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Thermal explosion with convection in porous media: a mathematical approach

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Abstract

This paper studies the interaction between natural convection and thermal explosion in porous media. The model consists of the heat equation with a nonlinear source term describing heat production due to an exothermic chemical reaction coupled with the Darcy law. The conditions for the existence of unique solutions of the energy equation are established by the Lipschitz continuity approach. The analytical solution is obtained via Olayiwola's generalized polynomial approximation method (OGPAM), which shows the influence of the parameters involved on the system. The effect of changes in values of parameters such as the Frank-Kamenetskii number, Rayleigh number, and inverse of Vadasz number are presented graphically and discussed. The results revealed that convection can change the conditions of thermal explosion.

Keywords and Phrases: convection; explosion; first-order reaction; OGPAM; porous medium; thermal explosion; mathematical approach

1 Introduction

An explosion describes the spontaneous development of the rapid rate of heat release by a chemical reaction in an initially nearly homogeneous system. The rate of reaction changes rapidly with temperature. Hence, the temperature may be used to describe the changes within an explosion process [5].

The theory of heat explosion began from the classical works by Semenov [20] and Frank-Kamenetskii [8]. In Semenov's theory, the temperature distribution in the vessel is supposed to be uniform. An average temperature in the vessel is described by the ordinary differential equation

$$\frac{d\theta}{dt} = \exp(\theta) - \lambda\theta .\tag{1}$$

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The first term on the right-hand side corresponds to heat production due to an exothermic chemical reaction, and the second term to heat loss through the boundary of the vessel. In Frank-Kamenetskii's theory, the spatial temperature distribution is taken into account. The model consists of the reaction-diffusion equation,

$$\frac{d\theta}{dt} = \Delta\theta + F_K \exp(\theta), \tag{2}$$

where the first term on the right-hand side describes heat diffusion, F_K is called the Frank-Kamenetskii parameter. This equation is considered in a bounded domain with the zero boundary condition for the dimensionless temperature.

In both models, heat explosion was treated as an unbounded growth of temperature (blow-up solution). Thus, the problem of heat explosion was reduced to the investigation of the existence, stability, and bifurcations of stationary solutions of differential equations.

The effect of natural convection on heat explosion was first studied in [11, 16]. It was shown that the critical value of the Frank-Kamenetskii parameter increases with the Rayleigh number and explosion can be prevented by vigorous convection. These works were continued by [4, 6, 7, 14] where new stationary and oscillating regimes were found. The authors showed how complex regimes appeared through successive bifurcations leading from a stable stationary temperature distribution without convection to a stationary symmetric convective solution, stationary asymmetric convection, periodic in-time oscillations, and finally periodic oscillations. Oscillating heat explosion, where the temperature grows and oscillates, was discovered. The effects of natural convection and consumption of reactants on heat explosion in a closed spherical vessel were studied in [15]. The influence of stirring on the limit of the thermal explosion was investigated in [10]. Heat explosion with convection in a horizontal cylinder was considered in [19].

All these works study heat explosion in a gaseous or liquid medium with its motion described by the Navier-Stokes equations under the Boussinesq approximation. Thermal ignition in a porous medium is investigated in [13]. The Darcy law in a quasi-stationary form under the Boussinesq approximation is used to describe fluid motion. It is shown that convection decreases the maximal temperature and increases the critical value of the Frank-Kamenetskii parameter. The interaction of free convection and exothermic chemical reaction is studied in [21]. The authors consider zero-order exothermic reactions in a rectangular domain and find the onset of convection by an approximate analytical method. A similar problem with the depletion of reactants is investigated in [9]. The ignition time of heat explosion in a porous medium with convection is found in [22]. Heat explosion in one-dimensional flow in a porous medium is studied in [3].

In this paper, an approximate analytical solution capable of predicting the temperature distribution in a process of thermal explosion with convection in porous media is presented.

2 Model formulation

Here, we consider the first-order reaction,

$$A \xrightarrow{K(T)} B, \tag{3}$$

and the temperature dependence of the reaction rate $K(T)$ given by the Arrhenius law:

$$K(T) = k_0 \exp\left(-\frac{E}{RT}\right), \tag{4}$$

where E is the activation energy, T the temperature, R the universal gas constant, and k_0 the pre-exponential factor.

The system is considered in a $2D$ square domain, $0 \leq x \leq L$, $0 \leq y \leq L$. Depletion of reactants in the heat balance equation is neglected. It is a conventional assumption in the theory of heat explosion. The model consists of the $2D$ reaction-diffusion equation with convective terms, continuity, and non-stationary Darcy equations for an incompressible fluid:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \tag{5}$$

$$\frac{\partial u}{\partial t} + \frac{\mu}{K} u + \frac{\partial p}{\partial x} = 0, \tag{6}$$

$$\frac{\partial v}{\partial t} + \frac{\mu}{K} v + \frac{\partial p}{\partial y} = g\beta\rho(T - T_0), \tag{7}$$

