UPPER AND LOWER BOUNDS FOR A REACTIVE-DIFFUSE SYSTEM WITH ARRHENIUS KINETICS

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Comparison arguments are used to study a problem in combustion theory consisting of a nonlinear parabolic equation together with initial and boundary conditions. Upper and lower bounds for the problem are constructed. The lower solutions are used to determine whether the solution of the problem is increasing in time for certain initial condition. Numerical results are presented for the slab, infinite cylinder, and unit sphere. The bounds are compared with the existing ones in the literature for the slab geometry.

1. Introduction

In this paper we consider the nonlinear parabolic equation, which describes the reactive-diffusive problem for a nonisothermal permeable catalyst pellet with first-order Arrhenius kinetics. The governing equation in the nondimensional form is

$$\frac{\partial\theta}{\partial t} = \nabla^2\theta + \lambda^2(\beta-\theta)e^{\delta(\theta/(1+\theta))}, \quad \mathbf{x}\in\Omega,\ t>0, \tag{1.1}$$

subject to homogeneous boundary condition of Dirichlet type and initial condition

$$\theta(\mathbf{x},0) = r(\mathbf{x}) \geq 0. \tag{1.2}$$

Here Ω is a bounded domain of $\mathbb{R}^N$ and $\partial\Omega$ is the smooth enough boundary of Ω. $\theta(\mathbf{x},t)$ is the temperature of the reacting species, and β, δ, and λ are nonnegative parameters which represent the chemical heat release, the activation energy of the reaction, and the Thiele modulus, respectively. All variables are considered nondimensionalized. The full derivation of the system and extensive literature for early work can be found in [3]. The steady-state problem has been studied by many authors for the Dirichlet and Robin boundary conditions, see [5–9], and here is a summary of previous work. Kapila and Matkowsky [7] considered the problem on the slab and infinite cylinder and derived asymptotic expansion for the solution with large δ. They found that the behavior of the solution is

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similar for both geometries and therefore only presented the results for the infinite cylinder. For the slab geometry the steady-state system has been reduced to a single equation by integrating the governing differential equation twice, see [5]. The literature shows that for certain values of δ and β there exist λ_o and λ^o such that the steady-state system has multiple solutions for $\lambda_o \leq \lambda \leq \lambda^o$. Here λ_o and λ^o correspond to extinction and ignition limits, respectively, and the corresponding steady-state solutions are known as the middle solutions, whereas for $\lambda > \lambda_o$ and $\lambda < \lambda_o$ the unique steady-state solutions are known as the upper and lower solutions, respectively. The number of middle solutions depends on the geometry of the domain Ω and the boundary conditions [6–8]. Of interest are the values of λ_o and λ^o. An attempt to evaluate these values was made in [7] for the slab and infinite cylinder geometries using asymptotic expansion approach. Recently, Al-Refai [1] has considered the problem with Dirichlet boundary conditions. He proved the existence of a nonnegative solution and derived sharp upper and lower bounds for the values of λ and δ using comparison theory. Also in [2] he derived analytical upperand lower bounds for the extinction and ignition limits for the three geometries: slab, infinite cylinder, and unit sphere. Although the steady-state problem may have more than one solution, the problem with time-dependent has a unique solution provided that $0 \leq \theta(\mathbf{x},0) \leq \beta$ (see [10, page 42]).

In this paper, we study the time-dependent problem in the slab $[0,1]$, in the unit sphere, and infinite cylinder. In Section 2, we write some preliminary results for the system which will be used through the text. In Section 3, we construct upper and lower solutions for the problem (1.1)-(1.2). In Section 4, we present some numerical results in the three geometries. Finally, we write some concluding remarks in Section 5.

2. A preliminary result

We have the problem

$$P\theta = \frac{\partial\theta}{\partial t} - \nabla^2\theta - \lambda^2 g(\theta) = 0, \quad \mathbf{x} \in \Omega,\ t > 0,$$
$$\theta(\mathbf{x},t) = 0, \quad \mathbf{x} \in \partial\Omega, \tag{2.1}$$
$$\theta(\mathbf{x},0) = r(\mathbf{x}) \geq 0,$$

where $g(\theta) = (\beta - \theta)e^{\delta(\theta/(1+\theta))}$. A well known result for the system is that $0 \leq \theta(\mathbf{x},t) \leq \beta$ provided that $r(x) \leq \beta$. If $\delta\beta \leq 1$, then

$$g'(\theta) = -\frac{e^{\delta(\theta/(\theta+1))}}{(\theta+1)^2}\left[\theta^2 + (2+\delta)\theta + 1 - \delta\beta\right] < 0, \tag{2.2}$$

and the corresponding steady-state problem has a unique solution, see [2, 10]. While, for $\delta > 4 + 4/\beta$, the steady-state problem may have more than one solution. The following result will be used in this paper.

