Int. J. Nonlinear Anal. Appl. 9 (2018) No. 2, 47-57
ISSN: 2008-6822 (electronic)
http://dx.doi.org/10.22075/ijnaa.2017.1538.1402

Multiple solutions of a nonlinear reactive transport model using least square pseudo-spectral collocation method

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(Communicated by M. Eshaghi)

Abstract

The recognition and the calculation of all branches of solutions of the nonlinear boundary value problems is difficult obviously. The complexity of this issue goes back to the being nonlinearity of the problem. Regarding this matter, this paper considers steady state reactive transport model which does not have exact closed–form solution and discovers existence of dual or triple solutions in some cases using a new hybrid method based on pseudo–spectral collocation in the sense of least square method. Furthermore, the method usages Picard iteration and Newton method to treat nonlinear term in order to obtain unique and multiple solutions of the problem, respectively.

Keywords: Pseudo–spectral collocation method, Least square method, Newton iteration method, Picard iteration, Chebyshev–Gauss–Lobatto points.
2010 MSC: Primary 65L10; Secondary 34L05.

1. Preliminaries and problem formulation

Chebyshev polynomials [20] are extremely functional as orthogonal polynomials on the interval $[-1, 1]$. These polynomials which appear frequently in several fields of mathematics, physics and engineering have very good properties in the approximation of functions. Spectral collocation methods [10, 23] based on Chebyshev polynomials (also is called pseudo-spectral method) in the context of numerical schemes for differential equations, belong to the family of weighted residual methods

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Received: August 2016 *Revised:* October 2017

(WRMs), which are traditionally regarded as the foundation of many numerical methods such as finite element, spectral, finite volume, boundary element [14]. Spectral collocation methods have been widely used to solve numerically differential equations by many authors, (see for instance [8, 12, 16, 18]). This method is accomplished successfully by generating approximations for the higher–order derivatives through successive differentiation of the approximate solution.

The least square method is a fundamental notion in the theory of approximation [9]. In general, the study of approximation theory involves two general types of problems. One problem arises when a function is given explicitly, but we wish to find a simpler type of function, such as polynomial, that can be used to determine approximated values of the given function. The other problem in approximation theory is concerned with fitting functions to given data and finding the best function in a certain class to represent the data.

It is common that numerical methods usually converge to only one solution that is exactly meaning of *convergence*. Once the given nonlinear boundary value problem admits multiple solutions, it is consequential to gain all branches of solutions in engineering and physical sciences [2, 3, 5]. Based on this important matter the present paper is going to present a procedure based on pseudo–spectral in the sense of least square using Picard and Newton iteration method to obtain unique, dual and triple solutions of a kind of generalization of the nonlinear reaction–diffusion model in porous catalysts so called one dimensional steady state reactive transport model in some cases.

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

$$D\mathbf{U}'' - V\mathbf{U}' - r(\mathbf{U}) = 0, \quad 0 \le x \le L, \quad \mathbf{U}'(0) = 0, \quad \mathbf{U}(L) = \mathbf{U}_s, \tag{1.1}$$

where D is the diffusivity, V is the advective velocity and $r(\mathbf{U})$ denotes reaction process [7, 11, 13, 15, 24]. 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 these nondimensional quantities into equation (1.1), we get

$$U'' - PU' - R(U) = 0, \quad 0 \le x \le 1, \quad U'(0) = 0, \quad U(1) = 1, \tag{1.2}$$

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 [13, 22]. Furthermore, if we consider $R(U)$ as Michaelis–Menten reaction term then the model is converted to

$$U''(x) - \frac{\alpha U(x)}{\beta + U(x)} = 0, \quad 0 \le x \le 1, \tag{1.3}$$

with the boundary condition

$$U'(0) = 0, \quad U(1) = 1, \tag{1.4}$$

where α, characteristic reaction rate, and β is half saturation concentration. The problem (1.2) 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 [21] and Homotopy analysis method [1, 2]. Subsequently, S. Abbasbandy and E. Shivanian [4] have considered almost the same problem arising in heat transfer and have successfully obtained the exact analytical solution in the implicit form and proved the existence of dual solutions on some domain of x.

