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Bounds and critical parameters for a combustion problem

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Abstract

A model from combustion theory consisting of a nonlinear elliptic equation and boundary conditions of Dirichlet type, is considered. Upper and lower solutions for the problem are obtained by solving linear elliptic equations. These solutions are used to obtain analytical bounds for the extinction and ignition limits. Numerical results are presented for the slab, cylindrical and spherical geometries. Results compare very well with existing ones in the literature.

MSC: 34C10; 80A25; 35J25

Keywords: Comparison theory; Combustion theory; Elliptic equations

1. Introduction

A well-known problem in combustion theory which describes the steady reactive diffusive problem for a nonisothermal permeable catalyst pellet with first-order Arrhenius kinetics, is the nonlinear elliptic equation

$$\nabla^2\theta + \lambda^2(1+\beta-\theta)\mathrm{e}^{\delta(\theta-1)/\theta} = 0 \quad \text{in } \Omega, \tag{1}$$

$$\theta = 1 \quad \text{on } \partial\Omega. \tag{2}$$

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Here Ω is a bounded domain, and $\partial\Omega$ is the boundary of Ω, θ is the temperature of the reacting species, and β, δ, and λ are nonnegative parameters which represent, respectively, the chemical heat release, the activation energy of the reaction, and the Thiele modulus. All variables are considered nondimensionalized. The full derivation of the system and extensive literature for early work can be found in [2], and discussions on the system can be found in [4,5,8]. Recently, Al-Refai [1] has shown the existence of a nonnegative solution for the problem, and derived upper and lower solutions using comparison theory. By asking that $g(\theta)/\theta$ be a decreasing function of θ, a necessary and sufficient condition for the uniqueness of θ has been derived in [3], where $g(\theta) = \lambda^2(1 + \beta - \theta)e^{\delta(\theta-1)/\theta}$. The condition is $\delta < 4 + 4/\beta$. An interesting phenomenon of the system is the multiplicity of its steady-state solutions. The literature shows that for some domain of δ and β there exists λ_0 and λ^0 such that the system has multiple solutions for $\lambda_0 \leqslant \lambda \leqslant \lambda^0$. The multiplicity bounds λ_0 and λ^0 correspond to extinction and ignition limits, respectively. For $\lambda > \lambda^0$ there exists a unique solution called the upper branch solution or explosion branch, and for $\lambda < \lambda_0$ the lower branch solution is unique and it is known as the quenching branch.For $\lambda_0 \leqslant \lambda \leqslant \lambda^0$ the multiple solutions are known as the middle solutions. The number of middle solutions depends on the geometry of the domain Ω. For the infinite slab and circular cylinder there are three middle solutions. This result was found in [6] by drawing the graph of the response (maximum of θ on Ω) versus λ, and noticing that the graph has the S shape. Similar discussions are made in [7] for the spherical geometry, and it is noted that the number of middle solutions may be very large. Of interest are the values of λ_0 and λ^0. An attempt to evaluate these values was made in [6,7] for the three geometries, by deriving asymptotic expansion of the solution for large δ.

In this paper, we consider the problem in the slab [0, 1], circular cylinder with radius 1, and unit sphere. We focus on the values of δ and β for which multiple solutions may occur. In Section 2, we construct upper and lower solutions for the problem using comparison theory. And then derive a lower bound λ_* for λ_0 and an upper bound λ^* for λ^0, where $\lambda_* \leqslant \lambda_0 \leqslant \lambda^0 \leqslant \lambda^*$. In Section 3, we present some numerical results for the problem in the three geometries. Finally, we write some concluding remarks in Section 4.

2. Upper and lower solutions

We substitute $u = \theta - 1$ into (1) and (2) and obtain

$$Pu = \nabla^2 u + \lambda^2 g(u) = 0, \quad \mathbf{x} \in \Omega, \tag{3}$$

$$u = 0, \quad \mathbf{x} \in \partial\Omega, \tag{4}$$

where $g(u) = (\beta - u)e^{\delta u/(1+u)}$. We use the Maximum Principle for elliptic equations to construct upper and lower solutions for the problem, see [9, p. 151]. Let v and w be such that

$$Pv \leqslant 0 \leqslant Pw, \quad \mathbf{x} \in \Omega' \quad \text{and} \quad w \leqslant 0 \leqslant v, \quad \mathbf{x} \in \partial\Omega,$$

then v and w are upper and lower solutions for u, respectively. The following lemma from comparison theory of elliptic equations [9, p. 64] will be used throughout this paper.

