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Research Article



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Analysis of the Parameter-Dependent Multiplicity of Steady-State Profiles of a Strongly Nonlinear Mathematical Model Arising From the Chemical Reactor Theory

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Abstract

In this paper, we study the uniqueness and multiplicity of the solutions of a strongly nonlinear mathematical model arising from chemical reactor theory. The analysis is based on the reproducing kernel Hilbert space method. The main aim of this work is to find how much information can be predicted using numerical computations. The dependence of the number of solutions on the parameters of the model is also studied. Furthermore, the analytical approximations of all branches of solutions can be calculated by the proposed method. The convergence of the proposed method is proved. Some numerical simulations are presented.

Keywords : Multiple solutions; Reproducing kernel Hilbert space; Strongly nonlinear problem; Adiabatic tubular chemical reactor; Iterative technique; Convergence.

1 Introduction

Boundary value problems arising in adiabatic tubular chemical reactors, have attracted the attention of many researchers [17, 21]. Approximate the solutions of the nonlinear problems are challenging even when we know the number of solutions. There is considerable lit-

erature that discusses the multiplicity of solutions of the boundary value problems, such as [23, 1, 2, 3, 18, 19, 4, 20, 6]. Here, we investigate the multiplicity of the solutions and their dependence on the various parameter of the model, numerically. Besides, the method is capable of calculating analytical approximations for all branches of solutions. The prediction of the number of branches of solutions and approximate them accurately is very important in the numerical method for nonlinear boundary value problems. The main aim of this work is to find how much information can be predicted using numerical computations. We approximate the solutions of a nonlinear boundary value problem via the shooting reproducing kernel Hilbert space (SRKHS) method. We will consider the depen-

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dence of the number of solutions to each parameter of the model separately. In the following, we consider a strongly nonlinear boundary value problem, which describes the steady-states of an adiabatic tubular chemical reactor,

$$\beta u'' - u' + b(c - u) \exp\left(\frac{-k}{1 + u}\right) = 0, \quad (1.1)$$

for $x \in [0, 1]$ under the following two-point boundary conditions,

$$u'(0) - \alpha u(0) = 0, u'(1) = 0, \quad (1.2)$$

where u is the dimensionless temperature in the reactor, and β, α, c and k are some given constant. The nonlinear term is the Arrhenius reaction rate given by

$$f(u) = b(c - u) \exp\left(\frac{-k}{1 + u}\right), \quad (1.3)$$

where $c > 0, k > 0$, which represents the rate of heat generation. It has been known from experimental and theoretical data that reactions modeled by (1.1)-(1.2) exhibit unique or multiple steady states, depending on the constants β, b and k . Reproducing kernel theory has important applications in numerical analysis and computational methods for differential equations. Recently, the numerical methods based on the reproducing kernel Hilbert spaces have been successfully applied to the various nonlinear problems, such as the nonlinear system of boundary value and initial value problems, boundary value problems with nonlinear and multi-point boundary conditions, fractional integro-differential equations and singularly perturbed turning point problems [13, 15, 5, 7, 8, 9, 14, 16, 10, 11, 22]. In this paper, we use the reproducing kernel Hilbert space method combined with the shooting technique. The shooting technique is well-known for transforming the boundary value problems into initial value problems. In this way, we derive an efficient and accurate iterative method to handle strongly nonlinear boundary value problem (1.1)-(1.2). Furthermore, we prove the convergence of the proposed iterative method. The main contribution of the current work is to investigate the effect of the parameters of the model on the multiplicity of solutions. Furthermore, we calculate

the approximate solutions for all branches of solutions. The advantages of the utilized approach lie in the following; firstly, it can produce good globally smooth numerical solutions, and with the ability to solve many problems with complex constraints conditions, which are difficult to solve; secondly, the numerical solutions and their derivatives converge uniformly to the exact solutions and their derivatives, respectively; thirdly, the numerical solutions and all their derivatives are applicable for each arbitrary point in the given domain. We illustrate some numerical experiments to demonstrate the validity of the procedure.

