Fixed-bed Solid Fuel Arrhenius Combustion: Modelling and Simulation

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Abstract

In this paper, we study coupled heat transport in Arrheniusly reactive porous medium using a homogeneous description at the Darcy-scale. We assume that there is a perfect contact between gas and solid phases. By method of upper and lower solution, we prove the existence of solution of the model. We show that temperature is non-decreasing function of time. We obtain the time-dependent temperature profiles through analytical method.

***Keywords* :** Arrhenius combustion, pyrolysis, fixed-bed, solid fuel, Darcy-scale.

1. Introduction

Oil shale in its natural state contains kerogen, a precursor to petroleum. Kerogen is the solid, insoluble, organic material in the shale that can be converted to oil and other petroleum products by pyrolysis and distillation. The kerogen in oil shale does not flow naturally and must be subjected to heat treatment to be released from the shale [1].

One of the converting methods is to burn a part of them to pyrolyze the other with the generated heat. This method can be applied in-situ or in a reactor after mining extraction [2].

The processing of oil shale involves numerous chemical reactions, not only those leading directly to oil and gas generation but also those required for process heat. The most important reaction in oil shale processing is that leading to shale oil. The pyrolysis reactions generate gas as well as oil. The composition of the gas depends on the processing time and the way the shale is heated [3].

In the literature, there are only few authors who attempted numerical simulation at a microscopic scale. Ohlemiller [4] gave a very detailed review of the chemical and physical processes implied in fixed-bed solid fuel combustion. He proposed a complete mathematical model taking into account all transport mechanisms and all complex chemical processes at grain scale. Then he estimated that the complete problem was not approachable.

Lu and Yortsos [5] presented numerical simulations where the porous medium had been represented by capillaries network. Work is done at the pore scale in off-line solids with a local approach for transport. Redl [6] come near this objective. He used a Lattice–Boltzmann type of approach in a three-dimensional space. He solved transport equations in each phase at the microscopic scale.

Debenest et al. [7, 8] adopted an original approach which was based on a detailed three-dimensional description at the microscopic scale. They carry out direct simulation in order to characterize various modes of propagation and to determine transport effective parameters at the Darcy-scale.

Lapene et al. [2] modeled coupled mass and heat transport in reactive porous medium using a homogeneous description at the Darcy-scale. Local non equilibrium transport of heat was treated with a two field temperature model, one for the gas phase and one for the solid phase.

This present paper focuses on further development of the model used in [2]. The Arrhenius heat generation and chemical reaction is introduced into the system of equation. We consider the pressure gradient to be parabolic. We prove the existence of solution. We also examine the properties of solution. To simulate the flow, we assume that there is a perfect contact between gas and solid phases.

2. Mathematical Model

Here, we extend Lapene et al. [2] model to a situation where there is Arrhenius heat generation and chemical reaction. Then we have

The gas phase energy equation

$$\varepsilon_g\left(\rho C_p\right)_g\frac{\partial T_g}{\partial t}+\left(\rho C_p\right)_g v\frac{\partial T_g}{\partial x}=\frac{\partial}{\partial x}\left(\lambda_g\frac{\partial T_g}{\partial x}\right)+\Gamma\left(T_g-T_s\right)+Q_g+$$

$$h\left(T_{amb}-T_g\right)+QAe^{-\frac{E}{RT_g}} \tag{2.1}$$

The solid phase energy equation

$$\varepsilon_s\left(\rho C_p\right)_s\frac{\partial T_s}{\partial t}=\frac{\partial}{\partial x}\left(\lambda_s\frac{\partial T_s}{\partial x}\right)-\Gamma\left(T_g-T_s\right)+Q_s+h\left(T_{amb}-T_s\right)+QAe^{-\frac{E}{RT_g}} \tag{2.2}$$

The Darcy's equation

$$v=-\frac{k}{\mu}\frac{\partial P}{\partial x} \tag{2.3}$$

The initial and boundary conditions at the inlet and outlet of the reactor were formulated as follows:

Initial condition:

At $t = 0$ and $\forall\ x$

$$T_g = T_0, \qquad T_s = T_0 \tag{2.4}$$

Boundary conditions:

$$\left.\begin{array}{l} T_g\big|_{x=0} = T_g\big|_{x=L} = T_0 \\ T_s\big|_{x=0} = T_s\big|_{x=L} = T_0 \end{array}\right\}, \tag{2.5}$$

where Q is the heat of reaction, A is frequency factor, E is activation energy, R is perfect gas constant, ε_g is gas phase porosity, ε_s is solid phase porosity, λ_g is effective thermal conductivity of gas phase, λ_s is effective thermal conductivity of solid phase, C_{pg} is the heat capacity of gas phase, ρ_g is gas phase density, ρ_s is solid phase density, v is filtration velocity, Γ is the exchange term between both phases, T_g is temperature of gas phase, T_s is temperature of solid phase, t is time, x is position, Q_g is the heat source term in gas phase, Q_s is the heat source term in solid phase, h is thermal exchange coefficient, T_{amb} is ambient temperature, k is permeability, μ is dynamic viscosity, P is pressure.

We emphasize here that the exponential term in the equations is due to Arrhenius reaction and assume that there is a perfect contact between gas and solid phases so that one can make the hypothesis of local thermal equilibrium between the phases:

$$T_g = T_s = T \tag{2.6}$$

Using (2.3) and adding (2.1) and (2.2), gives

$$\frac{\partial T}{\partial t} - \frac{(\rho C_p)_g}{\rho C_p}\frac{k}{\mu}\frac{\partial P}{\partial x}\frac{\partial T}{\partial x} = \frac{1}{\rho C_p}\frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) + \frac{Q_v}{\rho C_p} + \frac{h^*}{\rho C_p}\left(T_{amb} - T\right) + \frac{Q^* A}{\rho C_p} e^{-\frac{E}{RT}} \tag{2.7}$$

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

where

$\rho C_p = \varepsilon_g (\rho C_p)_g + \varepsilon_s (\rho C_p)_s, \quad \lambda = \lambda_g + \lambda_s, \quad h^* = 2h, \quad Q_v = Q_g + Q_s, \quad Q^* = 2Q$

are respectively, the overall thermal capacity per unit volume, the overall thermal conductivity, the overall thermal exchange coefficient, the overall heat source term and the overall heat of reaction.

3. Method of Solution

In this analysis, we let λ, ρC_p, $(\rho C_p)_g$, Q_v, h^* be constant and consider the pressure gradient to be parabolic i.e.

$$\frac{\partial P}{\partial x} = f(x) = \frac{x}{L}\left(1 - \frac{x}{L}\right) \tag{3.1}$$

By introducing the following dimensionless variables:

$$\theta = \frac{E}{RT_o^2}(T - T_o), \quad \in = \frac{RT_0}{E}, \quad x' = \frac{x}{L}, \quad t' = \frac{t}{t_{out}}, \tag{3.2}$$

where t_{out} is the time at which the combustion front leaves the reactor.

Equation (2.7) (after dropping prime) become

$$\frac{\partial \theta}{\partial t} - k_1 x(1-x)\frac{\partial \theta}{\partial x} = \lambda_1 \frac{\partial^2 \theta}{\partial x^2} - \alpha\theta + \beta + \delta e^{\frac{\theta}{1+\in\theta}} \tag{3.3}$$

$$\theta(x,0) = 0, \qquad \theta(0,t) = 0, \qquad \theta(1,t) = 0, \tag{3.4}$$

where

$k_1 = \dfrac{k t_{out} (\rho C_p)_g}{(\rho C_p)\mu L}$ is the permeability parameter

$\lambda_1 = \frac{t_{out}\lambda}{(\rho C_p)L^2}$ is the scaled thermal conductivity

$\delta = \frac{Q^* A t_{out}.e^{-\frac{E}{RT_0}}}{\in T_0(\rho C_p)}$ is the Frank-Kamenetskii parameter

$$\alpha = \frac{t_{out}h^*}{(\rho C_p)}, \qquad \beta = \frac{t_{out}(Q_v + h^*(T_{amb} - T_0))}{\in T_0(\rho C_p)}$$

3.1 Existence of Solution

To prove the existence of solution of problem (3.3), it suffices to show that there exists upper and lower solution.

