A Numerical Treatment of an Exothermic Reactions
Model with Constant Heat Source in a Porous Medium
Using Finite Difference Method

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Abstract

The flow patterns and concentration profiles are needed for fluid behavior simulation in the underground. The exothermic reaction models in porous medium can be described that requirement. The model is focused on the driving force problem which due to the temperature and concentration gradients at the system boundaries. In this research, the numerical computation of conduction solutions is presented. The governing equation is the steady-state energy balance equation of the temperature profile in conduction state with constant heat source. A finite difference technique for solving the equation is proposed. The computed results are second order accurate without instability problem.

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1 Introduction

In biological systems, energy is obtained from chemical bonds. When bonds are broken, energy is required. When bonds are formed, energy is released. Each type of bond has a specific bond energy. It can be predicted whether a
chemical reaction will release or require heat by using bond energies. When there is more energy used to form the bonds than to break the bonds, heat is given off. This is known as an exothermic reaction. When a reaction requires an input of energy, it is known as an endothermic reaction. Activation energy is the ability to break bonds.

Convection is driven by buoyancy has found increased applications in underground coal gasification, solar energy conversion, oil reservoir simulation, ground water contaminant transport, geothermal energy extraction and many areas. Most of interest is focused on the driving force problem which due to the temperature and concentration gradients at system boundaries.

The research of [2], [3], [4] and [5] were concerned with the study of Rayleigh-Bernard-type of convection. [15] focus on the convective instabilities that induced by exothermic reactions occurring inside a porous medium. The heat released by an exothermic reaction creates density differences within the fluid and induces natural convection, which give affects the rate reaction. A major factor in many of the stabilities observed in reactions flows are convection and reaction.

The non uniform flow are responsible for preventing thermal explosions. The condition for the onset of reaction-driven convection in a fluid confined between parallel plates are determined by [6]. The convective motion generated by internal heat sources are proposed by [7]. The chemically driven convection in a horizontal layer of initially quiescent, dissociating fluid is analyzed by [8].

The numerical analysis of natural convection for a zeroth-order reaction occurring in a closed porous cylindrical container of equal height and diameter is presented by [9]. The numerical computation of two-dimensional chemically driven convection in a rectangular geometry for a zeroth-order reaction is given by [11]. In [12], they considered the case of an open rectangular box, but their analysis was restricted to the case of identical mass and thermal diffusivities (Le=1.0). In [13], they investigated the onset of three-dimensional reaction-driven convection in closed geometries of a finite cylinder and a rectangular box. The numerical study for a closed rectangular box using orthogonal collocation has been proposed.

The case of convection due to internal heat generation are considered by [14]. [15] use a two-dimensional model of an open rectangular box and examine in detail the stability of the conduction solutions with respect to convective perturbations. They present some numerically computed flow patterns, isotherms and concentration profiles corresponding to the various convective solutions.

In the conductive solution in the base case, it is assumed that convection is neglected and that the solution id governed by diffusion and reaction only. In this research, the numerical computation of conduction solutions is proposed. The governing equation is the steady-state energy balance equation of the temperature profile in conduction state with constant heat source.
2 Governing Equation

A simple pseudohomogeneous model for describing convection driven by an exothermic reaction is proposed in this section. The usual assumptions in the continuity and momentum balance are required. Assuming that Darcy’s law is valid, Bossinesq approximation holds. That are density variations are small and effect only the body force term. Assuming that the porous medium Prandtl number is large. That is the acceleration terms in the momentum balance are negligible. The governing equations with the above assumptions are [15]

\[ \nabla \cdot \mathbf{u} = 0, \]  
\[ \nabla p = -\left(\frac{\mu_0}{\kappa}\right)\mathbf{u} - \rho_f[1 - b(T - T_0)]g e_z, \]  
\[ \rho_m C_{pm} \frac{\partial T}{\partial t} + \rho_f C_{pf} \mathbf{u} \cdot \nabla T = k_{eff} \nabla^2 T + (-\Delta H)r, \]  
\[ \epsilon \frac{\partial c_{Af}}{\partial t} + \mathbf{u} \cdot \nabla c_{Af} = D_{eff} \nabla^2 c_{Af} - r, \]

where the reaction rate for a first-order reaction is given by

\[ r = k(T)c_{Af}, \]  
\[ k(T) = k_0 \exp\left(-\frac{E}{RT}\right) = k(T_0) \exp\left(-\frac{E}{RT_0}\right). \]

