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A fractional calculus approach to the dynamic optimization of biological reactive systems. Part II: Numerical solution of fractional optimal control problems

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HIGHLIGHTS

- Fractional optimal control problems are formulated for biological reactive systems.
- Combines numerical/analytical strategies are proposed for solving FOCP.
- One approach combines optimality conditions for a FOCP and the gradient method.
- Second approach combines an NLP solver, shooting method and Laplace transformation.
- Resulting profiles show the effect of the fractional orders in the optimal results.

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ABSTRACT

This second paper of our series is concerned with the formulation and solution strategies of fractional optimal control problems (FOCP). Given the sets of fractional differential equations representing the behavior of fermentation and thermal hydrolysis reactive systems, here we formulate the corresponding FOCP's and describe suitable techniques for solving them. An analytical/numerical strategy that combines the optimality conditions and the gradient method for FOCP as well as the predictor–corrector fractional integrator is used to obtain optimal dilution rate profiles for the fermentation case-study. For the case of the thermal hydrolysis, the strategy involves discretization of the FOCP to formulate it as a Non-Linear Programming problem; then, the solution algorithm involves the use of an NLP solver and the shooting technique coupled to an inverse Laplace transformation subroutine. The optimal profiles show the performance of the numerical solution approaches proposed and the effect of the fractional orders in the optimal results.

1. Introduction

Optimal control problems (OCP) have been extensively studied in the literature. Several references and classical books provide the theoretical basis and fundamentals of this area (see for instance the books by Stengel, 1994; Sethi and Thompson, 2000; Diwekar, 2008 and the work by Poznyak, 2002).

In summary, an OCP is defined by the system of Eqs. (1)–(4):

$$\underset{u}{\text{Optimize}} \quad J = \phi(x(t_f), t_f) + \int_{t_0}^{t_f} L(x(t), u(t), t)dt \tag{1}$$

Subject to:

$$\frac{d(t)x}{dt} = f(x(t), u, t) \quad x(0) = x_0 \tag{2}$$

$$h(x, u, t) = 0 \tag{3}$$

$$g(x, u, t) \leq 0 \tag{4}$$

Solution techniques for an OCP involve the use of calculus of variation, dynamic programming and the maximum principle of

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Pontryagin. The use of the calculus of variations provides the optimality conditions for an OCP (also known as Euler–Lagrange equations). The optimality conditions involve a two-point boundary value problem whose solution provides the optimal profiles for the state and control variables.

1.1. A fractional optimal control problem (FOCP)

If the system dynamics of an OCP (Eq. (2)) is represented instead in terms of a set of differential equations of fractional order α,

$$ {}_0^C D_t^\alpha y(x) = f(x(t), u(t), t) \tag{5}$$

the resulting optimization problem is then a fractional optimal control problem (FOCP). Eq. (5) represents the fractional dynamics of a system in terms of the Caputo definition.

Interesting and promising applications of fractional calculus have been proposed in the area of process control (Moreau et al., 2002; Podlubny, 1999, 2002; Delavari et al., 2013), mostly related to the design and tuning of controllers. However, in the area of dynamic optimization or optimal control, the fractional calculus literature is limited. Still, recent advances propose numerical solution approaches to the solution of FOCP's. Agrawal (2002, 2004) uses calculus of variations and the formula for fractional integration by parts to derive the optimality conditions of an FOCP; the author provides the Euler–Lagrange equations for FOCP based on the Riemann–Liouville definition of a fractional derivative and developed an approximate numerical solution based on the transformation of the problem into a set of algebraic equations (by using Legendre polynomials). In later works, Agrawal (2008), Agrawal et al. (2010) also derived the optimality conditions when the Caputo definition for the fractional derivatives is used and proposed numerical solution techniques based on the Grünwald–Letnikov approximation. Numerical schemes for the solution of FOCP are also proposed in Tangpong and Agrawal (2009) and in Tricaud and Chen (2010). Tricaud and Chen (2010) solved classical FOCP's by using the Oustaloup recursive approximation to reformulate an FOCP as an OCP. These authors then used the RIOTS95 (Schwartz et al., 1997) solution algorithm for solving the resulting OCP.

1.1.1. Optimality conditions (Euler–Lagrange equations) for an FOCP (Agrawal, 2004)

The derivation of the optimality conditions for an FOCP is described in detail on the work of Agrawal (2004). The author used a simplified formulation of an FOCP as follows:

$$ \underset{u}{\text{Minimize}} \quad J(u) = \int_0^1 F(x, u, t)\, dt \tag{6}$$

subject to:

$$ {}_a D_t^\alpha\, x = G(x, u, t) \quad x(0) = x_0 \tag{7}$$

where the fractional derivative in Eq. (7) corresponds to the left hand side Riemann–Liouville definition. The goal is finding an optimal control profile $u(t)$ to minimize the integral Eq. (6); F and G are arbitrary continuous functions. Also notice that the integration limits have been set to 0 and 1 and it is further assumed that $0 < \alpha < 1$; these considerations do not affect the generalization of the derivation procedure. The derivation includes a calculus of variations approach and the formula for fractional integration by parts developed by Riewe (1996) and Samko et al. (1993). Agrawal (2004) demonstrates that the minimization of the Lagrangean objective function requires:

$$ {}_0 D_t^\alpha x = G(x, u, t) \quad x(0) = x_0 \tag{8}$$

$$ {}_t D_1^\alpha \lambda = \frac{\partial F}{\partial x} + \lambda \frac{\partial G}{\partial x} \quad \lambda(1) = 0 \tag{9}$$

and

$$ \frac{\partial F}{\partial u} + \lambda \frac{\partial G}{\partial u} = 0 \tag{10}$$

The fractional boundary value system of fractional Eqs. (8)–(10) are the Euler–Lagrange optimality conditions for FOCP's based on the left hand side Riemann–Liouville definitions for fractional derivatives. Following a similar procedure, Agrawal (2008) derived the Euler–Lagrange optimality conditions for FOCP's based on the Caputo definition for the fractional derivatives. The result of the derivations is given by Eqs. (11)–(13):

$$ {}_0^C D_t^\alpha x = G(x, u, t) \quad x(0) = x_0 \tag{11}$$

$$ {}_t^C D_1^\alpha \lambda = \frac{\partial F}{\partial x} + \lambda \frac{\partial G}{\partial x} \quad \lambda(1) = 0 \tag{12}$$

$$ \frac{\partial F}{\partial u} + \lambda \frac{\partial G}{\partial u} = 0 \tag{13}$$

If the order of the fractional derivatives, α, becomes 1, the system of Eqs. (11)–(13) reduces to the classical optimality condition equations for an OCP.

