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连续发酵过程分数阶非线性时滞最优控制

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摘要:针对连续发酵甘油转化 1,3-丙二醇(1,3-PD)的过程可能存在的时滞现象,考虑用分数阶时滞系统描述发酵过程,讨论系统状态关于参数的灵敏度。以甘油稀释速率和注入浓度为优化变量,以使灵敏度函数值较小为约束条件,以及使终端时刻 1,3-PD 浓度最大为性能指标,构建分数阶时滞系统最优控制模型。利用协态方法,得到性能指标和约束关于优化变量及参数的梯度,构造了基于序列二次规划(SQP)方法的优化算法。数值结果验证了优化策略的有效性。

关键词:分数阶导数;最优控制;时滞;连续发酵

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分数阶系统可以表示许多机械和生物动力学行为^[1-2],如记忆功能、遗传特征、扩散和粘塑性^[3-4], 在数学、工程等领域吸引了许多研究者的关注^[5-6]。时滞系统出现在许多实际工程问题中^[7-8],能够更 好地描述系统演化过程,根据一组给定实验数据估计未知的时滞是研究的关键问题之一^[9-10]。相比整 数阶最优控制,分数阶最优控制理论和应用起步较晚。Aghayan 等^[11]通过构建 Lyapunov-Krasovskii (LK)函数,讨论了执行器饱和条件下分数阶时滞系统的稳定性。Chen 等^[12]基于 Caputo 导数提出了具 有时滞系统的 SEIR 传染病模型,并讨论系统的分岔及病变时的平衡条件。Heydari 等^[13]研究 HIV/ AIDS 与疟疾合并感染的变阶分数阶时滞系统的最优控制问题,并构造 Grünwald-Letnikov 非标准有限差 分格式求解分数阶系统。Chen 等^[14]利用 Dickson 多项式处理分数阶时滞系统,采用直接轨迹优化方法 求解问题。Hassani 等^[15]考虑癌症治疗模型的非线性分数阶最优控制,采用广义移位勒让德多项式逼 近最优控制问题的数值解。

本文用分数阶时滞系统描述连续发酵甘油转化1,3-PD的过程。考虑到甘油稀释速率和注入浓度 对系统参数可能存在影响,讨论了分数阶意义下系统状态关于参数的灵敏度;为提高目标产物,以甘油 稀释速率和注入浓度为优化变量,以使终端时刻1,3-PD浓度最大为性能指标,使灵敏度函数值较小为 约束条件,构建分数阶非线性时滞系统连续发酵最优控制模型;进一步给出性能指标和约束关于优化变 量及参数的梯度公式,构造基于 SQP 方法的优化算法。经过数值计算得到的终端时刻目标产物高于已 有研究结果,验证了本文所提优化策略的有效性。

1 预备知识

设 *I* = [*a*,*b*] (−∞≤ *a* < *b* < +∞) 为 **R** 上的有限区间, *f*(*t*) (*t* ∈ *I*) 为给定函数。 定义 1 给定 α > 0, *f* 在 *I* 上的 Riemann-Liouville 意义下的左、右分数阶积分分别表示为:

$${}_{a}I^{\alpha}_{\iota}f(t) = \frac{1}{\Gamma(\alpha)}\int_{a}^{t}(t-\tau)^{\alpha-1}f(\tau) \,\mathrm{d}\tau, {}_{\iota}I^{\alpha}_{b}f(t) = \frac{1}{\Gamma(\alpha)}\int_{\iota}^{b}(\tau-t)^{\alpha-1}f(\tau) \,\mathrm{d}\tau,$$