Proposition 2.1. *Consider the problem in (2.1) with $g'(\theta)$ being bounded.*

(i) *If $(\partial\theta/\partial t)(\mathbf{x},0) < 0$, then $(\partial\theta/\partial t)(\mathbf{x},t) < 0$ for all $\mathbf{x} \in \Omega$, and $t \geq 0$.*

(ii) *If $(\partial\theta/\partial t)(\mathbf{x},0) > 0$, then $(\partial\theta/\partial t)(\mathbf{x},t) > 0$ for all $\mathbf{x} \in \Omega$, and $t \geq 0$.*

For the proof one can see [4, 12].

3. Upper and lower bounds

To construct upper and lower bounds for the problem we use maximum principle for parabolic equations, see [11, page 187]. Let $w(\mathbf{x},t)$ and $u(\mathbf{x},t)$ satisfy

$$\begin{gathered} Pw \leq 0 \leq Pu, \quad \mathbf{x} \in \Omega,\ t > 0, \\ w(\mathbf{x},t) \leq 0 \leq u(\mathbf{x},t), \quad \mathbf{x} \in \partial\Omega, \\ w(\mathbf{x},0) \leq r(\mathbf{x}) \leq u(\mathbf{x},0). \end{gathered} \tag{3.1}$$

Then $w(\mathbf{x},t)$ and $u(\mathbf{x},t)$ are lower and upper solutions for the problem in (2.1), respectively, $w(\mathbf{x},t) \leq \theta(\mathbf{x},t) \leq u(\mathbf{x},t)$, as long as both exist.

Let λ_1 be the first eigenvalue and ϕ_1 the corresponding normalized, with respect to L^2-norm, eigenfunction of

$$\begin{gathered} \nabla^2\phi = -\lambda\phi, \quad \mathbf{x} \in \Omega, \\ \phi = 0, \quad \mathbf{x} \in \partial\Omega. \end{gathered} \tag{3.2}$$

It is easily obtained that $\phi_1 = \sqrt{2}\sin(\pi x)$, $(1/\sqrt{2\pi})(\sin(\pi x)/x)$, and $J_0(\gamma_0 x)$, for the slab, spherical, and cylindrical geometries, respectively. Here $J_0(\gamma_0 x)$ is the Bessel function of order zero, $\gamma_0 = 2.404825\ldots$ is the first zero of $J_0(x)$, and $0 \leq x \leq 1$. In all cases, the first eigenfunction ϕ_1 is nonnegative in Ω.

3.1. Bounds when $g(\theta)$ is decreasing. We derive upper and lower solutions for the problem when $\delta\beta \leq 1$ and so $g(\theta)$ is decreasing. The function $g(\theta)$ has only one inflection point $\theta^0 = (\delta\beta - 2\beta - 2)/(\delta + 2 + 2\beta)$, and $g(\theta)$ is concave up for $\theta < \theta^0$ and concave down for $\theta > \theta^0$. For $\delta\beta \leq 1$, we have $\theta^0 < 0$, and therefore, $g(\theta)$ is concave down on $[0,\beta]$.

Theorem 3.1. *Let ϕ_1 and λ_1 be as defined in (3.2) and let ϕ_{1m} be the maximum of ϕ_1 on Ω. Let $k(t)$ be the solution of the IVP*

$$\begin{gathered} k'(t) = \lambda^2 g(k(t)) - \lambda_1 k(t), \\ k(0) = k_0. \end{gathered} \tag{3.3}$$

Then $k_0 \leq k(t) \leq k_m$ and $w(\mathbf{x},t) = k(t)(\phi_1(\mathbf{x})/\phi_{1m})$ is a lower solution of (2.1). Here k_m is the unique solution of $g(k_m) = (\lambda_1/\lambda^2)k_m$ and $k_0 = k(0)$ is chosen such that $k_0(\phi_1(\mathbf{x})/\phi_{1m}) \leq r(\mathbf{x})$.

Proof. Since $g(0) = \beta > 0$, we have $(\lambda_1/\lambda^2)u \leq g(u)$ for $0 \leq u \leq k_m$ and $(\lambda_1/\lambda^2)u \geq g(u)$ for $k_m \leq u \leq \beta$. If $k_0 < k_m$, then $k'(t) \geq 0$ and $k(t)$ is increasing with equilibrium value k_m, and therefore, $k_0 \leq k(t) \leq k_m$. The analogous result is obtained if $k_m \leq k_0 \leq \beta$, but $k(t)$ is decreasing. Now,

$$\begin{aligned} Pw &= k' \frac{\phi_1}{\phi_{1m}} + \lambda_1 k \frac{\phi_1}{\phi_{1m}} - \lambda^2 g\left(k \frac{\phi_1}{\phi_{1m}}\right) \\ &= \frac{\phi_1}{\phi_{1m}} \lambda^2 g(k) - \lambda^2 g\left(k \frac{\phi_1}{\phi_{1m}}\right) \leq \lambda^2 \left[g(k) - g\left(k \frac{\phi_1}{\phi_{1m}}\right)\right]. \end{aligned} \tag{3.4}$$