Definition 1: A smooth function $\underline{u}$ is said to be a lower solution of the problem

$$Lu = f(x,t,u)$$

where

$$L = \frac{\partial}{\partial t} + a(x,t)\frac{\partial^2}{\partial x^2} + b(x,t)\frac{\partial}{\partial x} + c(x,t)$$

if $\underline{u}$ satisfies

$$L\underline{u} \le f(x,t,\underline{u})$$

$$\underline{u}(x,0) \le f(x), \quad \underline{u}(0,t) \le h_1(t), \quad \underline{u}(L,t) \le h_2(t)$$

Definition 2: A smooth function $\bar{u}$ is said to be an upper solution of the problem

$$Lu = f(x,t,u)$$

where

$$L = \frac{\partial}{\partial t} + a(x,t)\frac{\partial^2}{\partial x^2} + b(x,t)\frac{\partial}{\partial x} + c(x,t)$$

if $\bar{u}$ satisfies

$L\bar{u} \geq f(x,t,\bar{u})$

$\bar{u}(x,0) \geq f(x), \quad \bar{u}(0,t) \geq h_1(t), \quad \bar{u}(L,t) \geq h_2(t)$

Theorem 1

Let $k_1 > 0,\ \lambda_1 > 0,\ \alpha > 0,\ \beta > 0,\ \delta > 0,\ \in > 0$. Then the equation (3.3) with the boundary and initial conditions (3.4) has a solution for all $t \geq 0$.

Proof:

Equation (3.3) can be written as

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

where

$$L\theta \equiv \frac{\partial \theta}{\partial t} - k_1 x(1-x)\frac{\partial \theta}{\partial x} - \lambda_1 \frac{\partial^2 \theta}{\partial x^2} + \alpha\theta$$

$$f(x,t,\theta) \equiv \beta + \delta e^{\frac{\theta}{1+\in\theta}}$$

Consider

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

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

Clearly,

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

Now,

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

This implies

$$L\underline{\theta} = \frac{\partial \underline{\theta}}{\partial t} - k_1 x(1-x)\frac{\partial \underline{\theta}}{\partial x} - \lambda_1 \frac{\partial^2 \underline{\theta}}{\partial x^2} + \alpha\underline{\theta} = 0 - 0 - 0 + 0 = 0$$

$f(x,t,\underline{\theta}) = \beta + \delta$

Hence

$L\underline{\theta} < f(x,t,\underline{\theta})$

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

Also consider

$$\overline{\theta}(x,t) = \left(\beta + \delta e^{\frac{1}{\epsilon}}\right)t$$

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

Clearly,

$$\overline{\theta}(x,0) = 0, \quad \overline{\theta}(0,t) = \left(\beta + \delta e^{\frac{1}{\epsilon}}\right)t, \quad \overline{\theta}(1,t) = \left(\beta + \delta e^{\frac{1}{\epsilon}}\right)t$$

Now,

$$\frac{\partial \overline{\theta}}{\partial t} = \left(\beta + \delta e^{\frac{1}{\epsilon}}\right)$$

$$\frac{\partial \overline{\theta}}{\partial x} = 0$$

$$\frac{\partial^2 \overline{\theta}}{\partial \eta^2} = 0$$

This implies

$$L\overline{\theta} = \frac{\partial \underline{\theta}}{\partial t} - k_1 x(1-x)\frac{\partial \underline{\theta}}{\partial x} - \lambda_1 \frac{\partial^2 \underline{\theta}}{\partial x^2} + \alpha \underline{\theta}$$

$$= \left(\beta + \delta e^{\frac{1}{\epsilon}}\right) - 0 - 0 + \alpha\left(\beta + \delta e^{\frac{1}{\epsilon}}\right)t$$

$$= \left(\beta + \delta e^{\frac{1}{\in}} \right) (1 + \alpha t)$$

$$f(x,t,\bar{\theta}) = \beta + \delta e^{\frac{\bar{\theta}}{1+\in\bar{\theta}}} \leq \beta + \delta e^{\frac{1}{\in}}$$