Lemma 1. *Let y satisfy the differential inequality*

$$(L + h)[y] = L[y] + h(\mathbf{x})y \geqslant 0,$$

where $h(\mathbf{x}) \leqslant 0$, is a bounded function and L is uniformly elliptic in a bounded domain Ω with bounded coefficients. If y attains a nonnegative maximum M at an interior point of Ω, then $y = M$.

A well-known result for the solution u which can be proved using Lemma 1 is that $0 \leqslant u \leqslant \beta$.

2.1. Lower solution and bound for the extinction limit

We use comparison theory to construct a lower solution for the problem. A similar discussion is given in [10] for another problem in combustion theory.

Lemma 2. *Let λ_1 and ϕ_1 be the first eigenvalue and the corresponding normalized eigenfunction of*

$$\nabla^2 \phi = -\lambda \phi, \quad \mathbf{x} \in \Omega,$$

$$\phi(\mathbf{x}) = 0, \quad \mathbf{x} \in \partial\Omega.$$

Let $\phi_{1\mathrm{m}} > 0$ be the maximum of ϕ_1 on Ω, and k be the solution (the smallest solution if there is more than one) of

$$\frac{\lambda_1 k}{\lambda^2} = g(k), \tag{5}$$

then $w = k\phi_1/\phi_{1\mathrm{m}}$ is a lower solution of (3) *and* (4).

Proof. Let $r(u) = (\lambda_1/\lambda^2)u$. Since $r(0) = 0$ and $g(0) = \beta \geqslant 0$, we have $r(u) = (\lambda_1/\lambda^2)u \leqslant g(u)$, for $u \leqslant k$, and hence $(\lambda_1/\lambda^2)k\phi_1/\phi_{1\mathrm{m}} \leqslant g(k\phi_1/\phi_{1\mathrm{m}})$, see Fig. 1. Now,

$$P\left(k\frac{\phi_1}{\phi_{1\mathrm{m}}}\right) = -\lambda_1 k \frac{\phi_1}{\phi_{1\mathrm{m}}} + \lambda^2 g\left(k\frac{\phi_1}{\phi_{1\mathrm{m}}}\right) \geqslant 0,$$

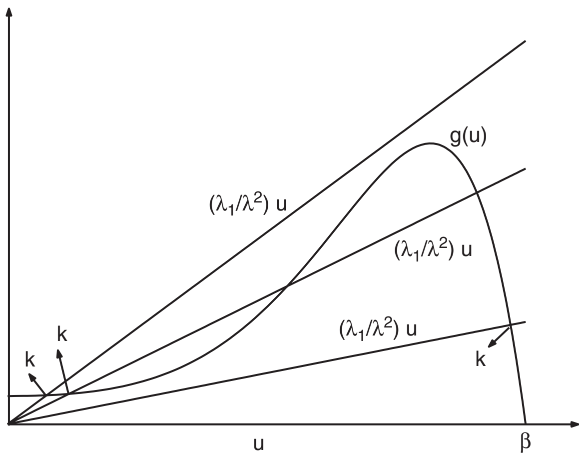

Fig. 1. All possible cases for the value of k, obtained by plotting $(\lambda_1/\lambda^2)u$ and $g(u)$ versus u.

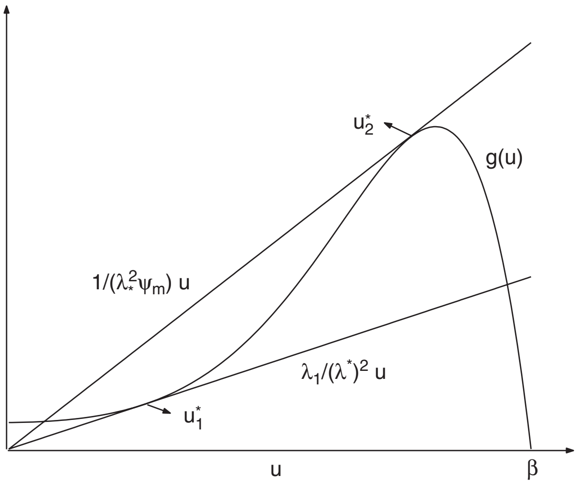

Fig. 2. Values of u_1^* and u_2^*, obtained by plotting $g(u)$, $(\lambda_1/(\lambda^*)^2)u$ and $(1/\lambda_*^2\psi_{\mathrm{m}})u$ versus u.