Since $k(t)(\phi_1/\phi_{1m}) \leq k(t)$ and g is decreasing, we have $Pw \leq 0$, which together with $w(\mathbf{x},0) \leq r(\mathbf{x})$ proves that w is a lower solution of (2.1). □

Theorem 3.2. *Let ψ be the solution of*

$$\begin{aligned} \nabla^2 \psi &= -1, \quad \mathbf{x} \in \Omega, \\ \psi &= 0, \quad \mathbf{x} \in \partial\Omega. \end{aligned} \tag{3.5}$$

Then $\psi \geq 0$, and $u(\mathbf{x},t) = h(t)\psi(x)$ is an upper solution of (2.1), where

$$h(t) = h_0 - \frac{1}{\lambda^2 g'(0)} \left[1 - e^{\lambda^2 g'(0) t}\right], \tag{3.6}$$

and $h_0 = h(0)$ is chosen such that $h_0 \geq \lambda^2 \beta$ and $h_0 \psi(\mathbf{x}) \geq r(\mathbf{x})$.

Proof. To show that $\psi \geq 0$, let $\xi = -\psi$, then ξ satisfies $\nabla^2 \xi = 1 \geq 0$, and $\xi = 0$ on $\partial\Omega$. Using maximum principle of elliptic equations (see [11, page 64]), we have $\xi \leq 0$, and hence $\psi \geq 0$. Since $g'(0) = \delta\beta - 1 \leq 0$, it is not difficult to see that $h(t)$ is increasing with

$$h_0 \leq h(t) \leq h_0 + \frac{1}{\lambda^2 (1 - \delta\beta)}, \tag{3.7}$$

and it is the unique solution of the IVP

$$\begin{aligned} h'' - \lambda^2 g'(0) h' &= 0, \\ h(0) = h_0 > 0, \qquad h'(0) &= 1. \end{aligned} \tag{3.8}$$

Now, $Pu = h'\psi + h - \lambda^2 g(h\psi)$ and

$$\frac{\partial Pu}{\partial t} = h''\psi + h' - \lambda^2 h' \psi g'(h\psi) = \left(h'' - \lambda^2 h' g'(h\psi)\right)\psi + h'. \tag{3.9}$$

Since $h(t)\psi \geq 0$ and g' is decreasing, we have

$$\frac{\partial Pu}{\partial t} \geq \left(h'' - \lambda^2 h' g'(0)\right)\psi + h'(t) = h'(t). \tag{3.10}$$

Integrate the above inequality from 0 to t to get

$$Pu - Pu(0) \geq h(t) - h(0), \tag{3.11}$$

or

$$Pu \geq \psi + h(t) - \lambda^2 g(h_0\psi) \geq h(t) - \lambda^2\beta \geq 0, \tag{3.12}$$

which together with $u(\mathbf{x},0) = h_0\psi(\mathbf{x}) \geq r(\mathbf{x}) \geq 0$ proves that u is an upper solution of (2.1). □

3.2. Lower solutions for $\delta > 4 + 4/\beta$**.** When $\delta > 4 + 4/\beta$, the inflection point $\theta^0 = (\beta(\delta-2)-2)/(\delta+2+2\beta) \in [0,\beta]$. Let $\theta^* \in [0,\beta]$ be the smallest solution of $(\lambda_1/\lambda^2)\theta = g(\theta)$ and $\lambda_1/\lambda^2 = g'(\theta)$, and let λ^* be the corresponding value of λ, see Figure 3.1. For the exact values of θ^* and λ^*, one is referred to [2]. We have the following.

Proposition 3.3. (1) $\theta^0 = (\beta(\delta-2)-2)/(\delta+2\beta+2) > \theta^* = (\beta(\delta-2)-\sqrt{\beta\delta(\beta\delta-4\beta-4)})/2(\beta+\delta)$ *for* $\delta > 4+4/\beta$.

(2) *The function* $h(\theta) = g(\theta) - (\lambda_1/\lambda^2)\theta$ *is decreasing in* $[0,\theta^*]$ *for* $\lambda \leq \lambda^*$.

Proof. (1) It is enough to show that

$$\frac{\beta(\delta-2)-2}{\delta+2+2\beta} > \frac{\beta(\delta-2)}{2(\beta+\delta)}, \tag{3.13}$$

or

$$2(\beta+\delta)[\beta(\delta-2)-2] > \beta(\delta-2)(\delta+2\beta+2). \tag{3.14}$$

The last inequality is equivalent to

$$\beta\delta^2 - \delta(4\beta+4) \geq 0. \tag{3.15}$$

Now, $4\beta+4 < \beta\delta$ and hence $-\delta(4\beta+4) > -\beta\delta^2$, which proves (3.15).