Where, \( p \) is the pressure, \( T \) is the temperature, and \( c_{Af} \) is the concentration on the fluid; \( \mathbf{u} \) is the superficial, \( \epsilon \) is the porosity of the bed or fractional volume of the fluid phase, \( b \) is the coefficient of density of the fluid at ambient temperature \( T_0 \), and \( e_z \) is the unit vector pointing vertically upward. Here

\[ \rho_m C_{pm} = \epsilon \rho_f C_{pf} + (1 - \epsilon) \rho_s C_{ps} \]

is the effective heat capacity per unit volume of the bed and \( \rho_f C_{pf} \) and \( \rho_s C_{ps} \) are the heat capacities of the fluid and solid, respectively, per unit volume. The effective thermal conductivity and diffusivity of the bed is denoted by \( k_{eff} \) and \( D_{eff} \) respectively. The permeability of the medium is denoted by \( \kappa \). The reaction terms appears as a source in Eq.(3) and as a sink in Eq.(4). The constant \( (-\Delta H) \) is the heat of reaction per mole of extent and \( r \) is the reaction rate per unit volume.

In writing Eq.(3) and Eq.(4), the interphase temperature and concentration gradients are ignored. A single temperature and concentration is used to describe the system. This pseudohomogeneous description is valid for vanishingly small-particle heat and mass Damkohler numbers, which are defined as,

\[ Da_{ph} = \frac{k(T_0)P_f0c_{0f}d_p}{h_c}, \]
Here, $d_p$ is the particle size, $k_c$ is the local mass transfer coefficient, and $h_c$ is the local heat transfer coefficient. In Eq.(2), the density variation with concentration is ignored. This assumption is reasonable if the reaction does not involve a change in number of moles.

The case of a rectangular box ($0 < x' < L, 0 < z' < H$) is considered. The following boundary conditions at the side walls and the bottom of the box,

$$ u \cdot e_n = 0, $$

$$ \nabla T \cdot e_n = 0, $$

$$ \nabla c_{Af} \cdot e_n = 0, $$

where $e_n$ is the unit outward normal. At the top, the box is open to the atmosphere, we can obtain the simple Dirichlet boundary conditions,

$$ \rho = \rho_0, $$

$$ T = T_0, $$

$$ c_{Af} = c_{Af0}, $$

at $z' = H$.

To transform the system of equations in dimensionless form, the following quantities are defined,

$$ z = \frac{z'}{H}, x = \frac{x'}{L}, \tau = \frac{u^* t}{\sigma H}, $$

$$ \theta = \frac{T - T_0}{T_0}, x = \frac{c_{Af}}{c_{Af0}}, \Pi = \frac{\kappa (p - p_a)}{\mu \lambda_m}, $$

$$ \lambda_m = \frac{k_{eff}}{\rho_f C_{pf}}, u^* = \frac{\lambda_m}{H}, v = \frac{u}{\sigma u^*}, $$

$$ \alpha = \frac{L}{H}, \sigma = \frac{\epsilon \rho_f C_{pf}}{\rho_m C_{pm}}, Le = \frac{\lambda_m}{D_{eff}}, $$

$$ \phi^2 = \frac{k(T_0) H^2}{\lambda_m}, Ra = \frac{\rho_f^2 C_{pf} g H b T_0 \kappa}{\gamma \mu k_{eff}}, $$

where $x$ and $z$ are the dimensionless coordinate axes in the horizontal and vertical direction, respectively, and $\tau$ is the dimensionless time. The three dimensionless state variables are $\theta$, the temperature, $c$, the concentration, and $\Pi$, the pressure. We also define a reference velocity, $u^*$, and use it to nondimensionalize the velocity $u$.