which together with $w=0$ on $\partial\Omega$, proves that w is a lower solution for any solution of (3) and (4). We have assumed that $\phi_{1\mathrm{m}}>0$, otherwise, $\phi_1(x)\leqslant 0$, and we choose $-\phi_1(x)$ to be the first eigenfunction. $\square$

In the following, we use Lemma 2 to derive an upper bound for λ^0. Let $u_1^*\in[0,\beta]$ be the smallest solution of $\lambda_1 u/\lambda^2=g(u)$ and $\lambda_1/\lambda^2=g'(u)$, see Fig. 2. Solving the two equations simultaneously, we have

$$u_1^*=\frac{\beta(\delta-2)-\sqrt{\beta\delta(\beta\delta-4\beta-4)}}{2(\beta+\delta)} \tag{6}$$

and the corresponding value of λ,

$$(\lambda^*)^2=\frac{\lambda_1 u_1^*}{\beta-u_1^*}\mathrm{e}^{-\delta u_1^*/(1+u_1^*)}. \tag{7}$$

The values of k in Eq. (5) are between 0 and β. By saying k is large we mean k is close to β, and it is small, when it is close to 0. Let $\|f\|_\Omega=\sup\{f(x)\,:\,x\in\Omega\}$ denotes the supremum norm on Ω, and $\zeta=\inf\{\|u_i^{\mathrm{m}}\|_\Omega\}$, where $u_i^{\mathrm{m}}:i=1,2,\ldots$ denote the middle solutions of the problem. Let u^{q} and u^{p} denote the quenching and upper branch solutions, respectively. Therefore, we have $w=k\phi_1/\phi_{1\mathrm{m}}\leqslant u^{\mathrm{q}}\leqslant\zeta\leqslant u^{\mathrm{p}}$. The temperature of u^{q} and ζ are too low, see [7]. Hence for large k, $w=k\phi_1/\phi_{1\mathrm{m}}$ is a lower solution only for u^{p}, that is, the quenching branch and middle solutions do not exist. It is clear from Fig. 2 that if $\lambda>\lambda^*$, then Eq. (5) has a unique solution, where the value of k is large. Hence the unique upper branch solution is obtained, and this implies that λ^* is an upper bound for λ^0. Moreover, if $\delta<4+4/\beta$, then the real solutions u_1^* and λ^* do not exist, and the solution u is unique.This is exactly the same result which has been obtained in [3]. A remarkable note here is that u_1^* does not depend on λ.

2.2. Upper solution and bound for the ignition limit

Let u_2^* be the largest solution of $u/(\psi_m\lambda^2)=g(u)$ and $1/(\psi_m\lambda^2)=g'(u)$, see Fig. 2. Then

$$u_2^*=\frac{\beta(\delta-2)+\sqrt{\beta\delta(\beta\delta-4\beta-4)}}{2(\beta+\delta)} \tag{8}$$

and the corresponding value of λ,

$$\lambda_*^2=\frac{u_2^*}{\psi_m(\beta-u_2^*)}\mathrm{e}^{-\delta u_2^*/(1+u_2^*)}. \tag{9}$$

It is rapidly seen that the values of λ_* and λ^* depend on β, δ and the bounded domain Ω.

Lemma 3. *The function $g(u)=(\beta-u)\mathrm{e}^{\delta u/(1+u)}$ is an increasing function on $[0,u_2^*]$, for $\delta>4+4/\beta$.*

Proof. The function

$$g'(u)=-\mathrm{e}^{\delta u/(1+u)}\left[\frac{u^2+(2+\delta)u+1-\delta\beta}{(1+u)^2}\right]$$

has only one positive root $u^+=\left(-(2+\delta)+\sqrt{\delta(\delta+4+4\beta)}\right)/2$. Since $g'(0)=-(1-\delta\beta)>0$ and $g'(\infty)<0$, we have g is increasing on $[0,u^+]$ and decreasing otherwise. Now, $g'(u_2^*)=1/(\psi_m\lambda^2)>0$, and hence $u_2^*\in[0,u^+]$. $\square$

The following lemma helps us in deriving a lower bound for λ_0.

