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Numerical Solution of Fractional Boundary Value Problem in Chemical Engineering using the Shooting Method

Resolução Numérica de Problemas de Valor no Contorno Fracionários em Engenharia Química usando o Método do Chute Simples

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ABSTRACT

This work presents a systematic approach to solving Fractional Ordinary Differential Equations (FODEs) of boundary value problems using the Shooting Method. This approach converts a boundary value problem into an initial value problem by defining sensitivity equations. The Predictor-Corrector Method with Caputo-type fractional derivative is used to integrate this system. The proposed approach is evaluated considering three case studies in Chemical Engineering. The results demonstrate that the proposed approach is a good alternative to solve this class of problems. In addition, as expected, the obtained profiles were dependent on fractional order.

Keywords: Fractional Ordinary Differential Equations. Boundary Value Problem. Shooting Method. Numerical Method.

RESUMO

Este trabalho tem por objetivo apresentar uma metodologia sistemática para a resolução numérica de Equações Diferenciais Ordinárias Fracionárias (EDOF) de valor no contorno usando o Método do Chute Simples. Nesta abordagem o problema de valor no contorno é transformado em um problema de valor inicial via dedução das equações de sensibilidade. Para integrar este sistema utiliza-se o Método Preditor-Corretor Fracionário (MPCF) considerando a derivada fracionária de Caputo. A metodologia proposta é aplicada em três estudos de caso clássicos de Engenharia Química. Os resultados obtidos demonstram que a abordagem proposta se configura como uma boa alternativa para a resolução dessa classe de problemas. Além disso, como esperado, os perfis obtidos são dependentes da ordem fracionária.

Palavras-chave: Equações Diferenciais Ordinárias Fracionárias. Problemas de Valor no Contorno. Chute Simples. Método Numérico.

1. INTRODUCTION

Many physical, chemical, and biological phenomena present inherently non-linear behavior, which implies that modeling these phenomena is complex (GHANDEHARI; RANJABAR, 2013). The complexities can be incorporated into the models by the hypotheses definition, as well as by the generalization of traditional differential models that present integer order for the fractional context, generated in the so-called Fractional Ordinary Differential Equation (FODE) (RODRIGUES; OLIVEIRA, 2015).

The FODEs Systems have been widely applied to Engineering areas such as Fluid Mechanics, Viscoelasticity, Electrochemistry, Heat Transfer, and Control Theory since they can evaluate phenomena with time delay and memory effect (OLIVEIRA; MACHADO, 2014). They have received attention due to their more accurate modeling for systems in which memory and heredity effects are relevant (SUN et al., 2019).

Solving a fractional differential equation problem (analytically or numerically) can be difficult since it is a generalization of traditional differential equations with integer order. Thus, one must choose the type of approximation for the fractional derivative to solve this problem. Liu and Hou (2017) proposed an approach based on the Finite Difference Method for solving partial differential equations using fractional order. Lobato et al. (2020) proposed the extension of the Orthogonal Collocation Method (OCM) to solve fractional partial differential equations as an alternative to minimize the effect of the number of discretization points and, consequently, the dimension of the problem to be analyzed.

The specialized literature presents several definitions concerning fractional derivatives. One of them is the Grünwald-Letnikov proposal, which represents a summation of an infinite series in which the entire order is replaced by an arbitrary order α (LORENZO; HARTLEY, 1998). In addition, there are also those derived from Marchaud, Chen, Hadamard, Riesz, Weyl, Osler, Hilfer, Davidson-Essex, Coimbra, Canavati, Cossar, Jumarie, Caputo-Hadamard, and Hilfer-Katugampola (OLIVEIRA; OLIVEIRA, 2014). These derivatives can approximate fractional terms, transforming the original problem into a purely algebraic equivalent (PODLUBNY, 1999). Riemann-Liouville and Caputo are the most common fractional derivatives, and they are similar. The Caputo-type fractional derivative modifies the definition of the fractional derivative proposed by Riemann-Liouville by changing the order of the derivative and integral operators (CAPUTO, 1993; OLIVEIRA; MACHADO, 2014).

In this context, we propose a systematic approach for the numerical resolution of fractional boundary value problems using the Caputo-type fractional derivative by the Shooting Method associated with the Fractional Predictor-Corrector Method (GARRAPPA, 2009). This work is organized as follows. Section 2 briefly describes the Shooting Method. Section 3 addresses important concepts about Fractional Calculus. The proposed approach is described in Section 4. The results for the three case studies based on Chemical Engineering problems are reported in Section 5. The last section presents the conclusions of this work.