其中,Γ(·)是Γ函数。

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定义 2 给定 $\alpha > 0$, *f* 在 *I* 上的 Riemann-Liouville 意义下的左、右分数阶积分分别表示为:

$${}_{a}\mathrm{D}_{t}^{\alpha}f(t) = \frac{1}{\Gamma(n-\alpha)} \left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^{n} \int_{a}^{t} (t-\tau)^{n-\alpha-1} f(\tau) \,\mathrm{d}\tau,$$
$${}_{t}\mathrm{D}_{b}^{\alpha}f(t) = \frac{(-1)^{n}}{\Gamma(n-\alpha)} \left(-\frac{\mathrm{d}}{\mathrm{d}t}\right)^{n} \int_{t}^{b} (\tau-t)^{n-\alpha-1} f(\tau) \,\mathrm{d}\tau_{\circ}$$

定义3 给定 $\alpha > 0$, $f \in I$ 上的 Caputo 意义下的左、右分数阶积分分别表示为:

$${}^{C}_{a} \mathrm{D}^{\alpha}_{t} f(t) = \frac{1}{\Gamma(n-\alpha)} \int_{a}^{t} (t-\tau)^{n-\alpha-1} f^{(n)}(\tau) \,\mathrm{d}\tau,$$
$${}^{C}_{t} \mathrm{D}^{\alpha}_{b} f(t) = \frac{(-1)^{n}}{\Gamma(\alpha)} \int_{t}^{b} (\tau-t)^{n-\alpha-1} f^{(n)}(\tau) \,\mathrm{d}\tau,$$

其中, $n = [\alpha] + 1$, $[\alpha] 是 \alpha$ 的整数部分。

性质 1 令
$$\alpha \in (0,1), f,g \in C^{1}([a,b],\mathbf{R}), 则有:$$

$$\int_{a}^{b} g(t) \cdot \binom{c}{a} D_{\iota}^{\alpha} f(t) dt = \int_{a}^{b} f(t) \cdot \binom{c}{l} D_{b}^{\alpha} g(t) dt + \binom{c}{a} I_{\iota}^{1-\alpha} g(t) \cdot f(t) \Big|_{a}^{b},$$
$$\int_{a}^{b} g(t) \cdot \binom{c}{l} D_{b}^{\alpha} f(t) dt = \int_{a}^{b} f(t) \cdot \binom{c}{a} D_{\iota}^{\alpha} g(t) dt + \binom{c}{a} I_{\iota}^{1-\alpha} g(t) \cdot f(t) \Big|_{a}^{b}.$$

2 连续发酵分数阶时滞系统

在连续发酵实验中,持续以恒定速率将底物注入到发酵罐中,同时以相同速率将反应物流出,发酵 罐中的菌群细胞始终在一种细微的振荡环境中生长,各反应物浓度不仅与当前时刻的生物量浓度有关, 还与之前某一时刻的生物量浓度有关,因此,模拟发酵过程中应考虑时滞现象。根据文献[16]的相关 定理与性质,采用分数阶导数直接替代整数阶导数进行建模,构造如下分数阶时滞系统:

$$\begin{cases} {}^{C}_{0} D_{t}^{\alpha_{1}} x_{1}(t) = \mu x_{1}(t-\xi) - U x_{1}, \\ {}^{C}_{0} D_{t}^{\alpha_{2}} x_{2}(t) = U(C_{so} - x_{2}) - q_{2} x_{1}(t-\xi), t \in [0,T], \\ {}^{C}_{0} D_{t}^{\alpha_{i}} x_{i}(t) = q_{i} x_{1}(t-\xi) - U x_{i}, i = 3, 4, 5, \end{cases}$$

其中: x_1 是生物量的质量浓度; x_2 , x_3 , x_4 , x_5 分别为甘油、1,3-PD、乙酸和乙醇的物质的量浓度; ξ 是时滞量, T 是终端时刻; U 是甘油的流加速率(即稀释速率), C_{so} 是初始甘油浓度, 根据实际发酵实验, U 和 C_{so} 在不同的实验条件下可取不同的实验值, $[U, C_{so}] \in U_c$: = [0.08,0.5] × [110.96,1883] $\in \mathbb{R}^2$; 细胞比生 长速度 μ , 底物比消耗率 q, 和产物比生成率 q_i (i = 3, 4, 5) 分别为^[17]

$$\mu = \mu_m \frac{x_2}{x_2 + k_s} \prod_{i=2}^5 \left(1 - \frac{x_i}{x_i^*} \right), q_2 = m_2 + \frac{\mu}{Y_2} + \Delta_2 \frac{x_2}{x_2 + K_2},$$
$$q_i = m_i + \mu Y_i + \Delta_i \frac{x_2}{x_2 + K_i}, i = 3, 4, 5_{\circ}$$