In the following sections, the fractional models developed for the biological reactive systems described in Toledo-Hernandez et al. (2014) will be reformulated as FOCP's. Then analytical/numerical solution strategies will then be proposed to solve those problems. Finally, results are presented and a final discussion is provided.

2. Case studies: Formulation of illustrative FOCP's

This section presents three illustrative examples of FOCP's. The first example is the fractional version of the classical time invariant problem (Agrawal, 2004); this case is used to test the numerical strategy that we have implemented to solve the fractional boundary value problem (optimality conditions) based on Caputo definitions for the fractional derivatives. The second and third examples correspond to the fermentation and thermal hydrolysis reactive systems described in Toledo-Hernandez et al. (2014); a performance index was incorporated to those fractional dynamic formulations, resulting in two FOCP's.

2.1. Fractional time invariant problem

The fractional version of the classical time invariant problem was proposed by Tricaud and Chen (2010) and Agrawal (2004); in those references, such formulation was approached by considering the Riemann–Liouville definition of fractional derivative. In this paper, however, we will consider the alternative approach based on the Caputo fractional derivative definition presented by Agrawal (2008).

The time invariant problem consists of finding the optimal control, $u(t)$, that minimizes the function:

$$ J(u) = \frac{1}{2} \int_0^1 [x^2(t) + u^2(t)] dt \tag{14}$$

subject to:

$$ {}_0^C D_t^\alpha x = -x + u \quad x(0) = 1 \tag{15}$$

The Hamiltonian functions for this problem is given by:

$$ \mathscr{H} = 1/2(x^2 + u^2) + \lambda(-x + u)$$

By obtaining the optimality conditions defined by Eqs. (11)–(13), the Euler–Lagrange equations for the fractional time invariant

problem are given by Eqs. (16) through (18):

$${}_0^C D_t^{\alpha} x = -x + u \quad x(0) = 1 \tag{16}$$

$${}_t^C D_0^{\alpha} \lambda = x - \lambda \quad \lambda(1) = 0 \tag{17}$$

$$u + \lambda = 0 \tag{18}$$

which constitute a two-point boundary value problem including a set of fractional order differential equations.

2.2. Fermentation fractional model

Consider here the fractional fermentation model for the Tequila production process presented in our companion paper (Toledo-Hernandez et al., 2014). To formulate an FOCP, we define the objective function of the optimization problem as the maximization of the end concentration of the product. Using the fitted parameters provided in that reference, the cell death/inhibition term will be omitted (k_m=0) for simplicity. The dilution rate, R, representing the ratio between the substrate feed flow rate, u, and the reactor volume, V, is assumed as the control variable:

$$R = \frac{u}{V}$$

An enhancer/inhibition term containing R is then added to each of the fractional differential equations of the model. The FOCP for the case of the fermentation is given by Eqs. (19)–(22):

$$\text{Maximize } J = P(t_f) \tag{19}$$

subject to

$${}_0^C D_t^{\alpha_1} B = k_c BS - R\,B \quad B(0) = 0.5 \tag{20}$$

$${}_0^C D_t^{\alpha_2} S = -k_s BS + R(S_0 - S) \quad S(0) = 90 \tag{21}$$

$${}_0^C D_t^{\alpha_3} P = k_p BS - R\,P \quad P(0) = 2.5 \tag{22}$$

P, B and S are product, biomass and substrate concentrations, respectively. The initial concentrations are all given in g/l.

2.2.1. The Euler–Lagrange optimality conditions for the fermentation FOCP

The Hamiltonian function for this problem is given by the expression:

$$\mathscr{H} = \lambda_1(k_c BS - RB) + \lambda_2[-k_s BS + R(S_0 - S)] + \lambda_3[k_p BS - RP]$$

From Eq. (20), the adjoint fractional equations for this problem are:

$${}_t^C D_0^{\alpha_1} \lambda_1 = -\lambda_1 k_c S + R\lambda_1 + \lambda_2 k_s S - \lambda_3 k_p S \quad \lambda_1(t_f) = 0 \tag{23}$$

$${}_t^C D_0^{\alpha_2} \lambda_2 = -\lambda_1 k_c B + \lambda_2 k_s B + R\lambda_2 - \lambda_3 k_p B \quad \lambda_2(t_f) = 0 \tag{24}$$

$${}_t^C D_0^{\alpha_3} \lambda_3 = R\lambda_3 \quad \lambda_3(t_f) = 1 \tag{25}$$

The end boundary conditions for the adjoint variables in Eqs. (23)–(25) come from the known equality

$$\lambda_i(t_f) = \left.\frac{\partial \phi}{\partial x_i}\right|_{t_f}$$

and the fact that, in this example, the salvage function ϕ is the product concentration, P; that is, $\phi(x(t_f), t_f) = x_3(t_f) = P(t_f)$ (see Eq. (1) and Eq. (19)).

Further, the use of Eq. (13) for this example results in Eq. (26):

$$-\frac{\lambda_1 B}{V} + \frac{\lambda_2(S_0 - S)}{V} - \frac{\lambda_3 P}{V} = 0 \tag{26}$$

In summary, the optimal control profiles for the fractional version of the fermentation model are obtained by the solution of the boundary value problem defined by Eqs. (20) through (25) and Eq. (26).