2. SHOOTING METHOD

The Shooting Method is a numerical approach proposed to solve a boundary value problem. This method transforms a boundary value problem into an initial value problem by defining sensitivity equations (DAVIS, 1984). The main advantage is the powerful numerical methods used for solving initial value problems. However, the main disadvantage is that it is not as robust as finite difference or collocation methods (DAVIS, 1984).

To characterize the problem of interest, consider the second-order boundary value problem described as:

$$\frac{d^2y}{dx^2} = F\left(x, y, \frac{dy}{dx}\right), \quad a \leq x \leq b \tag{1}$$

subject to the following boundary conditions:

$$a_0 y(a) - a_1 \left.\frac{dy}{dx}\right|_a = \alpha \tag{2}$$

$$b_0 y(a) + b_1 \left.\frac{dy}{dx}\right|_b = \beta \tag{3}$$

where y is the vector of dependent variables, x is the independent variable, F is the right-hand side of the ordinary differential equations, a and b are the lower and upper limits of the domain, a_0, a_1, b_0, b_1, α, and β are constants that define the characteristics of the boundary value problem.

The above model can be rewritten as an initial value problem represented by Eq.(4)-(6):

$$\frac{d^2u}{dx^2} = f\left(x, u, \frac{du}{dx}\right), \quad a \leq x \leq b \tag{4}$$

$$u(a) = a_1 s - c_1 \alpha \tag{5}$$

$$\left.\frac{du}{dx}\right|_a = a_0 s - c_0 \alpha \tag{6}$$

where u is the vector of dependent variables, f is the right-hand side of the ordinary differential equations, c_0 and c_1 are constants that define the characteristics of the problem, and s is a real parameter. In this problem, the following relation should be satisfied (DAVIS, 1984):

$$a_1 c_0 - a_0 c_1 = 1 \tag{7}$$

Thus, the solution of the model described by Eq.(4)-(6) will be the solution of the model described by Eq.(1)-(3) if the parameter s satisfies the original boundary condition ($\emptyset$) given by:

$$\emptyset(s) \equiv b_0 u(b,s) + b_1 \left.\frac{du}{dx}\right|_{(b,s)} = \beta \tag{8}$$

To find the numerical solution of the second-order ordinary differential equations given by Eq.(4)-(6), it is necessary to convert them into first-order ordinary differential equations defined as:

$$\frac{d\omega}{dx} = v, a \leq x \leq b \tag{9}$$

$$\frac{dv}{dx} = f(x, \omega, v), a \leq x \leq b \tag{10}$$

$$w(a) = a_1 s - c_1 \alpha \tag{11}$$

$$v(a) = a_0 s - c_0 \alpha \tag{12}$$

where ω and v are the auxiliary dependent variables. It is important to mention that this model is defined at the lower limit of the domain ($x = a$), i.e., both boundary conditions are defined at $x = a$ due to the insertion of the parameter s.

Finally, to integrate the initial value problem given by Eq.(9)-(12), it is necessary to inform the value of the parameter s since the other parameters (a_0, a_1, b_0, b_1, c_0, c_1, α, and β) are known or easily calculated for a particular case study. Thus, an initial value of the parameter s is defined, and the differential model is solved. Since the initial value will not likely be the optimal value for the parameter s, i.e., the boundary condition in Eq.(8) will not be satisfied, this value should be adjusted. For this purpose, Newton's Method is considered, and the parameter s is updated as expressed in Eq.(13):

$$s^{i+1} \equiv s^i - \frac{(\emptyset)^i}{\left(\frac{d\emptyset}{ds}\right)^i} \tag{13}$$

where the first value of s^1 is user-defined. To find the derivative of $\emptyset$ with respect to s ($\emptyset'(s)$) it is necessary to define the sensitivity equations for the system of interest. These sensitivity equations are given by:

$$\xi(x) = \frac{\partial \omega(x,s)}{\partial s} \tag{14}$$

$$\eta(x) = \frac{\partial v(x,s)}{\partial s} \tag{15}$$

Differentiating Eq.(9) and Eq.(10) with respect to s we obtain:

$$\frac{\partial \xi}{\partial x} = \eta \tag{16}$$

$$\frac{\partial \eta}{\partial x} = \frac{\partial f}{\partial v}\eta + \frac{\partial f}{\partial w}\xi \tag{17}$$

