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Equivalent Models, Maximum Principle and Optimal Control of Continuous Biotechnological Process: *Peculiarities and Problems*

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Abstract: *A Brunovsky normal form model is introduced by using some differential geometry results for reduction of a non-linear kinetic model into equivalent linearised form. The transformed model is implemented for optimal control determination with the maximum principle.*

Keywords: *Brunovsky normal form, Optimal control, Continuous biotechnological process, Differential geometry*

Introduction

The biosynthesis process description belongs to the class of non-linear, non-stationary, complex systems. The implementation of optimisation methods as well as Pontryagin's maximum principle-based method is problematic when a non-linear model is used. A differential geometric technique permits the utilisation of a new non-linear transformation of a biotechnological kinetic model into an equivalent model. The model investigated in this paper permits exact linearization to the Brunovsky normal form. In certain cases this transformation technique allows to obtain an equivalent model, which substantially simplifies the mathematical derivations leading to the optimal control law. All these peculiarities, together with the complex formula of the latter dependence cause difficulties when implementing this differential geometric technique. However, in other cases this peculiarity becomes an advantage, which permits interesting new solutions. In this paper we discuss the possibilities for utilisation of these equivalent models in order to determine the optimal control solutions.

Transformations and equivalent models

We discuss yeast's *C.blankii 35* continuous cultivation process [6, 8]. As usual, the first step in such investigations is identifying an adequate kinetic model. Consider the lactose utilising yeast's *C.blankii 35* continuous cultivation process, described by a non-linear kinetic model as follows [6, 7, 9]:

$$\begin{aligned}
&\dot{x} = \mu x - xD,\\
&\dot{S} = -\frac{1}{y}\mu x + (So - S)D,\\
&\dot{\mu} = m(\mu_m \frac{S}{K_S + S + S^2 K_0} - \mu) + v,\\
&\dot{a} == k_2 \mu x - Da,
\end{aligned} \qquad (\boldsymbol{A})$$

where x denotes biomass concentration [g/l], S - limiting substrate (residual lactose) concentration [g/l], μ - the specific growth rate [h^{-1}], a denotes acetate concentration [g/l], So - initial concentration of limiting substrate, D - the dilution rate (model input) in the same dimension as the specific growth rate, v - white noise. Coefficients are as follows: μ_{max} – maximal specific growth rate [h^{-1}], K_S – constant [g/l], K_o – inhibitory effects constant [-], m – correction constant [-]. The system parameters are as follows: μ_m=0.776 [h^{-1}], K_S= 14.81 [g/l], K_o=1/1231 [–], m=3.51 [–], S_e=0.2625 [g/l], S_0=9 [g/l], y=0.5584 [–], D_e=0.01 [h^{-1}]. The fourth equation in (***A***) is equivalent to the first one, which is seen by implementing the simple transformation:

$$x = \frac{1}{k_2} a.$$

Finally the non-linear kinetic model describes the continuous cultivation process:

$$\begin{aligned} \dot{x} &= \mu x - Dx, \\ \dot{S} &= -\frac{1}{y}\mu x + (So - S)D, \\ \dot{\mu} &= m(\mu_m \frac{S}{K_S + S + S^2 K_0} - \mu) + v. \end{aligned} \tag{1}$$

In another form this model is $d(x,S,\mu)'/dt=\mathbf{f_0}+\mathbf{f_1}D$. The basis of the appropriate linear space of the model (1) is $\{\mathbf{f_1}\}$ and $\mathbf{f_0}$ determines the affine space [1, 4, 6]. The first step leading to the Brunovsky normal form is a simplification of the basis of the affine model space. The common integral of the field $\mathbf{f}_1$ is a solution of the equation:

$$-\frac{\dot{x}}{x} = \frac{\dot{S}}{(S_o - S)}. \tag{2}$$

Taking into account the established results in [1] and the solution of equation (2), the model (1) is transformed with the diffeomorphic transformation:

$$\begin{aligned} x_1 &= x, \\ x_2 &= \frac{x}{(S - S_0)}, \\ x_3 &= \mu, \end{aligned} \tag{3}$$

where the new affine model has the form $d\mathbf{x}/dt=\mathbf{f}_0+\mathbf{f}_1 D$, $\mathbf{x}=(x_1, x_2, x_3)$:

$$\mathbf{f}_0 = \begin{pmatrix} x_3.x_1 \\ x_3(.x_1 + k_1 x_2^2) \\ m.\mu_m \dfrac{x_2}{K_s + x_2 + x_2^2 K_0} - x_3 \end{pmatrix}, \tag{4}$$

$$\mathbf{f}_1 = \begin{pmatrix} -x_1 \\ 0 \\ 0 \end{pmatrix}. \tag{5}$$

Now the field $\mathbf{f}_1$ has a simple form and it is easy to determine the *t*-differential forms. The dual spaces defined by the *t*-differential forms and their range determine the equivalent system [1, 4, 6]. In this case the system obtains the Brunovsky normal form:

$$\begin{aligned} \dot{x} &= y, \\ \dot{y} &= z, \\ \dot{z} &= \mathrm{V}. \end{aligned} \tag{6}$$

