Int. J. Nonlinear Anal. Appl. 8 (2017) No. 1, 69-80
ISSN: 2008-6822 (electronic)
http://dx.doi.org/10.22075/ijnaa.2017.1653.1436

A spline collocation method for integrating a class of chemical reactor equations

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(Communicated by S. Abbasbandy)

Abstract

In this paper, we develop a quadratic spline collocation method for integrating the nonlinear partial differential equations PDEs of a plug flow reactor model. The method is proposed in order to be used for the operation of control design and/or numerical simulations. We first present the Crank-Nicolson method to temporally discretize the state variable. Then, we develop and analyze the proposed spline collocation method for the spatial discretization. The design of the collocation method is interpreted as one order error convergent. This scheme is applied on some test examples, the numerical results illustrate the efficiency of the method and confirm the theoretical behavior of the rates of convergence.

Keywords: Partial differential equations; Distributed parameter systems; Plus flow reactors; Perturbed systems; Spline collocation method.
2010 MSC: Primary 58J10; Secondary 65D07.

1. Introduction and preliminaries

The plug flow reactor models are nowadays a necessity in chemical engineering and different catalytic processes with special needs have been lead to a wide variety of this class of tubular reactor models, since it reveal more informations about the reactor performance, and they can also be used for simulating steady-state and control operations (see eg., [12], [17]).

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Received: October 2016 *Revised:* January 2017

Usually, a dynamic tubular reactor model consists of PDEs and the practical method to integrate is to reduce them into a set of ordinary differential equations ODEs by spatial discretization, and to use well-known algorithms to solve the time-dependent model. This kind of systems are called distributed parameter systems DPSs and can be found in process control described by PDEs, e.g., robotics, bio-reactors, flexible structures, and vibrations (see e.g.,[1], [14]). These methods and algorithms are well described in several chemical engineering textbooks, (for example in [18, 7, 15]). Various numerical techniques have been developed and compared for solving the ODEs (see [3, 9]). Besides of the lack of knowledge of the connection between the original distributed parameter (infinite dimensional) model and its (finite dimensional) discretised version, the approximation methods may require extensive computation studies in order to try to capture the dynamic behavior of the DPS. For instance, the number of ODEs required in the finite differences method to obtain satisfactory model approximation many becomes excessively high (see [3]). Even when the methods of characteristics is able to provide an exact representation of the original model (see [9]) this attempt requires also a high number of collocation points which is difficult to implement in practical control and monitoring applications. The main objective of this study is to develop a user friendly, economical method which can work for solving a perturbed first-order hyperbolic PDEs model by using a quadratic splines collocation method.

Let us consider a chemical or a biological process taking place in a plug flow reactor whose mathematical model is given by

$$\left\{\begin{array}{rcll} \dfrac{\partial V}{\partial t}(z,t) & = & -\vartheta\dfrac{\partial V}{\partial z}(z,t)+Kf(V(z,t))+CV(z,t)+u(t), & (z,t)\in\Omega, \\ V(z,0) & = & \alpha(z), & z\in\Omega_z, \\ V(0,t) & = & \beta(t), & t\in\Omega_t, \end{array}\right. \tag{1.1}$$

In the above equations, $V(z,t)\in\mathbb{R}^H$ is the state vector, $f(V)\in\mathbb{R}^S$ is the nonlinearities vector and L_λ-Lipschitz ($L_\lambda \geq 0$), $K\in\mathbb{R}^{H\times S}$ denotes a matrix of known coefficients (e.g. stoichiometric or yield coefficients), $C\in\mathbb{R}^{H\times H}$ is the state matrix whose elements are known, $u(t)\in\mathbb{R}^H$ is a vector gathering the process inputs (e.g. mass and/or energy feeding rate vector) and/or other time-varying functions (e.g. gaseous outflow rate). Besides, t represents the time variable whereas z ($z\in[0,L]$) is the axial position, L is the reactor length, ϑ is considered as a positive and known constant describing the velocity of the inlet stream, $\beta(t)$ is a column vector which is a sufficiently smooth function of time and $\alpha(z)\in\mathcal{H}[(0,L),\mathbb{R}^H]$ where $\mathcal{H}^H[(0,L,\mathbb{R}^H)$ being the infinite dimensional Hilbert Space of H-dimensional-like vector functions defined on the interval $[0,L]$. The problem (1.1) can be formulated as the following problem