In [15], they introduce the streamfunction formulation,

$$ v_x = \alpha \frac{\partial \psi}{\partial z}, $$

$$ v_z = -\frac{\partial \psi}{\partial x}, $$

where $\psi$ is the streamfunction.
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and substitute Eq.(16) and Eqs.(17-18) into Eqs.(1-15) to get the equations,

\[ \frac{\partial^2 \psi}{\partial x^2} + \alpha^2 \frac{\partial^2 \psi}{\partial z^2} + Ra \frac{\partial \theta}{\partial x} = 0, \]  

(19)

\[ \frac{\partial \theta}{\partial \tau} = - \left( \frac{\partial \theta}{\partial x} \frac{\partial \psi}{\partial z} - \frac{\partial \psi}{\partial x} \frac{\partial \theta}{\partial z} \right) + \left( \frac{1}{\alpha^2} \frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial z^2} \right) + B \phi^2 c \exp\left( \frac{\gamma \theta}{\gamma + \theta} \right), \]  

(20)

\[ \text{Le} \sigma \frac{\partial c}{\partial \tau} = -\text{Le} \left( \frac{\partial c}{\partial x} \frac{\partial \psi}{\partial z} - \frac{\partial \psi}{\partial x} \frac{\partial c}{\partial z} \right) + \left( \frac{1}{\alpha^2} \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial z^2} \right) - \phi^2 c \exp\left( \frac{\gamma \theta}{\gamma + \theta} \right), \]  

(21)

subject to

\[ \psi = 0, \frac{\partial \theta}{\partial x} = 0, \frac{\partial c}{\partial x} = 0, \text{ at } x = 0, 1, \]  

(22)

\[ \psi = 0, \frac{\partial \theta}{\partial x} = 0, \frac{\partial c}{\partial z} = 0, \text{ at } z = 0, \]  

(23)

\[ \frac{\partial \psi}{\partial z} = 0, \theta = 0, c = 1, \text{ at } z = 1. \]  

(24)

Here, the Rayleigh number, Ra, is the ratio of characteristic time for heat diffusion to that of natural convection. The thermal Thiele modulus, \( \phi^2 \), is the ratio of characteristic time for diffusion to that of reaction. The parameter \( B \) is the maximum possible temperature in the absence of natural convection. The dimensionless activation energy, \( \gamma \), is a measure of the sensitivity of the reaction rate constant to changes in the temperature. The Lewis number, Le, is the ratio of heat to mass diffusivity. The parameter \( \sigma \) is the ratio of volume heat capacities and \( \alpha \) is the aspect ratio of the box.

In the base case, it is assumed that natural convection is completely absent (\( \psi = 0 \)) and that the solution is only governed by diffusion and reaction. Assuming that the basis of the lateral boundary conditions that the state variables \( \theta \) and \( c \) are dependent on the vertical coordinate. By the assumption, the equations describing the conduction(diffusion) state are

\[ \frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial z^2} + B \phi^2 c \exp\left( \frac{\gamma \theta}{\gamma + \theta} \right), \]  

(25)

\[ \text{Le} \sigma \frac{\partial c}{\partial \tau} = \frac{\partial^2 c}{\partial z^2} - \phi^2 c \exp\left( \frac{\gamma \theta}{\gamma + \theta} \right), \]  

(26)

subject to

\[ \frac{d \theta}{dz} = 0, \frac{dc}{dz} = 0, \text{ at } z = 0, \]  

(27)

\[ \theta = 0, c = 1, \text{ at } z = 1. \]  

(28)
At steady state, Eqs. (25-28) can be combined to
\[ c_0(z) = 1 - \frac{\theta_0(z)}{B}, \]  
(29)
where \( \theta_0 \) and \( c_0 \) are the steady-state temperature and concentration, respectively. Substituting this in the steady-state energy balance, Eq. (25), gives the two-point boundary value problem for the temperature profile of the diffusion state,
\[ \frac{d^2 \theta_0}{dz^2} + B \phi^2 (1 - \frac{\theta_0}{B}) \exp(\gamma \frac{\theta_0}{\gamma + \theta_0}) = 0. \]  
(30)
Here, the parameter \( B \) is the maximum possible temperature in the absence of natural convection, \( \phi^2 \) is the ratio of the characteristic time for diffusion of heat generator and \( \gamma \) is the dimensionless activation energy.