2. Solution Procedure

By the change of variable

$$x = \frac{1}{2}(\eta + 1),$$

we get $U_{xx} = 4u_{\eta\eta}$, then the problem (1.3)–(1.4) can be written as the differential equation with boundary conditions on interval $[-1, 1]$, i.e.

$$u_{\eta\eta} - \frac{\alpha}{4\beta}u = -\frac{1}{\beta}uu_{\eta\eta}, \ \beta \neq 0 \tag{2.1}$$

$$u_\eta(-1) = 0, \quad u(1) = 1. \tag{2.2}$$

So, as x goes from zero to one in the original problem continuously, η goes from -1 to 1 as well in the above differential equation, continuously. Now, having boundary conditions at interval $[-1, 1]$, we apply pseudo–spectral collocation method to handle the above problem as follows:

2.1. Pseudo–spectral collocation method

The method involves using the Chebyshev–Gauss–Lobatto point to discrete interval $[-1, 1]$, namely

$$\eta_j = \cos\left(\frac{\pi j}{N}\right), \quad j = 0, 1, 2, \ldots, N.$$

The unknown function $u(\eta)$ is approximated as a truncated series of Chebyshev polynomials

$$u(\eta) = \sum_{k=0}^{N} \tilde{u}_k T_k(\eta),$$

where $T_k(\eta)$ is the kth Chebyshev polynomial and $\tilde{u}_k$ are the Chebyshev coefficients which are determined by the formulations

$$\tilde{u}_k = \frac{2}{N\tilde{c}_k}\sum_{i=0}^{N}\frac{1}{\tilde{c}_i}u(\eta_i)\cos\left(\frac{\pi ik}{N}\right), \quad k = 0, 1, 2, \ldots, N,$$

where

$$\tilde{c}_k = \begin{cases} 2, & k = 0, \\ 1, & 1 \leq k \leq N, \\ 2, & k = N. \end{cases}$$

As it is well–known in Chebyshev pseudo–spectral method, first and second derivatives of the function $u(\eta)$ at the collocation points are presented as

$$\frac{\mathrm{d}u}{\mathrm{d}\eta}(\eta_j) = \sum_{i=0}^{N}\mathcal{D}_{ij}u(\eta_j), \tag{2.3}$$

$$\frac{\mathrm{d}^2u}{\mathrm{d}\eta^2}(\eta_j) = \sum_{i=0}^{N}\mathcal{D}_{ij}^2u(\eta_j). \tag{2.4}$$

In the above equations $\mathcal{D}$ is the Chebyshev differentiation matrix and $N + 1$ is the number of collocation points (nodes). The entries of the differentiation matrix $\mathcal{D}$ are

$$\mathcal{D}_{ij} = -\frac{1}{2}\frac{\tilde{c}_i}{\tilde{c}_j}\frac{(-1)^{i+j}}{\sin\left(\frac{\pi(j+i)}{2N}\right)\sin\left(\frac{\pi(j-i)}{2N}\right)}, \quad i \neq j$$

$$\mathcal{D}_{ii} = -\frac{1}{2}\frac{\eta_i}{\sin^2\left(\frac{\pi i}{2N}\right)}, \quad i \neq 0, N,$$

$$\mathcal{D}_{00} = -\mathcal{D}_{NN} = \frac{2N^2 + 1}{6}.$$

By employing derivatives formulation (2.3)–(2.4), equations (2.1)–(2.2) are transformed to the following expressions

$$\begin{cases} u(\eta_0)=1, \\ \sum_{j=0}^{N}\mathcal{D}^2_{ij}u(\eta_j)-\frac{\alpha}{4\beta}u(\eta_i)=-\frac{1}{\beta}u(\eta_i)\sum_{j=0}^{N}\mathcal{D}^2_{ij}u(\eta_j), \quad i=1,2,\ldots,N-1, \\ \sum_{j=0}^{N}\mathcal{D}_{Nj}u(\eta_j)=0. \end{cases} \tag{2.5}$$

Equation (2.5) is actually a system of nonlinear equations with number of $N+1$ equations and $N+1$ unknown parameters $u(\eta_0), u(\eta_1), u(\eta_2), \ldots, u(\eta_N)$.