(2) Since $\theta^* < \theta^0$, we have $g'(\theta)$ increasing in $[0,\theta^*]$ and hence $h'(\theta) = g'(\theta) - \lambda_1/\lambda^2 \leq g'(\theta^*) - \lambda_1/(\lambda^*)^2 = 0$, which proves the result. □

Theorem 3.4. *Let* ϕ_1 *and* λ_1 *be as defined in (3.2) and let* ϕ_{1m} *be the maximum of* ϕ_1 *on* Ω. *For* $\lambda \leq \lambda^*$, *let* $k(t)$ *be the solution of the IVP*

$$\begin{gathered} k'(t) = \frac{1}{\phi_{1m}}\{\lambda^2 g(k(t)\phi_{1m}) - \lambda_1 k(t)\phi_{1m}\}, \\ k(0) = k_0, \end{gathered} \tag{3.16}$$

where $k_0 \leq k_M$ *is chosen such that* $k_0\phi_1(\mathbf{x}) \leq r(\mathbf{x})$, *and* k_M *is the solution (the smallest solution if there is more than one) of* $\lambda^2 g(k_M\phi_{1m}) = \lambda_1 k_M\phi_{1m}$, *see Figure 3.1. Then* $k(t)$ *is an increasing function, with* $k_0 \leq k(t) \leq k_M$, *and* $w(\mathbf{x},t) = k(t)\phi_1(\mathbf{x})$ *is a lower solution of (2.1).*

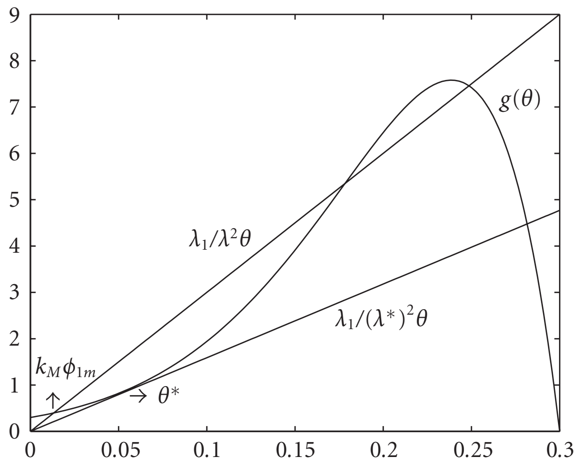

Figure 3.1. The values of θ^* and k_M, for $\beta = 0.3$ and $\delta = 25$.

Proof. Since $k_0 \le k_M$ and $(\lambda_1/\lambda^2)\phi_{1m}u \le g(\phi_{1m}u)$ for $0 \le u \le k_M$, we have $k(t)$ increasing with equilibrium value k_M, that is, $k_0 \le k(t) \le k_M$. Now,

$$\begin{aligned} Pw &= k'(t)\phi_1 + \lambda_1 k(t)\phi_1 - \lambda^2 g(k(t)\phi_1) \\ &= \frac{\phi_1}{\phi_{1m}}\{\lambda^2 g(k\phi_{1m}) - \lambda_1 k\phi_{1m}\} + \lambda_1 k\phi_1 - \lambda^2 g(k\phi_1) \\ &\le (\lambda^2 g(k\phi_{1m}) - \lambda_1 k\phi_{1m}) - (\lambda^2 g(k\phi_1) - \lambda_1 k\phi_1). \end{aligned} \tag{3.17}$$

Since $g(\theta) - (\lambda_1/\lambda^2)\theta$ is decreasing in $[0,\theta^*]$ for $\lambda \le \lambda^*$, we have $Pw \le 0$ and the result is obtained. □

Theorem 3.5. *For $\lambda > \lambda^*$, let $\epsilon(\lambda) > 1$ be such that $g(\theta^*) = \epsilon(\lambda_1/\lambda^2)\theta^*$, and let $k(t)$ be the solution of*

$$\begin{gathered} k'(t) = \frac{1}{\phi_{1m}}\{\lambda^2 g(k(t)\phi_{1m}) - \epsilon\lambda_1 k(t)\phi_{1m}\}, \\ k(0) = k_0, \end{gathered} \tag{3.18}$$

where $k_0 \le \theta^*/\phi_{1m}$ is chosen such that $k_0\phi_1(\mathbf{x}) \le r(\mathbf{x})$. Then the function $h(\theta) = g(\theta) - \epsilon(\lambda_1/\lambda^2)\theta$ is decreasing in $[0,\theta^*]$ and $w(\mathbf{x},t) = k(t)\phi_1(\mathbf{x})$ is a lower solution of (2.1).