For the nonlinear boundary value problems such as (1.1)-(1.2) the shooting reproducing kernel Hilbert space method is as follows. The boundary value problem (1.1)-(1.2) is replaced by the following initial value problem,

$$\begin{cases} \beta u'' - u' + f(u) = 0, x \in [0, 1] \\ u(0) = s, u'(0) = \alpha s, \end{cases} \quad (1.4)$$

where f is defined in (1.3) and s is unknown and should be determined such that $u(x)$ satisfies the condition $u'(1) = 0$. Here, we assume that the initial value problem (1.4) has a unique solution that is continuously dependent on its initial conditions. The existence and uniqueness of solutions of the initial value problems have been thoroughly investigated in the literature, for example, see [12] and the references therein. The solution of (1.4) is denoted by $u(x; s)$ where the parameter s is the initial value $u(0) = s$. Now, we obtain an accurate approximation for the initial value problem (1.4). Then s should be determined such that $u(x, s)$ satisfies the condition $u'(1, s) = 0$. Since the solution of the nonlinear problem (1.4) cannot be easily obtained, the reproducing kernel Hilbert space (RKHS) method is applied. To avoid the time consuming parametric computations a sequence $s_n \rightarrow s^*$ is used instead of the parameter s in a manner that $u'(1; s^*) = 0$ as $n \rightarrow \infty$. In the following, we describe how to obtain the approximate solution of (1.4) for a determined s . Let $Lu \equiv \beta u'' - u'$, after homogenization, the problem (1.4) can be converted into the following form:

$$\begin{cases} Lv = F(v; s), & x \in [0, 1], \\ v(0) = 0, v'(0) = 0, \end{cases} \quad (1.5)$$

where $u(x) = v(x) + s + \alpha sx$ and $F(v; s) = \alpha s - f(v(x) + s + \alpha sx)$. The reproducing kernel Hilbert spaces $W_2^m[0, 1]$, ($m \geq 3$) and $W_2^1[0, 1]$ are defined in the following, for more details and proofs, we refer to [13].

Definition 1.1. The inner product space $W_2^m[0, 1]$ is defined as $W_2^m[0, 1] = \{u(x) | u^{(m-1)}$ is absolutely continuous real valued functions, $u^{(m)} \in L^2[0, 1], u(0) = 0, u'(0) = 0\}$. The inner product in $W_2^m[0, 1]$ is given by

$$(u(\cdot), v(\cdot))_{W_2^m} = \sum_{i=0}^{m-1} u^{(i)}(0)v^{(i)}(0) + \int_0^1 u^{(m)}(x)v^{(m)}(x)dx, \quad (1.6)$$

and the norm $\|u\|_{W_2^m}$ is denoted by $\|u\|_{W_2^m} = \sqrt{(u, u)_{W_2^m}}$, where $u, v \in W_2^m[0, 1]$.

Definition 1.2. The inner product space $W_2^1[0, 1]$ is defined as $W_2^1[0, 1] = \{u(x) | u$ is absolutely continuous real valued functions, $u, u' \in L^2[0, 1]\}$. The inner product in $W_2^1[0, 1]$ is given by

$$(u(\cdot), v(\cdot))_{W_2^1} = u(0)v(0) + \int_0^1 u'(x)v'(x)dx, \quad (1.7)$$

and the norm $\|u\|_{W_2^1}$ is denoted by $\|u\|_{W_2^1} = \sqrt{(u, u)_{W_2^1}}$, where $u, v \in W_2^1[0, 1]$.

The inner product spaces $W_2^1[0, 1]$ and $W_2^m[0, 1]$ are reproducing kernel Hilbert spaces [13]. The reproducing kernel $R_x(\cdot) \in W_2^m[0, 1]$ can be denoted by

$$R_x(y) = \begin{cases} \sum_{i=1}^{2m} c_i(y)x^{i-1}, & x \leq y, \\ \sum_{i=1}^{2m} d_i(y)x^{i-1}, & x > y. \end{cases} \quad (1.8)$$

For the method of obtaining reproducing kernel $R_x(y)$, refer to [13, 15]. For any fixed $x_i \in [0, 1]$, let $\varphi_i(\cdot) = r_{x_i}(\cdot)$, where $r_x(\cdot)$ is the reproducing kernel of the Hilbert space $W_2^1[0, 1]$. Now assume that $\psi_i(\cdot) = (L^*\varphi_i)(\cdot)$, Where L^* is the adjoint operator of $L : W_2^m[0, 1] \rightarrow W_2^1[0, 1]$.