2.2. Multiple solutions of the model

The recognizability and the computation of all branches of solutions of nonlinear boundary value problems is a major topic in general. This part is devoted to show that the problem (2.1)–(2.2) and so, the original equations (1.3)–(1.4) admit unique or dual or even more, triple solutions for some values of the characteristic reaction rate, and half saturation concentration.

2.2.1. Unique solution–Picard iteration method

Consider the system (2.5) in the following matrix form

$$\mathbf{L}\mathbf{U}(\eta)=-\frac{1}{\beta}\mathbf{U}'(\eta)\circ\mathcal{D}'^2\mathbf{U}(\eta),$$

where "$\circ$" denotes the Hadamard product, $\mathbf{U}(\eta)=(u(\eta_0),u(\eta_1),u(\eta_2),\ldots,u(\eta_N))^t$ and

$$\mathbf{L}=\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ \mathcal{D}^2_{10} & \mathcal{D}^2_{11}-\frac{\alpha}{4\beta} & \mathcal{D}^2_{12} & \cdots & \mathcal{D}^2_{1(N-1)} & \mathcal{D}^2_{1N} \\ \mathcal{D}^2_{20} & \mathcal{D}^2_{21} & \mathcal{D}^2_{22}-\frac{\alpha}{4\beta} & \cdots & \mathcal{D}^2_{2(N-1)} & \mathcal{D}^2_{2N} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathcal{D}^2_{(N-1)0} & \mathcal{D}^2_{(N-1),1} & \mathcal{D}^2_{(N-1)2} & \cdots & \mathcal{D}^2_{(N-1)(N-1)}-\frac{\alpha}{4\beta} & \mathcal{D}^2_{(N-1)N} \\ \mathcal{D}_{N0} & \mathcal{D}_{N1} & \mathcal{D}_{N2} & \cdots & \mathcal{D}_{N(N-1)} & \mathcal{D}_{NN} \end{pmatrix}.$$

Also, $\mathcal{D}'^2=\mathcal{D}^2$ except that $\mathcal{D}'^2_{00}=-\beta$ and $\mathcal{D}'^2_{0j}=0$ for all $1\le j\le N$ and

$$\mathbf{U}'(\eta)_j=\begin{cases} 1 & j=0, \\ \mathbf{U}(\eta)_j & 1\le j\le N-1. \\ 0 & j=N. \end{cases}$$

Now, we provide a detailed description of the proposed nonlinear iterative method. The solution process known as Picard iterative method is as follows:

step 1. Choose an initial guess, $\mathbf{U_0}(\eta)$ to the nonlinear system (2.5).

step 2. Linearize the nonlinear system (2.5) in terms of $\mathbf{U}(\eta)$.

step 3. Solve the linear system by appropriate method.

The above three steps suggests the following process

$$\mathbf{U_{n+1}}(\eta)=\frac{1}{\beta}\mathbf{L}^{-1}\left[\mathbf{U'_n}(\eta)\circ\mathcal{D}'^2\mathbf{U_n}(\eta)\right]. \tag{2.6}$$

2.2.2. Multiple solutions–Newton iteration method

It is worth to mention that it is so difficult generally to solve system of nonlinear equations (2.5) even by Newton's method [17, 19]. The main difficulty with a such system is that how we can choose initial guess to handle Newton's method, in other words how many solutions the system of nonlinear equations admit. We think the appropriate way to discover proper initial guess (or initial guesses) is to solve system analytically for very small N (by using symbolic softwares' programs such as Mathematica or Maple) and then we can guess proper initial guesses and particularly multiplicity of solutions of such system, of course, if they converge to different solutions [6]. For example, let us take $N = 3$ in system (2.5), then having $u(\eta_0) = 1$ we stand to solve

$$\begin{cases} u(\eta_1)(-3\alpha - 8(8u(\eta_1) - 4u(\eta_2) + u(\eta_3) - 5)) + 8\beta(8u(\eta_1) - 4u(\eta_2) + u(\eta_3) - 5) = 0, \\ u(\eta_2)(8(4u(\eta_1) - 8u(\eta_2) + 5u(\eta_3) - 1) - 3\alpha) + 8\beta(4u(\eta_1) - 8u(\eta_2) + 5u(\eta_3) - 1) = 0, \\ -8u(\eta_1) + 24u(\eta_2) - 19u(\eta_3) + 3 = 0. \end{cases}$$