The boundary conditions for this system are given by:

$$\xi(a) = a_1 \tag{18}$$

$$\eta(a) = a_0 \tag{19}$$

In this case, solving the initial value problem given by Eq.(9)-(12) and Eq.(16)-(19) considering a pre-defined value for the parameter s, the derivative of $\emptyset$ can be evaluated. For this purpose, the following relation is used:

$$\frac{d\emptyset}{ds} = b_0\xi(b,s) + b_1\eta(b,s) \tag{20}$$

After calculating the value of this derivative, the parameter s can be updated using Eq.(13). This procedure is repeated until the absolute error for s in two consecutive iterations is less than a user-defined tolerance.

3. DEFINITIONS

This section presents some approximations to evaluate fractional derivatives. These mathematical tools approximate the term $d^\mu f(t)/dt^\mu$ (where μ is a fractional order in a fractional differential problem) in boundary value problems. The most common approaches are presented in Podlubny (1999), Demirci and Ozalp (2012), Rehman and Khan (2012), Aslefallah and Rostamy (2014), Liu and Hou (2017), Yang, Machado, and Baleanu (2017),

Yang et al. (2017), Li and Rui (2018), Liang et al. (2018), Zhang (2018), and Yang et al. (2019).

Definition 1

The Riemann–Liouville type fractional integral ($I^{\mu}f(t)$) of order μ ($\mu > 0$) of a generic function $f:(0,\infty) \to \mathbb{R}$ is given by:

$$I^{\mu}f(t) = \frac{1}{\Gamma(\mu)}\int_0^t (t-\tau)^{\mu-1} f(\tau)d\tau \tag{21}$$

where Γ denotes the Gamma function.

Definition 2

The Riemann–Liouville type fractional derivative ($D^{\mu}f(t)$) of order μ ($\mu > 0$) of a generic function $f:(0,\infty) \to \mathbb{R}$ is given by:

$$D^{\mu}f(t) = \frac{d^n}{dt^n}\frac{1}{\Gamma(n-\mu)}\int_0^t (t-\tau)^{n-\mu-1} f(\tau)d\tau \tag{22}$$

where n=[μ]+1 and [μ] is an operator that represents the integer part of μ.

Definition 3

The Caputo-type fractional derivative ($D^{\mu}f(t)$) of order μ ($\mu > 0$) of a generic function $f:(0,\infty) \to \mathbb{R}$ is given by:

$$D^{\mu}f(t) = \frac{1}{\Gamma(n-\mu)}\int_0^t (t-\tau)^{n-\mu-1} f^n(\tau)d\tau \tag{23}$$

where n=[μ]+1 and [μ] is an operator that represents the integer part of μ.

Definition 4

The Shifted Grunwald fractional derivative ($D^{\mu}f(t)$) of order μ ($1 < \mu < 2$) of a generic function $f:(0,\infty) \to \mathbb{R}$ is given by:

$$D^{\mu}f(t) = \frac{1}{h^{\mu}}\sum_{k=0}^{M}\left((-1)^k \frac{\Gamma(\mu+1)}{\Gamma(k+1)\Gamma(\mu-k+1)}\right) f(x-(k-1)h) \tag{24}$$

where M is the number of discretization points and $h = (t_f - t_0)/M$ is the integration step (t_0 and t_f represent the initial and final time, respectively).

Definition 5

If f is a continuous function with fractional order equal to $k\mu$ (where k is a positive integer and $1 < \mu < 2$), the fractional Taylor expansion for this function will be expressed as:

$$f(t+h) = \sum_{k=0}^{\infty} \frac{h^{k\mu}}{\Gamma(1+k\mu)} f^{k\mu}(t) \tag{25}$$

4. METHODOLOGY

This work investigates the influence of the fractional order $\gamma \in [0,2]$ on simulated profiles considering the Shooting Method. For this purpose, the integer derivatives of the initial value problem (Eq.(9)-(12) and Eq.(16)-(19)) are replaced by the following fractional derivatives:

$$\omega^{\gamma} = v, \omega(a) = a_1 s - c_1 \alpha \tag{26}$$
$$v^{\gamma} = f, \ \mathrm{v}(a) = a_0 s - c_0 \alpha \tag{27}$$
$$\xi^{\gamma} = \eta, \xi(a) = a_1 \tag{28}$$
$$\eta^{\gamma} = \frac{\partial f}{\partial v}\eta + \frac{\partial f}{\partial \omega}\xi, \eta(a) = a_0 \tag{29}$$

