A CUBIC SPLINE COLLOCATION METHOD FOR INTEGRATING A CLASS OF CHEMICAL REACTOR EQUATIONS

N. Barjes*, A. EL Hajaji**, A. Serghini***, K. Hilal* and E.B. Mermri****
*LMC Laboratory, FST, University of Sultan Moulay Slimane, Morocco
**LERSEM Laboratory, ENCGJ, University of Chouaïb Doukkali, Morocco.
***LANO Laboratoty, FSO-ESTO, University Mohammed First, Morocco.
****Department of Mathematics and Computer Science, Faculty of Science, University Mohammed Premier, Morocco.

ABSTRACT
In this paper, the cubic spline collocation method is implemented to find the numerical solution of 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 numerical simulations. We use the horizontal method of lines to discretize the temporal variable and the spatial variable by means of a Crank-Nicolson, and a cubic spline collocation method on meshes, respectively. The method is shown to be unconditionally stable and second order accurate with respect to both the variables. Numerical results are presented and compared with other collocation methods given in the literature.

KEYWORDS: Partial differential equations, Distributed parameter systems, Plug flow reactors, Cubic Spline collocation method.
MSC: 65D07.

RESUMEN
En este trabajo se implementa un método de colocación con splines cúbico para resolver numéricamente las ecuaciones en derivadas parciales que resultan de modelar el flujo de conexión de un reactor. Se discretiza la variable temporal mediante el método horizontal de líneas y las espaciales por el enfoque de Crank-Nicholson y el método de colocación de splines cúbico. Este enfoque es estable y tiene un grado de precisión de segundo orden con respecto a ambas variables. Los resultados obtenidos se comparan con otros métodos de este tipo que aparecen en la literatura.

PALABRAS CLAVE: Ecuaciones en derivadas parciales, sistemas de parámetros distribuidos, flujo de conexión de un reactor, método de colocación con splines cúbico

1. INTRODUCTION

In recent years much attention has been given to the numerical resolution of ODEs and particular interest has been given to resolte the nonlinear partial differential equations PDEs of a plug flow reactor models. These types of problems arise in various fields of science and engineering such as fluid mechanics, physics, chemistry, mechanics, chemical reactor theory, convection diffusion processes, optimal control and other branches of applied mathematics, 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]).

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 cubic B-spline collocation method is widely used in practice because it is computationally inexpensive, easy to implement and gives high-order accuracy. In our paper, we consider a cubic spline relative to a vector of multiple knots in the boundary and collocation points the mid-points of the knots to increase the number of control points and to avoid peaks at the ends, by against the authors (see [10]) used a cubic spline relative to a vector of knots simple, shows a series of peaks at the boundary. 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 cubic 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

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

In the above equations, $V = V(z,t) \in \mathbb{R}^H$ 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

$$\begin{cases} \dfrac{\partial V}{\partial t} + P\dfrac{\partial V}{\partial z} - CV &= I(V(z,t)), \quad (z,t) \in \Omega, \\ V(z,0) &= \alpha(z), \qquad z \in \Omega_z, \\ V(0,t) &= \beta(t), \qquad t \in \Omega_t, \end{cases} \tag{1.2}$$

where

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

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 $V \in C(\overline{\Omega}) \bigcap C^{2,1}(\Omega)$ 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 cubic spline collocation method for the spatial discretization. The scheme is two-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 cubic spline collocation method and we will give the stability and error analysis of proposed method. Next, the error bound of the spline solution is analyzed, some numerical results are given in Section 4 to validate monitoring tool and compare the method to the results given in [20]. Finally, the paper is closed with some concluding remarks and perspectives depicted in Section 5.

2. TIME DISCRETIZATION AND DESCRIPTION OF THE CRANK-NICOLSON SCHEME

The first step in the method is to consider the Crank-Nicolson scheme (CNS) to adequately represent the original equation. This method provides a precise framework to handel the nonlinearity providing a global linear behavior of the dynamic.
Let 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

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

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:

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

where, for any $m\geq 0$ 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 gives the order of convergence of the solution V^{m} to $V(z,t)$.

Theorem 2.1. *Problem (2.2) is second order convergent ie.*

$$\|V(z,t_{m})-V^{m}\|_{H}\leq Cte(\Delta t)^{2}.$$

Proof. The proof is similar the one of Theorem 2.1 in [20]. □

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

$$\left\{\begin{array}{rcl} PV'(z)+RV(z) & = & \widehat{f}(z)\in\mathbb{R}^{H}, \quad \forall z\in[0,L],\\ V(0) & = & \beta.I_{H}, \end{array}\right. \tag{2.3}$$

The second step will focus on the solution of problem (2.3).
The convenient of using this technique is that it transform the dynamic from a nonlinear distributed parameter system to a linear ODE system form, using a global linearization in contrast of several methods given until now. Furthermore, the method is shown to be second order accurate.