If we choose $\alpha = 0.5$ and $\beta = -0.1$, then after using $\eta = 2x-1$ in Chebyshev polynomial interpolation, we get two initial guesses as follow (plotted in Figure 1)

$$U_0(x) = 2x\left((2x-2)\left(0.2056 - 0.0659\left(2x - \frac{1}{2}\right)\right) + 0.4772\right) + 0.0454,$$

$$U_0(x) = 2x\left((2x-2)\left(0.0718 - 0.0006\left(2x - \frac{1}{2}\right)\right) + 0.1442\right) + 0.7115,$$

if $\alpha = 0.5$ and $\beta = -0.2$, then we have two other initial guesses (plotted in Figure 2)

$$U_0(x) = 2x\left((2x-2)\left(0.1744 - 0.0436\left(2x - \frac{1}{2}\right)\right) + 0.3925\right) + 0.2149,$$

$$U_0(x) = 2x\left((2x-2)\left(0.0865 - 0.0024\left(2x - \frac{1}{2}\right)\right) + 0.1755\right) + 0.6488,$$

and if we get $\alpha = 6$ and $\beta = 1$, then we are led to three initial guesses as follow (plotted in Figure 3)

$$U_0(x) = 2x\left((2x-2)\left(0.3698\left(2x - \frac{1}{2}\right) + 1.3986\right) + 2.4274\right) - 3.8549,$$

$$U_0(x) = 2x\left((2x-2)\left(0.7571 - 0.4758\left(2x - \frac{1}{2}\right)\right) + 1.99\right) - 2.9801,$$

$$U_0(x) = 2x\left((2x-2)\left(0.0409\left(2x - \frac{1}{2}\right) + 0.2071\right) + 0.3733\right) + 0.2533.$$

Now, what it remains is to solve the following linear system iteratively:

$$\mathbf{J_F}\left(\mathbf{U_n}(\eta)\right)(\mathbf{U_{n+1}}(\eta) - \mathbf{U_n}(\eta)) = -\mathbf{F}\left(\mathbf{U_n}(\eta)\right), \tag{2.7}$$

where

$$\mathbf{F}\left(\mathbf{U_n}(\eta)\right) = \mathbf{L}\mathbf{U}(\eta) + \frac{1}{\beta}\mathbf{U}'(\eta) \circ \mathcal{D}'^2\mathbf{U}(\eta)$$

and $\mathbf{J_F}\left(\mathbf{U_n}(\eta)\right)$ is the Jacobian matrix of $\mathbf{F}\left(\mathbf{U_n}(\eta)\right)$ which is in fact $\mathbf{J_F}\left(\mathbf{U_n}(\eta)\right) = \mathbf{L} + \frac{1}{\beta}\mathbf{N}(\eta)$ with

$$\mathbf{N}(\eta) = \begin{pmatrix} 0 & 0 & \cdots & 0 & 0 \\ u(\eta_1)\mathcal{D}^2_{10} & u(\eta_1)\mathcal{D}^2_{11} + \sum_{j=0}^{N}\mathcal{D}^2_{1j}u(\eta_j) & \cdots & u(\eta_1)\mathcal{D}^2_{1(N-1)} & u(\eta_1)\mathcal{D}^2_{1N} \\ u(\eta_2)\mathcal{D}^2_{20} & u(\eta_2)\mathcal{D}^2_{21} & \cdots & u(\eta_2)\mathcal{D}^2_{2(N-1)} & u(\eta_2)\mathcal{D}^2_{2N} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ u(\eta_{N-1})\mathcal{D}^2_{(N-1)0} & u(\eta_{N-1})\mathcal{D}^2_{(N-1)1} & \cdots & u(\eta_{N-1})\mathcal{D}^2_{(N-1)(N-1)} + \sum_{j=0}^{N}\mathcal{D}^2_{(N-1)j}u(\eta_j) & u(\eta_{N-1})\mathcal{D}^2_{(N-1)N} \\ 0 & 0 & \cdots & 0 & 0 \end{pmatrix}.$$