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} = \frac{k}{\rho c_p}\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) + \frac{qk_0}{\rho c_p}\exp\left(-\frac{E}{RT}\right). \tag{8}$$

The initial and boundary conditions are specified as:

$$\left.\begin{array}{c} u(x,y,0) = 0 \\ v(x,y,0) = 0 \\ T(x,y,0) = T_0(\in(x+y)+1), \quad \left.\frac{\partial T}{\partial x}\right|_{x=0} = 0, \ T(x,0,t) = T_0, \ \left.\frac{\partial T}{\partial x}\right|_{x=L} = 0, \ T(x,L,t) = T_0 \end{array}\right\} \tag{9}$$

Here u denotes the fluid velocity along the x-axis, v is the fluid velocity along the y-axis, p is the pressure, k the thermal conductivity, μ the kinematic viscosity, ρ the density, q the heat release, g is the acceleration due to gravity, T_0 the characteristic value of the temperature, U_0 the characteristic value of the velocity, K the permeability.

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3 Method of solution
3.1 Dimension analysis
Dimensionless variables are been introduced as:

$$x' = \frac{x}{L}, \quad y' = \frac{y}{L}, \quad t' = \frac{kt}{\rho c_p L^2}, \quad u' = \frac{\rho c_p L u}{k}, \quad v' = \frac{\rho c_p L v}{k},$$
$$p' = \frac{\rho c_p K p}{k\mu}, \quad \theta = \frac{E(T - T_0)}{RT_0^2}, \quad \in = \frac{RT_0}{E}, \tag{10}$$

Using (10), and after dropping the prime, equations (5) - (9) become

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \tag{11}$$

$$\sigma \frac{\partial u}{\partial t} + u + \frac{\partial p}{\partial x} = 0, \tag{12}$$

$$\sigma \frac{\partial v}{\partial t} + v + \frac{\partial p}{\partial y} = R_p \theta, \tag{13}$$

$$\frac{\partial \theta}{\partial t} + u \frac{\partial \theta}{\partial x} + v \frac{\partial \theta}{\partial y} = \left(\frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2} \right) + \delta \exp\left(\frac{\theta}{1 + \in \theta} \right), \tag{14}$$

$$\left. \begin{array}{c} u(x, y, 0) = 0 \\ v(x, y, 0) = 0 \\ \theta(x, y, 0) = (x + y), \quad \left.\frac{\partial \theta}{\partial x}\right|_{x=0} = 0, \quad \theta(x, 0, t) = 0, \quad \left.\frac{\partial \theta}{\partial x}\right|_{x=1} = 0, \quad \theta(x, 1, t) = 0 \end{array} \right\} \tag{15}$$

where

$\sigma = \dfrac{kK}{\rho c_p L^2 \mu} = \dfrac{1}{V_a}$ stands for the inverse of the Vadasz number, $V_a = \dfrac{P_r}{D_a}$, $P_r = \dfrac{\rho c_p \mu}{k}$ is the Prandtl

number and $D_a = \dfrac{K}{L^2}$ is the Darcy number, $\delta = \dfrac{q k_0 L^2}{k \in T_0} e^{-\frac{E}{RT_0}}$ is the Frank-Kamenetskii parameter,

$R_p = \dfrac{g\beta\rho K\rho c_p L \in T_0}{k\mu} = \dfrac{K\rho}{L^2} R_a$, $R_a = \dfrac{g\beta \in T_0 \rho c_p L^3}{k\mu}$ is the Rayleigh number.

Introducing the following new space variable (Olayiwola [18]):
$z = x + y$. \hfill (16)
Then, equations (11) – (15) reduce to
$$\frac{\partial U}{\partial z} = 0, \tag{17}$$

$$\sigma \frac{\partial U}{\partial t} + U + 2\frac{\partial p}{\partial z} = R_p \theta, \tag{18}$$

$$\frac{\partial \theta}{\partial t} + U \frac{\partial \theta}{\partial z} = 2\frac{\partial^2 \theta}{\partial z^2} + \delta \exp\left(\frac{\theta}{1+ \in \theta}\right), \tag{19}$$

$$\left.\begin{array}{l} U(z,0) = 0 \\ \theta(z,0) = z, \quad \left.\frac{\partial \theta}{\partial z}\right|_{z=0} + \theta(0,t) = 0, \quad \left.\frac{\partial \theta}{\partial z}\right|_{z=2} + \theta(2,t) = 0 \end{array}\right\}, \tag{20}$$

where

$$U = u + v.$$

3.2 Properties of solution

Theorem 1: Then there exists a unique solution $U(z,t),\ \ p(z,t),\ \ \theta(z,t)$ of (17) – (19) which satisfies (20).

Proof: Clearly $\delta \exp\left(\dfrac{\theta}{1+ \in \theta}\right)$ is Lipschitz continuous. Hence by Ayeni [2], the result follows. This completes the proof.

Theorem 2: Let $\theta(z,t) = \phi(z,t)\exp\left(\dfrac{U}{4}z - \dfrac{U^2}{8}t\right), \quad \eta = \sqrt{2}\,z$. Then $\dfrac{\partial \phi}{\partial t} \geq 0$.