Hence

$$L\bar{\theta} \geq f(x,t,\bar{\theta})$$

By definition 2, $\bar{\theta}(x,t) = \left(\beta + \delta e^{\frac{1}{\in}} \right) t$ is an upper solution.

Hence, there exists a solution of problem (3.3). This completes the proof.

3.2 Properties of Solution

Theorem 2

Let $\in > 0$, $\lambda_1 = 1$ *and* $k_1 = \alpha = \beta = 0$ in (3.3). Then $\frac{\partial \theta}{\partial t} \geq 0$.

In the proof, we shall make use of following Lemma of Kolodner and Pederson [9].

Lemma (Kolodner and Pederson [9])

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 $\in > 0$, $\lambda_1 = 1$ *and* $k_1 = \alpha = \beta = 0$ in (3.3). We obtain

$$\frac{\partial \theta}{\partial t} - \frac{\partial^2 \theta}{\partial x^2} - \delta e^{\frac{\theta}{1+\in\theta}} = 0$$

Differentiating with respect to t, we have

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

Let

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

Then

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

This can be written

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

where

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

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.

3.2 Analytical Solution

Here, we consider (3.3) when $\in\to 0$. Then (3.3) becomes

$$\frac{\partial \theta}{\partial t}-k_1x(1-x)\frac{\partial \theta}{\partial x}=\lambda_1\frac{\partial^2\theta}{\partial x^2}-\alpha\theta+\beta+\delta e^{\theta} \qquad (3.5)$$

Ayeni [10] has shown that $\exp(\theta)$ can be approximated as $1+(e-2)\theta+\theta^2$. In this paper we are going to take an approximation of the form

$$\exp(\theta)\approx 1+(e-2)\theta \qquad (3.6)$$

Then (3.5) can be written as

$$\frac{\partial\theta}{\partial t} - k_1 x(1-x)\frac{\partial\theta}{\partial x} = \lambda_1 \frac{\partial^2\theta}{\partial x^2} + \alpha_1\theta + \beta_1, \tag{3.7}$$

where

$\alpha_1 = (\delta(e-2) - \alpha)$ and $\beta_1 = \beta + \delta$

Using the asymptotic expansion

$$\theta = \theta_0 + \in\theta_1 + h.o.t., \tag{3.8}$$

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

Let

$$k_1 = \in k_0 \tag{3.9}$$

and equate the powers of $\in$, we have

$\in^0$:

$$\frac{\partial\theta_0}{\partial t} = \lambda_1 \frac{\partial^2\theta_0}{\partial x^2} + \alpha_1\theta_0 + \beta_1 \tag{3.10}$$

$$\theta_0(x,0) = 0, \qquad \theta_0(0,t) = 0, \qquad \theta_0(1,t) = 0$$

$\in^1$:

$$\frac{\partial\theta_1}{\partial t} = \lambda_1 \frac{\partial^2\theta_1}{\partial x^2} + \alpha_1\theta_1 + k_0 x(1-x)\frac{\partial\theta_0}{\partial x} \tag{3.11}$$

$$\theta_1(x,0) = 0, \qquad \theta_1(0,t) = 0, \qquad \theta_1(1,t) = 0$$

We obtain the solution of (3.10) and (3.11) as

$$\theta_0(x,t) = \sum_{n=1}^{\infty} \frac{2\beta_1\left(1-(-1)^n\right)}{n\pi(\alpha_1 - \lambda_1 n\pi)}\left(e^{(\alpha_1-\lambda_1 n\pi)t} - 1\right)\sin n\pi x \tag{3.12}$$