$$\left\{\begin{array}{rcll} \dfrac{\partial V}{\partial t}+P\dfrac{\partial V}{\partial z}-CV & = & I(V(z,t)), & (z,t)\in\Omega, \\ V(z,0) & = & \alpha(z), & z\in\Omega_z, \\ V(0,t) & = & \beta(t), & t\in\Omega_t, \end{array}\right. \tag{1.2}$$

where

$$\begin{array}{rcl} P & = & (diag(\upsilon.I_{j,j}))_{j=1,\ldots,H}\,, \\ I(V) & = & Kf(V)+u(t)\in\mathbb{R}^H, \end{array}$$

with $C_{i,j}\leq\widetilde{\gamma}<0$ on $\overline{\Omega}$ and f, u, α, β are sufficiently smooth functions.

Here we assume that the problem satisfies sufficient regularity and compatibility conditions which guarantee that the problem has a unique solution $u\in C(\overline{\Omega})\bigcap C^{2,1}(\Omega)$ satisfying (see, [10, 8, 11]):

$$\left|\frac{\partial^{i+j}V(x,t)}{\partial x^i\partial t^j}\right|\leq k \text{ on } \overline{\Omega};\quad 0\leq j\leq 3 \text{ and } 0\leq i+j\leq 4, \tag{1.3}$$

where k is a constant in $\mathbb{R}^H$.

In the present work, we present a numerical method for solving the general dynamical model for a class of plug flow reactors. The method is based on Crank-Nicolson scheme to discretize the temporal variable and a quadratic spline collocation method for the spatial discretization. The scheme is one-order convergent with respect to the spatial variable.

The organization of the paper is as follows. In Section 2, we discuss time semi-discretization. Section 3 is devoted to the spline collocation method for solving the general dynamical model for a class of plug flow reactors using a quadratic spline collocation method. Next, the error bound of the spline solution is analyzed. In order to validate the theoretical results presented in this paper, we present numerical tests on two known examples in Section 4. Finally, a conclusion is given in Section 5.

2. Time discretization and description of the Crank-Nicolson scheme

Discretize the time variable by setting $t^m = m\Delta t$ for $m = 0, 1, ..., M$, in which $\Delta t = \frac{T}{M}$ and then define

$$V^m(z) = V(z, t^m), \qquad m = 0, 1, ..., M.$$

Now by applying the Crank-Nicolson scheme on (1.2), we arrive at the following equation

$$\frac{V^{m+1} - V^m}{\Delta t} - \frac{1}{2}\mathcal{L}(V^{m+1} + V^m) = \frac{1}{2}\left(I(V^{m+1}) + I(V^m)\right).$$

One way is to replace V^{m+1} with V^m in the nonlinear terms. This leads to the following modified system:

$$V^{m+1} - \frac{\Delta t}{2}\mathcal{L}V^{m+1} = \frac{\Delta t}{2}\mathcal{L}V^m + V^m + \Delta t I(V^m). \tag{2.1}$$

For $m = 0, 1, ..., M$. The value of V at time level m will be of the form:

$$\left\{\begin{array}{rcll} P\dfrac{\partial V^{m+1}}{\partial z} + RV^{m+1} &=& J(V^m), & \forall z \in [0, L], \\ V^0(z) &=& \alpha(z), & \forall z \in [0, L], \\ V^{m+1}(0) &=& \beta^{m+1}, & 0 \le m < M. \end{array}\right. \tag{2.2}$$

where, for any $m \ge 0$ and for any $z \in [0, L]$, we have

$$\begin{array}{rcl} R &=& \left(\dfrac{2}{\Delta t}I - C\right), \\ J(V^m) &=& \mathcal{L}V^m + \dfrac{2}{\Delta t}V^m + 2I(V^m), \\ \mathcal{L} &=& -P\dfrac{\partial}{\partial z} + CI, \end{array}$$

V^{m+1} is solution of (2.2), at the $(m+1)$ th-time level.

The following theorem proves the order of convergence of the solution V^m to $V(z, t)$.