3. SPATIAL DISCRETIZATION

In this section we construct the totally discrete scheme by using a cubic spline collocation method in the spatial direction.

3.1. Description of Cubic 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 cubic spline which approximates the solution V of problem (2.3), in the interval $[0, L] \subset \mathbb{R}$.

Let $\Theta = \{0 = z_{-3} = z_{-2} = z_{-1} = z_0 < z_1 < \cdots < z_{n-1} < z_n = z_{n+1} = z_{n+2} = z_{n+3} = L\}$ 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 $h = \dfrac{L}{n}$. Denote by $\mathbb{S}_4([0, L], \Theta) = \mathbb{P}_3^2([0, L], \Theta)$ the space of piecewise polynomials of degree less than or equal to 3 over the subdivision Θ and of class C^2 everywhere on $[0, L]$. Let B_i, $i = -3, \cdots, n-1$, be the B-splines of degree 3 associated with Θ. These B-splines are positives and form a basis of the space $S_4([0, L], \Theta)$.
Consider the local linear operator Q_3 which maps the function V onto a cubic spline space $\mathbb{S}_4([0, L], \Theta)$ and which has an optimal approximation order. This operator is the discrete C^2 cubic quasi-interpolant (see [16]) defined by

$$Q_3 V = \sum_{i=-3}^{n-1} \mu_i(V) B_i,$$

where the coefficients $\mu_j(V)$ are determined by solving a linear system of equations given by the exactness of Q_3 on the space of cubic polynomial functions $\mathbb{P}_3([0, L])$. Precisely, these coefficients are defined as follows:

$$\begin{cases} \mu_{-3}(V) = V(z_0) = V(0), \\ \mu_{-2}(V) = \frac{1}{18}(7V(z_0) + 18V(z_1) - 9V(z_2) + 2V(z_3)), \\ \mu_j(V) = \frac{1}{6}(-V(z_{j+1}) + 8V(z_{j+2}) - V(z_{j+3})), -1 \leq j \leq n-3, \\ \mu_{n-2}(V) = \frac{1}{18}(2V(z_{n-3}) - 9V(z_{n-2}) + 18V(z_{n-1}) + 7V(z_n)), \\ \mu_{n-1}(V) = V(z_n) = V(L). \end{cases}$$

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

$$\|V^{(k)} - Q_3 V^{(k)}\|_H \leq C_k h^{2-k} \|V^{(2-k)}\|_H, \quad k = 0, 1, \tag{3.1}$$

By using the boundary conditions of problem (2.3), we obtain $\mu_{-3}(V) = Q_3 V(0) = V(0) = \beta.I_H$.
In order to uniquely determine a solution, by differentiating Eq. (2.3) with respect to variable $z = 0$, we get

$$\begin{cases} -12P\mu_{-2}(V) + (P + 3hR)\mu_{-1}(V) = 6h^2 \widehat{f}'(z) - (6P - 3hR)\beta.I_H, \\ 4hR\mu_{-2}(V) + (3P + hR)\mu_{-1}(V) = 6h\widehat{f}(z) - (-3P + hR)\beta.I_H. \end{cases}$$

Hence

$$Q_3 V = \mu_{-3}(V) B_{-3} I_H + \mu_{-2}(V) B_{-3} I_H + S,$$

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

$$PS^{(1)}(z_j) + RS^{(0)}(z_j) = g(z_j) + O(h^2).I_H, \;\; j = 0, ..., n \tag{3.2}$$

with

$$g(z_j) = \widehat{f}(z_j) - \beta(PB_{-3}^{(1)}(z_j) + RB_{-3}^{(0)}) - \mu_{-2}(PB_{-2}^{(1)}(z_j) + RB_{-2}^{(0)}(z_j)),$$

is element of $\mathbb{R}^H$, for $j = 0, ..., n$.