$$\theta_1(x,t)=\sum_{n=1}^{\infty}\left(\sum_{n=1}^{\infty}\frac{2\beta_1 k_0\left(1-(-1)^n\right)\left(1-(-1)^{2n}\right)}{n^2\pi^2(\alpha_1-\lambda_1 n\pi)}\left(te^{(\alpha_1-\lambda_1 n\pi)t}+\frac{1-e^{(\alpha_1-\lambda_1 n\pi)t}}{(\alpha_1-\lambda_1 n\pi)}\right)\right)\sin n\pi\, x \qquad (3.13)$$

Therefore,

$$\begin{aligned}\theta(x,t)=&\sum_{n=1}^{\infty}\frac{2\beta_1\left(1-(-1)^n\right)}{n\pi(\alpha_1-\lambda_1 n\pi)}\left(e^{(\alpha_1-\lambda_1 n\pi)t}-1\right)\sin n\pi\, x+\\ &\sum_{n=1}^{\infty}\left(\sum_{n=1}^{\infty}\frac{2\beta_1 k_0\left(1-(-1)^n\right)\left(1-(-1)^{2n}\right)}{n^2\pi^2(\alpha_1-\lambda_1 n\pi)}\left(te^{(\alpha_1-\lambda_1 n\pi)t}+\frac{1-e^{(\alpha_1-\lambda_1 n\pi)t}}{(\alpha_1-\lambda_1 n\pi)}\right)\right)\sin n\pi\, x\end{aligned} \qquad (3.14)$$

4. Results and Discussion

We have proved the existence of solution of the Problem by method of upper and lower solution. Also, we have shown that $\theta(x,t)$ is non-decreasing function of time, under certain conditions.

The temperature profiles are presented in Figures 1- 6. Figure 1 displays the graph of $\theta(x,t)$ against x and t for different values of δ. Figure 2 displays the graph of $\theta(x,t)$ against x for different values of δ. Figure 3 displays the graph of $\theta(x,t)$ against t for different values of δ. From Figures 1-3 it is seen that temperature increases as Frank-Kamenetskii number increases.

It is worth pointing out that the effect of δ as shown in Figures 1-3 indicating that there is increase in heat of reaction Q^*. When the heat of reaction is high, the rate of conversion of Kerogen into oil and other petroleum products by pyrolysis and distillation is high and consequently, the recovery rate is boosted. This is of great economic importance.

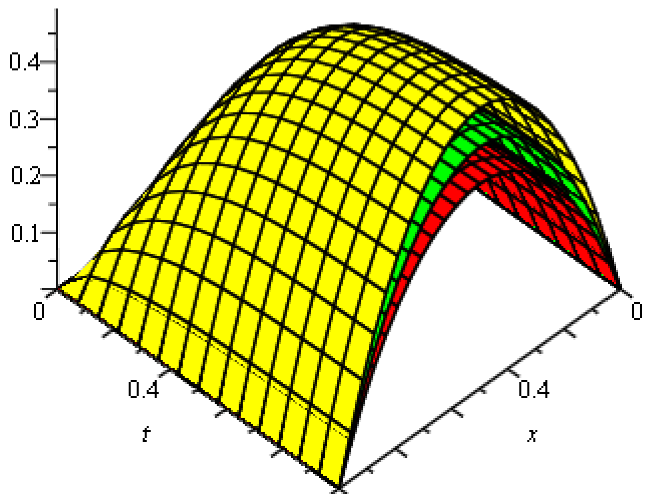

Figure 1: Plots of $\theta(x, t)$ against x and t for equation (3.5) for different values of δ and $\alpha = 2$, $\beta = 1$, $\lambda_1 = 0.3$, $e = 2.718$