令 $p = (\mu_m, k_s, m_2, \dots, m_5, K_2, \dots, K_5, Y_2, \dots, Y_5, \Delta_2, \dots, \Delta_5)^{\mathsf{T}} \in \mathbb{R}^{18}$ 为参数向量。参考文献[17]的辨 识结果,给定参数容许集合为

 $P = \left\{ \left(p_1, p_2, \cdots, p_{18} \right)^{\mathrm{T}} \in \mathbf{R}^{18} : p_{j_*} \leq p_j \leq p_j^*, j = 1, 2, \cdots, 18 \right\}_{\circ}$

由文献[17—18],取时滞量 ξ = 0.26,阶数 $\alpha_i \in (0,1), i = 1, 2, \cdots, 5$ 。 阶数辨识结果见表 1。

表 1 阶数辨识结果 ¹¹⁷ Tab.1 The identified results for the orders											
阶数	α_1	α2	α ₃	α_4	α ₅						
结果	0.699 451	0.782 464	0.774 484	0.763 372	0.672 697						

定义容许状态集为:

$$W_{ad} = \left\{ \boldsymbol{x} \in \mathbf{R}^{5} \mid x_{i} \in [x_{i_{*}}, x_{i}^{*}], i = 1, 2, \dots, 5 \right\},\$$

其中, x_{i_*} , x_i^* 分别表示上限和下限。

令 $z = (U, C_{so}, p) \in \mathbb{R}^{20}$,定义可行集为 $\kappa_{:} = \{z \in U_{c} \times P \mid x(t \mid z) \in W_{ad}, \forall t \in [0, T]\}$,则分数阶 时滞系统可表示为

$$\begin{cases} {}_{0}^{c} \mathbf{D}_{t}^{\alpha} \mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t), \mathbf{x}_{\xi}(t), \mathbf{z}), t \in [0, T], \\ \mathbf{x}(0) = \mathbf{x}^{0}, \end{cases}$$
(1)

其中, $\mathbf{x}^0 = (x_1^0, x_2^0, \cdots, x_5^0)^{\mathsf{T}}$ 是给定的初始状态, $\mathbf{x}_{\xi}(t) = \mathbf{x}(t - \xi)_{\circ}$

根据已有研究结果,**f**满足如下条件:

(a) f关于 x, x_{ε}, z 是 Lipschitz 连续的;

(b) 存在常数 K > 0, 使得 $\| f(\mathbf{x}(t), \mathbf{x}_{\xi}(t), \mathbf{z}) \| \leq K(1 + \|\mathbf{x}\| + \|\mathbf{x}_{\xi}\|)$, 其中 $\|\cdot\| \in Euclidean 范数$ 。

性质 2 对于任意的 $z \in U_e \times P$,记分数阶系统(1)的解为 x(t|z),满足

$$\boldsymbol{x}(t|\boldsymbol{z}) = \boldsymbol{x}_0 + \frac{1}{\Gamma(\alpha)} \int_0^T (t - \tau)^{\alpha - 1} \boldsymbol{f}(\boldsymbol{x}(t), \boldsymbol{x}_{\xi}(t), \boldsymbol{z}) \, \mathrm{d}\tau_0$$

性质3 任给 $z \in U_c \times P$,分数阶系统(1)的解x(t|z)是一致有界的,且关于z连续。

3 分数阶时滞最优控制模型

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3.1 分数阶时滞最优控制问题

据已有研究结果显示,在相同的实验条件下,不同的甘油流加速率和注入浓度对系统参数会产生影响,导致辨识结果产生较大的偏差。因此,在优化 U 和 C_{so} 时,需要考虑它们对系统参数的影响,为此引入系统状态对参数的灵敏度。