The corresponding non-linear transformation (diffeomorphism) is of the form:

$$\begin{aligned} x &= x_2\,, \\ y &= x_3\left(x_2 + k_1 x_2^2\right), \\ z &= m\left(\mu_m \frac{S}{K_S + S + S^2 K_o} - \mu\right)\left(x_2 + k_1 x_2^2\right) + x_3^2\left(x_2 + 3k_1 x_2^2 + 2k_1^2 x_2^3\right)\,, \end{aligned} \tag{7}$$

where S is substrate concentration, x_2 corresponds to $x'_1/(x'_2\text{-}S_0)$ and $\mathbf{x}'=(x_1', x_2', x_3')$, which are the state vector coordinates of model (1). The control input V of the model (6) is linked with the control input D of the model (1) by the formula [1, 6]:

$$\mathrm{V} = \left(x_2 + k_1 x_2^2\right)\left[m\frac{\left(k_S - k_0 S^2\right)}{k_S + S + S^2 k_0}\right]\left[-k_2 x_3 x_1 + \left(S_0 - S\right)D\right] + m^2\left(x_2 + k_1 x_2^2\right)\left(\frac{\mu_m S}{k_S + S + S_2 k_0} - x_3\right) +$$

$$+ 3m x_3\left(\frac{\mu_m S}{k_S + S + S^2 k_0} - x_3\right)\left(x_2 + 3k_1 x_2^2 + 2k_1^2 x_2^3\right) + x_3^3\left(x_2 + k_1 x_2^2\right)\left(1 + 6k_1 x_2 + 6k_1^2 x_2^2\right)\,. \tag{8}$$

The main conclusion after these transformations is that the model (1) and the model (6) are equivalent, in the sense that every solution of the model (1) with control D is a solution of model (6) with control V using transformations (3) and (7) [1]. There are many other non-linear transformations and the Brunovsky normal form is only one of them.

Maximum principle and optimal control

The optimisation problem is:

min $(x(t_1)\text{-}x^0)^2$, where the variable x is the first coordinate of the model (6) state vector and $t\in[0,t_1]$, $D\in[0,D_0]$. Here $\mathbf{x}^0$ is a chosen constant.

In agreement with the maximum principle, the following problem has to be solved:

$$\begin{aligned} \dot{\vec{\mathbf{x}}} &= \frac{\partial H(t,\vec{\mathbf{x}},D,\vec{\mathbf{\Psi}})}{\partial \vec{\mathbf{\psi}}},\ \vec{\mathbf{x}} = (x,y,z),\ \vec{\mathbf{\Psi}} = (\psi_1,\psi_2\psi_3)\,, \\ \dot{\vec{\mathbf{\Psi}}} &= -\frac{\partial H(t,\vec{\mathbf{x}},D,\vec{\mathbf{\Psi}})}{\partial \vec{\mathbf{x}}}\,, \\ \vec{\mathbf{\Psi}}(t_1) &= -\frac{\partial (x - x^0)^2}{\partial \vec{\mathbf{x}}}(t_1)\,, \\ \mathrm{H}(t,\vec{\mathbf{x}}(t),D(t),\vec{\mathbf{\Psi}}(t)) &= \max_D \mathrm{H}(t,\vec{\mathbf{x}}(t),D(t),\vec{\mathbf{\Psi}}(t))\,. \end{aligned} \tag{9}$$

The model's (6) Hamiltonian H(.) is:

$$\mathrm{H} = \Psi_1 y + \Psi_2 z + \Psi_3 \mathrm{V}\,,$$

$$\Psi_1 = C_1\,,$$

$$\Psi_2 = -C_1 t + C_2 \,, \tag{10}$$

$$\Psi_3 = C_1 \frac{t^2}{2} - C_2 t + C_3 \,.$$

But the problem is more complicated. The domain of the control input V(x, y, z, t,...) depend on variables (x, y, z). According the optimal control theory, $\Phi(t, x, y, z, \psi)=\max_{V(x, y, z)}H(t, x, y, z, D, \psi)$ must be put in the place of H(.) [3]. In addition, constants C_1, C_2, C_3 are calculated in the moment t_1. The constants C_1, C_2 and C_3 have the forms:

$$C_1 = 2(x - x_0) \,, \tag{11}$$

$$C_2 = -2(x - x^0)t_1 \,, \tag{12}$$

$$C_3 = 2(x - x^0)t_1^2 \,. \tag{13}$$

Finally, the optimal control law depends on formula max(Ψ_3V), where:

$$\Psi_3 \mathrm{V} = \left(x - x^0\right)\left(t_1 - t\right)^2 \mathrm{V},$$

$$\Psi_3 = C_1 \frac{t^2}{2} - C_2 t + C_3 \quad . \tag{14}$$

This part of V, which determines max(Ψ_3V) is negative /under the chosen initial conditions/. That is why only $\Psi_3(t)$ determines the control law. Concluding this section we emphasise that the Pontryagin′s conditions are not sufficient conditions. Some sufficient conditions can be determined with the Krotov′s function. Equations (9) determine only the derivative of the Krotov′s function [3].