Theorem 2.1. *problem* (2.2) *is second order convergent, i.e.*

$$\|V(z, t_m) - V^m\|_H \le Cte(\Delta t)^2.$$

Proof . We introduce the notation $e_m = V(z,t_m) - V^m$ the error at step m and

$$\|e_m\|_H = \sup_{z\in[0,L]} \max_{1\le i\le H} |e^i_m(z)|.$$

By Taylor series expansion of V, we have

$$V(z,t_{m+1}) = V(z,t_{m+\frac{1}{2}}) + \frac{\Delta t}{2}\frac{\partial V}{\partial t}(z,t_{m+\frac{1}{2}}) + \frac{(\Delta t)^2}{8}\frac{\partial^2 V}{\partial t^2}(z,t_{m+\frac{1}{2}}) + O((\Delta t)^3).I_H,$$

$$V(z,t_m) = V(z,t_{m+\frac{1}{2}}) - \frac{\Delta t}{2}\frac{\partial V}{\partial t}(z,t_{m+\frac{1}{2}}) + \frac{(\Delta t)^2}{8}\frac{\partial^2 V}{\partial t^2}(z,t_{m+\frac{1}{2}}) + O((\Delta t)^3).I_H.$$

By using these expansions, we get

$$\frac{V(z,t_{m+1}) - V(z,t_m)}{\Delta t} = \frac{\partial V}{\partial t}(z,t_{m+\frac{1}{2}}) + O((\Delta t)^2).I_H, \tag{2.3}$$

and by Taylor series expansion of $\dfrac{\partial V}{\partial t}$, we have

$$\frac{\partial V}{\partial t}(z,t_{m+1}) = \frac{\partial V}{\partial t}(z,t_{m+\frac{1}{2}}) + \frac{\Delta t}{2}\frac{\partial^2 V}{\partial t^2}(z,t_{m+\frac{1}{2}}) + \frac{(\Delta t)^2}{8}\frac{\partial^3 V}{\partial t^3}(z,t_{m+\frac{1}{2}}) + O((\Delta t)^3).I_H,$$

$$\frac{\partial V}{\partial t}(z,t_m) = \frac{\partial V}{\partial t}(z,t_{m+\frac{1}{2}}) - \frac{\Delta t}{2}\frac{\partial^2 V}{\partial t^2}(z,t_{m+\frac{1}{2}}) + \frac{(\Delta t)^2}{8}\frac{\partial^3 V}{\partial t^3}(z,t_{m+\frac{1}{2}}) + O((\Delta t)^3).I_H.$$

By using these expansions, and $\left|\dfrac{\partial^3 V}{\partial t^3}\right| \le c.I_H$ on $\overline{\Omega}$ (see relation (1.3)), we have

$$\frac{1}{2}\frac{\partial}{\partial t}[V(z,t_{m+1}) + V(z,t_m)] = \frac{\partial}{\partial t}V(z,t_{m+\frac{1}{2}}) + O((\Delta t)^2).I_H.$$

This implies

$$\begin{aligned}
\frac{\partial V}{\partial t}(z,t_{m+\frac{1}{2}}) &= \frac{1}{2}\frac{\partial}{\partial t}[V(z,t_{m+1}) + V(z,t_m)] + O((\Delta t)^2).I_H \\
&= \frac{1}{2}[\mathcal{L}V(z,t_{m+1}) + I(V(z,t_{m+1})) + \mathcal{L}V(z,t_m) + I(V(z,t_m))] + O((\Delta t)^2).I_H.
\end{aligned}$$

By using this relation in (2.3) we get

$$(1 - \frac{\Delta t}{2}\mathcal{L})V(z,t_{m+1}) = (1 + \frac{\Delta t}{2}\mathcal{L})V(z,t_m) + \frac{\Delta t}{2}[I(V(z,t_{m+1})) + I(V(z,t_m))] + O((\Delta t)^3).I_H,$$

by (2.1). Then, we obtain

$$(1 - \frac{\Delta t}{2}\mathcal{L})e_{m+1} = (1 + \frac{\Delta t}{2}\mathcal{L})e_m + \frac{\Delta t}{2}[I(e_{m+1}) + I(e_m)] + O((\Delta t)^3).I_H.$$

We may bound the term $O((\Delta t)^3)$ by $c(\Delta t)^3$ for some $c > 0$, and this upper bound is valid uniformly throughout $[0,T]$. Therefore, it follows from the triangle inequality that

$$\left\|(I - \frac{\Delta t}{2}\mathcal{L})e_{m+1}\right\|_H \le \left\|(I + \frac{\Delta t}{2}\mathcal{L})e_m\right\|_H + \frac{\Delta t}{2}(\|I(e_m)\|_H + \|I(e_{m+1})\|_H) + c(\Delta t)^3.$$