定义
$$\phi_j^i(t) = \frac{\partial x_i(t|z)}{\partial z_j} (i = 1, 2, \dots, 5, j = 3, 4, \dots, 20)$$
,满足如下辅助方程:

$$\begin{cases} {}^{C}_{0} D_t^{\alpha} \phi_j^i(t) = \left(\frac{\partial f_i(\boldsymbol{x}(t), \boldsymbol{x}_{\xi}(t), z)}{\partial \boldsymbol{x}}\right)^{\mathrm{T}} \phi_j(t) + \left(\frac{\partial f_i(\boldsymbol{x}(t), \boldsymbol{x}_{\xi}(t), z)}{\partial \boldsymbol{x}(t-\xi)}\right)^{\mathrm{T}} \frac{\partial \boldsymbol{x}(t-\xi)}{\partial z_j} + \frac{\partial f_i(\boldsymbol{x}(t), \boldsymbol{x}_{\xi}(t), z)}{\partial z_j}, t \in [0, T], \end{cases}$$
(2)

由文献[17],灵敏度函数 $\frac{\partial x_i(n_z)}{\partial z_i}$ 存在且连续, x 关于 z 的二阶偏导数满足:

$${}^{C}_{0}\mathrm{D}^{\alpha}_{i}\left(\frac{\partial^{2}x_{i}}{\partial z_{j}\partial z_{s}}\right) = \left(\frac{\partial f_{i}}{\partial \boldsymbol{x}}\right)^{\mathrm{T}}\frac{\partial^{2}\boldsymbol{x}}{\partial z_{j}\partial z_{s}} + \frac{\partial}{\partial z_{s}}\left(\frac{\partial f_{i}}{\partial \boldsymbol{x}}\right)^{\mathrm{T}}\frac{\partial \boldsymbol{x}}{\partial z_{j}} + \left(\frac{\partial f_{i}}{\partial \boldsymbol{x}_{\xi}}\right)^{\mathrm{T}}\frac{\partial^{2}\boldsymbol{x}_{\xi}}{\partial z_{j}\partial z_{s}} + \frac{\partial}{\partial z_{s}}\left(\frac{\partial f_{i}}{\partial \boldsymbol{x}_{\xi}}\right)^{\mathrm{T}}\frac{\partial \boldsymbol{x}_{\xi}}{\partial z_{j}\partial z_{s}} + \frac{\partial}{\partial z_{s}}\left(\frac{\partial f_{i}}{\partial \boldsymbol{x}_{\xi}}\right)^{\mathrm{T}}\frac{\partial \boldsymbol{x}_{\xi}}{\partial z_{s}} + \frac{\partial}{\partial z_{s}}\left(\frac{\partial f_{i}}{\partial \boldsymbol{x}_{\xi}}\right)^{\mathrm{T}}\frac{\partial \boldsymbol{x}_{\xi}}{\partial z_{s}} + \frac{\partial^{2} f_{i}}{\partial z_{j}\partial z_{s}}, \quad (3)$$

且 $\frac{\partial^2 x_i}{\partial z_j \partial z_s} \bigg|_{t=0} = 0$ 。因此,为最大化目标产物,建立如下分数阶时滞系统最优控制问题:

问题(P1): $\begin{cases} \min J(z) = -x_3(T) ,\\ \text{s.t.} \left\| \frac{\partial x_i(T|z)}{\partial z_j} \right\| \leq \varepsilon, z \in U_c \times P, \varepsilon$ 是充分小的常数, $i = 1, 2, \dots, 5, j = 3, 4, \dots, 20_o$

定理1 问题(P1)存在一个最优解 $z^* \in U_c \times P$,使得 $J(z^*) \leq J(z)$, $\forall z \in U_c \times P_o$