In summary, the proposed approach presents the following steps:

- For each application, the parameters a_0, a_1, b_0, b_1, c_0, c_1, α, and β, the fractional order (γ), the initial value of the parameter s, and the tolerance to stop the iterative process are defined.
- To solve the fractional initial value problem, the Fractional Predictor-Corrector Methodis considered (GARRAPPA, 2009).
- After solving this problem, the functions $\emptyset$ (Eq.(8)) and $\emptyset'$ (Eq.(20) are evaluated.
- The parameter s is updated considering the obtained values for $\emptyset$ and $\emptyset'$.
- If the absolute error of the parameters s in two consecutive iterations is less than a user-defined tolerance, the iterative process will be stopped. Otherwise, the procedure continues until to achieve convergence.

5. RESULTS AND DISCUSSION

This section presents the results of the proposed approach applied to three case studies considering Chemical Engineering problems. We evaluated different configurations for the fractional order and integration step size. The results are compared with those obtained by analytical and numerical solutions, the optimal value of the parameter s, the number of iterations, and the processing time (PT). The models are solved in an Intel Core i7-4770 Desktop microcomputer with 8GB of memory.

The fractional model's evaluation considering $\gamma > 1$ requires a new initial condition. Thus, the derivative of the vector of dependent variable with respect to the independent variable is equal to zero (when the independent variable is equal to the lower limit).

5.1 Cyclohexane Reactor Problem

Consider the dehydrogenation reaction of cyclohexane catalyzed by Pt/alumina spheres. The cyclohexane reactor problem evaluates the cyclohexane concentration profile in a porous catalyst pellet. The mathematical model formulation of this process considered the following hypotheses (DAVIS, 1984): *i*) steady state; *ii*) isothermal system; *iii*) diffusion as the main contribution; *iv*) first-order reaction; *v*) the concentration profile in the radial direction; and *vi*) constant physical properties. Based on these hypotheses, the dimensionless mathematical model for the cyclohexane concentration along the sphere is given by:

$$\frac{d^2C}{dR^2} + \frac{2}{R}\frac{dC}{dR} = \Theta^2 \frac{C}{C_0}, 0 \leq R \leq 1 \quad (30)$$

$$\frac{dC}{dR} = 0, R = 0 \quad (31)$$

$$C = 1, R = 1 \quad (32)$$

where C is the dimensionless cyclohexane concentration (defined as the relation between the cyclohexane concentration at any point on the sphere and the cyclohexane concentration at the surface of the sphere), R is the dimensionless radius (defined as the relation between a generic radius and the sphere radius), C_0 is the cyclohexane concentration atthe surface of the sphere, and Θ is the Thiele modulus.

The analytical solution for this problem is defined as:

$$C = \frac{sinh(\Theta R)}{R\, sinh(\Theta)} \quad (33)$$

To apply the Shooting Method, the second-order integer ordinary differential model is transformed into a first-order fractional ordinary differential model given by:

$$\omega^\gamma = v, \omega(0)=\mathrm{s} \quad (34)$$

$$v^\gamma = \frac{\Theta^2}{C_0}\omega - \frac{2}{R}v, v(0)=0 \quad (35)$$

$$\xi^\gamma = \eta, \xi(0)=1 \quad (36)$$

$$\eta^\gamma = \frac{\Theta^2}{C_0} - \frac{2}{R}\eta, \eta(0)=0 \quad (37)$$

where ω is equal to C, v is an auxiliary variable, and ξ and η represent the sensitivity variables.

Since the ω at $R = 0$ is unknown, the value of the parameter s should be estimated in which the value of ω at $R = 1$ will be satisfied. Thus, the values of $\emptyset$ and $\emptyset'$ must be calculated by both Eq.(8) and Eq.(20).