Proof. Since $\epsilon = (\lambda/\lambda^*)^2$, we have $h(\theta) = g(\theta) - (\lambda_1/(\lambda^*)^2)\theta$ and $h'(\theta) = g'(\theta) - \lambda_1/(\lambda^*)^2 \le g'(\theta^*) - \lambda_1/(\lambda^*)^2 = 0$. Using the same arguments as in the previous theorem, one can verify that $k(t)$ is increasing in $k_0 \le k(t) \le \theta^*/\phi_{1m}$. Since $g(\theta) - \epsilon(\lambda_1/\lambda^2)\theta$ is decreasing in $[0,\theta^*]$ and $\epsilon > 1$ we have

$$
\begin{aligned}
Pw &= k'(t)\phi_1 + \lambda_1 k(t)\phi_1 - \lambda^2 g(k(t)\phi_1)\\
&= \frac{\phi_1}{\phi_{1m}}\left(\lambda^2 g(k\phi_{1m}) - \epsilon\lambda_1 k\phi_{1m}\right) - \left(\lambda^2 g(k\phi_1) - \lambda_1 k\phi_1\right)\\
&\le \lambda^2 g(k\phi_{1m}) - \epsilon\lambda_1 k\phi_{1m} - \left(\lambda^2 g(k\phi_1) - \epsilon\lambda_1 k\phi_1\right)\\
&= \lambda^2\left(\left[g(k\phi_{1m}) - \epsilon\frac{\lambda_1}{\lambda^2}k\phi_{1m}\right] - \left[g(k\phi_1) - \epsilon\frac{\lambda_1}{\lambda^2}k\phi_1\right]\right) \le 0,
\end{aligned}
\tag{3.19}
$$

which proves the result. □

4. Numerical results

We consider the case where $g(\theta)$ is decreasing, and use Theorems 3.1 and 3.2 to obtain lower and upper solutions of (2.1). We present the bounds for different values of λ, β, δ and $0 \le t \le 0.2$, with initial condition $\theta(\mathbf{x},0) = \lambda^2\beta\psi(\mathbf{x})$, where $\psi(\mathbf{x})$ is defined in Theorem 3.2. Figures 4.1, 4.2, and 4.3 depict these bounds of the problem when Ω is the slab, unit sphere, and infinite cylinder, respectively, and $\beta = 0.5$, $\delta = 0.1$, and $\lambda = 0.5, 1, 2, 5$. In order for the condition $k_0(\phi_1/\phi_{1m}) \le r(\mathbf{x})$ to be satisfied in Theorem 3.1, we take $k_0 = \lambda^2\beta/8$, $\lambda^2\beta/18.9$, $\lambda^2\beta/6.4$, for the slab, sphere, and infinite cylinder, respectively. From the figures one can see that the upper bounds are increasing in time, where

$$
h(t) = \lambda^2\beta + \frac{1}{\lambda^2}\frac{1}{1-\delta\beta}\left[1 - e^{-\lambda^2(1-\delta\beta)t}\right],
\tag{4.1}
$$

whereas the lower bounds are decreasing or increasing in time, depending on the geometry k_0 and k_m. For example, the lower solutions are decreasing in time in the slab geometry since $k_0 > k_m$, while they are increasing with time for $\lambda = 0.5, 1, 2$ and decreasing for $\lambda = 5$ in the sphere. Table 4.1 shows k_0 and k_m, for $\beta = 0.5$, $\delta = 0.1$, and different values of λ. Also, the upper and lower solutions are close to each other and give good information about the exact solution θ.

From Proposition 2.1 we have that if $\theta_t(\mathbf{x},0) \ne 0$, then the solution θ is either increasing or decreasing in time. We now take $\theta(\mathbf{x},0) = c\phi_1(\mathbf{x})$ and ask the following: for what values of c the solution θ of (2.1) is increasing with respect to time? To answer the question, we substitute $k_0 = c\phi_{1m}$ in Theorem 3.1. Since $\theta(\mathbf{x},0) = w(\mathbf{x},0)$ and $w(\mathbf{x},t)$ is increasing in time for $c < k_m/\phi_{1m}$, then so is θ.

Finally, we compare our bounds with the bounds obtained in [10]. Consider the PDE

$$
\begin{gathered}
\frac{\partial v}{\partial t} = \nabla^2 v - \lambda^2 c_0 v + \mu_0\beta, \quad \mathbf{x} \in \Omega,\\
v(\mathbf{x},t) = 0, \quad \mathbf{x} \in \partial\Omega,\\
v(\mathbf{x},0) = r(\mathbf{x}) \ge 0,
\end{gathered}
\tag{4.2}
$$

where $c_0 = \max\{-\lambda^2 g'(v),\ 0 \le v \le \beta\}$. Let $\overline{v}(\mathbf{x},t)$ be the solution of (4.2) with $\mu_0 = c_0$, then $\overline{v}(\mathbf{x},t)$ is an upper solution of (2.1). A lower solution $\underline{v}(\mathbf{x},t)$ of (2.1) is obtained by solving (4.2) with $\mu_0 = \lambda^2$. For more details one can see [10, page 36]. For the slab