Theorem 1.1. Let $\{x_i\}_{i=1}^\infty$ is dense on $[0, 1]$, then $\{\psi_i(x)\}_{i=1}^\infty$ is the complete system of $W_2^m[0, 1]$ and $\psi_i(x) = L_y R_x(y)|_{y=x_i}$.

Proof. Let

$$\begin{aligned} \psi_i(x) &= (L^*\varphi_i)(x) = ((L^*\varphi_i)(y), R_x(y))_{W_2^m} \\ &= (\varphi_i(y), L_y R_x(y))_{W_2^1} = L_y R_x(y)|_{y=x_i}. \end{aligned}$$

Clearly $\psi_i \in W_2^m[0, 1]$, then for any $u \in W_2^m[0, 1]$ let

$$(u(\cdot), \psi_i(\cdot))_{W_2^m} = 0, \quad i = 1, 2, \dots$$

So

$$\begin{aligned} (u(x), \psi_i(x))_{W_2^m} &= (u(x), L_y K(x, y)|_{t=x_i})_{W_2^m} \\ &= L_y(u(x), K(x, y))_{W_2^m}|_{y=x_i} = (Lu)(x_i) = 0. \end{aligned}$$

Since $\{x_i\}_{i=1}^\infty$ is dense on $[0, 1]$ we have $(Lu)(x) = 0$. It is easy to see that the problem

$$\begin{cases} Ly = 0; & x \in [a, b], \\ y(0) = 0, y'(0) = 0, \end{cases}$$

has only the trivial solution $u = 0$. The proof is complete. \square

The orthonormal system $\{\bar{\psi}_i(x)\}_{i=1}^\infty$ of $W_2^m[0, 1]$ can be derived from Gram-Schmidt orthogonalization process of $\{\psi_i(x)\}_{i=1}^\infty$,

$$\bar{\psi}_i(x) = \sum_{k=1}^i \beta_{ik} \psi_k(x) \quad (\beta_{ii} > 0, i = 1, 2, \dots). \quad (1.9)$$

In the following an iterative reproducing kernel Hilbert space method is used to approximate the solution of (1.5) for any determined s ,

$$\begin{cases} v_0(x) = 0, \\ B_i = \sum_{k=1}^i \beta_{ik} F(v_{k-1}(x_k); s), \\ v_n(x; s) = \sum_{i=1}^n B_i \bar{\psi}_i(x). \end{cases} \quad (1.10)$$

Theorem 1.2. Suppose that the problem (1.5) has a unique solution and also suppose that $\|v_n\|_{W_2^m}$ in (1.10) is bounded. If $\{x_i\}_{i=1}^\infty$ is a dense set on the interval $[0, 1]$, then $v_n(\cdot; s)$ derived from (1.10) converges to the exact solution $v(\cdot; s)$ of the homogeneous initial value problem (1.5) and $v(x; s) = \sum_{i=1}^\infty B_i \bar{\psi}_i(x)$, where B_i is derived by (1.10).

Proof. For any fixed s , from (1.10) we can see that $v_{n+1}(x; s) = v_n(x; s) + B_{n+1} \bar{\psi}_{n+1}(x)$ and from the orthogonality of $\{\bar{\psi}_i\}_{i=1}^\infty$ we can see that $\|v_{n+1}\|^2 = \|v_n\|^2 + (B_{n+1})^2$ which concludes that $\|v_{n+1}\|^2 \geq \|v_n\|^2$. Since $\|v_n\|$ is bounded, so $\|v_n\|$ is convergent. It is easy to see that $v_n(\cdot; s)$ is a