Lemma 4. *Let ψ be the solution of*

$$\nabla^2\psi=-1,\quad \mathbf{x}\in\Omega,$$

$$\psi=0,\quad \mathbf{x}\in\partial\Omega,$$

and ψ_m be the maximum of ψ on Ω. For $\lambda<\lambda^*/\sqrt{\psi_m\lambda_1}$, let $k\in(0,u_2^*)$ be the solution (the smallest solution if there is more than one) of

$$\frac{k}{\lambda^2\psi_m}=g(k), \tag{10}$$

then $\psi\geqslant 0$, and $v=(k/\psi_m)\psi$ is an upper solution of (3) and (4).

Proof. To show that $\psi\geqslant 0$, let $\xi=-\psi$, then ξ satisfies $\nabla^2\xi=1\geqslant 0$, and $\xi=0$ on $\partial\Omega$. Applying Lemma 1, we get $\xi\leqslant 0$ and hence $\psi\geqslant 0$.

Since $(k/\psi_m)\psi\in[0,u_2^*]$ and $g(u)$ is increasing on this interval, we have

$$P\left(\frac{k}{\psi_m}\psi\right)=-\frac{k}{\psi_m}+\lambda^2 g\left(\frac{k}{\psi_m}\psi\right)\leqslant-\frac{k}{\psi_m}+\lambda^2 g(k)=0,$$

which proves v is an upper solution. $\square$

Note here that for $\lambda_* < \lambda < \lambda^*/\sqrt{\psi_m \lambda_1}$, Eq. (10) has two solutions in $[0, u_2^*]$, each of them leads to an upper solution of (3) and (4), and we choose the smallest one to have a better bound. For $\lambda < \lambda_*$, Eq. (10) has a unique solution, where the value of k is small. Therefore, $v = (k/\psi_m)\psi$ is an upper solution for the unique lower branch solution, that is λ_* is a lower bound for λ_0.

2.3. The more general case

When $\lambda > \lambda^*/\sqrt{\psi_m \lambda_1}$, Lemma 4 is not any more applicable to get an upper solution, since the value of k does not exist. The following lemma treats the problem.

Lemma 5. *Let ψ be a solution of*

$$\nabla^2 \psi + \lambda^2 (\beta - \psi) e^{\delta\beta/(1+\beta)} = 0, \tag{11}$$

$$\psi = 0 \quad \text{on } \partial\Omega, \tag{12}$$

then $0 \leqslant \psi \leqslant \beta$, and it is an upper solution of (3) *and* (4).

Proof. Let $w_1 = -\psi$, then w_1 satisfies

$$\nabla^2 w_1 - \lambda^2 e^{\delta\beta/(1+\beta)} w_1 = \lambda^2 \beta e^{\delta\beta/(1+\beta)} \geqslant 0,$$

$$w_1 = 0 \quad \text{on } \partial\Omega.$$

Applying Lemma 1, we have $w_1 \leqslant 0$ and $\psi \geqslant 0$.

Let $w_2 = \psi - \beta$, then w_2 satisfies

$$\nabla^2 w_2 - \lambda^2 e^{\delta\beta/(1+\beta)} w_2 = 0,$$

$$w_2 = -\beta \quad \text{on } \partial\Omega.$$

Again by Lemma 1, we have $w_2 \leqslant 0$, and $\psi \leqslant \beta$.

Using $0 \leqslant \psi \leqslant \beta$, we have

$$\lambda^2 (\beta - \psi) e^{\delta\beta/(1+\beta)} \geqslant \lambda^2 (\beta - \psi) e^{\delta\psi/(1+\psi)}$$

and hence

$$\nabla^2 \psi + \lambda^2 (\beta - \psi) e^{\delta\psi/(1+\psi)} \leqslant 0$$

and the result is obtained. □

3. Numerical results

For various values of β and δ, we compute λ_* and λ^*, where $\lambda_* \leqslant \lambda_0 \leqslant \lambda^0 \leqslant \lambda^*$. To facilitate the computation we assume that the Laplacian operator depends only on the radial coordinate for the unit sphere and