证明 由性质 3,分数阶时滞系统(1)的解关于 z 连续,因此,性能指标 J(z) 在 $U_c \times P$ 上连续;又由 于 κ 是非空紧集,由连续函数的性质,问题(P1)存在最优解。

3.2 状态约束近似转化

为显式表达状态约束,令

$$\begin{cases} g_i(\boldsymbol{x}(t|\boldsymbol{z})) := x_i(t|\boldsymbol{z}) - x_i^* \leq 0, \\ g_{i+5}(\boldsymbol{x}(t|\boldsymbol{z})) := x_{i_*} - x_i(t|\boldsymbol{z}) \leq 0, i = 1, 2, \cdots, 5, \end{cases}$$
(4)

约束(4)等价于

$$G(z) := \sum_{i=1}^{10} \int_{0}^{T} \max \{0, g_{i}(\boldsymbol{x}(t | \boldsymbol{z}))\} dt = 0_{\circ}$$
(5)

由于约束(5)不满足常规约束规范,下面使用近似平滑技术^[19]进行处理。定义

$$\tilde{g}_{\varepsilon,i}(\boldsymbol{x}(t|\boldsymbol{z})) = \begin{cases} 0, & g_i(\boldsymbol{x}(t|\boldsymbol{z})) < -\varepsilon, \\ \frac{(g_i(\boldsymbol{x}(t|\boldsymbol{z})) + \varepsilon)^2}{4\varepsilon}, & -\varepsilon \leq g_i(\boldsymbol{x}(t|\boldsymbol{z})) \leq \varepsilon, \\ g_i(\boldsymbol{x}(t|\boldsymbol{z})), & g_i(\boldsymbol{x}(t|\boldsymbol{z})) > \varepsilon, \end{cases}$$

其中, ε > 0 是足够小的常数。则约束(5)可以近似表示为

$$G_{\varepsilon,\gamma}(z) := \sum_{i=1}^{10} \int_{0}^{T} \widetilde{g}_{\varepsilon,i}(\boldsymbol{x}(t|z)) dt - \gamma \leq 0,$$

其中, γ > 0 是可调参数。从而问题(P1)可近似转化为下面问题:

问题(P2):
$$\begin{cases} \min J(z) = -x_3(T) ,\\ \text{s.t.} W_{ij}(z) = \left\| \frac{\partial x_i(T|z)}{\partial z_j} \right\| - \varepsilon \leq 0, i = 1, 2, \dots, 5, j = 3, 4, \dots, 20, \\ G_{\varepsilon, \gamma}(z) \leq 0, z \in U_c \times P_o \end{cases}$$

性质4 问题(P1)的可行解也是问题(P2)的可行解。 证明过程详见文献[20]。

4 优化算法

4.1 梯度公式

为利用基于梯度的优化方法,下面将讨论性能指标及约束关于优化变量 z 的梯度。 定义 Hamiltonian 函数 H_w 和 \tilde{H}_w 为:

$$H_w(\boldsymbol{x}(t),\boldsymbol{x}_{\xi}(t),\boldsymbol{z},\boldsymbol{\lambda}_w(t)) = \boldsymbol{\lambda}_w^{\mathrm{T}}(t) \boldsymbol{f}(\boldsymbol{x}(t),\boldsymbol{x}_{\xi}(t),\boldsymbol{z}),$$

$$\widetilde{H}_{w}(\boldsymbol{x}(t+\xi),\boldsymbol{x}_{\xi}(t),\boldsymbol{z},\widetilde{\boldsymbol{\lambda}}_{w}(t)) = \widetilde{\boldsymbol{\lambda}}_{w}^{\mathrm{T}}(t)\boldsymbol{f}(\boldsymbol{x}(t+\xi),\boldsymbol{x}_{\xi}(t),\boldsymbol{z})\boldsymbol{e}(T-t-\xi),$$