In the proof, we shall need the following lemma of Kolodner and Pederson [12].

Lemma (Kolodner and Pederson [12]): Let $u(y,t) = O\left(e^{\alpha|y|^2}\right)$ be a solution on $R^n \times [0,t_0)$ of the differential inequality

$$\frac{\partial u}{\partial t} - \Delta u + k(y,t)u \geq 0 \tag{21}$$

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

Proof of Theorem 2: Let $\theta(z,t) = \phi(z,t)e^{\left(\frac{U}{4}z - \frac{U^2}{8}t\right)}, \quad \eta = \sqrt{2}\,z, \quad p = \dfrac{\partial \phi}{\partial t}$.

Then

$$\frac{\partial p}{\partial t} - \frac{\partial^2 p}{\partial \eta^2} - \frac{\delta}{\left(1+ \in \phi(z,t)e^{\left(\frac{U}{4}z - \frac{U^2}{8}t\right)}\right)^2} e^{\frac{\phi(z,t)e^{\left(\frac{U}{4}z - \frac{U^2}{8}t\right)}}{1+\in \phi(z,t)e^{\left(\frac{U}{4}z - \frac{U^2}{8}t\right)}}} p \geq 0$$

$$p(\eta,0) \geq 0.$$

Now

$$-\frac{\delta}{\left(1+\in\phi(z,t)e^{\left(\frac{U}{4}z-\frac{U^2}{8}t\right)}\right)^2}e^{1+\in\phi(z,t)e^{\left(\frac{U}{4}z-\frac{U^2}{8}t\right)}}\phi(z,t)e^{\left(\frac{U}{4}z-\frac{U^2}{8}t\right)} \quad \text{is bounded.}$$

Hence by Kolodner and Pederson lemma $p(\eta,t)\geq 0$, i.e. $\dfrac{\partial\phi}{\partial t}\geq 0$. Hence $\phi(z,t)$ is a non-decreasing function of t.

3.3 Analytical solution via Olayiwola's generalized polynomial approximation method

Here, in the limit $\in\to 0$, and by introducing the following new space variable:

$$\eta=\frac{z}{2}. \tag{22}$$

Equations (17) – (20) can be solved analytically using Olayiwola's generalized polynomial approximation method (OGPAM) in [17]. Follow the idea in [1], that:

$$\exp(\theta)\approx 1+(e-2)\theta+\theta^2. \tag{23}$$

Take $\dfrac{\partial p}{\partial\eta}=b\exp(-\lambda t)$ and let $0<R_p\ll 1$, $\delta=aR_p$ such that

$$\left.\begin{aligned}U(\eta,t)&=U_0(\eta,t)+R_pU_1(\eta,t)+...\\ \theta(\eta,t)&=\theta_0(\eta,t)+R_p\theta_1(\eta,t)+...\end{aligned}\right\} \tag{24}$$

and using OGPAM in [17], we obtain the solutions to (17) - (20) as:

$$U(\eta,t)=\beta\left(e^{-\frac{1}{\sigma}t}-e^{-\lambda t}\right)+R_p\left(\frac{1}{\sigma}\sqrt{\frac{\pi}{m_0}}\left(3\eta-3\eta^2+\eta^3\right)\left(erf\left(\frac{m_2}{2\sqrt{m_0}}\right)+erf\left(\frac{2m_0t-m_2}{2\sqrt{m_0}}\right)\right)e^{\left(\frac{m_2^2}{4m_0}-\frac{1}{\sigma}t\right)}\right) \tag{25}$$

$$\theta(\eta,t)=3\theta_0\big|_{\eta=1}-3\theta_0\big|_{\eta=1}\eta+\theta_0\big|_{\eta=1}\eta^2+R_p\left(3\theta_1\big|_{\eta=1}-3\theta_1\big|_{\eta=1}\eta+\theta_1\big|_{\eta=1}\eta^2\right), \tag{26}$$