Table 1
The Laplacian operator, first eigenvalue, first eigenfunction, $\phi_{1\mathrm{m}}$, ψ and ψ_{m} for the three geometries

	Slab	Sphere	Cylinder
∇^2	$\frac{\partial}{\partial x^2}$	$\frac{\partial}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}$	$\frac{\partial}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}$
ϕ_1	$\sqrt{2}\sin(\pi x)$	$\frac{1}{\sqrt{2\pi}}\frac{\sin(\pi r)}{r}$	$J_0(\gamma_0 r)$
$\phi_{1\mathrm{m}}$	$\sqrt{2}$	$\sqrt{\pi/2}$	1
λ_1	π^2	π^2	γ_0^2
ψ	$\frac{1}{2}x(1-x)$	$\frac{1}{6}(1-r^2)$	$\frac{1}{4}(1-r^2)$
ψ_{m}	$\frac{1}{8}$	$\frac{1}{6}$	$\frac{1}{4}$

Table 2
The lower bound λ_* and the upper bound λ^* for $\beta=0.25$ and different values of δ

δ	λ_*			λ^*	
	Slab	Sphere	Cylinder	Slab+Sphere	Cylinder
20	0.930670	0.805983	0.658083	1.033712	0.791287
25	0.670551	0.580714	0.474151	0.870196	0.666117
30	0.458682	0.397231	0.324337	0.771595	0.590640
35	0.306023	0.265024	0.216391	0.701456	0.536950
40	0.200952	0.174029	0.142094	0.647911	0.495963
45	0.130487	0.113005	0.092269	0.605189	0.463260
50	0.084026	0.072769	0.059416	0.570029	0.436345
60	0.034214	0.029630	0.024193	0.515011	0.394230

Table 3
The lower bound λ_* and the upper bound λ^* for $\beta=0.5$ and different values of δ

δ	λ_*			λ^*	
	Slab	Sphere	Cylinder	Slab+Sphere	Cylinder
12	0.849581	0.735759	0.600745	0.943647	0.722343
15	0.612126	0.530117	0.432839	0.794377	0.608079
20	0.320372	0.277450	0.226537	0.659631	0.504934
25	0.159023	0.137718	0.112447	0.577540	0.442095
30	0.076705	0.066429	0.054239	0.520363	0.398327
35	0.036329	0.031461	0.025688	0.477498	0.365515
40	0.016988	0.014712	0.012012	0.443790	0.339712
50	0.003619	0.003134	0.002559	0.393489	0.301208

circular cylinder. The assumption of radially symmetric geometries has been used by many authors, see [6,7]. Table 1 shows ϕ_1, $\phi_{1\mathrm{m}}$, λ_1, ψ and ψ_{m} for the three geometries, where $J_0(\gamma_0 r)$ is the Bessel function of order zero, and $\gamma_0=2.404825\ldots$ is the first zero of $J_0(r)$. Tables 2 and 3 show the values of λ_* and λ^*

Table 4
The analytical bounds λ^* and λ_*, and the asymptotic bounds λ^0 and λ_0, for $\beta = 0.5$ and Ω is the circular cylinder

δ	λ^0	λ^*	λ_0	λ_*
100	0.200000	0.209494	2.467889×10^{-6}	8.843198×10^{-7}
150	0.163299	0.170153	8.898077×10^{-10}	2.617109×10^{-10}
200	0.141421	0.146975	2.851768×10^{-13}	7.282759×10^{-14}
250	0.126491	0.131256	8.568476×10^{-17}	1.960198×10^{-17}
300	0.115470	0.119697	2.471520×10^{-20}	5.166708×10^{-21}
400	0.100000	0.103529	1.903976×10^{-27}	3.451394×10^{-28}
500	0.089443	0.092529	1.375087×10^{-34}	2.231199×10^{-35}

Table 5
The analytical bounds λ^* and λ_*, and the asymptotic bounds λ^0 and λ_0, for $\beta = 0.5$ and Ω is the unit sphere