Cauchy sequence in $W_2^m[0, 1]$ and then the completeness of $W_2^m[0, 1]$ shows that $v_n(\cdot; s) \rightarrow \bar{v}(\cdot; s)$ in the sense of $\|\cdot\|_{W_2^3}$. Then we will prove that $\bar{v}(\cdot; s)$ is the solution of the problem (1.5). Taking limit in (1.10), we get $\bar{v}(x; s) = \sum_{i=1}^{\infty} B_i \bar{\psi}_i(x)$. Since $\bar{\psi}_i \in W_2^m[0, 1]$, clearly $\bar{v}(\cdot; s)$ satisfies the initial condition of the problem (1.5). Then we have

$$\begin{aligned} B_n &= (\bar{v}, \bar{\psi}_n) = (\bar{v}, \sum_{j=1}^n \beta_{nj} \psi_j) \\ &= \sum_{j=1}^n \beta_{nj} (\bar{v}, \psi_j) \\ &= \sum_{j=1}^n \beta_{nj} (\bar{v}, L^* \varphi_j) \\ &= \sum_{j=1}^n \beta_{nj} (L\bar{v}, \varphi_j) \\ &= \sum_{j=1}^n \beta_{nj} (L\bar{v})(x_j; s). \end{aligned} \tag{1.11}$$

From the definition of B_n in (1.10) and (1.11), it is easy to see that

$$(L\bar{v})(x_j; s) = F(x_j, v_{j-1}(x_j; s); s), \tag{1.12}$$

$(j = 1, 2, \dots).$

Since $\{x_j\}_{i=1}^{\infty}$ is dense in $[0, 1]$ for any $\bar{x} \in [0, 1]$, there exists a subsequence $\{x_{n_j}\}_{i=1}^{\infty}$ such that $x_{n_j} \rightarrow \bar{x}$. From (1.12) and continuity of $F(v; s)$ and $v(\cdot; s)$, we have $(L\bar{v})(\bar{x}; s) = F(\bar{x}, \bar{v}(\bar{x}; s); s)$. It means that $\bar{v}(x; s)$ is the solution of the initial value problem (1.5) and then from the uniqueness of solution of (1.5) we conclude that $v(x; s) = \sum_{i=1}^{\infty} B_i \bar{\psi}_i(x)$. \square

If we let $u(x; s) = v(x; s) + s + \alpha x$, then the shooting method for the problem (1.1)-(1.2) is coincide to the method of finding the root of the $G(s) = u'(1; s)$. In fact, for any root of $G(s) = u'(1; s)$ such as $s = s^*$ the $u(x) \equiv u(x; s^*)$ is a solution of problem (1.1)-(1.2) and also for any solution $u(x)$ of (1.1)-(1.2) the $s = u(0)$ is a root of $G(s)$. Thus the problem is reduced to finding the roots of $G(s)$. It follows from the strong maximum principle that every solution to (1.1)-(1.3) satisfies $0 \leq u(x) \leq c$ for $0 \leq x \leq 1$. So we can let $0 \leq u(0) = s \leq c$. To avoid of the time consuming parametric computation the successive bisection method is utilized for calculating s_n the root of $G_n(s) = u'_n(1; s) = 0$ and we will show that $s_n \rightarrow s^*$ such that $G_n(s_n) \rightarrow G(s^*) = u'(1; s^*) = 0$ as $n \rightarrow \infty$.

Theorem 1.3. [13] *Let $W_2^m[0, 1]$ is a reproducing kernel Hilbert space and $f_n, f \in W_2^m[0, 1]$ ($n = 1, 2, \dots$). If f_n converges to f in the sense of*

$\|\cdot\|_{W_2^m}$, then for $0 \leq k \leq m - 1$, $f_n^{(k)}$ converges to $f^{(k)}$ uniformly.