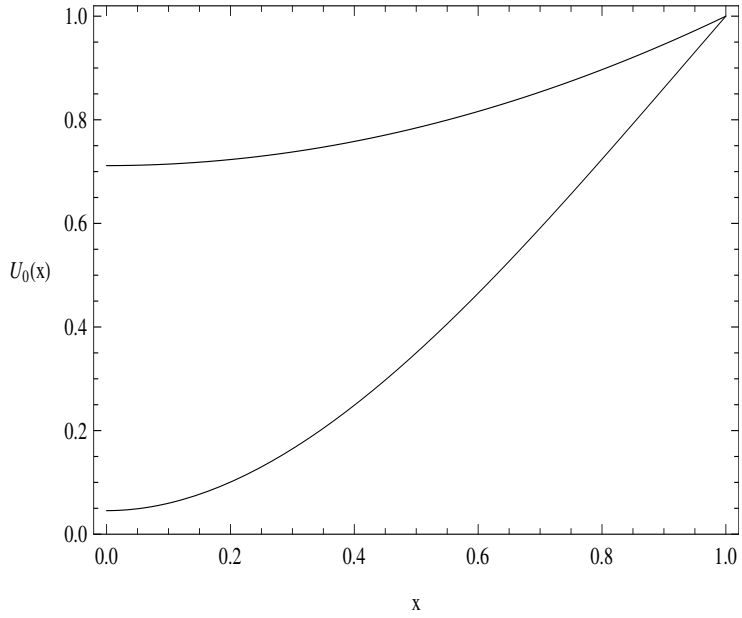

Figure 1: Initial guesses for system (2.5) when $\alpha = 0.5$ and $\beta = -0.1$.

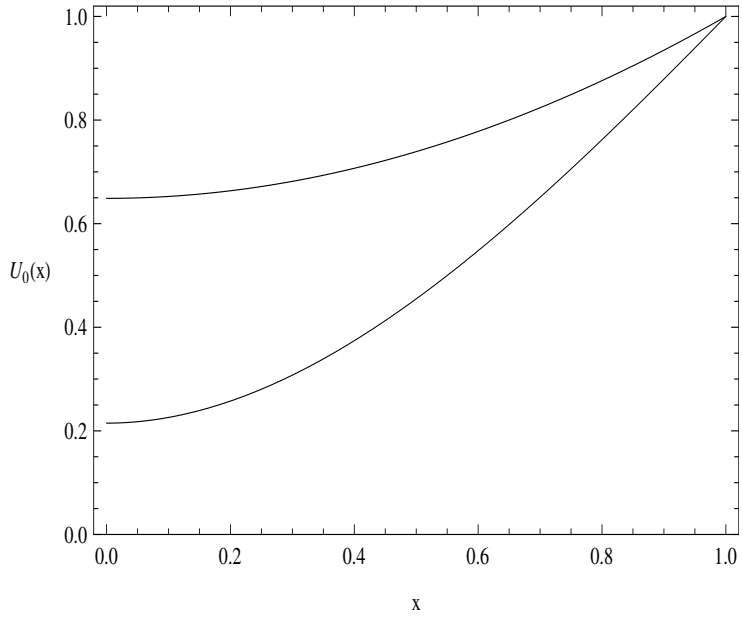

Figure 2: Initial guesses for system (2.5) when $\alpha = 0.5$ and $\beta = -0.2$.

2.3. Least square approximation

After obtaining the solutions of the systems (2.6) or (2.7) to the desired order of accuracy, to get more smooth function as approximate solution we use discrete $\mathcal{L}_2$ norm

$$\|u\|_{2,w} = \left(\sum_{j=0}^{N} w_j |u(\eta_j)|^2 \right)^{\frac{1}{2}}$$

which involves set of $N+1$ distinct Chebyshev–Gauss–Lobatto points $\eta_0, \eta_1, \ldots, \eta_N$ along with positive weight factors $w_0, w_1, \ldots, w_N$ (possibly all equal to 1). Then the smooth approximate function

