, t)$ against t for different values of D_1 and $\delta = 0.4, \sigma = 0.5, \epsilon = 0.01, e = 2.718, x = 1$

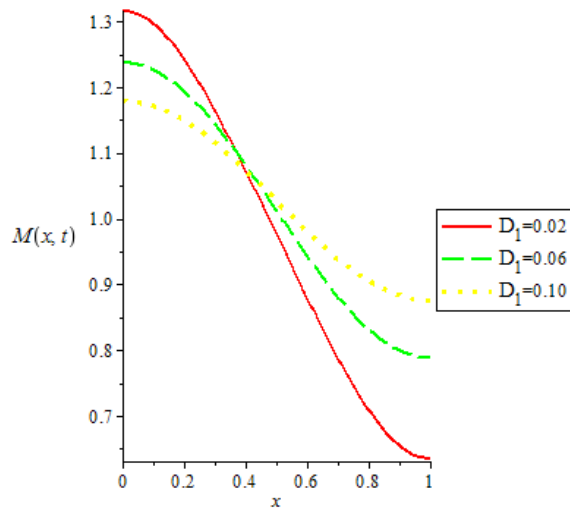


Figure 11: Plots of $M(x, t)$ against x for different values of D_1 and $\delta = 0.4, \sigma = 0.5, \epsilon = 0.01, e = 2.718, t = 1$

It is worth pointing out that the effect of δ as shown in Figures 1-6 physically means that the temperature rises and species is consumed. These occur as a result of increase in reaction enthalpy. When the heat of reaction is high, the rate of conversion of a monomer-initiator mixture into a polymer is high and consequently, the rate of formation of long chains of covalently bonded monomer units is boosted. This is of great economic importance.

CONCLUSION

To study a model for the free radical polymerization in the presence of the material diffusion, we used the parameter-expanding method to decouple the system of partial differential equations and analytical solution via direct eigenfunctions expansion is obtained. The governing parameters for the problem under study are the Frank-Kamenetskii number, material diffusion coefficient and thermal diffusivity of the mixture.

The mixture temperature and monomer concentration profiles are significantly influenced by the parameters involved. The results may be used as a preliminary predictive tool to study mathematically the free radical polymerization in the presence of the material diffusion. The work may be extended to more complex cases such as when the order of reaction is more than unity and therefore, recommended for further research.

NOMENCLATURE

n : order of reaction

E : activation energy

R : gas constant

A : Arrhenius constant

ΔH : reaction enthalpy

c : specific heat

T : temperature of the mixture

t : time

x : position

M : monomer concentration

k : thermal diffusivity of the mixture

D : material diffusion coefficient

Greek Letters

ρ : mixture density

\in : dimensionless activation energy $\left\{ = \frac{RT_0}{E} \right\}$

θ : dimensionless temperature

δ : Frank-Kamenetskii number for material

$$\left\{ = \frac{At_0 M_0^n q e^{-\frac{E}{RT_0}}}{\in T_0} \right\}$$

Subscripts

g : gas

0 : initial

REFERENCES

1. Salamone, J.C. 1996. *Polymeric materials Encyclopedia*. 3: 10-13.
2. Al-Harhi M. 2006. *Mathematical Modeling of Atom Transfer Radical Polymerization*. Ph.D. Thesis. University of Waterloo: Waterloo, Ontario, Canada.
3. Cardarelli, S.A., D. Golovaty, L.K. Gross, V.T. Gyrya, and J. Zhu. 2005. "A Numerical Study of One-Step Models of Polymerization: Frontal versus Bulk Mode". *Elsevier Physica D*. 206:145–165.
4. Odian, G. 1990. *Principles of Polymerization, 3rd Edition*. 198.
5. Rudin, A. 1999. "The Element of Polymer Science and Engineering". 189.
6. Almeida A.S., K. Wada, and A.R. Secchi. 2008. "Simulation of Styrene Polymerization Reactors: Kinetics and Thermodynamic Modeling". *Brazilian Journal of Chemical Engineering*. 25(2):337-349, April - June, 2008.
7. Kolodner, J. and R.H. Pederson. 1966. "Pointwise Bounds for Solutions of some Semi-Linear Parabolic Equations". *J. Diff. Equations*. 2:353-364.
8. Ayeni, R.O. 1982. "On the Explosion of Chain-Thermal Reactions". *J. Austral. Math. Soc. (Series B)*. 24:194-202.

ABOUT THE AUTHORS

Dr. R.O. Olayiwola, is a Lecturer in the Department of Mathematics and Statistics, Federal University of Technology, Minna, Nigeria. He holds a Ph.D. degree in Applied Mathematics from Ladoke Akintola University of Technology, Ogbomoso, Nigeria. His research interests are in areas of combustion, fluid mechanics, and mathematical modeling.

Dr. M.O. Durojaye, is a Lecturer in the Department of Mathematics, University of Abuja, Abuja, Nigeria. She holds a Ph.D. degree in Applied Mathematics from Ladoke Akintola University of Technology, Ogbomoso, Nigeria. Her research interests are in areas of fluid mechanics and computational fluid dynamics.

Mr. M. S. Immam, is an undergraduate student in the Department of Mathematics and Statistics, Federal University of Technology, Minna, Nigeria. His research interests are in modeling and combustion.

Mr. S. E. Shuaib, is an undergraduate student in the Department of Mathematics and Statistics, Federal University of Technology, Minna, Nigeria. His research interests are in modeling and combustion.

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