ARTICLE IN PRESS

Ain Shams Engineering Journal (2014) **xxx**, xxx–xxx

Ain Shams University

Ain Shams Engineering Journal

www.elsevier.com/locate/asej
www.sciencedirect.com

ENGINEERING PHYSICS AND MATHEMATICS

On the multiplicity of solutions of the nonlinear reactive transport model

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Received 17 August 2013; revised 24 November 2013; accepted 5 January 2014

KEYWORDS

Reactive transport model;
Michaelis–Menten reaction;
Exact analytical solution;
Multiple solutions

Abstract The generalization of the nonlinear reaction–diffusion model in porous catalysts the so called one dimensional steady state reactive transport model is revisited. This model, which originates also in fluid and solute transport in soft tissues and microvessels, has been recently given analytical solution in terms of Taylor's series for different families of reaction terms. This article considers the mentioned model without advective transport in the case of including Michaelis–Menten reaction term and shows that it is exactly solvable and furthermore, gives analytical exact solution in the implicit form for further physical interpretation. It is also revealed that the problem may admit unique or dual or even more triple solutions in some domains for the parameters of the model.

1. Introduction and the problem formulation

The governing boundary value problem of the one dimensional steady state reactive transport model can be written in dimensional variables as

$$D\mathbf{U}'' - V\mathbf{U}' - r(\mathbf{U}) = 0, \quad 0 \leqslant X \leqslant L, \qquad \mathbf{U}'(0) = 0, \quad \mathbf{U}(L) = \mathbf{U}_s, \tag{1}$$

where D is the diffusivity, V is the advective velocity and $r(\mathbf{U})$ denotes reaction process [1–5]. Now, by introducing nondimensional quantities $U(x) = \frac{\mathbf{U}(X)}{\mathbf{U}_s}$, $x = \frac{X}{L}$ and $R(U)$ as nondimensional reaction term and then substituting into Eq. (1), we get

$$U'' - PU' - R(U) = 0, \quad 0 \leqslant x \leqslant 1, \quad U'(0) = 0, \quad U(1) = 1, \tag{2}$$

where $P = \frac{VL}{D}$ is so-called Péclet number. Without advective transport, we have $P = 0$ and in this case the model has been used to study porous catalyst pellets as the model of diffusion and reaction [1,6]. Furthermore, if we consider $R(U)$ as Michaelis–Menten reaction term then the model is converted to

$$U''(x) - \frac{\alpha U(x)}{\beta + U(x)} = 0, \quad 0 \leqslant x \leqslant 1, \tag{3}$$

with the boundary condition

$$U'(0) = 0, \quad U(1) = 1, \tag{4}$$

where α, characteristic reaction rate, and β is half saturation concentration.

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Peer review under responsibility of Ain Shams University.

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http://dx.doi.org/10.1016/j.asej.2014.01.001

We mention here that $\alpha \in \mathbb{R}$, when $\alpha < 0$, it means that we look at the reactives instead of looking at the products of the reaction. Furthermore, half saturation concentration i.e. β is always positive and there is no physical interest for the case $\beta < 0$, but we consider this case too to better disclose the existence of multiple solutions from mathematical point of view.

The problem (2) without advective transport ($P = 0$) and with reaction term $R(U) = \phi^2 U^n$ (ϕ is Thiele modulus) has been studied by Adomian decomposition method [7] and Homotopy analysis method [8,9]. In this paper, we analyze the problem (3) and (4), which is arisen also as multiscale modeling of fluid and solute transport in soft tissues and microvessels [10], for different values of α and β, show that the differential equation is exactly solvable, and gives the exact analytical solution in the implicit form. Moreover, we prove that the boundary value problem (3) and (4) either admits unique solution, dual solutions, triple solutions or does not admit any solution in some domains of x for different values of α and β.

2. Existence results for corresponding initial value problem

Consider corresponding initial value problem of (3) and (4), which is read

$$U''(x) - \frac{\alpha U(x)}{\beta + U(x)} = 0, \quad 0 \leqslant x \leqslant 1, \tag{5}$$

$$U(0) = U_0, \quad U'(0) = 0. \tag{6}$$

It can be reformulated as a system of two first-order equations by introducing

$$y_1(x) = U(x), \quad y_2(x) = U'(x). \tag{7}$$

as

$$\begin{cases} y_1'(x) = y_2(x) & y_1(0) = U_0 \\ y_2'(x) = \frac{\alpha y_1(x)}{\beta + y_1(x)} & y_2(0) = 0 \end{cases} \tag{8}$$

Definition 1. Consider a two dimensional vector-valued function $\mathbf{F}$ defined for $(x, \mathbf{y})$ in some set S (x real, $\mathbf{y}$ in $\mathbb{R}^2$). We say that $\mathbf{F}$ satisfies a Lipschitz condition on $S \subseteq \mathbb{R}^3$ if there exists a constant $K > 0$ such that

$$\|\mathbf{F}(x,\mathbf{y}) - \mathbf{F}(x,\mathbf{z})\| \leqslant K\|\mathbf{y} - \mathbf{z}\| \tag{9}$$

for all $(x, \mathbf{y}), (x, \mathbf{z})$ in S, where $\|\cdot\|$ denotes L_1-norm defined by $\|\mathbf{y}\| = |y_1| + |y_2|$.