where

$$\theta_0\big|_{\eta=1}=2\eta e^{-\left(c_0t-m_0t^2-m_1t^3\right)}$$

$$\theta_1\big|_{\eta=1} = e^{-\left(c_0 - m_7 t - m_8 t^2\right)} \left(\begin{array}{c} \dfrac{a}{2A}\sqrt{\dfrac{\pi}{m_8}}\left(erf\left(\dfrac{2m_8 t + m_7}{2\sqrt{m_8}}\right) - erf\left(\dfrac{m_7}{2\sqrt{m_8}}\right)\right)e^{\frac{4c_0 m_8 + m_7^2}{4m_8}} - \\[2ex] \dfrac{3a(e-2)}{4A}\sqrt{\dfrac{\pi}{-m_{10}}}\left(erf\left(\dfrac{2m_{10} t - m_9}{2\sqrt{-m_{10}}}\right) + erf\left(\dfrac{m_9}{2\sqrt{-m_{10}}}\right)\right)e^{\frac{4c_0 m_{10} - m_9^2}{4m_{10}}} - \\[2ex] \dfrac{36a}{28A}\sqrt{\dfrac{\pi}{-m_{12}}}\left(erf\left(\dfrac{2m_{12} t - m_{11}}{2\sqrt{-m_{12}}}\right) + erf\left(\dfrac{m_{11}}{2\sqrt{-m_{12}}}\right)\right)e^{\frac{4c_0 m_{12} - m_{11}^2}{4m_{12}}} - \\[2ex] \dfrac{86}{240\sigma A}\sqrt{\dfrac{\pi}{-m_{15} m_0}}\left(erf\left(\dfrac{2m_0 t - m_2}{2\sqrt{m_0}}\right) + erf\left(\dfrac{m_2}{2\sqrt{m_0}}\right)\right) \\[2ex] \left(erf\left(\dfrac{2m_{10} t - m_{14}}{2\sqrt{-m_{10}}}\right) + erf\left(\dfrac{m_{14}}{2\sqrt{-m_{10}}}\right)\right)e^{\frac{4m_{13} m_{10} - m_{14}^2}{4m_{15}}} \end{array}\right),$$

$$A = \frac{11}{6}, \quad c_0 = \frac{1}{2A}, \quad \beta = \frac{b}{1-\sigma\lambda}, \quad c_1 = \frac{\beta}{A}\left(\frac{\sigma\lambda-1}{\sigma}\right), \quad c_2 = \frac{\beta}{A}\left(\frac{1}{2\sigma^2} - \frac{\lambda^2}{2}\right), \quad m_0 = \frac{c_1}{2}, \quad m_1 = \frac{c_2}{3},$$

$$m_2 = \left(\frac{1}{\sigma} - c_0\right), \quad m_3 = \beta\left(\frac{\sigma\lambda-1}{\sigma}\right), \quad m_4 = \beta\left(\frac{1}{2\sigma^2} - \frac{\lambda^2}{2}\right), \quad m_5 = \frac{m_2^2}{4m_0}, \quad m_6 = \left(\frac{1}{\sigma} + c_0\right), \quad m_7 = \frac{m_3}{A},$$

$$m_8 = \frac{m_4}{A}, \quad m_9 = (m_7 + c_0), \quad m_{10} = (m_0 - m_8), \quad m_{11} = (m_7 + 2c_0), \quad m_{12} = (2m_0 - m_8), \quad m_{13} = (m_5 + c_0),$$

$$m_{14} = (m_7 + m_6)$$

The computation was done on equations (25) and (26) using the computer symbolic algebraic package MAPLE 2021 version.

4 Results and discussion

The simulation was carried out to show the impact of the model parameters by employing Olayiwola's Generalized Polynomial Approximation Method (OGPAM) on the equations (17) – (20). We are concerned with the nature of the solutions obtained for different values of δ, R_p and σ. The computation of equations (25) and (26) was done using the MAPLE 2021 version.

Figure 1 shows the temperature history at $x = 1$, $y = 1$ for $\sigma = 2$, $R_p = 0.1$ $\delta = 0.4, 0.6, 0.8$. The graph displays an increase in maximum temperature with time as the Frank-Kamenetskii number increases. If δ is sufficiently large, the temperature becomes unbounded, which corresponds to the thermal explosion.

Figure 2 displays the temperature topography for $\sigma = 2$, $R_p = 0.1$ $\delta = 0.4, 0.6, 0.8$. The graph reveals a decrease in temperature along the spatial coordinates while this temperature increases as the Frank-Kamenetskii number increases.

Figure 3 shows the temperature history at $x = 1$, $y = 1$ for $\delta = 0.4$, $\sigma = 2$ $R_p = 0.1, 0.2, 0.3$. The graph displays an increase in maximum temperature with time as the Rayleigh number increases.

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Figure 4 depicts the velocity history at $x = 1$, $y = 1$ for $\delta = 0.4$, $\sigma = 2$ $R_p = 0.1, 0.2, 0.3$. After the first oscillation, the graph displays a rapid transition to a steady solution. Meanwhile, the graph displays an increase in maximum velocity with time as the Rayleigh number increases.

Figure 5 displays the velocity topography for $\delta = 0.4$, $\sigma = 2$ $R_p = 0.1, 0.2, 0.3$. The graph reveals a steady velocity along the spatial coordinates while this velocity increases as the Rayleigh number increases.

Figure 6 shows the temperature history at $x = 1$, $y = 1$ for $\delta = 0.4$, $R_p = 0.1$, $\sigma = 0.2, 2, 20$ which an increase in temperature exists when $\sigma \geq 2$. When $2 \leq \sigma < \infty$ (convection), the solution remains bounded (no explosion) but when $\sigma \to 0$, $U(x, y, t) \to \infty$ (convection), however, oscillations are generated (no explosion). It can be stationary or oscillating with convection. When $\sigma \to \infty$, $U(x, y, t) \to 0$ (no convection), then stationary solutions do not exist, and the solution of the evolution problem grows to infinity ($\theta(x, y, t) \to \infty$). This case corresponds to the thermal explosion.