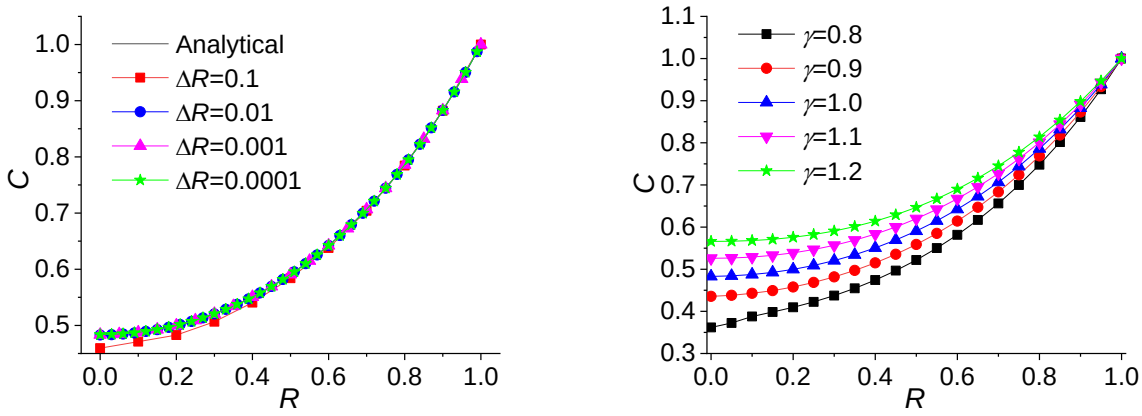
Table 1 presents the cyclohexane reactor problem results considering different values for the fractional order (γ) and different integration step sizes (ΔR). The initial value of the parameter s is equal to 1. The iterative process should stop when the absolute errorin two consecutive iterationsis less than 10^{-8} (tolerance). In addition, the average absolute error ($\sum$) considering analytical and numerical solutions is also estimated.

Table 1. Results for the cyclohexane reactor problem ($\Theta = 2.236$ and $C_0 = 1$).

γ	ΔR	s^1	s^k	Iteration	$\sum$	PT (s)
1	0.1000	1	0.4595	18.0	1.37×10^{-4}	0.1404
	0.0100		0.4829	16.0	1.85×10^{-8}	0.4681
	0.0010		0.4835	16.0	9.97×10^{-13}	1.6380
	0.0001		0.4835	16.0	3.75×10^{-20}	5.2572
0.8	0.0100	1	0.3617	24.0	-	0.5056
0.9			0.4356	19.0	-	0.4808
1			0.4829	16.0	1.85×10^{-8}	0.4681
1.1			0.5258	14.0	-	0.4496
1.2			0.5659	13.0	-	0.4184

From Table 1, we can observe that, for the integer order (γ equal to 1), a decrease in the value of ΔR decreased the average absolute error ($\sum$). This result was expected since the integration step size is related to the refinement level (see Table 1 and Figure1(a)). Furthermore, regardless of the value of ΔR, the proposed approach always converged to the optimal value of s (0.4835) for γ equal to 1, as reported by Davis (1984). For the number of iterations, a similar result for each value of ΔR is achieved. However, the higher the refinement level, the longer the processing time. As expected, a more refined mesh means a greater number of evaluations of the mathematical model increasing the processing time.

For fractional order, we can observe that this parameter influences the concentration profile and, consequently, the value of the parameter s. Thus, the higher the value for fractional order, the higher the value of the parameter s. Finally, higher values of fractional order reduced the number of iterations required to find the optimal solution.



(a) Analytical × Numerical ($\gamma = 1$). (b) γ=[0.8;0.9;1;1.1;1.2] and $\Delta R = 0.01$.

Figure 1. Influence of the integration step size and fractional order for the cyclohexane reactor problem.

5.2 Rectangular Fin Problem

Consider a rectangular fin to increase the heat transfer area between the surface and a fluid. The structure is welded to a vertical wall where the temperature (T) at $X = 0$ is equal to T_w, and the system is thermally insulated at $x = L$ (length of fin). The following hypotheses are considered in the mathematical model formulation (Davis, 1984): *i*) steady state; *ii*) conduction in the *x*-directionas the main heat contribution; *iii*) constant thermal conductivity; *iv*) constant convection heat transfer coefficient; and*v*) no phase change. The dimensionless mathematical model is given by:

$$\frac{d^2\theta}{dX^2} = H^2\theta, 0 \leq X \leq 1 \quad (38)$$

$$\theta = 1, X = 0 \quad (39)$$

$$\frac{d\theta}{dX} = 0, X = 1 \quad (40)$$

where θ is the dimensionless temperature (defined forthe wall and the room temperatures), X is the dimensionless length (defined in terms of a generic length and length of fin), and H is a dimensionless defined in function of the thermal conductivity, the convection heat transfer coefficient, and the length and thickness of fin.