Lemma 1. *Suppose* $\mathbf{F}$ *is a two dimensional vector-valued function as*

$$\mathbf{F}(x,\mathbf{y}) = \left(y_2, \frac{\alpha y_1}{\beta + y_1}\right)^T, \tag{10}$$

defined for $(x, \mathbf{y})$ *on a set* S *of the form*

$$0 \leqslant x \leq 1, \quad \|\mathbf{y}\| < \infty. \tag{11}$$

If $\beta y_1(x) > 0$ *on* $0 \leqslant x \leq 1$, *then* $\mathbf{F}$ *satisfies a Lipschitz condition on* S.

Proof. Let $(x, \mathbf{y}), (x, \mathbf{z})$ be fixed points in S, and define the vector-valued function $\mathcal{F}$ for real $s, 0 \leqslant s \leq 1$, by

$$\mathcal{F}(s) = \mathbf{F}(x, \mathbf{z} + s(\mathbf{y} - \mathbf{z})) = \begin{pmatrix} z_2 + s(y_2 - z_2) \\ \frac{\alpha(z_1 + s(y_1 - z_1))}{\beta + (z_1 + s(y_1 - z_1))} \end{pmatrix} \tag{12}$$

This is a well-defined function since the points $(x, \mathbf{z} + s(\mathbf{y} - \mathbf{z}))$ are in S for $0 \leqslant s \leq 1$. Clearly $0 \leqslant x \leq 1$, and if

$\|\mathbf{y}\| < \infty, \|\mathbf{z}\| < \infty,$

then

$$\|\mathbf{z} + s(\mathbf{y} - \mathbf{z})\| \leqslant (1 - s)\|\mathbf{z}\| + s\|\mathbf{y}\| \leqslant \|\mathbf{z}\| + \|\mathbf{y}\| < \infty, \tag{13}$$

We now have

$$\mathcal{F}'(s) = (y_2 - z_2, q(s))^T, \tag{14}$$

where

$$q(s) = \frac{\alpha(y_1 - z_1)(\beta + (z_1 + s(y_1 - z_1))) - \alpha(y_1 - z_1)(z_1 + s(y_1 - z_1))}{(\beta + z_1 + s(y_1 - z_1))^2} \tag{15}$$

It is not difficult to see $(\beta + z_1 + s(y_1 - z_1))^2 > \beta^2$. Also, suppose $|z_1 + s(y_1 - z_1)| < M_1$, then

$$\begin{aligned} |q(s)| &\leqslant \frac{|\alpha||y_1 - z_1|(|\beta| + M_1) + |\alpha||y_1 - z_1|M_1}{\beta^2} \\ &= M|y_1 - z_1| \end{aligned} \tag{16}$$

where $M = \frac{|\alpha|(|\beta| + M_1) + |\alpha|M_1}{\beta^2}$, therefore

$$\begin{aligned} \|\mathcal{F}'(s)\| &= |y_2 - z_2| + |q(s)| \leqslant |y_2 - z_2| + M|y_1 - z_1| \\ &\leqslant M|y_2 - z_2| + M|y_1 - z_1| = M\|\mathbf{y} - \mathbf{z}\|. \end{aligned} \tag{17}$$

Thus, since

$$\mathbf{F}(x,\mathbf{y}) - \mathbf{F}(x,\mathbf{z}) = \mathcal{F}(1) - \mathcal{F}(0) = \int_0^1 \mathcal{F}'(s)\,\mathrm{d}s, \tag{18}$$

we have

$$\|\mathbf{F}(x,\mathbf{y}) - \mathbf{F}(x,\mathbf{z})\| \leqslant M\|\mathbf{y} - \mathbf{z}\|, \tag{19}$$

which was to be proved. □

Suppose $\mathbf{y}_0 = (U_0, 0)^T$ and consider a successive approximations $\Phi_0(x), \Phi_1(x), \Phi_2(x), \ldots$, where

$$\Phi_0(x) = \mathbf{y}_0,$$

$$\Phi_{k+1}(x) = \mathbf{y}_0 + \int_{U_0}^{x} \mathbf{F}(t, \Phi_k(t))\mathrm{d}t, \quad k = 0, 1, 2, \ldots. \tag{20}$$

Now since $\mathbf{F}(x, \mathbf{y})$ defined by (10) is continuous on

$$S: \quad 0 \leqslant x \leq 1, \ \|\mathbf{y}\| < \infty, \tag{21}$$

for $\beta U(x) > 0$ then it is bounded there, that is, there is a positive constant M such that

$\|\mathbf{F}(x,\mathbf{y})\| \leqslant M.$

On the other hands, Lemma 1 reveals that $\mathbf{F}$ satisfies a Lipschitz condition on S. All these confirm that the hypotheses of the following theorem hold.

Theorem 1. *Let* $\mathbf{F}(x,\mathbf{y})$ *be a real-valued continuous function on* S *defined by* (21) *such that*

$\|\mathbf{F}(x,\mathbf{y})\| \leqslant M.$

Suppose there exists a constant $K > 0$ *such that*

$$\|\mathbf{F}(x,\mathbf{y}) - \mathbf{F}(x,\mathbf{z})\| \leqslant K\|\mathbf{y} - \mathbf{z}\|, \tag{22}$$

Please cite this article in press as: Shivanian E, On the multiplicity of solutions of the nonlinear reactive transport model, Ain Shams Eng J (2014), http://dx.doi.org/10.1016/j.asej.2014.01.001