If the heat source is constant, then Eq. (30) becomes
\[ \frac{d^2 \theta_0}{dz^2} + B \phi^2 (1 - \frac{\theta_0}{B}) = 0, \]  
(31)
subject to
\[ \frac{d \theta_0}{dz} = 0, \text{ at } z = 0, \]  
(32)
\[ \theta_0 = 0, \text{ at } z = 1. \]  
(33)

3 Numerical Techniques

Consider Eq. (31) in a form
\[ \theta_0'' = p(z) \theta_0' + q(z) \theta_0 + r(z), \]  
(34)
where \( p(z) = 0, q(z) = \phi^2 \) and \( r(z) = -B \phi^2 \). First, we select an integer \( N > 0 \) and divide the interval \([a, b]\) into \( N + 1 \) equal subintervals, whose endpoints are the mesh points \( z_i = a + ih \), for all \( i = 0, 1, \ldots, N \), where \( h = \frac{(b-a)}{N} \). At the interior mesh points, \( z_i \) for all \( i = 0, 1, \ldots, N-1 \), the differential equation to be approximated is
\[ \theta_0''(z_i) = p(z_i) \theta_0'(z_i) + q(z_i) \theta_0(z_i) + r(z_i). \]  
(35)
Expanding \( y \) in a third Taylor polynomial about \( z_i \) evaluated at \( z_{i+1} \) and \( z_{i-1} \), we have
\[ \theta_0(z_{i+1}) = \theta_0(z_i + h) = \theta_0(z_i) + h \theta_0'(z_i) + \frac{h^2}{2} \theta_0''(z_i) + \frac{h^3}{6} \theta_0'''(z_i) \]  
\[ + \frac{h^4}{24} \theta_0^{(4)}(\xi_i), \]  
(36)
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Using the central difference method, we can obtain
\[ Eqs.(39)-(40) \] results in the equation
\[ \theta_0(z_{i-1}) = \theta_0(z_i - h) = \theta_0(z_i) - h\theta'_0(z_i) + \frac{h^2}{2}\theta''_0(z_i) - \frac{h^3}{6}\theta'''_0(z_i) \]
\[ + \frac{h^4}{24}\theta^{(4)}_0(\xi^-), \] (37)

for some \( \xi \in (z_{i-1}, z_i) \), assuming \( \theta_0 \in C^4[z_{i-1}, z_{i+1}] \). If these equations are added, the terms involving \( c'(z_i) \) and \( c''(z_i) \) are eliminated and simple algebraic manipulation gives
\[ \theta''_0(z_i) = \frac{1}{h^2}[\theta_0(z_{i+1}) - 2\theta_0(z_i) + \theta_0(z_{i-1})] - \frac{h^2}{24}[\theta^{(4)}_0(\xi^+) + \theta^{(4)}_0(\xi^-)]. \] (38)

The intermediate value theorem can be used to simplify this even further
\[ \theta''_0(z_i) = \frac{1}{h^2}[\theta_0(z_{i+1}) - 2\theta_0(z_i) + \theta_0(z_{i-1})] - \frac{h^2}{12}[\theta^{(4)}_0(\xi_i)], \] (39)

for some \( \xi_i \in (z_{i-1}, z_{i+1}) \). A centered-difference formula for \( y'(z_i) \) is obtained in a similar manner resulting in
\[ \theta'_0(z_i) = \frac{1}{2h}[\theta_0(z_{i+1}) - \theta_0(z_{i-1})] - \frac{h^2}{6}[\theta'''_0(\eta_i)], \] (40)