It follows from the Lipschitz condition we have

$$\begin{aligned}\|(I-\frac{\Delta t}{2}\mathcal{L})e_{m+1}\|_H &\leq \|(I+\frac{\Delta t}{2}\mathcal{L})e_m\|_H+\frac{\Delta t}{2}\left(\|I(e_m)\|_H+\|I(e_{m+1})\|_H\right)+c(\Delta t)^3,\\ &\leq \|(I+\frac{\Delta t}{2}\mathcal{L})\|_H\|e_m\|_H+\frac{\Delta t}{2}\|K\|_H\|f\|_H\left(\|e_m\|_H+\|e_{m+1}\|_H\right)+c(\Delta t)^3.\end{aligned}$$

Clearly, the operator $\left(I_H\pm\frac{\Delta t}{2}\mathcal{L}\right)$ satisfies a maximum principle (see, [4, 5]) and consequently

$$\left\|\left(I_H\pm\frac{\Delta t}{2}\mathcal{L}\right)^{-1}\right\|_H\leq\left(\frac{1}{1+\frac{\Delta t}{2}\widetilde{\gamma}}\right).$$

Since we are ultimately interested in letting $\Delta t\to 0$, there is no harm in assuming that $\Delta t.\eta<2$, with $\eta=(\|\mathcal{L}\|_H+\|K\|_H\|f\|_H)$. We can thus deduce that

$$\|e_{m+1}\|_H\leq\left(\frac{1+\frac{1}{2}\Delta t.\eta}{1-\frac{1}{2}\Delta t.\eta}\right)\|e_m\|_H+\left(\frac{c}{1-\frac{1}{2}\Delta t.\eta}\right)(\Delta t)^3. \tag{2.4}$$

We now claim that

$$\|e_m\|_H\leq\frac{c}{\eta}\left[\left(\frac{1+\frac{1}{2}\Delta t.\eta}{1-\frac{1}{2}\Delta t.\eta}\right)^m-1\right](\Delta t)^2. \tag{2.5}$$

The proof is by induction on m. When $m=0$ we need to prove that $\|e_0\|_H\leq 0$ and hence that $e_0=0$. This is certainly true, since at $t_0=0$ the numerical solution matches the initial condition and the error is zero.
For general $m\geq 0$, we assume that (2.5) is true up to m and use (2.4) to argue that

$$\begin{aligned}\|e_{m+1}\|_H &\leq \frac{c}{\eta}\left(\frac{1+\frac{1}{2}\Delta t.\eta}{1-\frac{1}{2}\Delta t.\eta}\right)\left[\left(\frac{1+\frac{1}{2}\Delta t.\eta}{1-\frac{1}{2}\Delta t.\eta}\right)^m-1\right](\Delta t)^2+\left(\frac{c}{1-\frac{1}{2}\Delta t.\eta}\right)(\Delta t)^3,\\ &\leq \frac{c}{\eta}\left[\left(\frac{1+\frac{1}{2}\Delta t.\eta}{1-\frac{1}{2}\Delta t.\eta}\right)^{m+1}-1\right](\Delta t)^2.\end{aligned}$$

This advances the inductive argument from m to $m+1$ and proves that (2.5) is true. Since $0<\Delta t.\eta<2$, it is true that

$$\left(\frac{1+\frac{1}{2}\Delta t.\eta}{1-\frac{1}{2}\Delta t.\eta}\right)=1+\left(\frac{\Delta t.\eta}{1-\frac{1}{2}\Delta t.\eta}\right)\leq\sum_{l=0}^{\infty}\frac{1}{l!}\left(\frac{\Delta t.\eta}{1-\frac{1}{2}\Delta t.\eta}\right)^l=exp\left(\frac{\Delta t.\eta}{1-\frac{1}{2}\Delta t.\eta}\right).$$

Consequently, relation (2.5) yields

$$\|e_m\|_H\leq\frac{c(\Delta t)^2}{\eta}\left(\frac{1+\frac{1}{2}\Delta t.\eta}{1-\frac{1}{2}\Delta t.\eta}\right)^m\leq\frac{c(\Delta t)^2}{\eta}exp\left(\frac{m\Delta t.\eta}{1-\frac{1}{2}\Delta t.\eta}\right).$$