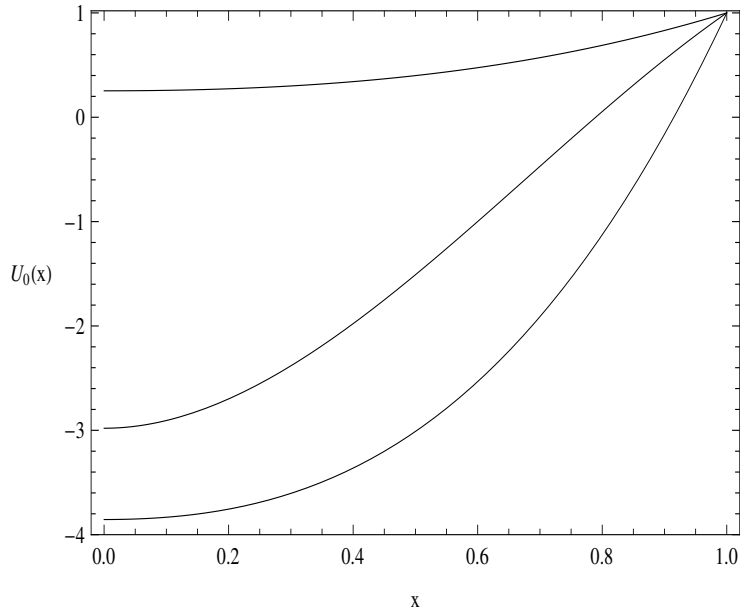

Figure 3: Initial guesses for system (2.5) when $\alpha = 6$ and $\beta = 1$.

will be the solution of the least square problem as $\varphi(\eta)$ from an $(N+1)$–dimensional linear space

$$\Phi_{N+1} = \left\{ \varphi : \varphi(\eta) = \sum_{j=0}^{N} c_j \pi_j(\eta), c_j \in \mathbb{R} \right\}$$

where $\pi_j(\eta) = \eta^j$, $j = 0, 1, 2, \ldots, N$.

3. Numerical experiments

In this section, some results of the implementation of the aforementioned procedure are shown for some values of the characteristic reaction rate, and half saturation concentration. In all computations the stopping criteria, once the systems (2.6) and (2.7) are handled iteratively, has been considered as $\left\| \mathbf{U_{n+1}}(\eta) - \mathbf{U_n}(\eta) \right\|_\infty \leq 10^{-10}$, where $\left\| u(\eta) \right\|_\infty = \max_{0 \leq j \leq N} \left| u(\eta_j) \right|$. Also, we have gotten $w_j = 1$ for all $0 \leq j \leq N$ in the least square problem. Finally, after getting best approximate solution in the sense of the least square, we use the change of variable $\eta = 2x - 1$ to shift the approximate solution from the interval $[-1, 1]$ to the $[0, 1]$. The Figures 4 and 5 show the dimensionless reactant concentration profiles for different values of parameters α and β. As it is clear from these Figures, the reactant concentration at zero increases with the increasing of β while it decreases with the increasing of α. Now, we turn to see some multiple profiles which have been gathered in Figures 6 and 7 for those specified values of α and β in subsection 2.2.2. Figure 6 indicates that the original problem (1.3)–(1.4) admits dual solutions in the case $\alpha = 0.5$ and $\beta = -0.2, -0.1$. Also, Figure 7 indicates that the original problem (1.3)–(1.4) admits triple solutions in the case that characteristic reaction rate is six and half saturation concentration is one. Furthermore, the numerical results corresponding to the Figures 6 and 7 have been given in the Tables 1 and 2, respectively.

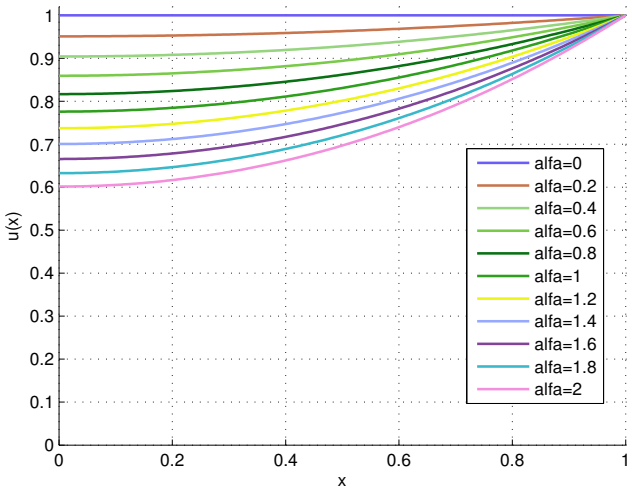

Figure 4: Dimensionless reactant concentration profiles with $\beta = 1$.