2.3. Thermal hydrolysis of Agave for Mezcal production as an FOCP

As explained in Toledo-Hernandez et al. (2014), this example not only represents a challenge from the modeling point of view, but will also require a non-conventional numerical solution strategy.

As suggested in the work by Garcia-Soto et al. (2011), the practical goal in this case is to maximize the end concentration of the reducing sugars, whereas temperature can be defined as the control variable. Therefore, in order to define an FOCP, we have not only to define a performance index in terms of the reducing sugars concentration, but also need to assume the kinetics parameters as being functions of temperature.

The FOCP could then be defined as:

$$\underset{T}{Maximize} \;\; J = M(t_f) \tag{27}$$

subject to:

$$\frac{dP}{dt} = -k_h\, {}_0D_t^{1-\alpha_1}\, P(t) \tag{28}$$

$$\frac{dM}{dt} = k_h\, {}_0D_t^{1-\alpha_1}\, P(t) - k_d\, {}_0D_t^{1-\alpha_2}\, M(t) \tag{29}$$

$$\frac{dD}{dt} = k_d\, {}_0D_t^{1-\alpha_2}\, M(t) \tag{30}$$

$$k_h = k_1 e^{(-A_1/T_i)} \tag{31}$$

$$k_d = k_2 e^{(-A_2/T_i)} \tag{32}$$

Notice that Arrhenius type of expression is assumed then for the kinetics constants behavior (Eqs. (31) and (32)). Because of the fractionalized Eqs. (28)–(30), the solution approach based on the calculus of variation as proposed by Agrawal (2004, 2008) cannot be used to obtain the optimality conditions of the FOCP. Therefore, in this case-study, the set of fractional order differential Eqs. (28)–(30) representing the dynamics was transformed to the Laplace domain:

$$\hat{P}(s) = \frac{P0}{s + k_h(T_i)\, s^{1-\alpha_1}} \tag{33}$$

$$\hat{M}(s) = \frac{1}{s + k_d(T_i)\, s^{1-\alpha_2}} \left\{ k_h(T_i)[s^{1-\alpha_1} \hat{P}(s)] + M0 \right\} \tag{34}$$

$$\hat{D}(s) = \frac{1}{s} \left\{ k_d(T_i)[s^{1-\alpha_2}\, \hat{M}(s)] + D0 \right\} \tag{35}$$

Notice that the transformed equations are time dependent algebraic equations (although represented in the Laplace domain). Therefore, after the transformation, the original FOCP becomes an NLP problem given by Eqs. (36)–(44):

$$\underset{T_i}{Maximize} \quad J = M(t_f) \tag{36}$$

subject to:

$$P(t) = \mathscr{L}^{-1}\{\hat{P}(s)\} \tag{37}$$

$$M(t) = \mathscr{L}^{-1}\{\hat{M}(s)\} \tag{38}$$

$$D(t) = \mathscr{L}^{-1}\{\hat{D}(s)\} \tag{39}$$

$$\hat{P}(s) = \frac{P0}{s + k_h(T_i)\, s^{1-\alpha_1}} \tag{40}$$

$$\hat{M}(s)=\frac{1}{s+k_d(T_i)\,s^{1-\alpha_2}}\left\{k_h(T_i)[s^{1-\alpha_1}\hat{P}(s)]+M0\right\} \tag{41}$$

$$\hat{D}(s)=\frac{1}{s}\left\{k_d\,(T_i)[s^{1-\alpha_2}\hat{M}(s)]+D0\right\} \tag{42}$$

$$k_h=k_1e^{(-A_1/T_i)} \tag{43}$$

$$k_d=k_2e^{(-A_2/T_i)} \tag{44}$$

The problem can be discretized into time intervals to optimize a nonlinear algebraic system of equations and to obtain the optimal profiles. A complication however arises, since the equations in the Laplace domain have to be transformed back to the time domain (Eqs. (37)–(39)) during the iterative solution scheme; then, an inverse Laplace transformation is required. T_i represents the control variable at each time interval. To illustrate our approach, in this example the temperature was bounded so that $369.15\ \mathrm{K} < T_i < 379.15\ \mathrm{K}$. k_h and k_d depend on the temperature but they will be assumed as constants at each time interval of constant temperature.

3. Numerical solution techniques for FOCP

Ford and Morgado (2011) considered boundary value problems of fractional order; they studied the existence and uniqueness of the solution and presented a comparison among alternative methods for their numerical solution. The authors focused on problems involving fractional differential equations and boundary conditions of the type $y(a)=y_a$. Therefore, the numerical solution techniques involved the shooting method to estimate the initial condition $y(0)=y_0$; then a fractional integrator for an initial value problem (IVP) could be used to test that the given boundary at point a is achieved. The predictor–corrector method described by Diethelm et al. (2002) showed the best performance as the IVP solver. Later, Ford et al. (2014) proposed a similar strategy for the same problem but, instead of the predictor–corrector method, a collocation technique was incorporated to the numerical solution approach.

In this paper we used two different numerical strategies for solving FOCP's. The numerical solution strategies for the boundary value problem describing the time invariant problem and the fermentation optimality condition are solved by combining the classical gradient method and the predictor-method for fractional integration (Diethelm et al., 2002; Diethelm and Ford, 2004; Diethelm, 2010). For the thermal hydrolysis problem, our numerical algorithm is quite related to the one discussed by Ford and Morgado (2011). We also combine the shooting technique with the predictor–corrector method described by Diethelm et al. (2002). However, we emphasize that our problem is a two-point boundary value problem, where an initial condition and a terminal condition are given. Our numerical approach for the hydrolysis problem involves the combined use of an NLP solver, an inverse Laplace transformation subroutine and the shooting method. The computer implementations of all of the numerical algorithms have been developed by using the Matlab® environment.