This bound is true for every nonnegative integer m such that $m\Delta t < T$. Therefore

$$\|e_m\|_H \leq \frac{c(\Delta t)^2}{\eta} exp\left(\frac{T.\eta}{1-\frac{1}{2}\Delta t.\eta}\right).$$

We deduce that

$$\|V(x,t_m) - V^m\|_H \leq Cte(\Delta t)^2.$$

In other words, problem (2.2) is second order convergent. $\square$

For any $m \geq 0$, problem (2.2) has a unique solution and can be written on the following form:

$$\begin{cases} PV'(z) + RV(z) &= \widehat{f}(z) \in \mathbb{R}^H, \quad \forall z \in [0,L], \\ V(0) &= \beta.I_H, \end{cases} \tag{2.6}$$

In the sequel of this paper, we will focus on the solution of problem (2.6).

3. Spatial discretization and quadratic spline collocation method

Let $\otimes$ denotes the notation of Kronecker product, $\|\ .\ \|$ the Euclidean norm on $\mathbb{R}^{n+1+H}$ and $S^{(k)}$ the k^{th} derivative of a function S.

In this section we construct a quadratic spline which approximates the solution V of problem (2.6), in the interval $[0,L] \subset \mathbb{R}$.

Let $\Theta = \{0 = z_{-2} = z_{-1} = z_0 < z_1 < \cdots < z_{n-1} < z_n = z_{n+1} = z_{n+2} = L\}$ be a subdivision of the interval $[0,L]$. Without loss of generality, we put $z_i = a + ih$, where $0 \leq i \leq n$ and $h = \frac{L}{n}$. Denote by $\mathbb{S}_3([0,L],\Theta) := \mathbb{P}_2^1([0,L],\Theta)$ the space of piecewise polynomials of degree less than or equal to 2 over the subdivision Θ and of class C^1 everywhere on $[0,L]$. Let B_i, $i = -2,\cdots,n-1$, be the B-splines of degree 2 associated with Θ. These B-splines are positives and form a basis of the space $S_3([0,L],\Theta)$.

Consider the local linear operator Q_2 which maps the function V onto a quadratic spline space $\mathbb{S}_3([0,L],\Theta)$ and which has an optimal approximation order. This operator is the discrete C^1 quadratic quasi-interpolant (see [16]) defined by

$$Q_2V = \sum_{i=-2}^{n-1} \mu_i(V) B_i,$$

where the coefficients $\mu_j(V)$ are determined by solving a linear system of equations given by the exactness of Q_2 on the space of quadratic polynomial functions $\mathbb{P}_2([0,L])$. Precisely, these coefficients are defined as follows:

$$\begin{cases} \mu_{-2}(V) = V(z_0) = V(0), \\ \mu_{-1}(V) = \frac{1}{6}(-2V(z_0) + 9V(z_1) - V(z_2)), \\ \mu_j(V) = \frac{1}{8}(-V(z_{j-1}) + 10V(z_j) - V(z_{j+1})), \text{ for } j = 0,...,n-3, \\ \mu_{n-2}(V) = \frac{1}{6}(-V(z_{n-2}) + 9V(z_{n-1}) - 2V(z_n)), \\ \mu_{n-1}(V) = V(z_n) = V(L). \end{cases}$$

It is well known (see e.g. [6], chapter 5) that there exists constants C_k, $k = 0,1,2$, such that, for any function $V \in C^3([0,L])$,

$$\|V^{(k)} - Q_2V^{(k)}\|_H \leq C_k h^{3-k} \|V^{(3-k)}\|_H, \qquad k = 0,1,2, \tag{3.1}$$

By using the boundary conditions of problem (2.6), we obtain $\mu_{-2}(V) = Q_2V(0) = V(0) = \beta.I_H$. Hence

$$Q_2V = \beta B_{-2}I_H + S,$$

where

$$S = \left[\sum_{j=-1}^{n-1} \mu_j(V_1)B_j, \cdots, \sum_{j=-1}^{n-1} \mu_j(V_H)B_j\right]^T.$$