其中, $\lambda_w(\cdot)$ 和 $\tilde{\lambda}_w(\cdot)$ 分别是 $H_w(\cdot)$ 和 $\tilde{H}_w(\cdot)$ 的协态, 且 $\tilde{\lambda}_w(t) = \lambda_w(t + \xi)$, $e(\cdot)$ 是单位阶跃函数。下 面将约束 $W_u(z)$ 整合为一个函数 W(z), 并转化为如下形式:

$$W(\boldsymbol{z}) = \sum_{i=1}^{5} \sum_{j=3}^{20} \left\| \frac{\partial x_i(T|\boldsymbol{z})}{\partial z_j} \right\| + \int_0^T \left[H_w(\boldsymbol{x}(t), \boldsymbol{x}_{\xi}(t), \boldsymbol{z}, \boldsymbol{\lambda}_w(t)) - \boldsymbol{\lambda}_w^{\mathrm{T}}(t) \boldsymbol{f}(\boldsymbol{x}(t), \boldsymbol{x}_{\xi}(t), \boldsymbol{z}) \right] \mathrm{d}t_{\circ}$$
(6)

由链式法则,可得

$$\frac{\partial W(z)}{\partial z} = \sum_{i=1}^{5} \sum_{j=3}^{20} \left. \frac{\partial}{\partial z} \left(\left\| \frac{\partial x_i(T | z)}{\partial z_j} \right\| \right) + \int_0^T \left[\Delta H_w(\boldsymbol{x}(t), \boldsymbol{x}_{\xi}(t), \boldsymbol{z}, \boldsymbol{\lambda}_w(t)) - \boldsymbol{\lambda}_w^{\mathrm{T}}(t) \left({}_0^C \mathrm{D}_t^{\alpha} \Delta \boldsymbol{x}(t) \right) \right] \mathrm{d}t, \quad (7)$$

其中,

$$\Delta H_w(\boldsymbol{x}(t), \boldsymbol{x}_{\xi}(t), \boldsymbol{z}, \boldsymbol{\lambda}_w(t)) = \frac{\partial H_w}{\partial \boldsymbol{x}} \Delta \boldsymbol{x}(t) + \frac{\partial H_w}{\partial \boldsymbol{x}(t-\xi)} \Delta \boldsymbol{x}(t-\xi) + \frac{\partial H_w}{\partial \boldsymbol{z}}, \ \Delta \boldsymbol{x}(t) = \frac{\partial \boldsymbol{x}(t|\boldsymbol{z})}{\partial \boldsymbol{z}},$$

选择适当 $\lambda_w(t)$ 满足下列协态方程:

$$\begin{cases} {}_{t} D_{T}^{\alpha} \boldsymbol{\lambda}_{w}^{\mathrm{T}}(t) = \frac{\partial H_{w}(\boldsymbol{x}(t|\boldsymbol{z}), \boldsymbol{x}_{\xi}(t|\boldsymbol{z}), \boldsymbol{z}, \boldsymbol{\lambda}_{w}(t))}{\partial \boldsymbol{x}} + \frac{\partial \widetilde{H}_{w}(\boldsymbol{x}(t+\xi|\boldsymbol{z}), \boldsymbol{x}_{\xi}(t|\boldsymbol{z}), \boldsymbol{z}, \widetilde{\boldsymbol{\lambda}}_{w}(t))}{\partial \boldsymbol{x}}, \\ {}_{t} I_{T}^{1-\alpha} \boldsymbol{\lambda}_{w}(t) \mid_{t=T} = \sum_{i=1}^{5} \sum_{j=3}^{20} \left. \frac{\partial}{\partial \boldsymbol{z}} \left(\left\| \frac{\partial x_{i}(T|\boldsymbol{z})}{\partial \boldsymbol{z}_{j}} \right\| \right)_{\circ} \right) \end{cases}$$

$$(8)$$

由 H_w 和 \tilde{H}_w 的定义,可得

$$\int_{0}^{T} \frac{\partial H_{w}(\boldsymbol{x}(t), \boldsymbol{x}_{\xi}(t), \boldsymbol{z}, \boldsymbol{\lambda}_{w}(t))}{\partial \boldsymbol{x}(t - \xi)} \Delta \boldsymbol{x}(t - \xi) dt = \int_{0}^{T} \frac{\partial \widetilde{H}_{w}(\boldsymbol{x}(t + \xi), \boldsymbol{x}_{\xi}(t), \boldsymbol{z}, \widetilde{\boldsymbol{\lambda}}_{w}(t))}{\partial \boldsymbol{x}} \Delta \boldsymbol{x} dt, \qquad (9)$$