3.1. Solving the optimality conditions of the FOCP: Numerical solution approach to the two-point boundary value problem

We solved the two-point boundary value problem through a numerical iterative procedure based on the gradient method for conventional OCP. The algorithmic steps are as follows:

(a) Set the iteration counter $k=0$; Provide the initial value for the state variables $x(t_0)$ and an initial guess for the control profile u_0.
(b) Perform forward integration of the state variables x from t_0 to t_f.
(c) Similarly, given the final condition $\lambda(t_f)$, perform backward integration of the adjoint variables λ from t_f to t_0.
(d) Update the control profiles by using:

$$u_{k+1}=u_k-\varepsilon_k\left[\frac{\partial\mathscr{H}}{\partial u}\right]_k$$

where ε_k is a small positive number and $\mathscr{H}$ is the Hamiltonian function.
(e) If $u_{k+1}-u_k$ is greater than a specified tolerance, set $k=k+1$ and go back to step b) using u_{k+1} as new guess for the control profile. Otherwise, the solution has been obtained.

The integration steps (b) and (c) of the solution algorithm involve numerical integration of fractional differential equations. As mentioned before, that steps are completed by using the integration method provided by Diethelm (2010), which is a generalization of the Adams–Bashforth–Moulton method for its application to fractional order equations. The main algorithm steps of the predictor–corrector method were provided in the companion paper of this series of two (Toledo-Hernandez et al., 2014). One of the algorithmic decisions consists of fixing the value of parameter ε_k, which has a significant impact on the convergence of the method. Small values might cause a large number of iterations and an increase in computational effort; large values might cause divergence of the algorithm.

This numerical technique is used to solve the two-point boundary value problems formulated for the time invariant and the fermentation problems.

3.2. Optimizing fractionalized dynamic systems: Numerical solution of the NLP including constraints in the Laplace domain

Similar to the non-linear fitting algorithm reported in Toledo-Hernandez et al. (2014), the dynamic optimization of the thermal hydrolysis system (Eqs. (36)–(44)) requires the inverse Laplace transformations defined by Eqs. (37)–(39).

Further, the representation of the kinetics constants as functions of temperature (Arrhenius-like Eqs. (43) and (44)) also causes an additional complexity. Eqs. (43) and (44) are non-linear; therefore, if they are substituted into Eqs. (40)–(42), the inversion of the Equations defined by (37)–(39) would not be possible. However, as a numerical approximation, the NLP can be discretized so that each time period can be associated to one value of temperature; the kinetics parameters can then be considered constants at each time interval.

An additional issue to consider is the fact that fractional derivatives are defined using integrals, so they are non-local operators. The fractional derivative in time contains information about the function at earlier points, so it possesses a memory effect. Therefore, fractional differential equation implies non-local dynamics and involves memory effects. Then, in order to evaluate a fractional derivative at time t, the behavior at the whole interval $[0,t]$ must be considered. Several works describe and/or study the non-locality and memory effect of fractional calculus operators (Herrmann, 2011; Sun et al., 2011; Constantinescu and Stoicescu, 2011; Du et al., 2013).

Rather than focusing on the concept of the non-locality of fractional differential equations, an illustration of the implications of this issue and how it affects our solution approach is given next. Consider the ordinary differential equation given by Eq. (45):

$$\frac{dX}{dt}=-kX \tag{45}$$

Analytical integration of Eq. (45) in a time interval starting from t_0 up to t_n results in:

$$X_n = X_0 \exp[-k \times (t_n - t_0)] \tag{46}$$

Let us now consider the time discretization from $t_0=0$ to t_n in N time intervals of constant length Δt shown in Fig. 1. If one tries to find the value of X at each time point from $t_0=0$ to t_n, due to local behavior of ordinary differentiation, Eq. (46) can be used; however, the initial conditions would vary for each time interval. Then, Eq. (46) may be re-written as:

$$X_{i+1} = X_i \exp[-k \times (t_{i+1} - t_i)] = X_i \exp[-k \times (\Delta t)] \quad i = 0 \ldots n-1 \tag{47}$$

Eq. (47) has been expressed in terms of a constant time increment $\Delta t = t_{i+1} - t_i$. Successive calculation for each period would involve only the variation of the initial condition at each interval, X_i. That occurs because an ordinary differential equation implies local dynamics. That is, the calculation of X_i at each interval depends only on the information of such interval. Observe consistency of the results by either using Eq. (46) or successively using Eq. (47). Calculation of X_2 by using Eq. (46) results in:

$$X_2 = X_0 \exp[-k \times (t_2 - t_0)]$$

On the other hand, the same result can be obtained by the successive use of Eq. (47):

$$X_1 = X_0 \exp[-k \times (t_1 - t_0)]$$

$$X_2 = X_1 \exp[-k \times (t_2 - t_1)]$$

and the substitution of X_1 in X_2:

$$\begin{aligned} X_2 &= X_1 \exp[-k \times (t_2 - t_1)] \\ &= X_0 \exp[-k \times (t_1 - t_0)] \exp[-k \times (t_2 - t_1)] \\ &= X_0 \exp[-k \times (t_2 - t_0)] \end{aligned}$$

Let us now consider a fractional differential equation (non-local dynamics) similar to Eq. (45):

$$\frac{d^\alpha X}{dt^\alpha} = -kX \tag{48}$$

Analytical solution to Eq. (48) gives:

$$X = X_0 E_a(-k \times \Delta t^\alpha) \tag{49}$$

where $\Delta t = t_n - t_0$ and X_0 is the initial value of X at the beginning of the time period. In the previous expression, $E_a(t)$ is the Mittag–Leffler function defined as follows:

$$E_a(t) = \sum_{k=0}^{\infty} \frac{t^k}{\Gamma(\alpha k + 1)} \tag{50}$$

where Γ is the gamma function.