From equation: (3.1), we can easily see that the spline S satisfies the following equation

$$PS^{(1)}(z_j) + RS^{(0)}(z_j) = g(z_j) + O(h).I_H, \quad j = 0, ..., n \tag{3.2}$$

with

$$g(z_j) = \widehat{f}(z_j) - (P\beta B_{-2}^{(1)}(z_j) + R\beta B_{-2}^{(0)}(z_j)) \in \mathbb{R}^H, \quad j = 0, ..., n.$$

The goal of this section is to compute a quadratic spline collocation $\widetilde{Sp}_i = \sum_{j=-2}^{n-1} \widetilde{c}_{j,i}B_j,\ i = 1, ..., H$ which satisfies the equation (2.6) at the points $\tau_j,\ j = 0, ..., n+2$ with $\tau_0 = z_0,\ \tau_j = \dfrac{z_{j-1} + z_j}{2}$, $j = 1, \cdots, n$, $\tau_{n+1} = z_{n-1}$ and $\tau_{n+2} = z_n$.
Then, it is easy to see that

$$\widetilde{c}_{-2,i} = \beta, \text{ for } i = 1, ..., H$$

Hence

$$\widetilde{Sp}_i = \beta B_{-2}I_H + \widetilde{S}_i, \qquad \text{where} \quad \widetilde{S}_i = \sum_{j=-1}^{n-1} \widetilde{c}_{j,i}B_j, \text{ for } i = 1, ..., H$$

and the coefficients $\widetilde{c}_{j,i}$, $j = -1, ..., n-1$ and $i = 1, ..., H$ satisfy the following collocation conditions :

$$P\widetilde{S}^{(1)}(\tau_j) + R\widetilde{S}^{(0)}(\tau_j) = g(\tau_j), \quad j = 1, ..., n+1, \tag{3.3}$$

where

$$\widetilde{S} = [\widetilde{S}_1, ..., \widetilde{S}_H]^T,$$
$$g(\tau_j) = \widehat{f}(\tau_j) - (P\beta B_{-2}^{(1)}(\tau_j) + R\beta B_{-2}^{(0)}(\tau_j)) \in \mathbb{R}^H, \quad j = 1, ..., n+1.$$

Taking

$$C = [\mu_{-1}(V_1), ..., \mu_{n-1}(V_1), ..., \mu_{-1}(V_H), ..., \mu_{n-1}(V_H)]^T \in \mathbb{R}^{n+1+H},$$
$$\widetilde{C} = [\widetilde{c}_{-1,1}, ..., \widetilde{c}_{n-1,1}, ..., \widetilde{c}_{-1,H}, ..., \widetilde{c}_{n-1,H}]^T \in \mathbb{R}^{n+1+H},$$

and using equations (3.2) and (3.3), we get:

$$\left(P \otimes A_h^{(1)} + R \otimes A_h^{(0)}\right) C = F + E, \tag{3.4}$$

and

$$\left(P \otimes A_h^{(1)} + R \otimes A_h^{(0)}\right) \widetilde{C} = F, \tag{3.5}$$

with

$$F = [g_1, ..., g_{n+1}]^T \text{ and } g_j = \frac{1}{\Delta t} g(\tau_j) \in \mathbb{R}^H,$$
$$E = [O(\frac{h}{\Delta t}), ..., O(\frac{h}{\Delta t})]^T \in \mathbb{R}^{n+1+H},$$
$$A_h^{(k)} = (B_{-2+p}^{(k)}(\tau_j))_{1 \le j,p \le n+1}, \quad k = 0, 1.$$

It is well known that $A_h^{(k)} = \dfrac{1}{h^k} A_k$ for $k = 0, 1$ where matrices A_0 and A_1 are independent of h, with the matrix A_1 is invertible [13].

Then, relations (3.4) and (3.5) can be written in the following form

$$(P \otimes A_1)(I + U)\, C = hF + hE, \tag{3.6}$$

$$(P \otimes A_1)(I + U)\, \widetilde{C} = hF, \tag{3.7}$$

with

$$U = h(P \otimes A_1)^{-1}(R \otimes A_0). \tag{3.8}$$

In order to determine the bounded of $\| C - \widetilde{C} \|_\infty$, we need the following Lemma.