Figure 7 depicts the temperature topography for $\delta = 0.4$, $R_p = 0.1$, $\sigma = 0.2, 2, 20$. The graph reveals a decrease in temperature along the spatial coordinates while this temperature tends to zero when $\sigma \to \infty$ and it is at maximum value when $\sigma \to 0$.

Figure 8 shows the velocity history at $x = 1$, $y = 1$ for $\delta = 0.4$, $R_p = 0.1$, $\sigma = 0.2, 2, 20$ which there is a rapid transition to a steady solution when $\sigma = 0.2$ and $\sigma = 2$. Stable solutions exist after oscillation and are achieved faster when $\sigma = 0.2$, $\sigma = 2$ than when $\sigma = 20$.

Figure 9 displays the velocity topography for $\delta = 0.4$, $R_p = 0.1$, $\sigma = 0.2, 2, 20$. The graph reveals a steady velocity along the spatial coordinates while this velocity tends to zero when $\sigma \to \infty$ and it is at maximum value when $\sigma \to 0$.

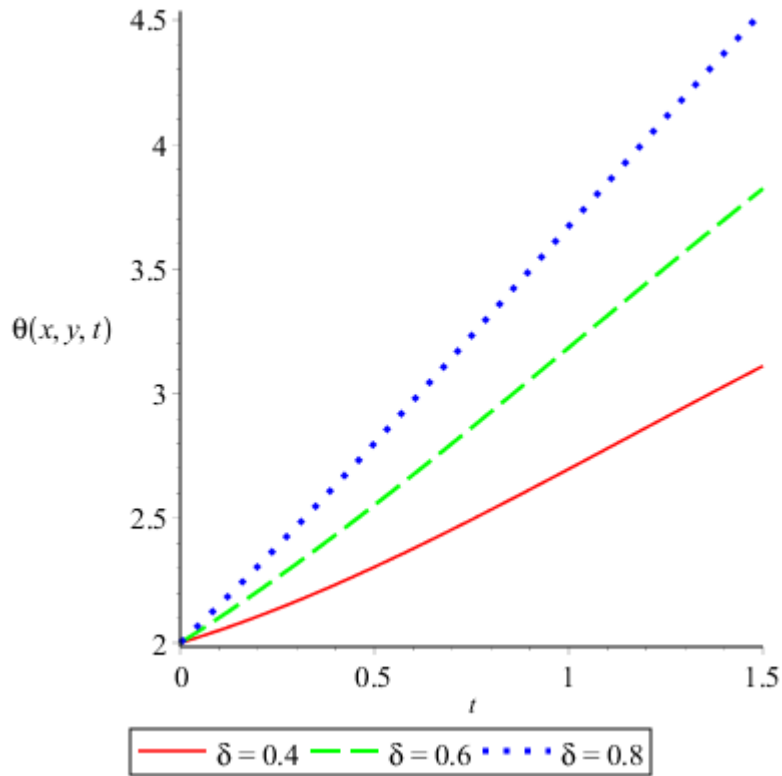**Figure 1**: Temperature history at $x = 1$, $y = 1$ for $\sigma = 2.0$, $R_p = 0.1$, $\delta = 0.4$, 0.6, 0.8.
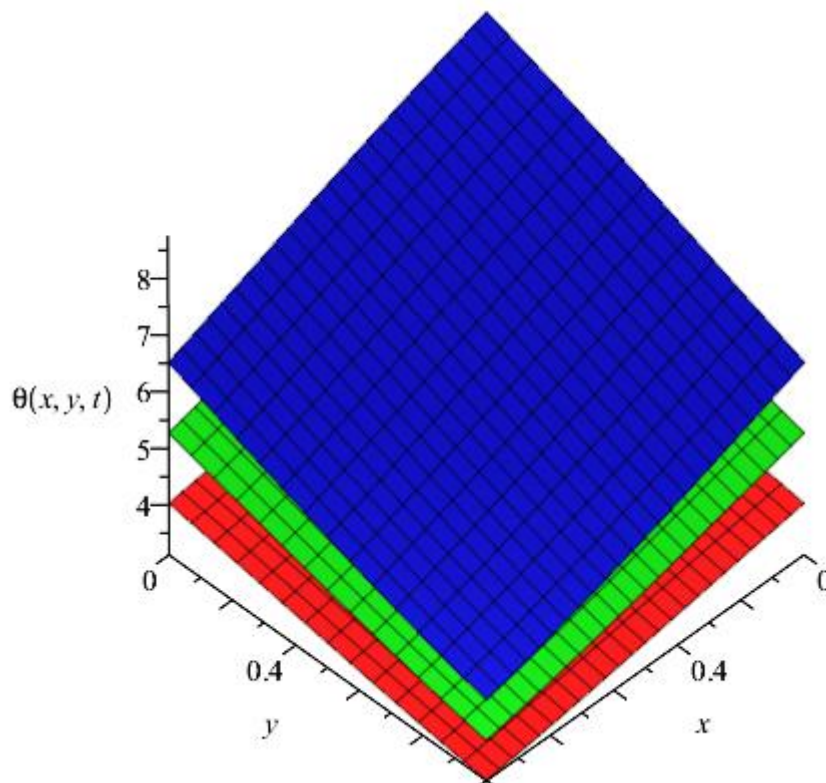