If we intend to apply Eq. (49) for the numerical evaluation of X_i at each of the time intervals of Fig. 2 (as we did in the ordinary case), the resulting expression would be:

$$X_{i+1} = X_i E_a(-k \times (t_{i+1} - t_i)^\alpha) \tag{51}$$

however, in this case the numerical result would be different if one applies either Eq. (49) or successively applies Eq. (51). Calculation of X_2 by using Eq. (49) results in:

$$X_2 = X_0 E_a[-k \times (t_2 - t_0)^\alpha]$$

On the other hand, the successive use of Eq. (51) results in:

$$X_1 = X_0 E_a[-k \times (t_1 - t_0)^\alpha]$$

$$X_2 = X_1 E_a[-k \times (t_2 - t_1)^\alpha]$$

and by substituting X_1 in X_2:

$$\begin{aligned} X_2 &= X_1 E_a[-k \times (t_2 - t_1)^\alpha] \\ &= X_0 E_a[-k \times (t_1 - t_0)^\alpha] E_a[-k \times (t_2 - t_1)^\alpha] \\ &\neq X_0 E_a[-k \times (t_2 - t_0)^\alpha] \end{aligned}$$

An incorrect result is obtained by the successive use of Eq. (51). Observe, however that, in the limiting case when $\alpha=1$, the Mittag–Leffler function reduces to the exponential function (therefore, the ordinary local-dynamics behavior is recovered in that case). As a consequence of the previous analysis, assume for instance that we are numerically integrating Eq. (48) from 0 to 20. A value is obtained if we consider just one interval ($\Delta t = 20$) but, by taking two time intervals ($\Delta t = 10$) and using the same approach as in the ordinary differential equation, a different value is obtained for X at time 20 after successive calculation of the two intervals.

This simple exercise shows the non-local behavior of fractional integration. Recall that the definition of a fractional derivative includes an integral expression, representing the memory effects of fractional calculus. As a consequence, for any time interval i, Eq. (49) implies considering the total time period $\Delta t = t_i - t_0$.

This property of fractional derivatives makes the numerical optimization algorithm for Eqs. (36)–(44) more computational intensive. For each time interval, besides solving the discretized set of equations corresponding to the interval, we propose an iterative numerical strategy to find the initial state conditions needed to maintain consistency of the solution; the shooting method was used for that purpose. In summary, to find the optimal profiles that maximize the end concentration of reducing sugars, the numerical strategy includes an inverse Laplace transformation function, the shooting method and an NLP solver.

Fig. 2 is used to illustrate the proposed numerical approximation. Consider the constraints (37) through (44). Eq. (36) is the objective function and the decision variable is the temperature at

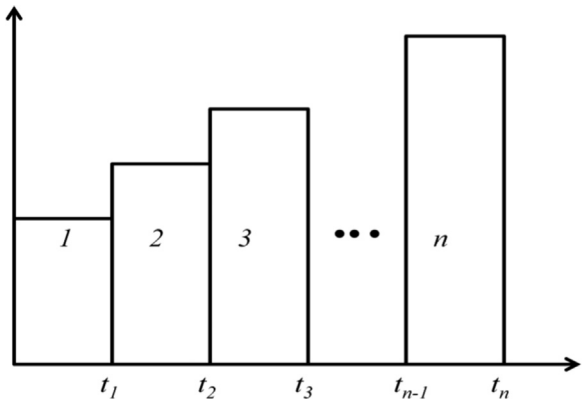

Fig. 1. Time discretization in N intervals.

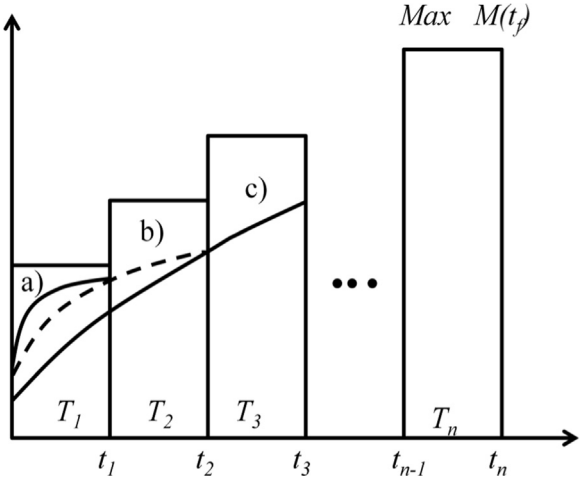

Fig. 2. Iterative numerical solution strategy for the discretization-NLP approach.

each time interval T_i. Since the model is a time dependent model, the system of equations is discretized in the N intervals of Fig. 2. At $t=0$, the discretized equations of the first interval (t_1,t_0) are solved considering the decision value T_1. For the second time interval the equations are the same as in the first interval, but the decision value is now T_2. Because of the non-local property of fractional dynamics, calculations in interval 2 requires to consider the total time period from t_0 to t_2 and the decision T_2.

As a numerical approximation to the solution of the system, the following numerical strategy is proposed. We propose to find the initial conditions of the state variables used for interval 2 so that consistency of the solution is preserved; that is, $P(t_1,T_1)=P(t_1,T_2)$, $M(t_1,T_1)=M(t_1,T_2)$ and $D(t_1,T_1)=D(t_1,T_2)$. An iterative shooting method is implemented following path (a) of Fig. 2. Once the consistency conditions are achieved, the discretized equations are solved for interval 2, using the decision T_2, the time period from t_0 to t_2 and the state initial conditions found by the shooting method.

A similar procedure is applied for the rest of the time intervals. Initial state conditions for interval 3 from t_0 to t_3 are calculated using T_3 so that $P(t_2,T_2)=P(t_2,T_3)$, $M(t_2,T_2)=M(t_2,T_3)$ and $D(t_2,T_2)=D(t_2,T_3)$; the shooting method would now follow path (b) in Fig. 2.

As a final note, it is important to emphasize that the proposed numerical method is intended to:

(1) Keep consistency in the values of the decision variable used; T_i is assumed constant only in interval i and is used for the calculations in interval i.
(2) Keep consistency in the numerical solution so that $P(t_i,T_i)=P(t_i,T_{i+1})$, $M(t_i,T_i)=M(t_i,T_{i+1})$ and $D(t_i,T_i)=D(t_i,T_{i+1})$.
(3) Consider the non-local property for the fractional derivative, so that the calculation at each interval i considers the whole time period (t_0,t_i).