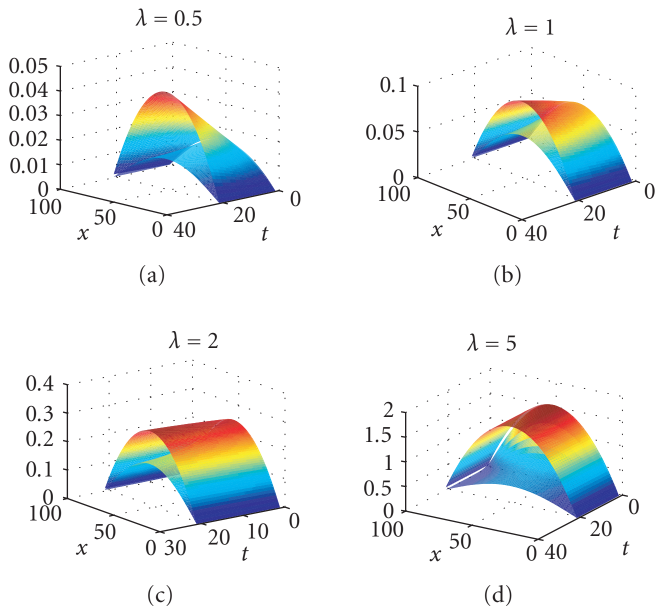

Figure 4.1. Upper and lower bounds for the slab geometry, when $\beta = 0.5$, $\delta = 0.1$, and $\lambda = 0.5, 1, 2, 5$.

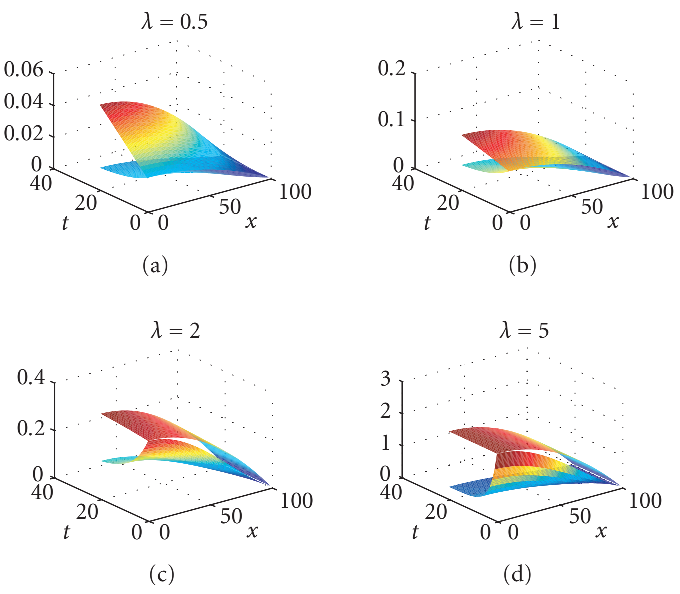

Figure 4.2. Upper and lower bounds for the spherical geometry, when $\beta = 0.5$, $\delta = 0.1$, and $\lambda = 0.5, 1, 2, 5$.

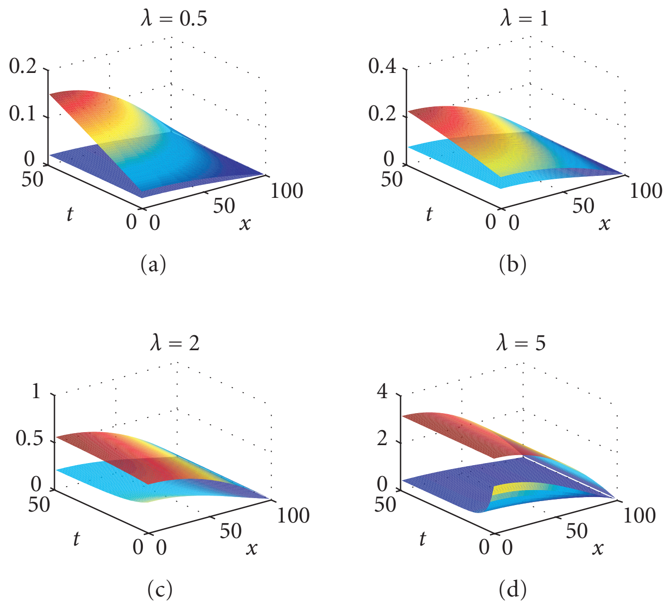

Figure 4.3. Upper and lower bounds for the cylindrical geometry, when $\beta = 0.5$, $\delta = 0.1$, and $\lambda = 0.5, 1, 2, 5$.

Table 4.1. The values of k_0 and k_m, for $\beta = 0.5$ and $\delta = 0.1$, in the three geometries.