The goal of this section is to compute a cubic spline collocation $\widetilde{Sp}_i = \sum_{j=-2}^{n-1} \widetilde{c}_{j,i} B_j, i = 1, ..., H$ which satisfies the equation (2.3) at the points τ_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

$$\widetilde{c}_{-3,i} = \beta, \text{ for } i = 1, ..., H$$

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

Hence

$$\widetilde{Sp}_i = \beta B_{-3} I_H + \widetilde{c}_{-2,i} B_{-2} I_H + \widetilde{S}_i,$$

where $\widetilde{S}_i = \sum_{j=-1}^{n-1} \widetilde{c}_{j,i} B_j$, 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

$$\begin{aligned}
&\widetilde{S} = [\widetilde{S}_1, ..., \widetilde{S}_H]^T, \\
&g(\tau_j) = \widehat{f}(\tau_j) - \beta(PB_{-2}^{(1)}(\tau_j) + RB_{-2}^{(0)}(\tau_j)) \\
&-\widetilde{c}_{-2,i}(PB_{-2}^{(1)}(\tau_j) + RB_{-2}^{(0)}(\tau_j)) \in \mathbb{R}^H, \quad j = 1, ..., n+1.
\end{aligned}$$

Taking

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

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

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

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 3.1. *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*

$$\|c - \widetilde{c}\| \leq cte\ h^2. \tag{3.10}$$

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 $E = O(\dfrac{h^2}{\triangle t})$, then there exists a constant K_1 such that $\|E\| \leq K_1\dfrac{h^2}{\triangle t}$. This implies that

$$\begin{aligned}
\|c - \widetilde{c}\| &\leq h\|(I+U)^{-1}\|_\infty \|(P \otimes A_1)^{-1}\|_\infty \|E\| \\
&\leq \frac{h\rho}{\triangle t}\|(I+U)^{-1}\|_\infty K_1 h^2 \\
&\leq \|(I+U)^{-1}\|_\infty K_1 h^2. \\
&\leq \frac{1}{1-\|U\|_\infty} K_1 h^2. \\
&\leq cte\ h^2.
\end{aligned}$$

Finally, we deduce that

$$\|c - \widetilde{c}\| \leq cte\ h^2.$$

□

3.2. Convergence analysis

Proposition 3.2. *The cubic-spline approximation $\widetilde{Sp}$ converges quadratically to the exact solution V of problem (2.3), i.e., $\|V - \widetilde{Sp}\|_H = O(h^2)$.*

Proof. From the relation (3.1), we have
$\|V - Q_3(V)\|_H = O(h^2)$, so $\|V - Q_3(V)\|_H \leq Kh^2$, where K is a positive constant. On the other hand we have

$$Q_3(V_i(z)) - \widetilde{Sp}_i(z) = \sum_{j=-1}^{n-1} (\mu_j(V_i) - \widetilde{c}_{j,i}) B_j(x), \text{ for } i = 1, ..., H$$

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

$$|Q_3(V_i(z)) - \widetilde{Sp}_i(z)| \leq \|c - \widetilde{c}\| \sum_{j=-1}^{n-1} B_j(z) \leq \|c - \widetilde{c}\| \leq K_1 h^2, \text{ for } i = 1, ..., H.$$

Since $\|Q_3(V) - \widetilde{Sp}\|_H \leq \|V - Q_3(V)\|_H + \|Q_3(V) - \widetilde{Sp}\|_H$, we deduce the stated result.

Theorem 3.1. *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 according to the proposed method, then we have,

$$\|V - V_c\|_\infty = \begin{cases} C_1(\triangle t^2 + h), \text{ for quadratic spline (see, [20]),} \\ C_2(\triangle t^2 + h^2), \text{ for cubic spline .} \end{cases}$$

where C_1 and C_2 are finite constants. 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 $O(\triangle t^2 + h)$ and $O(\triangle t^2 + h^2)$.

□

3.3. Stability analysis

We will now show that the fully discretized collocation cubic spline method is stable.
The collocation procedure for solving boundary value problem (2.3) given by (3.7), i.e.,

$$A\widetilde{c} = G \text{ where } A = (P \otimes A_1)(I + U) \text{ and } G = hF,$$

is said to be stable if for a perturbation of the data, i.e.,

$$(A + \Gamma)\widetilde{\widetilde{c}} = G + \delta \text{ and } \widetilde{\widetilde{S}}(t_i) = \widetilde{S}(t_i) + \delta_i \text{ for } i = 1, ..., n+1$$

there exists positive constants k_1, k_2 and k_3 independent of n and G in $\overline{\Omega}_x$, such that for all sufficiently large n

$$(A+\Gamma)\tilde{\tilde{c}} = G + \delta. \tag{3.12}$$

The equation (3.12) has a unique solution for $\|\Gamma\|_\infty \le k_1$ and

$$\|\tilde{\tilde{S}} - \tilde{S}\|_\infty \le k_2\|\Gamma\|_\infty + k_3\|\tilde{\delta}\|_\infty$$

where, $\delta = (\delta_1, \delta_2, ..., \delta_{n+1})$ and $\tilde{\delta} = (\delta_0, \delta_1, ..., \delta_{n+2})$.
The functions $\tilde{S}$ and $\tilde{\tilde{S}}$ are uniquely determined by $\tilde{c}_j$ and $\tilde{\tilde{c}}_j$, $-2 \le j \le n-2$ in (3.7) and (3.12) respectively.