Discussion

Because the maximum principle does not give sufficient conditions the control law needs supplementary verifications. Here Belman′s principle [2] is very useful. It states that the control law is optimal in every time subinterval. And now we note that the optimisation problem discussed in the previous section, in view of the Belman′s principle becomes "**reach for minimal time the state x^0**". The result is shown in fig.1. Now in the formula max(Ψ_3V) the sign sgn(x (t)-x^0) is taken into account at every moment t.

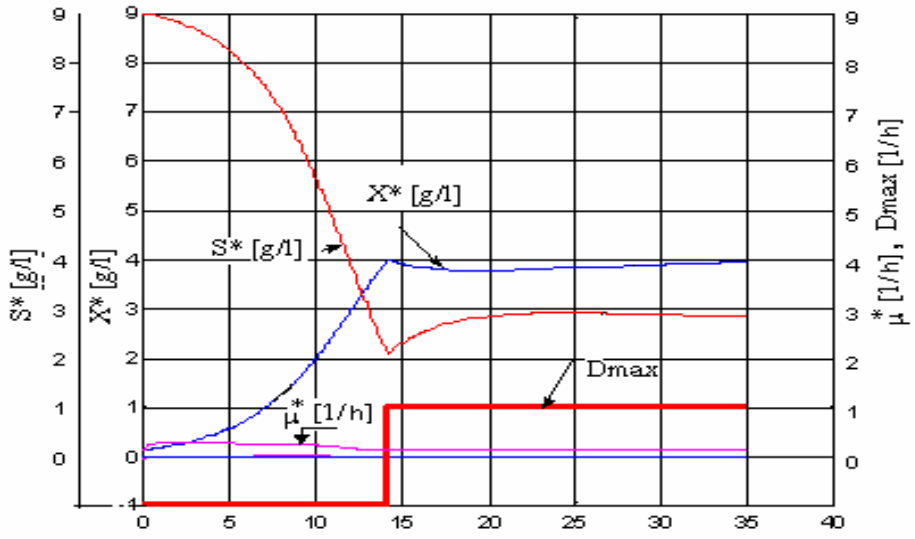

Fig. 1 Optimal control where x is by model (6)

The use of Belman′s principle needs cumulative criteria. Such a criterion is for example the maximum biomass in the end of a fed-batch biotechnological process [5]. It should be noted that other similar problems can be solved with this mathematical apparatus. An example is the achievement and stabilising of a biomass concentration x^0 by model (1):

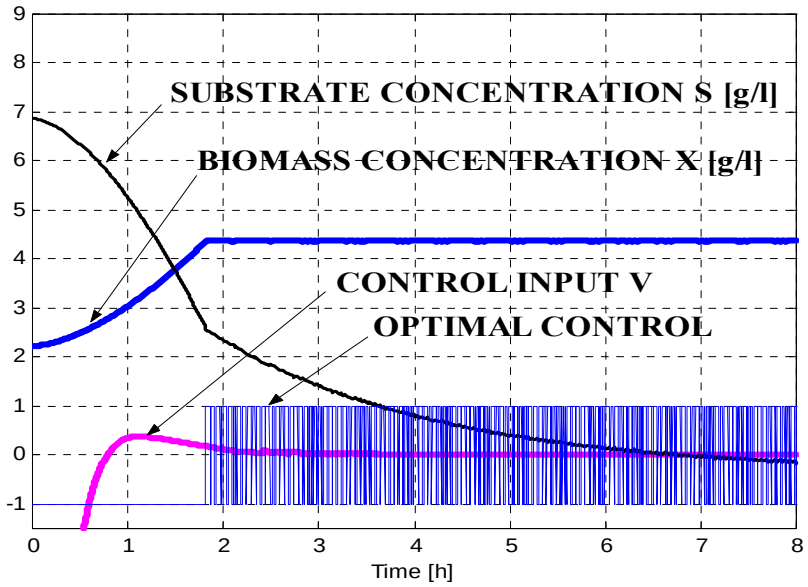

Fig. 2 Optimal control x - model (1)

The optimal control law is analytically determined by implementing the Belman′s principle. The optimal control is obtained by iterations of relatively small intervals $[t_i,t_{i+1}]$, solving the optimal problem in each subinterval.

Conclusions

The discussed biotechnological models were shown here to be equivalent in the sense that every solution to one of them is solution to the others.

The non-linear equivalent transformation proposed here to the Brunovsky normal form of the continuous biotechnological process permits obtaining a stationary linear model. This model is also easy for optimisation with the Pontryagin's maximum principle.

Some disadvantages of this approach are the complex formulae of the state vector (x, y, z) by model (6), and the complex formula of the control V(.). But with the use of Bellman′s principle these formulae permit analytical determination of new control laws.

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