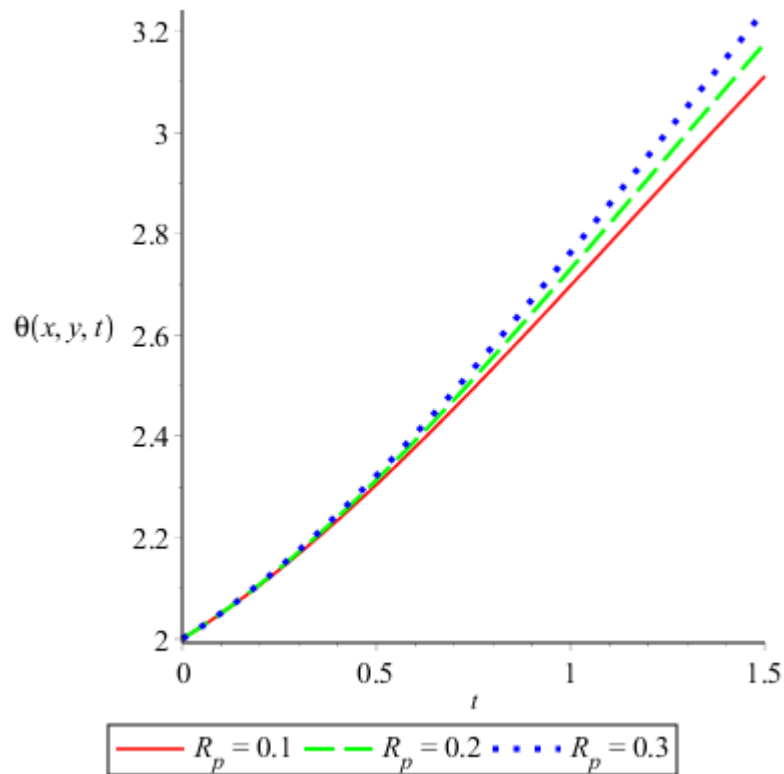**Figure 2**: Temperature topography for $\sigma = 2.0$, $R_p = 0.1$, $\delta = 0.4$, 0.6, 0.8.

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Figure 3: Temperature history at $x = 1,\ y = 1$ for $\sigma = 2.0,\ \delta = 0.4,\ R_p = 0.1, 0.2, 0.3$.
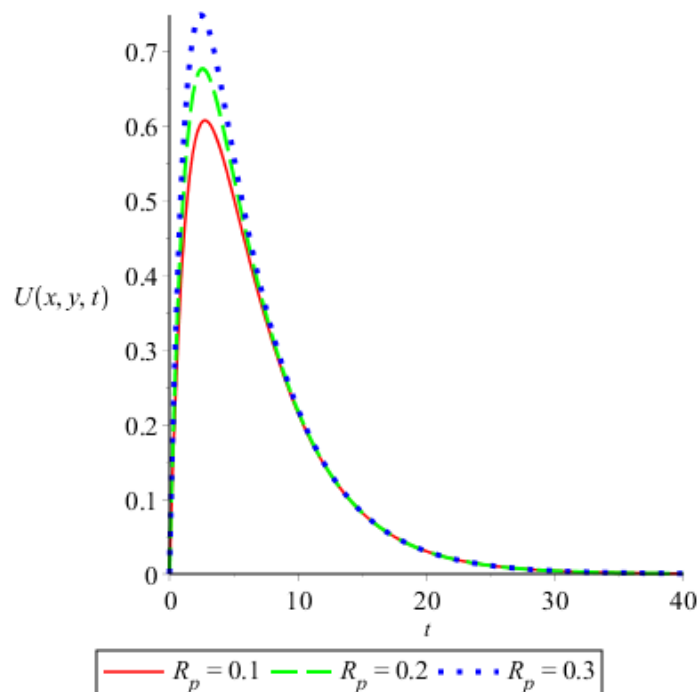
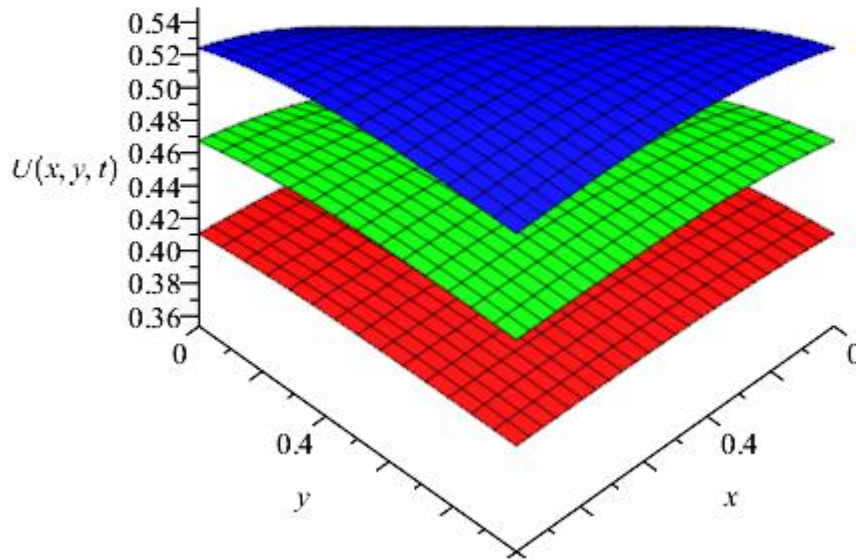**Figure 4**: Velocity history at $x = 1,\ y = 1$ for $\sigma = 2.0,\ \delta = 0.4,\ R_p = 0.1, 0.2, 0.3$.