Lemma 3.1. *If $h^2 \rho < \dfrac{\Delta t}{4}$, then $I + U$ is invertible, where $\rho = \|(P \otimes A_1)^{-1}\|_\infty$.*

Proof . From the relation (3.8) and $\|A_0\|_\infty \leq 1$, We have

$$\begin{aligned} \|U\|_\infty &\leq h\|(P \otimes A_1)^{-1}\|_\infty \|(R \otimes A_0)\|_\infty, \\ &\leq h\rho\|(R \otimes A_0)\|_\infty, \\ &\leq h\rho\|R\|_\infty. \end{aligned}$$

For h sufficiently small, we conclude

$$\|U\|_\infty < 1. \tag{3.9}$$

Therefore $I + U$ is invertible. □

From (3.7), we get $\widetilde{C} = h(I + U)^{-1}(P \otimes A_1)^{-1} F$.

Proposition 3.2. *If $h \leq \dfrac{\triangle t}{\rho}$, then there exists a constant K_1 which depends only on the functions p, q, l and g such that*

$$\|C - \widetilde{C}\| \leq cte\ h. \tag{3.10}$$

Proof . Assume that $h \leq \dfrac{\triangle t}{\rho}$. According to Lemma 3.1 and relations (3.6) and (3.7), we have $C - \widetilde{C} = h(I + U)^{-1}(P \otimes A_1)^{-1} E$. Since $E = O(\dfrac{h}{\triangle t})$, then there exists a constant K_1 such that $\|E\| \leq K_1 \dfrac{h}{\triangle t}$. This implies that

$$\begin{aligned} \|C - \widetilde{C}\| &\leq h\|(I + U)^{-1}\|_\infty \|(P \otimes A_1)^{-1}\|_\infty \|E\|, \\ &\leq \frac{h\rho}{\triangle t}\|(I + U)^{-1}\|_\infty K_1 h, \\ &\leq \|(I + U)^{-1}\|_\infty K_1 h, \\ &\leq \frac{1}{1 - \|U\|_\infty} K_1 h, \\ &\leq cte\ h. \end{aligned}$$

Finally, we deduce that

$$\|C - \widetilde{C}\| \leq cte\ h.$$

□

Now, we are in position to prove the main theorem of our work.

Proposition 3.3. *The quadratic-spline approximation $\widetilde{Sp}$ converges to the exact solution V of the boundary value problem (2.6) with order one by the $\|.\|_H$ norm, i.e., $\|V - \widetilde{Sp}\|_H = O(h)$.*

Proof . From the relation (3.1), we have
$\|V - Q_2(V)\|_H = O(h)$, so $\|V - Q_2(V)\|_H \leq Kh$, where K is a positive constant. On the other hand we have

$$Q_2(V_i(x)) - \widetilde{Sp}_i(x) = \sum_{j=-1}^{n-1} (\mu_j(V_i) - \widetilde{c}_{j,i}) B_j(x), \text{ for } i = 1, ..., H.$$

Therefore, by using (3.10) and $\sum_{j=-1}^{n-1} B_j(x) \leq 1$, we get

$$|Q_2(V_i(x)) - \widetilde{Sp}_i(x)| \leq \|C - \widetilde{C}\| \sum_{j=-1}^{n-1} B_j(x) \leq \|C - \widetilde{C}\| \leq K_1 h, \text{ for } i = 1, ..., H.$$

Since $\|Q_2(V) - \widetilde{Sp}\|_H \leq \|V - Q_2(V)\|_H + \|Q_2(V) - \widetilde{Sp}\|_H$, we deduce the stated result. $\square$

Theorem 3.4. If we assume that the discretization parameters h and Δt satisfy the following relation

$$h \leq \frac{\triangle t}{\rho}, \tag{3.11}$$

and we suppose that $V(z,t)$ is the solution of (1.1) and $V_c(z,t)$ is the approximate solution by our presented method, then we have,

$$\|V(z, t_m) - V_c(z, t_m)\|_\infty \leq cte(\triangle t^2 + h),$$

where cte, is finite constant. Therefore for sufficiently small $\triangle t$ and h, the solution of presented scheme (3.4-3.5) converges to the solution of initial boundary value problem (1.1) in the discrete L_∞-norm and the rates of convergence are $O(\triangle t^2 + h)$.