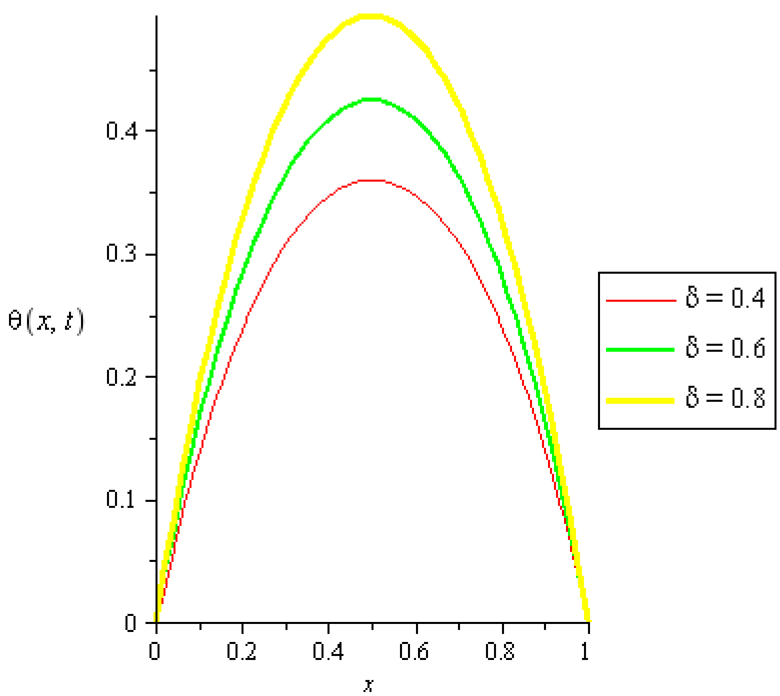

Figure 2: Plots of $\theta(x, t)$ against x for equation (3.5) for different values of δ and $\alpha = 2$, $\beta = 1$, $\lambda_1 = 0.3$, $e = 2.718$, $t = 1$

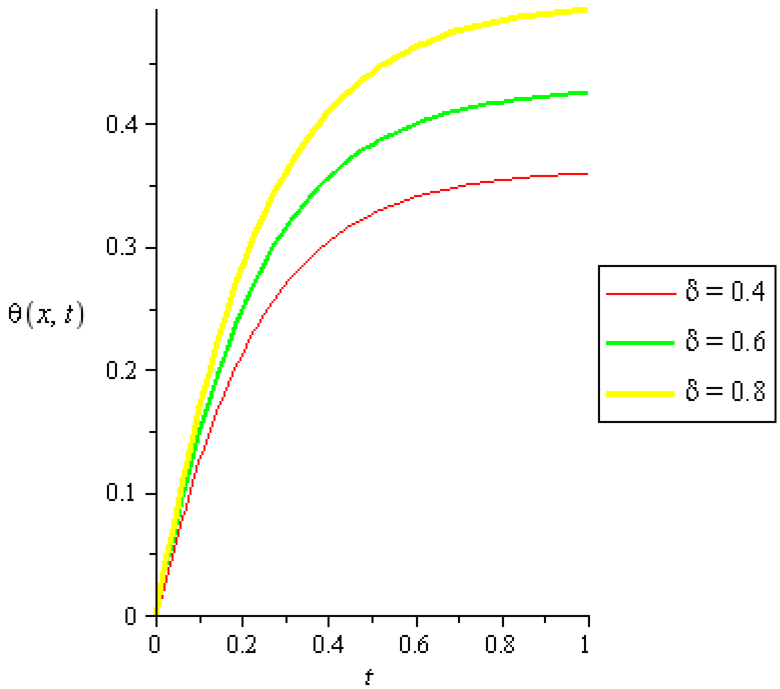

Figure 3: Plots of $\theta(x, t)$ against t for equation (3.5) for different values of δ and $\alpha = 2$, $\beta = 1$, $\lambda_1 = 0.3$, $e = 2.718$, $x = 0.5$

Figure 4 displays the graph of $\theta(x,t)$ against x and t for different values of λ_1. Figure 5 displays the graph of $\theta(x,t)$ against x for different values of λ_1. Figure 6 displays the graph of $\theta(x,t)$ against t for different values of λ_1. From Figures 4-6 it is evident that temperature increases as scaled thermal conductivity decreases.