由分数阶分部积分公式,可得

$$\int_{0}^{T} \boldsymbol{\lambda}_{w}^{\mathrm{T}}(t) \,_{0}^{c} \mathrm{D}_{\iota}^{\alpha} \,\Delta \boldsymbol{x}(t) \,\mathrm{d}t = \int_{0}^{T} \Delta \boldsymbol{x}(t) \,(_{\iota} \mathrm{D}_{T}^{\alpha} \,\boldsymbol{\lambda}_{w}(t) \,)^{\mathrm{T}} \mathrm{d}t + _{\iota} I_{T}^{1-\alpha} \boldsymbol{\lambda}_{w}^{\mathrm{T}}(t) \,\Delta \boldsymbol{x} \mid_{0}^{T}, \tag{10}$$

将式(8)~(10)代人式(7)中,且由于 $\Delta x(0) = 0$,可得

$$\frac{\partial W(z)}{\partial z} = \int_0^T \frac{\partial H_w(x(t), x_{\xi}(t), z, \lambda_w(t))}{\partial z} dt_{\circ}$$
(11)

同理,选取适合协态 $\lambda(t)$ 和 $\lambda_w(t)$,类似得到性能指标 J(z) 和约束函数 $G_{\varepsilon,\gamma}$ 关于 z 的梯度,其中:

$$\frac{\partial J(z)}{\partial z} = \int_0^T \frac{\partial H_w(\boldsymbol{x}(t), \boldsymbol{x}_{\xi}(t), \boldsymbol{z}, \boldsymbol{\lambda}_w(t))}{\partial z} dt, \qquad (12)$$

$$\frac{\partial G_{\varepsilon,\gamma}(z)}{\partial z} = \int_{0}^{T} \frac{\partial \widetilde{H}_{w}(\boldsymbol{x}(t), \boldsymbol{x}_{\xi}(t), \boldsymbol{z}, \boldsymbol{\lambda}_{w}(t))}{\partial z} dt_{o}$$
(13)

4.2 数值算法

利用 4.1 节的梯度公式,下面构造一个基于 SQP 方法的优化算法,具体步骤如下:

1) 给定参数 $z \in U_{\varepsilon} \times P, \varepsilon > 0, \gamma > 0$ 的初值,且设定 $\varepsilon, \overline{\gamma}$ 为参数 ε, γ 的临界值, $\beta_1, \beta_2 \in (0, 1)$ 为比例折减系数。

2) 利用 G-L 方法^[21] 以及分数阶短存储原理^[22] 计算式(1) ~ (3)、(10),得到状态方程、灵敏度函数 $\frac{\partial x_i(t|z)}{\partial z_j}$ 和 $\frac{\partial^2 x_i}{\partial z_j \partial z_s}$ 对应的协态方程的数值解;进一步应用式(11) ~ (13) 分别计算性能指标、约束关于

z的梯度。

3) 采用 SQP 方法求解最优参数 z_{\circ} 若不符合 SQP 停机准则,可转至步骤 2);否则,直接输出最优 解 z^{e,γ^*} 。

4)检查 $G(z^{\epsilon,\gamma^*}) = 0$ 的可行性。若 $G(z^{\epsilon,\gamma^*}) = 0$ 可行,转步骤 5);若 $G(z^{\epsilon,\gamma^*}) = 0$ 不可行,令 $\gamma_{:} = \beta_1 \gamma_{\circ}$ 若 $\gamma \leq \overline{\gamma}$,得到了异常解;否则,转步骤 2)。