Theorem 1.4. *If $G(s) = u'(1; s)$ has a first order root in interval I , then $u_n(x; s)$ converges to a exact solution $u(x)$ of nonlinear boundary value problem (1.1)-(1.2) such that for this solution $u'(0) = s \in I$.*

Proof. Suppose that for two determined values μ_1 and μ_2 we have $u'(1; \mu_1)u'(1; \mu_2) < 0$ such that $u'(1; \mu_1) < 0$ and $u'(1; \mu_2) > 0$, then from theorem (1.3), there exist a positive integer N such that for any $n > N$ we have $u'_n(1; \mu_1) < 0$ and $u'_n(1; \mu_2) > 0$. Then we use bisection method for $u'_n(1; s) = 0$ to find $s_n \in [\mu_1, \mu_2]$ such that $u'_n(1; s_n) = 0$. If we can show that $u'_k(1; s_n)u'(1; s_n) > 0$ for any $k > n$ then we can detect that the root of $G(s) = 0$ is belongs to $[\mu_1, s_n]$ or $[s_n, \mu_2]$. From theorem (1.3) and for any $k > n$ for enough large n we have

$$|u'(1; s_n) - u'_k(1; s_n)| \leq |u'(1; s_n) - u'_n(1; s_n)|,$$

and then since $u'_n(1; s_n) = 0$, we can see

$$|u'(1; s_n) - u'_k(1; s_n)| \leq |u'(1; s_n)|. \tag{1.13}$$

Suppose that $u'_k(1; s_n)u'(1; s_n) > 0$ is not true, i.e. $u'(1; s_n) > 0$ and $u'_k(1; s_n) < 0$. the opposite case can be treated in a similar way. So we have

$$\begin{aligned} &|u'(1; s_n) - u'_k(1; s_n)| \\ &\leq u'(1; s_n) \\ &\Rightarrow -u'(1; s_n) \leq u'(1; s_n) - u'_k(1; s_n) \\ &\leq u'(1; s_n) \\ &\Rightarrow -u'(1; s_n) + u'_k(1; s_n) \\ &\leq u'(1; s_n) \leq u'(1; s_n) + u'_k(1; s_n), \end{aligned} \tag{1.14}$$

the right-hand side inequality is in contradiction to the assumption obviously. Considering the method of obtaining $\{s_n\}$, it has subsequences $\{\gamma_n\}$ and $\{\beta_n\}$ such that

$$\begin{aligned} &\mu_1 < \gamma_1 < \gamma_2 < \dots < \gamma_n < \dots < s^* \\ &< \dots < \beta_n < \dots < \beta_2 < \beta_1 < \mu_2, \end{aligned} \tag{1.15}$$

which they are bounded monotone sequences, and so either of them are convergent to a root of $u'(1; s) = 0$. So if $u'(1; s) = 0$ has a simple root in $[\mu_1, \mu_2]$ then both sequences $\{\gamma_n\}$ and $\{\beta_n\}$ and then $\{\alpha_n\}$ are convergent to the root

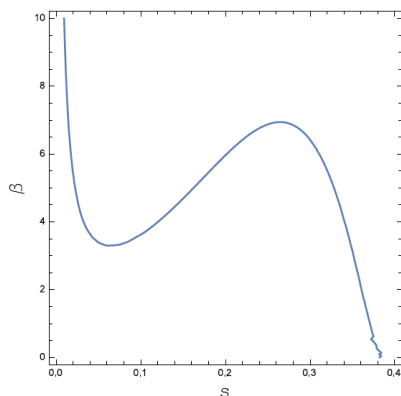


Figure 1: Graph of β versus s based on $u'_8(1; s) = 0$, where $\alpha = 0.2$ and $f(u) = 2(10^7)(0.4 - u) \exp\left(\frac{-20}{1+u}\right)$.

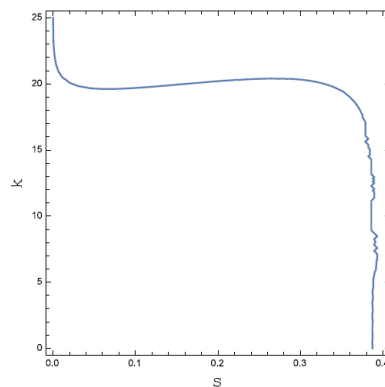


Figure 2: Graph of k versus s based on $u'_8(1; s) = 0$, where $\beta = 5, \alpha = 0.2$ and $f(u) = 2(10^7)(0.4 - u) \exp\left(\frac{-k}{1+u}\right)$.