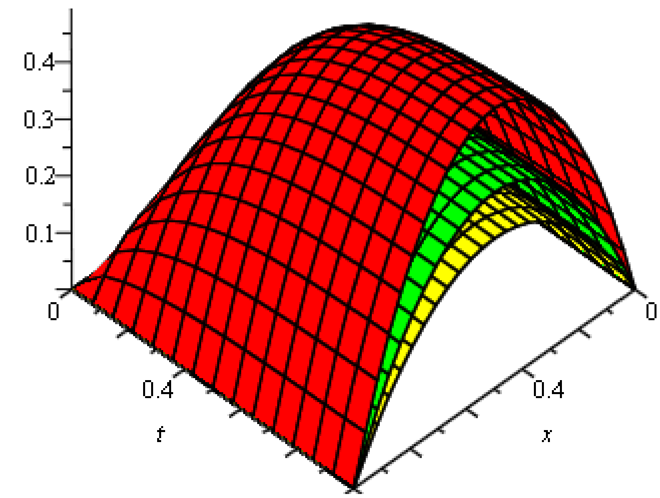

Figure 4: Plots of $\theta(x, t)$ against x and t for equation (3.5) for different values of λ_1 and $\alpha = 2$, $\beta = 1$, $\delta = 0.8$, $e = 2.718$

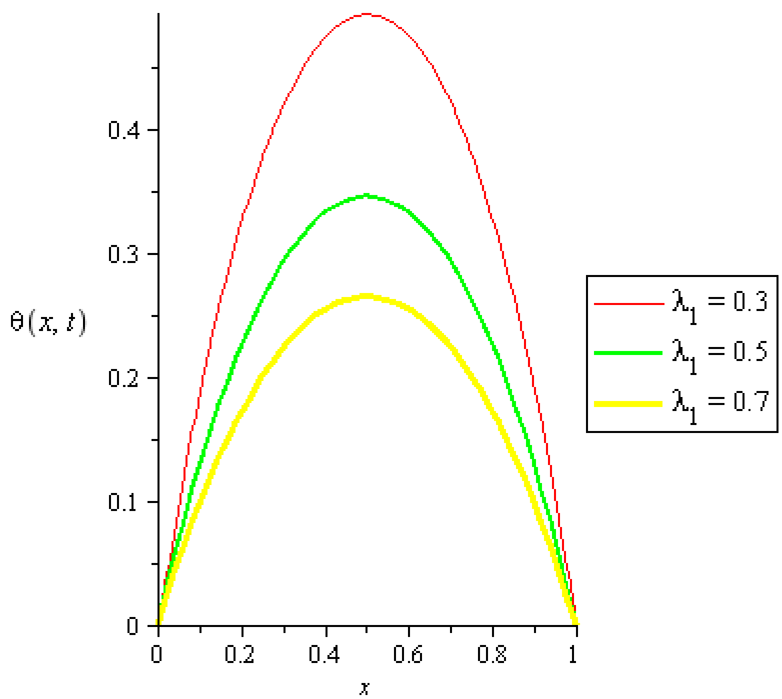

Figure 5: Plots of $\theta(x, t)$ against x for equation (3.5) for different values of λ_1 and $\alpha = 2$, $\beta = 1$, $\delta = 0.8$, $e = 2.718$, $t = 1$