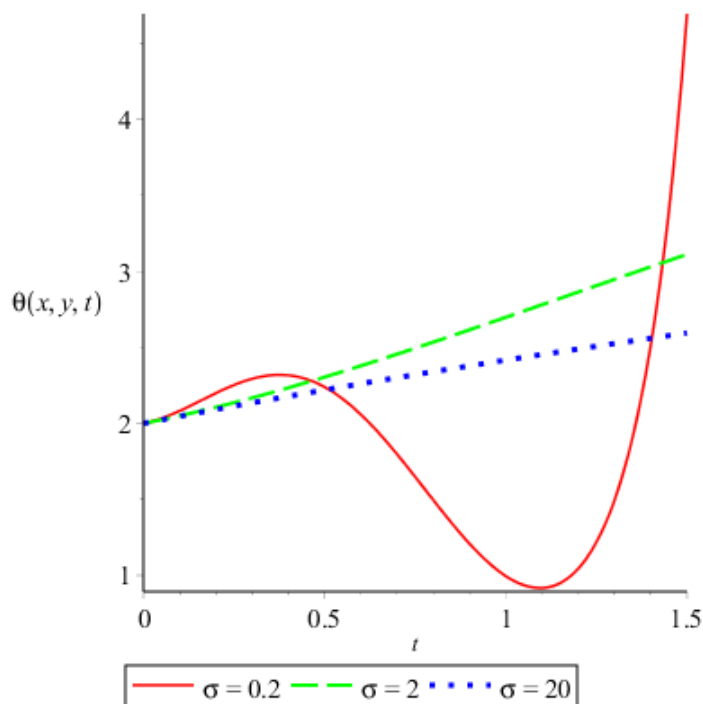**Figure 5**: Velocity topography for $\sigma = 2.0, \; \delta = 0.4, \; R_p = 0.1, 0.2, 0.3$.

Figure 6: Temperature history at $x = 1, \; y = 1$ for $\delta = 0.4, R_p = 0.1, \; \sigma = 0.2, 2, 20$.

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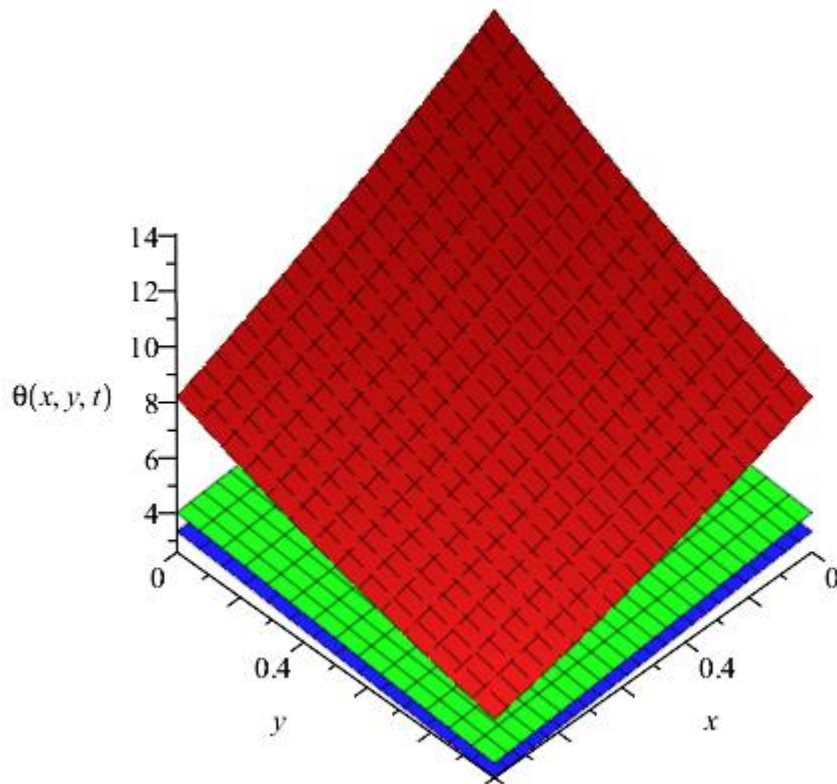
Figure 7: Temperature topography for $\delta = 0.4$, $R_p = 0.1$, $\sigma = 0.2, 2, 20$.
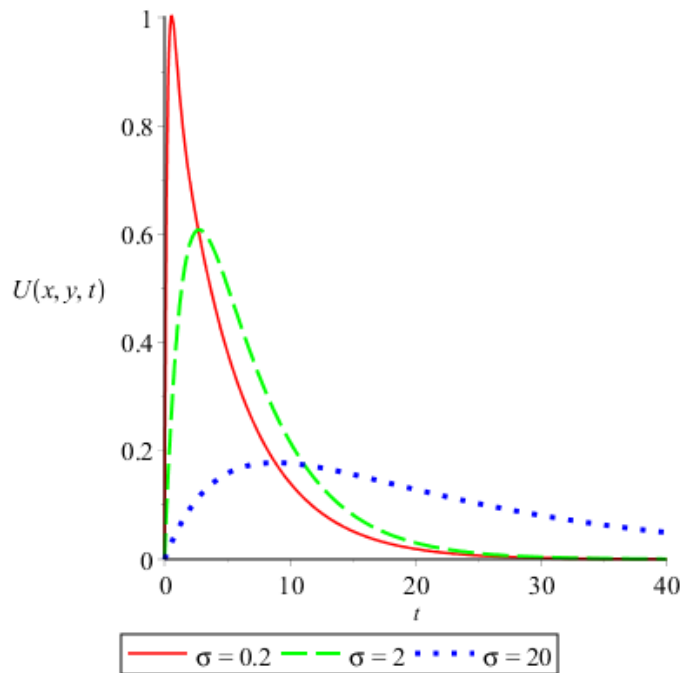