δ	λ^0	λ^*	λ_0	λ_*
100	0.253850	0.273677	3.631542×10^{-6}	1.250617×10^{-6}
150	0.207268	0.222282	1.309368×10^{-9}	3.701150×10^{-10}
200	0.179499	0.192004	4.196428×10^{-13}	1.029938×10^{-13}
250	0.160549	0.171469	1.260866×10^{-16}	2.772138×10^{-17}
300	0.146561	0.156369	3.636886×10^{-20}	7.306829×10^{-21}
400	0.126925	0.135247	2.801735×10^{-27}	4.881008×10^{-28}
500	0.113525	0.120877	2.023465×10^{-34}	3.155392×10^{-35}

for $\beta = 0.25$, 0.5 and different values of δ for the three geometries. From the tables one can see that, as δ increases, the difference $(\lambda^* - \lambda_*)$ increases as well. That is, the domain of λ for which the system may have multiple solutions increases with δ. Moreover, as δ becomes large, λ_* goes to zero, and the possibility of getting the quenching branch is reduced. Also, as β increases we need less values of δ to obtain multiple solutions. The values of λ_* and λ^* for large δ are presented in Tables 4 and 5, and compared with the values of λ^0 and λ_0 obtained in [6,7] using asymptotic expansion techniques.One can see that for all values of δ we have $\lambda_* < \lambda_0 < \lambda^0 < \lambda^*$, and the analytical bounds λ^* and λ_* are close to the asymptotic bounds λ^0 and λ_0, respectively.

Figs. 1–3 show the upper and lower solutions for the problem obtained by using Lemmas 2 and 4, for the three geometries. When $\beta = 0.25$ and $\lambda = 25$, the values of $\lambda^*/\sqrt{\psi_m \lambda_1}$ are 0.7833, 0.6783 and 0.5489, for the slab, sphere and cylinder, respectively, and $\lambda = 0.4 < \lambda^*/\sqrt{\psi_m \lambda_1}$. For the sphere and cylinder, the upper and lower solutions are monotonically decreasing functions, with maximum values occurring at $r = 0$, and we expect the exact solution to have the same behavior (Figs. 4 and 5). This agrees with the results obtained in [6,7]. For the slab, the maximum values of the upper and lower solutions occurring at $x = \frac{1}{2}$. In general the temperature is maximal at the center and decreases as we move towards the boundary in the three geometries.

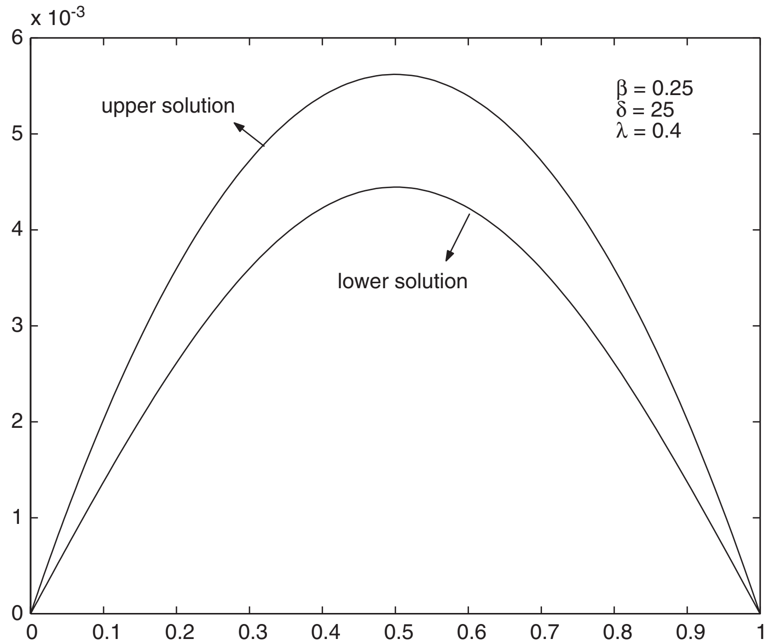

Fig. 3. Upper and lower solutions for $\beta = 0.25$, $\delta = 25$ and $\lambda = 0.4$, when Ω is the slab.