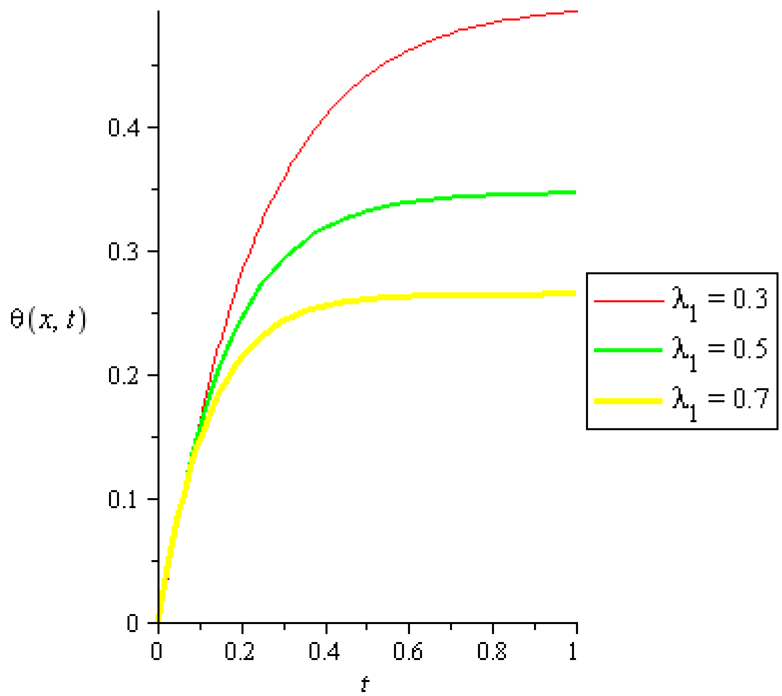

Figure 6: Plots of $\theta(x, t)$ against t for equation (3.5) for different values of λ_1 and $\alpha = 2$, $\beta = 1$, $\delta = 0.8$, $e = 2.718$, $x = 0.5$

5. Conclusion

For coupled heat transport in Arrheniusly reactive porous medium using a homogeneous description at the Darcy-scale, analytical solution has been presented for the case of high activation energy asymptotics. The governing parameters of the problem are the scaled thermal conductivity (λ_1) and Frank-Kamenetskii number (δ). The heat transfer increases as Frank-Kamenetskii number increases and scaled thermal conductivity decreases.

References

[1] Veil J.A. and Quinn J.J. (2008) “Water Issues Associated with Heavy Oil Production,” A report ANL/EVS/R-08/4 prepared for U.S. Department of Energy, National Energy Technology Laboratory. http://www.osti.gov/bridge

[2] Lapene A., Martins M.F., Debenest G., Quintard M. and Salvador S. (2007) “Numerical Simulation of Oil Shale Combustion in a fixed bed: Modelling and chemical,” Reactive Heat transfer in porous media, Albi, France, June 4 - 6.

[3] Burnham, A.K (1993) “Chemical Kinetics and Oil shale Process Design”, A paper prepared for submittal to the NATO Advanced study Institute : Composition : Geochemistry and conversion of oil shale, Akcay, Turkey.

[4] Ohlemiller T.J. (1985) “Modeling of Smoldering combustion propagation,” Progress in Energy and Combustion Science, 11, 277 – 310.

[5] Lu C. and Yortos Y. (2000) “The dynamics of combustion in porous media at the pore-network scale,” ECMOR VII (Baveno, Italie).

[6] Redl C. (2002) “In situ Combustion Modeling in Porous Media Using Lattice Boltzmann Methods,” A paper presented at 8th European Conference on the Mathematics of Oil Recovery – Freiberg, Germany, 1 - 8.

[7] Debenest G., Mourzenko V.V. and Thovert J.F. (2005) “ Smouldering in fixed beds of oil shale grains. A three-dimensional microscale numerical model “, Combustion Theory and Modelling, 9, 113 – 135.

[8] Debenest, G., Mourzenko, V.V and Thovert J.F (2005) “ Smouldering in fixed beds of oil shale grains. Governing parameters and global regimes “, Combustion Theory and Modelling, 2, 301 – 321.

[9] Kolodner J. and Pederson R.H. 1966. “Pointwise bounds for solutions of some semi-linear parabolic equations”, J. Diff equations 2, 353-364.

[10] Ayeni R.O. (1982) “On the Explosion of Chain-thermal Reactions,” J. Austral. Math. Soc. (Series B), 24, 194-202.