5) 令 $\varepsilon_{:=}\beta_{2}\varepsilon_{,}\gamma_{:=}\beta_{2}\gamma_{o}$ 若 $\varepsilon \leq \varepsilon$,转步骤 2);否则输出 $z^{*} = z^{\varepsilon,\gamma^{*}}$,即得到最优解 $J(z^{*})$ 及 z^{*} 。

5 数值结果

依据发酵实验原理进行操作,给定初值条件为 x^0 = (0.405,440.8578,0,0,0)^T,发酵终止时间 T = 70 h。应用算法数值求解时,选取步长为1/3600,利用分数阶短存储原理得到节点数n = 600,且 SQP 粒子数为288,其他参数取值详见表2。以C++为编程语言,在并行机上完成了8次数值试验,平均 耗时5 h/次,试验得到优化的甘油流速率为0.08,优化的甘油初始浓度为703.371 mmol·L⁻¹,并由此得 到终端时刻1,3-PD 浓度为772.843 mmol·L⁻¹。最优参数的辨识结果详见表3,反应器中的各物质随 时间变化曲线详见图1、2。相比文献[23]的最大浓度710.1 mmol·L⁻¹,本文的结果优于文献[23]。由 图1、2 可以看出,发酵初期各物质浓度比较震荡,后期趋于稳定,与实际发酵过程比较吻合,显示了数值 模拟结果的可参考性。

Tab.2 Parameters values													
参数	$(-\varepsilon)^-$	$\overline{\gamma}$	$oldsymbol{eta}_1$	β_2	$M_{ m sup}$	$M_{\rm iter}$	$w_{\rm max}$	w_{\min}	c_1	c_2			
取值	í 1.0×10	⁻⁸ 1.0×10 ⁻²	0.5	0.1	5×10 ⁷	300	0.9	0.4	2.0	2.0			
				表 3 :	参数辨识结	果							
Tab.3 The identified results for the parameters													
参数	$\mu_{\scriptscriptstyle m}$	k_s	m_2	Y_2	Δ_2	K_2	n	n ₃	Y_3	Δ_3			
结果	0.704 814	0.350 162	1.226 5	0.012 012 8	27.417 8	12.987	8 -2.8	96 99	87.863 3	31.156 5			
参数	<i>K</i> ₃	m_4	Y_4	Δ_4	K_4	m_5]	Y ₅	Δ_5	K ₅			
结果	22.365 8	-0.865 612	18.423 1	8.079 09	72.000 9	6.446 3	31 16.4	474 9	0.333 15	-0.068 669 6			



表 2 参数取值 Tab.2 Parameters values

(c) 乙酸





6 结论

本文针对微生物连续发酵生产1,3-PD 过程,通过引入分数阶微积分思想,建立新的分数阶非线性时滞系统模型。为使终端时刻1,3-PD 浓度最大,以参数的灵敏度函数为约束,以甘油的流加速率和初始注入浓度为控制变量,构造了连续发酵分数阶时滞系统的最优控制模型,并利用 SQP 算法,通过优化计算得到最优流加策略,为实际发酵过程提供参考。

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Optimal Control of Fractional Nonlinear Time-delay System in Continuous Fermentation Process

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Abstract: Considering that there may be a time-delay in the conversion of glycerol to 1,3-propanediol (1,3-PD) in continuous culture, a fractional order time-delay system is considered to describe the fermentation process, and the sensitivity of system states with respect to the parameters is discussed. The optimal control model of the fractional time-delay system for the continuous fermentation was formulated with a small sensitivity as the constraint, the glycerol dilution rate and feeding concentration as the optimization variable, and the maximum concentration of 1,3-PD at the terminal time as the performance index. By using the co-state method, the gradients of performance index and constraints with respect to optimization variables and parameters were obtained, and a optimization algorithm based on sequential quadratic programming (SQP) method was constructed. Finally, the numerical results were used to verify the effectiveness of the optimization strategies.

Keywords: fractional derivative; optimal control; time-delay; continuous fermentation

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