Theorem 3.2. *The collocation procedure (3.7) for solving boundary value problem (2.3) is stable.*

Proof. As we know that $\|A^{-1}\|_\infty \le \|(P\otimes A_1)^{-1}\|_\infty \| \left(I+U\right)^{-1}\|_\infty \le \dfrac{\rho}{1-\|U\|_\infty} = k$, for $n \ge n_0$, where n_0 is sufficiently large positive real number and k is a constant. Choose a positive constant $k_1 < \frac{1}{2k}$. Then whenever $\|\Gamma\|_\infty \le k_1$, $(A+\Gamma)^{-1} = (I + A^{-1}\Gamma)^{-1}A^{-1}$ exists because

$$\|A^{-1}\Gamma\|_\infty \le \|A^{-1}\|_\infty\|\Gamma\|_\infty \le \frac{1}{2}.$$

and in fact $\|(A+\Gamma)^{-1}\|_\infty \le 2k,$ for $n \ge n_0$. After subtracting (3.7) from (3.12), we get

$$(A+\Gamma)\tilde{\tilde{c}} - A\tilde{c} - \Gamma\tilde{c} = \delta - \Gamma\tilde{c},$$

involving that

$$\|\tilde{\tilde{c}} - \tilde{c}\|_\infty \le 2k(\|\delta\|_\infty + \|\Gamma\|_\infty\|\tilde{c}\|_\infty).$$

As it is assumed that f, u, α and β are sufficiently smooth on $\overline{\Omega}$ and

$$\left|\frac{\partial^i V(z,t)}{\partial z^i}\right| \le k \text{ on } \overline{\Omega} \text{ for } 0 \le i \le 4,$$

so f^{m+1}, u^{m+1}, α^{m+1} and β^{m+1} will be sufficiently smooth on $\overline{\Omega}$ and

$$\left|\frac{\partial^i V^{m+1}}{\partial z^i}\right| \le k \text{ on } \overline{\Omega} \text{ for } 0 \le i \le 4, \text{ and } m = 0, 1, ..., M-1.$$

Further, since $V(\tau_i) = S(\tau_i)$ for all $i = 1, ..., n+1$ and the inverse of the collocation matrix is bounded, i.e., $\|A^{-1}\|_\infty \le k$ and $\|\tilde{c}\|_\infty \le r$, with $r > 0$, So

$$\|\tilde{\tilde{c}} - \tilde{c}\|_\infty \le 2k(\|\delta\|_\infty + r\|\Gamma\|_\infty). \tag{3.13}$$

Now, since (3.13) therefore with the help of relation $\tilde{\tilde{S}} = \tilde{S} + \delta_i$ for $i = 0, .., n+2$, we have

$$\max_{-2\le j\le n-2} |\tilde{\tilde{c}}_j - \tilde{c}_j| \le 2kr\|\Gamma\|_\infty + (1+2k)\|\delta\|_\infty.$$

Further,

$$\tilde{\tilde{S}}(z) - \tilde{S}(z) = \sum_{-2\le j\le n-2} (\tilde{\tilde{c}}_j - \tilde{c}_j)B_j(z).$$

So

$$|\tilde{\tilde{S}}(\tau_i) - \tilde{S}(\tau_i)| \le \max_{-2\le j\le n-2} |\tilde{\tilde{c}}_j - \tilde{c}_j| \sum_{-2\le j\le n-2} |B_j(\tau_i)|, \text{ for } i = 1, ..., n+1,$$

and like $\displaystyle\sum_{-2\le j\le n-2} |B_j(\tau_i)| \le 1$, therefore

$$\|\tilde{\tilde{S}} - \tilde{S}\|_\infty \le k_2\|\Gamma\|_\infty + k_3\|\tilde{\delta}\|_\infty,$$

where $k_2 = kr$ and $k_3 = 1 + 2k$. □

4. NUMERICAL IMPLEMENTATION 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:

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

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

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

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 $1 \leq i \leq H$. As examples, in this parer we are only considering chemical reactor examples in numerical resolution. Nevertheless such technic can be also applied to bio-reactors where biological process are taking place.