of $u'(1; s) = 0$ in $[\mu_1, \mu_2]$ and since the solution of the initial value problem (1.4) is continuously dependent on its initial conditions, $u_n(x; s_n)$ converges to a solution $u(x)$ of nonlinear boundary value problem (1.1)-(1.2) such that for this solution $u'(0) = s \in [\mu_1, \mu_2]$. \square

2 Results and discussion

In this section, we apply the proposed method to the boundary value problem (1.1)-(1.2). Define the residual error of the approximate solution v at a point $x \in [0, 1]$ as

$$Res(x, v) = \beta v'' - v' + f(v).$$

Then the square root of integral of residual is defined as follows

$$E(v) = \sqrt{\int_0^1 (Res(x, v))^2 dx}. \tag{2.16}$$

We apply the proposed method in $W_2^4[0, 1]$ and the following results are obtained. The Fig. 1 is the graph of β versus s based on $u'_n(1; s) = 0$, where $n = 8, \alpha = 0.2$ and

$$f(u) = 2(10^7)(0.4 - u) \exp\left(\frac{-20}{1+u}\right),$$

which indicate that for some value of β we have unique solutions and for some value of β we have three solutions. The Fig. 2 is the graph of k versus s based on $u'_n(1; s) = 0$, where $n = 8, \beta =$

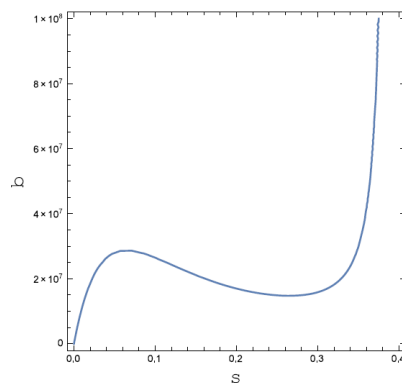


Figure 3: Graph of b versus s based on $u'_8(1; s) = 0$, where $\alpha = 0.2$ and $f(u) = b(0.4 - u) \exp\left(\frac{-20}{1+u}\right)$.

$5, \alpha = 0.2$ and

$$f(u) = 2(10^7)(0.4 - u) \exp\left(\frac{-k}{1+u}\right),$$

which shows the multiplicity of solutions for some value of k . The Fig. 3 is the graph of b versus s based on $u'_n(1; s) = 0$, where $n = 8, \beta = 5, \alpha = 0.2$ and

$$f(u) = b(0.4 - u) \exp\left(\frac{-20}{1+u}\right),$$

which shows the multiplicity of solutions for some value of b .

Example 2.1. Consider problem (1.1)-(1.2) with $\beta = 5, \alpha = 0.2$ and

$$f(u) = 2(10^7)(0.4 - u) \exp\left(\frac{-20}{1+u}\right).$$

Table 1: Square root of integral of the squared residual error for example (2.1)

Number of iteration	$n = 10$	$n = 25$	$n = 50$	$n = 100$
First solution	8.10583×10^{-6}	8.28762×10^{-7}	1.15327×10^{-7}	7.82974×10^{-9}
Second solution	1.99622×10^{-4}	1.83693×10^{-5}	2.56265×10^{-6}	2.14811×10^{-7}
Third solution	1.9028×10^{-4}	1.44628×10^{-5}	2.19408×10^{-6}	4.12512×10^{-7}

Table 2: Square root of integral of the squared residual error for example (2.2)

Number of iteration	$n = 10$	$n = 25$	$n = 50$	$n = 100$
$E(u_n)$	1.86366×10^{-3}	1.63077×10^{-4}	2.45307×10^{-5}	3.10783×10^{-6}

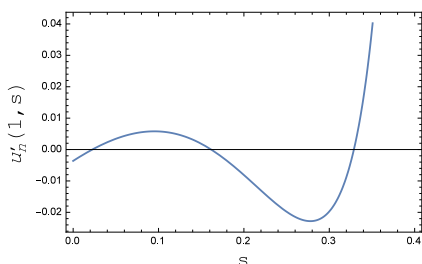


Figure 4: Graph of $u'_{10}(1; s)$ for example (2.1) which shows the problem has three solutions.