The analytical solution for this problem is given by:

$$\theta = \frac{cosh(H(1-X))}{cosh(H)} \quad (41)$$

The correspondent first-order fractional ordinary differential model for this case studyis defined as:

$$\omega^{\gamma} = v, \omega(0)=1 \quad (42)$$
$$v^{\gamma} = H^2\omega, v(0) = s \quad (43)$$
$$\xi^{\gamma} = \eta, \xi(0)=0 \quad (44)$$
$$\eta^{\gamma} = H^2\xi, \eta(0)=1 \quad (45)$$

where ω is equal to θ, v is an auxiliary variable, and ξ and η represent the sensitivity variables.

In this model, the value of v at X equal to 0 is unknown. Thus, we should find the value of the parameter s in which the constraint v ($X = 1$) will be satisfied.

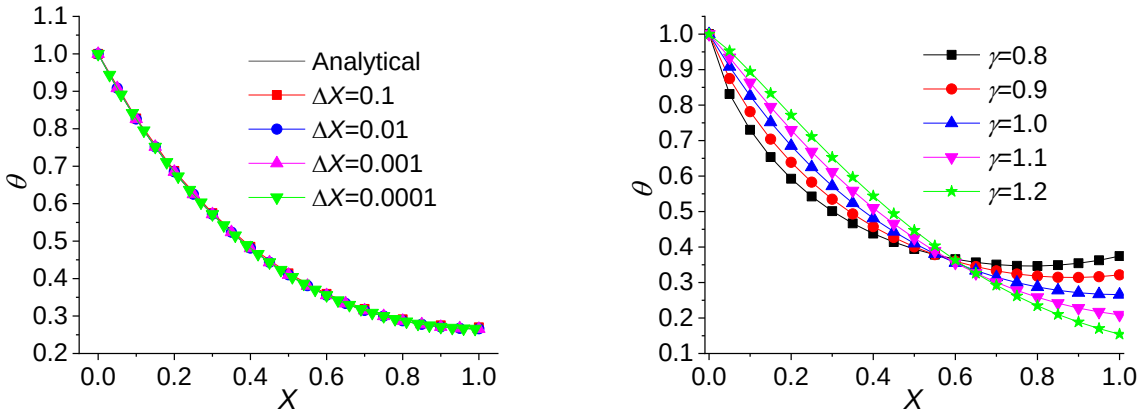
Table 2 presents the results for the rectangular fin problem considering different configurations for γ and ΔX (the tolerance is set to 10^{-8}).

Table 2. Results for the rectangular fin problem ($H = 2$).

γ	ΔX	s^1	s^k	Iteration	$\sum$	PT (s)
1	0.1000	1	-1.9261	3.0	1.07×10^{-5}	0.0468
	0.0100		-1.9280	3.0	8.52×10^{-10}	0.0936
	0.0010		-1.9280	3.0	4.27×10^{-16}	0.3120
	0.0001		-1.9280	3.0	8.78×10^{-21}	2.2301
0.8	0.0100	1	-1.9441	3.0	-	0.0936
0.9			-1.9330	3.0	-	0.1092
1			-1.9280	3.0	8.52×10^{-10}	0.0936
1.1			-1.9300	3.0	-	0.1248
1.2			-1.9382	3.0	-	0.1248

For the influence of the parameter ΔX, smaller values led to smaller average absolute errors ($\sum$) (see Table2), which is similar to the first case study results. The result for integer order presented in Figure 2(a) was consistent with those reported by Davis (1984) ($s = -1.9280$).

Figure 2(b) shows that the increase in the value of γ decreased the dimensionless temperature for X equal to 1. The same number of iterations is required for all meshes considered. This indicates that, for this application, ΔX does not influence the number of iterations required to solve the problem. As expected, the increase in the number of mesh points increased the processing time. Finally, the fractional order influenced the dimensionless temperature profiles, similar to the first case study.



(a) Analytical × Numerical ($\gamma = 1$). (b) γ=[0.8; 0.9; 1; 1.1;1.2] and $\Delta X = 0.01$.

Figure 2. Influence of the integration step size and fractional order for the Rectangular Fin problem.