4.1. Example 1: isothermal plug flow reactor

Consider the model state equations representing material balances in the isothermal plug flow reactor reactor with length $L = 20m$ where irreversible consecutive reactions $x \to y \to z$ take place in liquid phase. If the volume of the reactor, densities and heat capacities are constants, if the heat losses, diffusion and dispersion are negligible and under conditions of perfect radial mixing, the model state equations representing material blances in the reactor (see [19]) exactly match the mathematical model (1.1) with:

$\Omega = (0,10) \times (0,1)$, and $\vartheta = 2$,

$V(z,t) = [c_x(z,t) \;\; c_y(z,t)]^T$,

$f(V(z,t)) = c_x(z,t)^2$,

$u(t) = [0 \;\; 0]^T$,

$K = [-2.63 \;\; 0.00109]^T$,

$\alpha(z) = [-0.1z + 1.5 \;\; 0.05z + 0.5]^T$,

$\beta(t) = [4.10^{-3}t^2 - 0.09t + 1.5 \;\; 0]^T$,

$$C = \begin{bmatrix} 0 & 0 \\ 0 & -0.00109 \end{bmatrix}.$$

Where $c_x(z,t)$ and $c_y(z,t)$ denote the concentration of x and y within the reactor.

We now use the cubic spline collocation method (3.7) in this paper and the quadratic spline collocation method in (see [20]) to solve the above problem numerically. For comparison, Table 1 lists the maximum error (max_error) obtained in the numerical experiments for different time of Δt, and spatial h. It is seen from Table 1 that the cubic spline collocation method (3.7) given here is more accurate than the quadratic spline collocation method in (see [20]) for the same spatial step h. We also see from Table 1 that the cubic spline collocation method (3.7) in this paper possesses the second order spatial accuracy, whereas the quadratic spline collocation method in (see [20]) has only the first-order spatial accuracy.

4.2. Example 2: nonisothermal plug flow reactor

Now; let us consider the mathematical model of a nonisothermal plug flow reactor where a first-order reaction of the form $x \to y$ takes place in liquid phase (see [2]). The dynamic exactly matches the mathematical model (1.1) with:

$\Omega = (0, 10) \times (0, 1)$ and $\vartheta = 2$,

$V(z,t) = [c_x(z,t) \;\; T(z,t)]^T$,

$f(V(z,t)) = 5.10^{12} c_x(z,t)$,

$u(t) = [0.01 \;\; 74585.07455507456]^T$,

$K = [-1 \;\; -17065.897]^T$,

$\alpha(z) = [0.5 \;\; 300]^T$,

$\beta(t) = [0.5 \sin(0.1t + 2000) + 2 \;\; 0.1625t + 300]^T$,

$$C = \begin{bmatrix} -0.1 & 0 \\ 0 & -240.6002405002405 \end{bmatrix}.$$

As in the previous example, satisfactory results are given in Table 2. In both the examples, the initial and boundary conditions are considered axial varying and time-varying respectively, but one may reproduce the simulation results by considering constant values for these conditions.

Table 2 shows values of the maximum error (max_error) obtained in the 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 3.1 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. Furthermore, it is important to remark that this monitoring tool is also able to handel nonlinearity, caused by disturbances, providing satisfactory monitoring results.

Table 1: Numerical results for Example 1.

N	10	20	40	80	160
M	5	10	20	40	80
our max_error	1.056×10^{-3}	2.639×10^{-4}	0.659×10^{-4}	0.164×10^{-4}	0.411×10^{-5}
max_error in [20]	2.660×10^{-2}	1.140×10^{-2}	5.225×10^{-3}	2.493×10^{-3}	1.217×10^{-3}

Table 2: Numerical results for Example 2.

N	10	20	40	80	160
M	5	10	20	40	80
our max_error	1.024×10^{-3}	0.255×10^{-3}	0.639×10^{-4}	1.595×10^{-5}	0.398×10^{-5}
max_error in [20]	2.100×10^{-2}	0.900×10^{-2}	4.125×10^{-3}	1.968×10^{-3}	0.960×10^{-3}

5. CONCLUSION

In this paper, a cubic spline collocation approach is prosed in the context to be used for reducing a nonlinear PDEs plug flow reactors models for numerical simulation. Some efforts have been made to handel the nonlinear behaviour. After a brief review of the nonlinear tubular reactor model in consideration, we present the details of the given monitoring which consists of first discretizing in time (by Crank-Nicolson scheme) and then collocating in space (by a cubic spline collocation method). In spite of the large number of the discretization points required by the SCM. The two test problems which are studied in this paper demonstrate that this approach is an efficient alternative since it is unconditionally stable and confirm the theoretical behavior of the rates of convergence.

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