From Fig. 4 we see that there exists three solutions for example (2.1). The approximations of these three branches of solutions have been shown in Fig. 5. Table 1 shows the square root of integral of the squared residual error of all three approximate branches of SRKHS solutions for example (2.1).

Example 2.2. Consider problem (1.1)-(1.2) with $\beta = 2, \alpha = 0.2$ and

$$f(u) = 2(10^7)(0.4 - u) \exp\left(\frac{-20}{1 + u}\right).$$

From Fig. 6 we see that there exists a unique solution for example (2.2) and the approximation of this solution has been shown. Table 2 shows the square root of integral of the squared residual error of the approximate SRKHS solution for example (2.1).

3 Conclusions

In this manuscript, we considered a nonlinear boundary value problem, which arises in adiabatic tubular reactors. The shooting reproducing

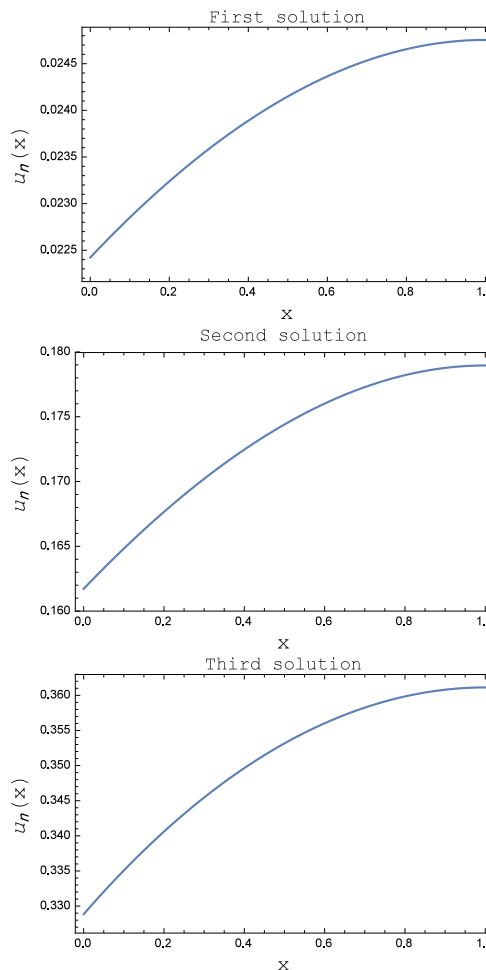


Figure 5: Graph of three approximate solutions $u_{50}(x)$ for example (2.1).

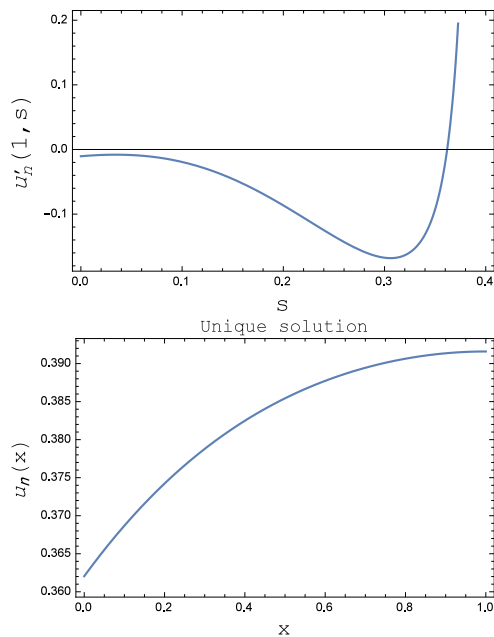


Figure 6: Graph of $u'_{10}(1; s)$ for example (2.2), which shows the uniqueness of solution and its approximation $u_{50}(x)$.

kernel Hilbert space (SRKHS) method is used to study the existence and uniqueness or multiplicity of the solutions of nonlinear boundary value problem (1.1)-(1.3). We showed the dependence of the number of solutions to the values of various parameters of the problem. In addition, the analytical approximations of all branches of solutions are calculated by the proposed method. We proved the convergence of the method. The implementation of the presented method is easy. Some numerical simulations have been given to show the high applicability of the SRKHS method.

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