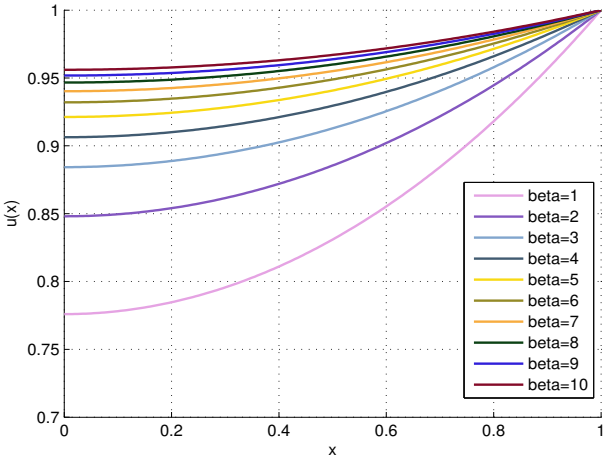

Figure 5: Dimensionless reactant concentration profiles with $\alpha = 1$.

Table 1: The numerical results obtained by stopping criteria $\left|U_{n+1}(x_j) - U_n(x_j)\right| \leq 10^{-10}$ in which $x_j = \frac{1}{2}(\eta_j + 1)$

Shifted GL Points	First branch, $\beta = -0.2$	Second branch, $\beta = -0.2$	First branch, $\alpha = -0.1$	Second branch $\alpha = -0.1$
x_0	1.000000000000000	1.000000000000000	1.000000000000000	1.000000000000000
x_1	0.992762689539665	0.995815852869048	0.992470497398321	0.996491945595226
x_2	0.971369461829524	0.983506753436129	0.970191374981000	0.986178749388718
x_3	0.936757383483006	0.963784428115971	0.934074829035453	0.969676390161860
x_4	0.890426279604282	0.937775517864263	0.885578078630867	0.947956563380994
x_5	0.834351011799216	0.906937100699585	0.826620037615376	0.922269299953068
x_6	0.770868575208694	0.872947758188667	0.759466680991504	0.894044230420183
x_7	0.702548780922441	0.837582619525251	0.686607916264933	0.864779099336968
x_8	0.632058283028987	0.802582121512899	0.610619876404679	0.835925290916968
x_9	0.562027706979890	0.769524965969476	0.534040999555540	0.808780479665386
x_{10}	0.494930590273862	0.739715983497967	0.459249308179152	0.784398026726932
x_{11}	0.432980520213731	0.714099279858313	0.388374510663231	0.763521389571351
x_{12}	0.378048960680408	0.693205883786545	0.323218439057115	0.746549612500604
x_{13}	0.331599354417182	0.677142655249737	0.265225526311520	0.733536998191860
x_{14}	0.294620664435374	0.665625063664073	0.215453805179060	0.724226543187005
x_{15}	0.267521624623586	0.658050837817300	0.174605438812733	0.718113053502620
x_{16}	0.249931005059686	0.653605569055702	0.143029835982671	0.714528576356617
x_{17}	0.240435572139193	0.651386769913537	0.120793087881347	0.712740408965591
x_{18}	0.236600385477486	0.650530874755133	0.107642778057771	0.712050804005151
x_{19}	0.235676364871992	0.650328350418943	0.102651459152635	0.711887642043874
x_{20}	0.235613688137102	0.650314669351559	0.102176507060695	0.711876620209264

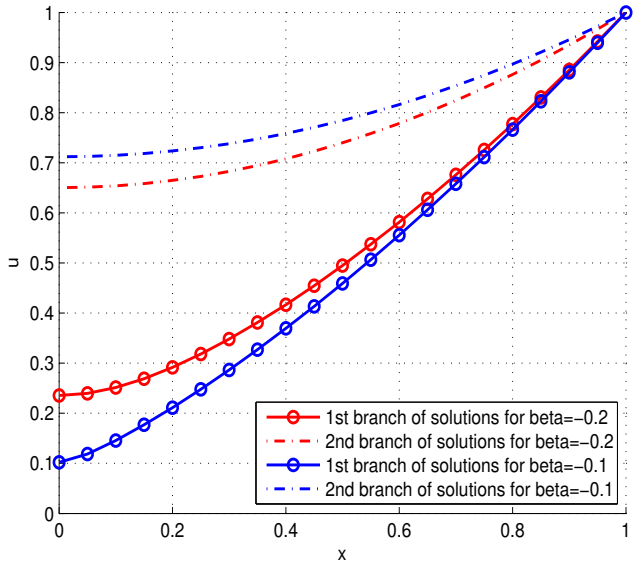

Figure 6: Dimensionless dual reactant concentration profiles when $\alpha = 0.5$.