Figure 8: Velocity history at $x = 1$, $y = 1$ for $\delta = 0.4$, $R_p = 0.1$, $\sigma = 0.2, 2, 20$.
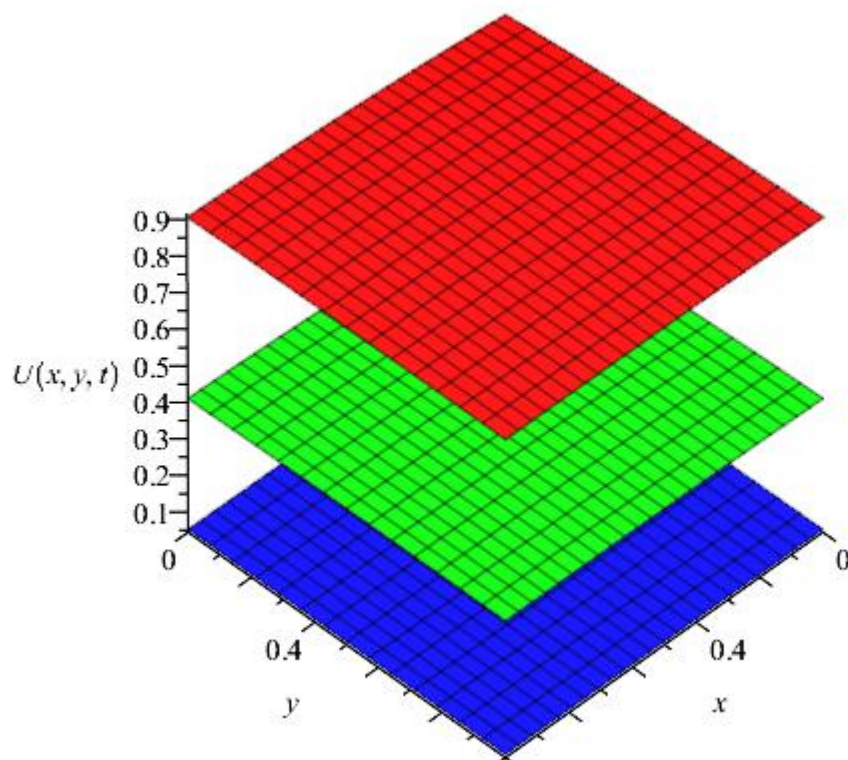
Figure 9: Velocity topography for $\delta = 0.4$, $R_p = 0.1$, $\sigma = 0.2, 2, 20$.

It is worth pointing out that the effects observed in Figures 1 - 9, are important to guide explosive materials manufacturers to provide safety precautions during storage and usage.

5 Conclusion

Here, we have presented the model describing the interaction between natural convection and thermal explosion in porous media, established the conditions for the existence of a unique solution of the model, and provided the approximate analytical solution. The existence of a unique solution to the problem implies that the problem represents a physical situation under specific conditions. The simulation results revealed the impact of the model parameters and the following conclusion can be drawn:

Temperature is a non-decreasing function of time.
If the Frank-Kamenetskii number is sufficiently large, a thermal explosion can occur.
Convection can change the conditions of a thermal explosion.

Therefore the established conditions and the results obtained are not expected to guide manufacturers of explosive materials but provide safety precautions during storage and usage.

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