5.3 Thin Film Flow Problem

The last case considers a thin film flow of third-order fluid on a moving belt governed by the following boundary value problem (SAJID and HAYAT, 2008):

$$\frac{d^2v_\delta}{dx^2} + \frac{6(\beta_2+\beta_3)}{\lambda}\left(\frac{dv_\delta}{dx}\right)^2\frac{d^2v_\delta}{dx^2} - \frac{\rho g}{\lambda} = 0 \tag{46}$$

$$v_\delta = U_0, x = 0 \tag{47}$$

$$\frac{dv_\delta}{dx} = 0, x = \delta \tag{48}$$

where v_δ is the fluid velocity, ρ is the density, λ is dynamic viscosity, β_2 and β_3 are the material moduli of third-order fluid, g is the acceleration due to gravity, and δ the thickness of the thin layer.

The dimensionless variables are defined as:

$$V = \frac{v_\delta}{U_0} \tag{49}$$

$$X = \frac{x}{\delta} \tag{50}$$

and after some manipulations, the dimensionless mathematical model is given by:

$$\frac{d^2V}{dX^2} + \varepsilon\left(\frac{dV}{dX}\right)^2\frac{d^2V}{dX^2} - K = 0 \tag{51}$$

$$V = 1, X = 0 \tag{52}$$

$$\frac{dV}{dX} = 0, X = 1 \tag{53}$$

where

$$\varepsilon = \frac{6(\beta_2+\beta_3)U_0^2}{\lambda\delta^2} \tag{54}$$

$$K = \frac{\rho g \delta^2}{\lambda U_0} \tag{55}$$

The correspondent first-order fractional ordinary differential model for this case study is defined as:

$$V^{\gamma} = Q, V(0)=1 \tag{56}$$

$$Q^{\gamma} = \frac{K}{1+\varepsilon Q^2}, Q(0) = s \tag{57}$$

$$\xi^{\gamma} = \eta, \xi(0)=0 \tag{58}$$

$$\eta^{\gamma} = \left(\frac{-2K\varepsilon Q}{(1+\varepsilon Q^2)^2}\right)\eta, \eta(0)=1 \tag{59}$$

where ω is equal to V, Q is an auxiliary variable, and ξ and η represent the sensitivity variables.

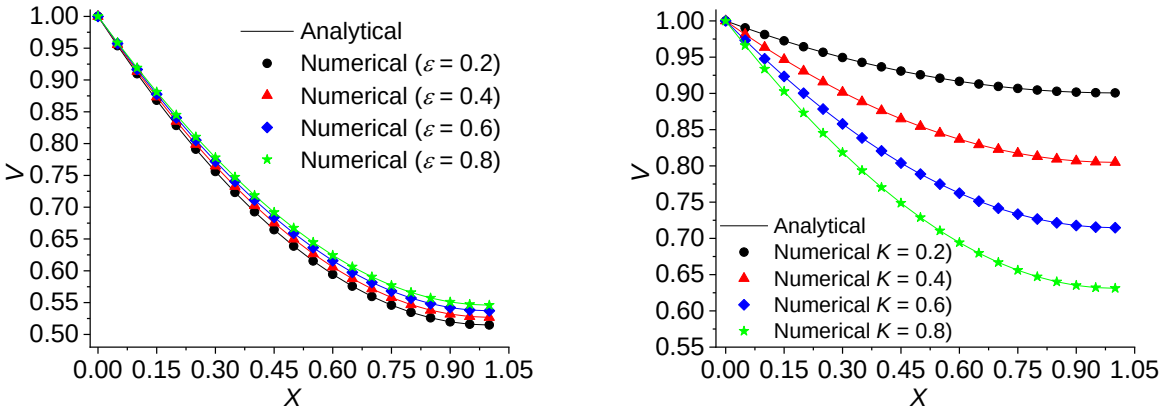
In this case, the value of Q at X equal to 0 is unknown. Thus, we should find the value of the parameter s in which the constraint $Q(X=1)$will be satisfied. The analytical solution of this case study is unknown. Thus, we obtained the numerical solution considering the Normal Collocation Method with 50 collocation points (for integer order) to compare the results. The average absolute error ($\sum$) was calculated by the difference between both numerical solutions.

Table 3 presents the thin film flow problem results considering different values for the parameters K and ε and fractional order equal to 1 ($\Delta X = 0.01$). From this table, we can observe that the combination between K and ε led to different values of the parameter s. For K equal to 1, an increase in the value of the parameter ε increased the parameter s, while, for ε equal to 1, an increase in the value of the parameter K decreased the parameter s. The number of iterations did not change with the combination of the parameters considered. The average absolute error demonstrates the accuracy of the results for the Normal Collocation Method. Finally, the processing time required by the proposed approach was more sensitive for variation of the parameter ε, i.e., it is observed a fluctuation in these values for parameter K.