Because of issue (3), the initial state conditions found for each time interval (shooting method) from the 2nd to nth are fictitious but are also needed to preserve the consistency described in (2). They would represent the initial conditions that would apply if the ith decision variable, T_i, were kept constant for the whole period (t_0,t_i). In that sense, the initial values found with constant T_i are equivalent to the given (real) initial conditions X_0 used when the decision variable values are different at each time interval. This approximate iterative procedure avoids specialized discretization approaches recently suggested for FDE.

The computational effort of the approach is significant; recall that this iterative procedure is embedded in an optimization scheme (NLP solution algorithm) which will find the optimal values for the decision profiles T_i; an algorithm which is also iterative in nature.

4. Results

This section provides the optimal profiles for the FOCP's described in Section 2. First, we show the results for the invariant time and the fermentation problems obtained by using the gradient method (and the predictor–corrector fractional integrator). Then, the optimal profiles for the thermal hydrolysis are presented.

Calculations were performed in a computer running under Microsoft Windows 7 operating system with an Intel Core i5 processor (2.53 GHz). Depending upon both the initial guesses for the control and state variables and the value of the parameter used to update the optimal profile (ε), the numerical iterative procedure based on the gradient method uses a computational time ranging from 15 to 30 min (the FOCP for fermentation is used as case-study). As described before, the value of ε has a significant impact on the convergence of the method. On the other hand, for the hydrolysis case-study, the combined use of an NLP solver, the inverse Laplace transformation subroutine and the shooting method makes the numerical approach for this case more computationally intensive. Computations times depend strongly on the number of time intervals used for the solution and, in our calculations, they varied from three to six hours for such a simple FOCP. We should clarify, however, that our code was not developed by considering numerical efficiency in the computations, since our goal was not to compare the computational effort of our approach with respect to alternative solution techniques.

4.1. The invariant time problem

The invariant time problem is a classical illustrative example that has been solved for both the ordinary and fractional cases. Therefore, here we use it just as a test problem to verify our computational implementation of the gradient method and the predictor–corrector fractional integrator. Caputo definitions are used for the fractional derivatives.

Results for the optimal time profiles of the state, $X(t)$, and the control variables, $u(t)$, are shown in Fig. 3 for different values of the fractional order for the derivative. The results are identical to those presented by Agrawal (2008) for the same problem, so that our numerical strategy is validated and can be used for solving the fermentation problem (for which results are not available in the literature for the FOCP).

4.2. Fermentation for production of Tequila

Optimal profiles for this problem have not been provided in the literature neither for the ordinary dynamic optimization nor for the FOCP. The optimal profile for the control variable is presented in Fig. 4. Fig. 5 shows the optimal profiles for the product, substrate and biomass. Since the reactor volume is a constant value, Fig. 4 shows the optimal substrate feed flow rate instead of the dilution rate (R). It is suggested for the substrate feed flow rate to display an initial rate increase up to roughly 22 l/h after 20 h of operation; from that, the flow rate decreases until a minimum value (practically zero) is reached after roughly 40 h operation. In practice this would mean that an initial fed-batch operation mode switches to a batch operation mode. The behavior is consistent with an initial high rate for biomass growth in the system.

The maximum product concentration (objective function) is $P(T)=38.4548\ g/l$. In Table 1, this value is compared against the final concentrations of the fermentation product obtained by using different non optimal control variable profiles.

4.3. Thermal hydrolysis of Agave for Mezcal production

Maximum concentration for the reducing sugars achieved for this case is $(T)=182.0344\ g/l$. Table 2 compares this optimal value with final reducing sugars concentrations obtained by using two non optimal profiles of constant temperature (the lower and upper values of temperature); as expected, the optimal profile results is a higher concentration. Fig. 6 shows the optimal dynamic profile for the state variables (furans, fructans and reducing sugars). These optimal profiles are typical profiles of a thermal hydrolysis process. Fructans concentration decreases as reducing sugars are produced; furans are obtained from reducing sugars and their concentration also increases as reducing sugars concentration increases. Six temperature intervals were used for the numerical optimization of the process. The optimal temperature profiles are shown in Fig. 7. The discretization approach is evident, since optimal constant values of temperature for each interval are attained. Maximum value allowed for the temperature is suggested at the beginning of the process and then a decreasing

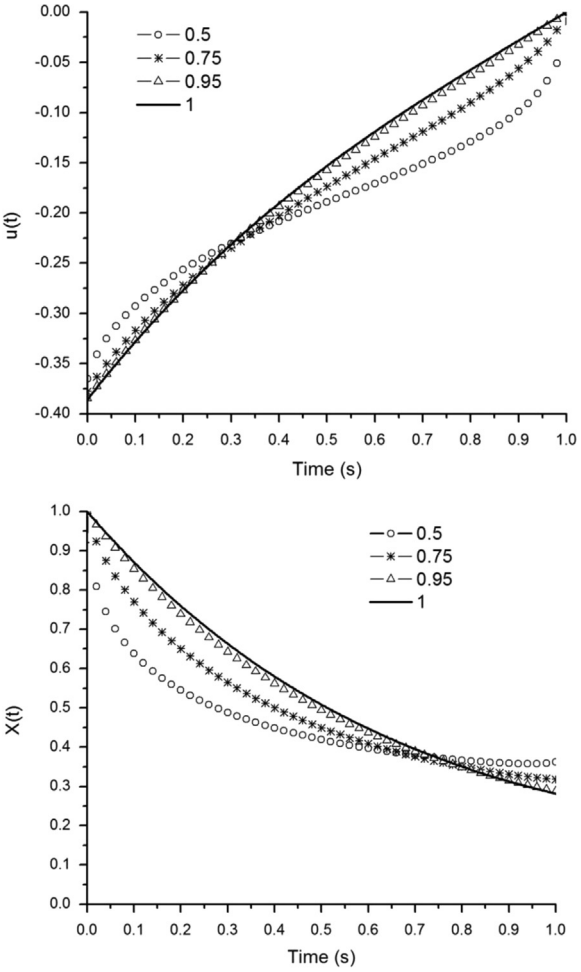

Fig. 3. Optimal profiles for the Fractional time invariant problem.