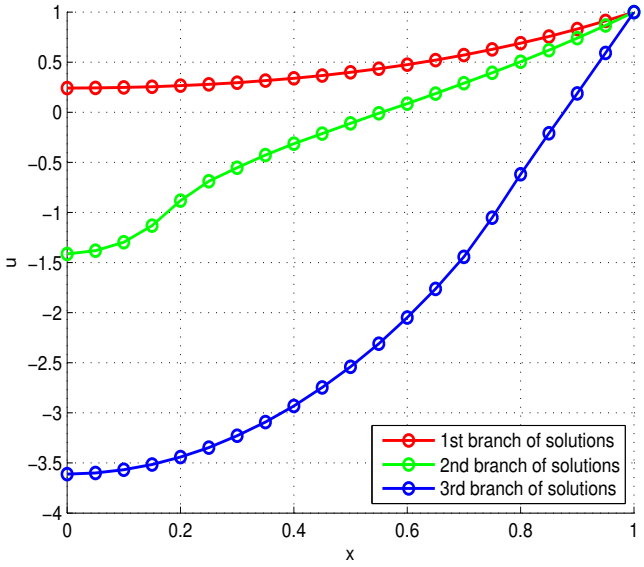

Figure 7: Dimensionless triple reactant concentration profiles when $\alpha = 6$ and $\beta = 1$.

4. Conclusions

This article, in general looking, leaves the the calculation of all branches of solutions of nonlinear boundary value problems by numerical method with high accuracy as a research challenging opportunity. The complexity of finding multiple solutions of the nonlinear differential equations has suggested us to consider steady state reactive transport model so that we have discovered existence of unique, dual or triple solutions. It has been used a simple technique to get initial guess or guesses to apply Newton method on the system arisen from applying pseudo–spectral collocation method, to get approximate solutions. We have also applied discrete least square method to obtain more smooth polynomial as more accurate solutions.

Table 2: The numerical results obtained by stopping criteria $\left|U_{n+1}(x_j) - U_n(x_j)\right| \leq 10^{-10}$ in which $x_j = \frac{1}{2}(\eta_j + 1)$

Shifted GL Points	First branch	Second branch	Third branch
x_0	1.000000000000000	1.000000000000000	1.000000000000000
x_1	0.988738357399405	0.983199428562339	0.949537204419829
x_2	0.955896743914803	0.933603977446942	0.799349888005267
x_3	0.904180186516632	0.854586016610016	0.555667476804374
x_4	0.837701331786638	0.750502923405602	0.224980871366515
x_5	0.761456096290749	0.627332334556379	-0.182045988889929
x_6	0.680716971565579	0.490436156623909	-0.670896050548213
x_7	0.600445354233793	0.345523765808495	-1.241559952395031
x_8	0.524817173797971	0.195791426529886	-1.736733950971937
x_9	0.456927301539902	0.044170450620247	-2.166202035099350
x_{10}	0.398693495113621	-0.110628922066492	-2.540879769993515
x_{11}	0.350933197250186	-0.269164601914809	-2.853548584268253
x_{12}	0.313552721582670	-0.438943105375970	-3.104634149346748
x_{13}	0.285779489772151	-0.623133543934853	-3.294925927675300
x_{14}	0.266383703475706	-0.853078832172846	-3.430651253281671
x_{15}	0.253864783204669	-1.147793462336315	-3.519458262589144
x_{16}	0.246604836634713	-1.306116704988593	-3.571847594583344
x_{17}	0.243005305250908	-1.375635070920413	-3.598144121329155
x_{18}	0.241621100679336	-1.404795944292564	-3.608654020329617
x_{19}	0.241293916871000	-1.412397193011418	-3.611299372274864
x_{20}	0.241271819556713	-1.413871855911548	-3.611632825779648

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