Figure 3(a) shows the variation of the velocity field for large values of the third-order parameter ε considering integer order. The velocity decreased for the large values of the parameter ε. Figure 3(b) presents the effects of the parameter K on the velocity field considering integer order. From this figure, we can observe that the velocity decreased with an increase in the parameter K. Finally, it is important to mention that these profiles agree with those obtained by Sajid and Hayat (2008).

Table 3. Results for the thin film flow problem considering different values for the parameters K and ε and fractional order equal to 1 ($\Delta X = 0.01$).

K	ε	s^1	s^k	Iteration	$\sum$	PT (s)
1	0.2	1	-0.9439	6.0	1.44×10^{-9}	0.3120
	0.4		-0.9021	6.0	4.54×10^{-9}	0.2340
	0.6		-0.8688	6.0	6.77×10^{-9}	0.2496
	0.8		-0.8412	6.0	3.44×10^{-9}	0.3900
0.2	1	1	-0.1974	5.0	5.42×10^{-9}	0.2184
0.4			-0.3815	6.0	7.84×10^{-9}	0.2184
0.6			-0.5458	6.0	1.22×10^{-9}	0.2028
0.8			-0.6903	6.0	6.56×10^{-9}	0.1872



(a) K=1 and$\varepsilon = [0;\ 0.2;\ 0.4;\ 0.6;\ 0.8]$ (b) $K = [0;\ 0.2;\ 0.4\ ;0.6;\ 0.8]$ and $\varepsilon = 1$.

Figure 3. Influence of the parameters K and ε considering integer order for the thin film flow problem.

Table 4 presents the thin film flow problem results considering the parameters K and ε equal to 0.5 and different values for the fractional order. From this table, we can observe that the increase in the value of the parameter γ increased the parameter s. The number of iterations did not change, and the processing time was different for each fractional order.

Figure 4 presents the influence of the fractional order in the dimensionless velocity profile. It is possible to observe that the increase in this parameter converted a nonlinear profile into (approximately) a linear one.

Table 4. Results for the thin film flow problem considering different values for the fractional order (ΔX =0.01, $K = 0.5$ and $\varepsilon = 0.5$).

γ	s^1	s^k	Iteration	$\sum$	PT (s)
0.8		-0.5203	6.0	-	0.4836
0.9		-0.5019	6.0	-	0.2808
1	1	-0.4814	6.0	6.45×10^{-9}	0.1716
1.1		-0.4593	6.0	-	0.3432
1.2		-0.4360	6.0	-	0.2184

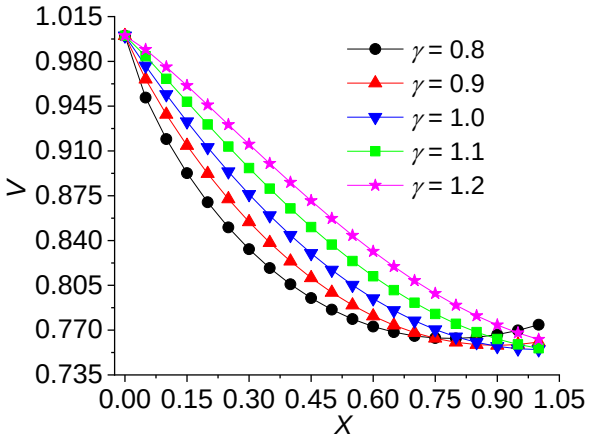


Figure 4. Influence of the fractional order considering $\Delta X = 0.01$, $K = 0.5$, and $\varepsilon = 0.5$ for the thin film flow problem.

6. CONCLUSIONS

This work proposed and solved three fractional boundary value ordinary differential problems. The Shooting Method transformed the original boundary value problem into an initial value problem. The final model was rewritten as a fractional model. The Fractional Predictor-Corrector Method associated with Caputo-type fractional derivative integrated the fractional model.

In general, the proposed approach achieved consistent results compared to the analytical or numerical solutions for fractional order equal to 1. From the physical point of view, it is evident that the variation in the value of the fractional order changes the profiles. In practice, the fractional order variation allows a greater adherence between model and experimental points in a given application since, in the fractional context, there is an increase in the number of degrees of freedom.

For future work, inverse and optimal control problems will be investigated, as well as the solution of fractional partial differential equations.

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