	λ	0.5	1.0	2.0	5.0
Slab	k_0	0.015625	0.062500	0.250000	1.562500
	k_m	0.012367	0.046185	0.145507	0.361155
Sphere	k_0	0.006614	0.026455	0.105820	0.661380
	k_m	0.012367	0.046185	0.145507	0.361155
Cylinder	k_0	0.019531	0.078125	0.312500	1.953100
	k_m	0.020759	0.074147	0.206504	0.408257

geometry we have

$$\begin{aligned} \overline{v}(x,t) &= \frac{2\beta}{\pi}\sum_{n=1}^{\infty}\frac{1-(-1)^n}{n}\left(\frac{\lambda^2}{n^2\pi^2}e^{-r_n t}+\frac{\mu_0}{r_n}\left(1-e^{-r_n t}\right)\right)\sin(n\pi x), \\ \underline{v}(x,t) &= \frac{2\beta\lambda^2}{\pi}\sum_{n=1}^{\infty}\frac{1-(-1)^n}{n}\left(\frac{1}{n^2\pi^2}e^{-r_n t}+\frac{1}{r_n}\left(1-e^{-r_n t}\right)\right)\sin(n\pi x), \end{aligned} \tag{4.3}$$

where $r_n = n^2\pi^2 + \lambda^2\mu_0$ and $\mu_0 = 1.033895$.

Figures 4.4 and 4.5 on the left show the upper solutions u and $\overline{v}$ and on the right the difference between them. For $\lambda = 0.1$ and 0.5 we have $\overline{v} - u \geq 0$, that is, the upper

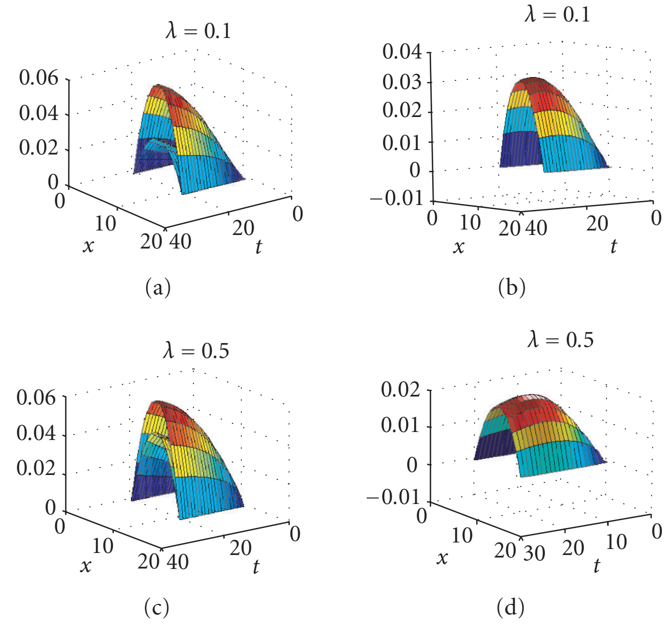

Figure 4.4. The upper solutions $u(\mathbf{x},t)$ and $\overline{v}(\mathbf{x},t)$ and the difference $\overline{v}(\mathbf{x},t)-u(\mathbf{x},t)$ for the slab geometry, when $\beta = 0.5$, $\delta = 0.1$, and $\lambda = 0.1, 0.5$.

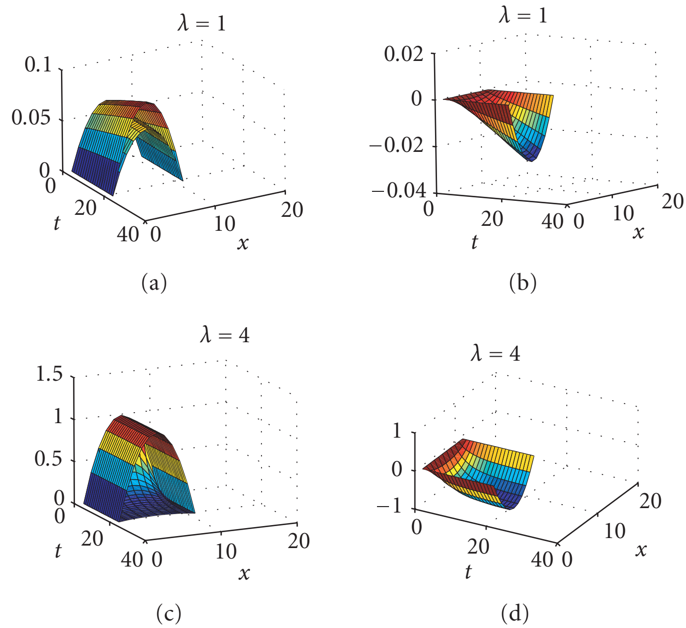

Figure 4.5. The upper solutions $u(\mathbf{x},t)$ and $\overline{v}(\mathbf{x},t)$ and the difference $\overline{v}(\mathbf{x},t)-u(\mathbf{x},t)$ for the slab geometry, when $\beta = 0.5$, $\delta = 0.1$, and $\lambda = 1, 4$.