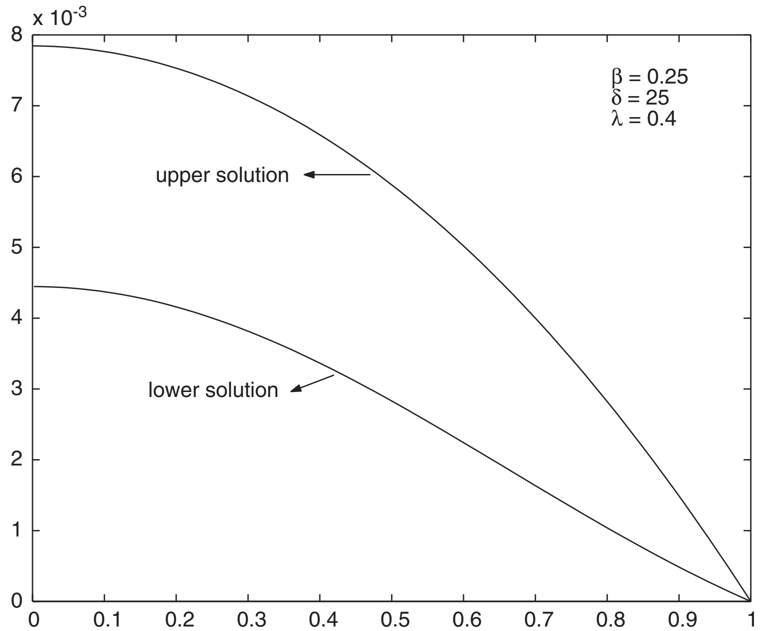

Fig. 4. Upper and lower solutions for $\beta = 0.25$, $\delta = 25$ and $\lambda = 0.4$, when Ω is the unit sphere.

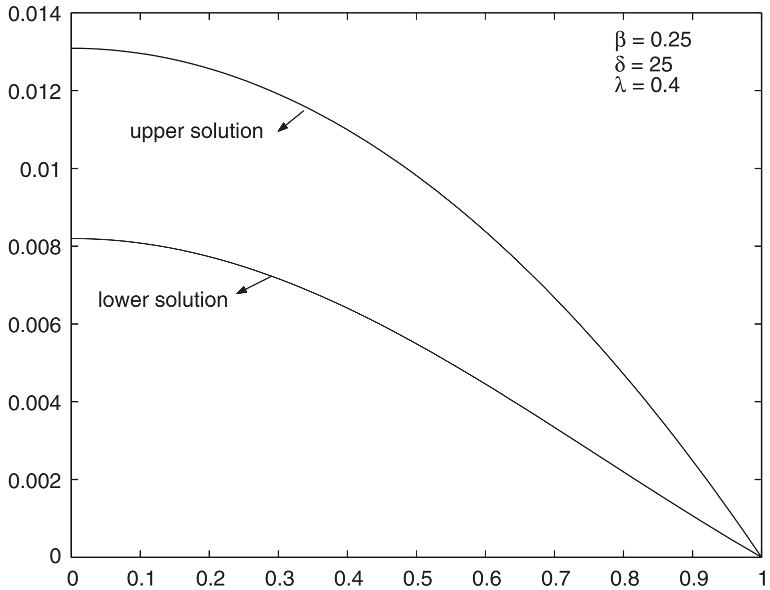

Fig. 5. Upper and lower solutions for $\beta = 0.25$, $\delta = 25$ and $\lambda = 0.4$, when Ω is the circular cylinder.

4. Concluding remarks

We have used comparison theory to study a nonlinear elliptic equation arising from the theory of catalyst pellets reaction, for the case where multiple solutions may occur. We constructed a lower solution for the problem using the first eigenfunction of the associated Laplacian operator with homogeneous Dirichlet boundary conditions. This solution is used to obtain an analytical upper bound λ^* for the ignition limit λ^0. We also, constructed an upper solution for $\lambda < \lambda^*/\sqrt{\psi_m \lambda_1}$, and used it to obtain a lower bound λ_* for the extinction limit λ_0. A general upper solution which does not depend on the value of λ is given by approximating the nonlinear term $f(u)$, and solving a linear elliptic equation. The bounds λ^* and λ_* are easily constructed as shown in (7) and (9), and depend on β, δ and the domain Ω. They give us sufficient conditions to obtain the quenching and explosion branches. They also estimate very well the values of λ_0 and λ^0 as shown in Tables 4 and 5. Many properties of the system are illustrated through the text, and in all cases there is good agreement with previous results.

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