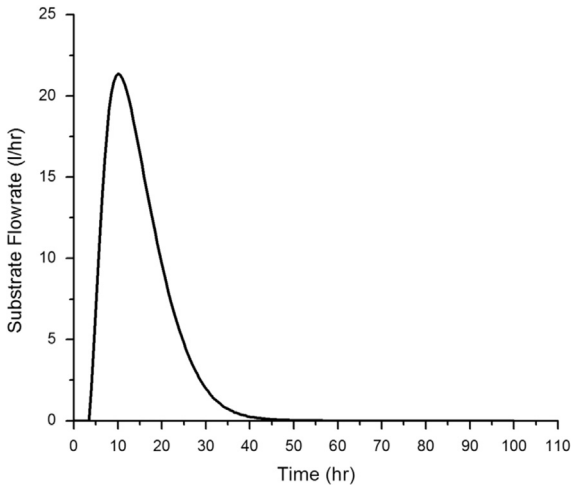

Fig. 4. Optimal control variable profile in the fermentation case-study.

behavior is predicted until the minimum value allowed is reached. That behavior seems reasonable and similar profiles are often suggested in practice.

5. Summary and conclusions

This paper focuses on the solution of fractional optimal control problems corresponding to the dynamic optimization of biological

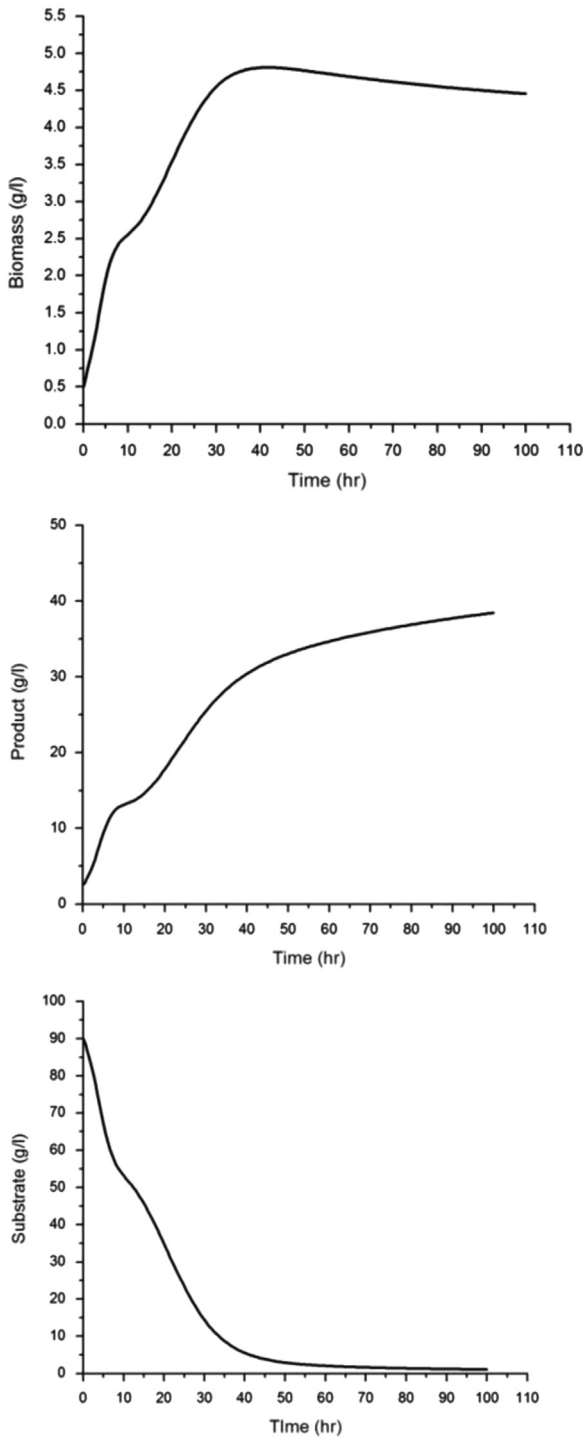

Fig. 5. Optimal time profiles for the state variables in the fermentation case-study.

Table 1
Final concentrations of the fermentation product by using different control variable profiles.

Substrate feed flow rate u (t) (l/h)	$P(T)$ (g/l)
6 (constant)	23.018
24 (constant)	13.2875
$\sqrt{t}$	20.2118
$t^{1/16}$	34.9605
u^*_{ord}	37.4689
u^*_{frac}	38.4548

Table 2
Thermal hydrolysis of Agave: final concentrations of reducing sugars by using different temperature profiles.

$T(t)$(K)	$M(T)$(g/l)
369.15 (constant)	174.2954
379.15 (constant)	180.3795
T^*	182.0344

reactive systems. The first goal of the paper is to describe practical dynamic optimization problems where mathematical tools of fractional calculus can be applied to achieve optimal system behavior.

The illustrative biological systems are represented by models that, although both of them are posed as FOCP, require quite different approaches to their solution. Therefore, the second goal of the paper is to provide numerical solution techniques for the solution of the resulting FOCP's.

The reactive systems used as the case-studies include a fermentation process for the production of Tequila and a thermal hydrolysis reaction as the first step in the production of Mezcal.

In the fermentation process, the Euler–Lagrange optimality conditions for FOCP were derived, so that the task reduces to solving a two-point boundary value problem. The classical gradient method for solving boundary value problems was used as the basis of the numerical solution technique; as a necessary change to the conventional algorithm, a fractional differential equation integrator is used instead of ordinary integration techniques. The predictor–corrector method of Diethelm (2010) was used for this step.