4. Numerical examples

In this section we verify experimentally theoretical results obtained in the previous section. If the exact solution is known, then at time $t \leq T$ the maximum error E^{max} can be calculated as:

$$E^{max} = \max_{z \in [0,L], t \in [0,T], 1 \leq i \leq H} | S_i^{M,N}(z,t) - V_i(z,t) | .$$

Otherwise it can be estimated by the following double mesh principle:

$$E^{max}_{M,N} = \max_{z \in [0,L], t \in [0,T], 1 \leq i \leq H} | S_i^{M,N}(z,t) - S_i^{2M,2N}(z,t) |,$$

where $S_i^{M,N}(z,t)$ is the numerical solution on the $M+1$ grids in space and $N+1$ grids in time, and $S_i^{2M,2N}(z,t)$ is the numerical solution on the $2M+1$ grids in space and $2N+1$ grids in time, for $1 \leq i \leq H$.

We present two examples to better illustrate the use of the quadratic spline collocation approach and the proposed evaluation methodology in concrete situations. These examples are concerned with isothermal and nonisothermal plug flow reactor respectively.

4.1. Example 1: isothermal plug flow reactor

Consider the model state equations representing material balances in the reactor (see [19]) exactly match the mathematical model (1.1) with:

$$
\begin{aligned}
&\Omega = (0,10)\times(0,1), \text{ and } \vartheta = 2,\\
&V(z,t) = [c_x(z,t) \;\; c_y(z,t)]^T,\\
&f(V(z,t)) = c_x(z,t)^2,\\
&u(t) = [0 \;\; 0]^T,\\
&K = [-2.63 \;\; 0.00109]^T,\\
&\alpha(z) = [-0.1z+1.5 \;\; 0.05z+0.5]^T,\\
&\beta(t) = [4.10^{-3}t^2 - 0.09t + 1.5 \;\; 0]^T,\\
&C = \begin{bmatrix} 0 & 0 \\ 0 & -0.00109 \end{bmatrix}.
\end{aligned}
$$

Table 1: Numerical results for Example 1.

N	10	20	40	80	160
M	5	10	20	40	80
max_error	2.660×10^{-2}	1.140×10^{-2}	5.225×10^{-3}	2.493×10^{-3}	1.217×10^{-3}

Table 1 shows values of the maximum error (max_error) obtained in our numerical experiments for different values of N, and M, we note the convergence of the solution S to the function V depends on the discretization parameters h, and Δt. Theorem 3.4 is shown the convergence of the method provided that the parameters h and Δt satisfy the relation (3.11). Moreover, the numerical error estimates behave like which confirms what we are expecting.

4.2. Example 2: nonisothermal plug flow reactor

Consider the mathematical model of the plug flow reactor (see [2]) exactly matches the mathematical model (1.1) with:

$$
\begin{aligned}
&\Omega = (0,10)\times(0,1) \text{ and } \vartheta = 2,\\
&V(z,t) = [c_x(z,t) \;\; T(z,t)]^T,\\
&f(V(z,t)) = 5.10^{12}c_x(z,t),\\
&u(t) = [0.01 \;\; 74585.07455507456]^T,\\
&K = [-1 \;\; -17065.897]^T,\\
&\alpha(z) = [0.5 \;\; 300]^T,\\
&\beta(t) = [0.5\sin(0.1t+2000)+2 \;\; 0.1625t+300]^T,\\
&C = \begin{bmatrix} -0.1 & 0 \\ 0 & -240.6002405002405 \end{bmatrix}.
\end{aligned}
$$

Table 2: Numerical results for Example 2.

N	10	20	40	80	160
M	5	10	20	40	80
max_error	2.100×10^{-2}	0.900×10^{-2}	4.125×10^{-3}	1.968×10^{-3}	0.960×10^{-3}

Table 2 shows values of the maximum error (max_error) obtained in our numerical experiments for different values of N and M, we note the convergence of the solution S to the function V depends on the discretization parameters h and Δt. Theorem 3.4 is shown the convergence of the method provided that the parameters h and Δt satisfy the relation (3.11). Moreover, the numerical error estimates behave like which confirms what we are expecting.

5. Conclusion

In this paper, a quadratic spline collocation approach is prosed in the context to be used for reducing a nonlinear PDEs plug flow reactors models for numerical simulation and/or control design. After a brief review of the nonlinear tubular reactor model in consideration, we present the details of our methodology which consists of first discretizing in time (by Crank-Nicolson scheme) and then collocating in space (by a quadratic spline collocation method). The two test problems which are studied in this paper demonstrate that this approach is an efficient alternative and confirm the theoretical behavior of the rates of convergence.

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