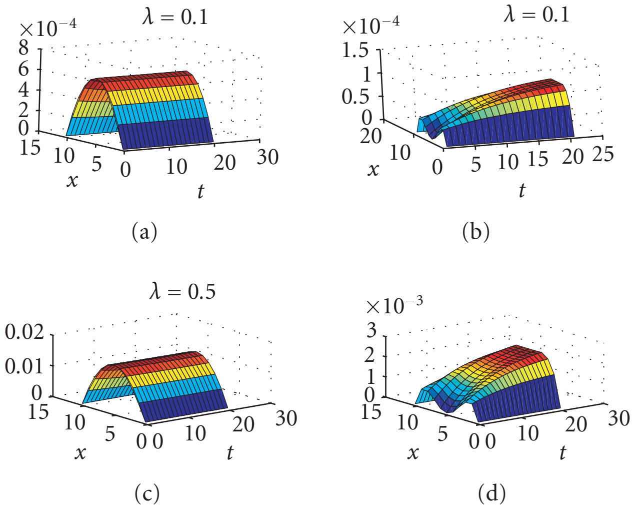

Figure 4.6. The lower solutions $w(\mathbf{x},t)$ and $\underline{v}(\mathbf{x},t)$ and the difference $\underline{v}(\mathbf{x},t) - w(\mathbf{x},t)$ for the slab geometry, when $\beta = 0.5$, $\delta = 0.1$, and $\lambda = 0.1, 0.5$.

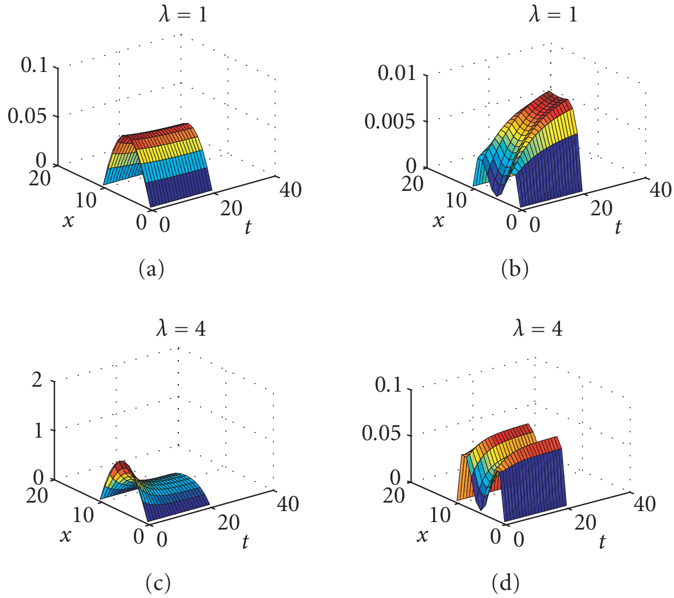

Figure 4.7. The lower solutions $w(\mathbf{x},t)$ and $\underline{v}(\mathbf{x},t)$ and the difference $\underline{v}(\mathbf{x},t) - w(\mathbf{x},t)$ for the slab geometry, when $\beta = 0.5$, $\delta = 0.1$, and $\lambda = 1, 4$.

solution u is better than $\overline{v}$. Whereas for $\lambda = 1$ and 4 we have $u \geq \overline{v}$, and the upper solution $\overline{v}$ is better than u. Figures 4.6 and 4.7 on the left show the lower solutions w and $\underline{v}$ and on the right the difference between them. One can see that the two bounds are close to each other and for all values of λ we have $\underline{v} \geq w$, that is, the lower solution $\underline{v}$ is better than w.

5. Concluding remarks

We have used comparison arguments to study a nonlinear parabolic equation arising from the theory of catalyst pellets reaction. For $\delta\beta \leq 1$, a lower solution of the form $w(\mathbf{x},t) = k(t)(\phi_1/\phi_{1m})$ is obtained, where ϕ_1 is the first normalized eigenfunction of the associated Laplacian operator, ϕ_{1m} is the maximum of ϕ_1 in Ω, and $k(t)$ is the solution of an IVP. Depending on the initial condition $k(0)$, the function $k(t)$ might be decreasing or increasing. An upper solution of the form $u(\mathbf{x},t) = h(t)\psi(\mathbf{x})$ is obtained by solving a second-order linear IVP for $h(t)$ and a linear PDE for ψ, where $h(t)$ is increasing in time. The lower solution is used to give a sufficient condition for the solution θ to be increasing in time for certain initial condition. For the case where $\delta > 4 + 4/\beta$, we have constructed a lower solution $w(\mathbf{x},t) = k(t)\phi_1(\mathbf{x})$, where $k(t)$ is increasing and depends on the value of λ^*. We present the upper and lower solutions for certain parameters in the three geometries numerically. These upper and lower solutions are compared with the ones obtained by Pao [10] for the slab geometry.

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