Our implementation of the gradient method was first tested by solving the classical time invariant problem with satisfactory results. As an important note, in our model we use the Caputo definition for fractional derivatives, so that the results differ from those of Agrawal (2004) and Tricaud and Chen (2010), but agree with those of Agrawal (2008) which used the same fractional derivative definition.

Once our numerical strategy has been validated, we used it to solve the fermentation problem. Our results could not be compared to literature (since no similar results have been reported) but the results are consistent with the expected physicochemical behavior of the system. Biomass growth behavior is fundamental and affects both production yield and substrate consumption. Also, we compared our results with the results obtained by assuming several different arbitrary control variable profiles and all of them resulted in lower values of the objective function.

The model for the second illustrative reactive system was derived by using a fractionalization approach to preserve consistency with the mass balance constraints (Toledo-Hernandez et al., 2014). As a result, the model dynamics involve fractional as well as ordinary differentiation operators. Therefore, the optimality conditions for the problem could not be derived from the approach provided by Agrawal (2008).

We propose then to represent the model dynamics in the Laplace domain, so that it becomes an algebraic model. Still, since the constraints are time dependent constraints, the operation time is discretized. The discretization approach calls for a shooting method to ensure that the non-local nature of fractional dynamics is taken into consideration. In summary, the solution technique for the thermal hydrolysis model involves the use of a NLP solver to attain optimal temperature profiles, and the combined use of an inverse Laplace function and the shooting method to solve the equations for each interval of the discretized time domain. Since optimal results have not been reported in the literature, the maximum reducing sugars concentration achieved was compared to the concentration obtained by using two control policies of constant values of temperature. Results are consistent with temperature profiles suggested in practice. As an alternative method to approach this problem, we are currently analyzing the feasibility of representing both the ordinary and the fractional derivative operators in terms of finite differences in the time domain, so that a simpler approach based just on an NLP solver can be applied.

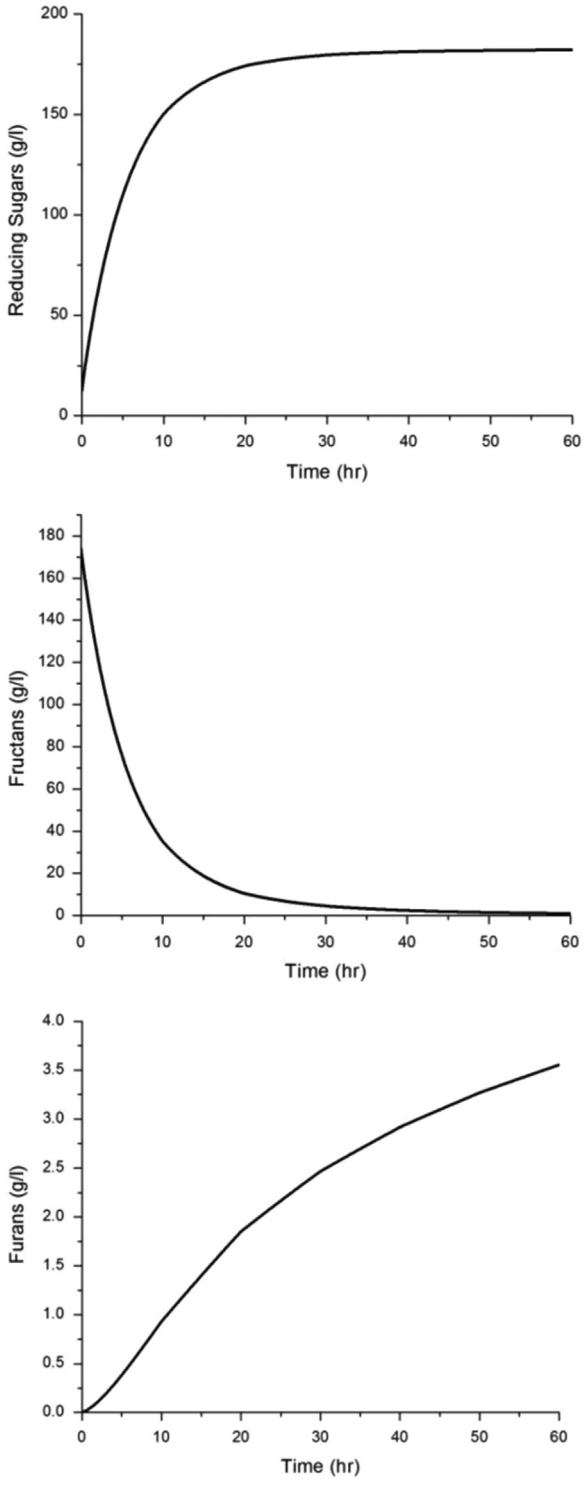

Fig. 6. Optimal profiles for the state variables in the thermal hydrolysis of Agave.

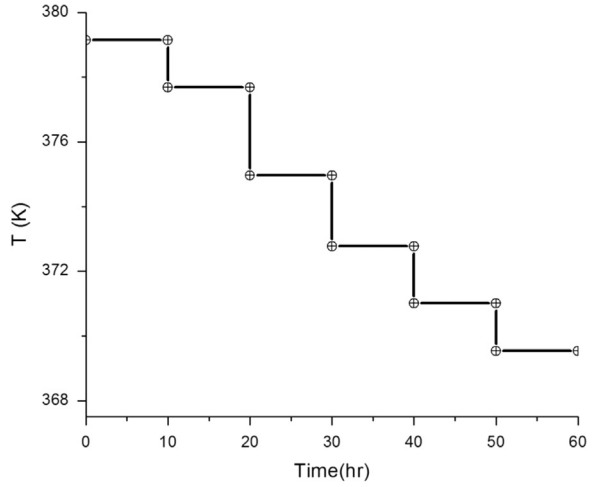

Fig. 7. Optimal temperature (control) profiles for the thermal hydrolysis of Agave.

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