for some \( \eta_i \in (z_{i-1}, z_{i+1}) \). The use of these centered-difference formulas in Eqs.-(39)-(40) results in the equation
\[ \frac{\theta_0(z_{i+1}) - 2\theta_0(z_i) + \theta_0(z_{i-1})}{h^2} = \frac{p(z_i)[\theta_0(z_{i+1}) - \theta_0(z_{i-1})]}{2h} + q(z_i)\theta_0(z_i) \]
\[ + r(z_i) - \frac{h^2}{12}[2p(z_i)\theta'''_0(\eta_i) - \theta^{(4)}(\xi_i)]. \] (41)

A finite difference method with truncation error [1] of order \( O(h^2) \) results by using the Eq.-(41) together with the boundary conditions \( \theta_0(b) = 0 \) and a Neumann boundary condition \( \theta'_0(a) = 0 \) become
\[ \theta_{0-1} = \theta_0, \] (42)
\[ \theta_N = 0. \] (43)

Using the central difference method, we can obtain
\[ \left( \frac{2\theta_0 - \theta_{0-1} - 2\theta_{0-1}}{h^2} \right) + \frac{p(z_i)[\theta_0(z_{i+1}) - \theta_0(z_{i-1})]}{2h} + q(z_i)\theta_0(z_i) = -r(z_i), \] (44)
\[ -(1 + \frac{h}{2}p(z_i)\theta_{0-1}) + (2 + h^2q(z_i))\theta_0 - (1 - \frac{h}{2}p(z_i))\theta_{0+1} = -h^2r(z_i), \] (45)
\[ [K] = \begin{bmatrix}
2 + h^2 q(z_0) & -2 & & & & \\
-(1 + \frac{h}{2} p(z_1)) & 2 + h^2 q(z_1) & -(1 - \frac{h}{2} p(z_1)) & & & \\
& -(1 + \frac{h}{2} p(z_2)) & 2 + h^2 q(z_2) & -(1 - \frac{h}{2} p(z_2)) & & \\
& & \ddots & \ddots & \ddots & \\
& & & -(1 + \frac{h}{2} p(z_{N-1})) & 2 + h^2 q(z_{N-1}) & 
\end{bmatrix} \] (47)

and the resulting system of equation is expressed in the tridiagonal \( N \times N \)-matrix form

\[ [K]\{\theta_0\} = \{G\}, \] (46)

where

\[ \{\theta_0\} = \begin{bmatrix}
\theta_{0_1} \\
\theta_{0_2} \\
\theta_{0_3} \\
\vdots \\
\theta_{0_{N-2}} \\
\theta_{0_{N-1}} 
\end{bmatrix}, \quad \{G\} = \begin{bmatrix}
-h^2 r(z_0) \\
-h^2 r(z_1) \\
-h^2 r(z_2) \\
\vdots \\
-h^2 r(z_{N-2}) \\
-h^2 r(z_{N-1}) 
\end{bmatrix}, \] (48)

where \( p(z) = 0, q(z) = \phi^2 \) and \( r(z) = -B\phi^2 \).

4 Numerical Example

Assume that the maximum temperature in the absence of natural convection \( B \) is 12.00 and the ratio of the characteristic time for conduction to heat generation \( \phi^2 \) is 0.5. Since the heat source is constant, we have the dimensionless activation energy \( \gamma \) is 0. Given \( h = 0.25, 0.1 \) and 0.05 and using Eq.(46), the steady-state temperature is shown in Table 1 and Fig.1

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<th>( \theta_0 )</th>
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Conclusion

In this paper, one has described a numerical method for solving exothermic reaction models in porous medium with constant heat source. The results reveal that for each mesh point sizes, the steady state temperature decrease as the dimensionless coordinate axis in vertical direction increase to the endpoint. This finite difference technique for solving the equation is easy to use and the computed results are second order accurate without instability problem. The open problem is a numerical treatment of the steady-state energy balance equation of the temperature profile in conduction state with non-constant heat source.

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References


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