THE EFFECT OF ALGEBRAIC EQUATIONS ON THE STABILITY OF PROCESS SYSTEMS

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Abstract: The effect of the algebraic constitutive equations on local stability of lumped process models is investigated in this paper using local linearization and eigenvalue checking. Case studies are used to systematically show the influence of algebraic equations on the open loop local stability of process systems using illustrative examples of a continuous fermentation process model and a countercurrent heat exchanger.

Keywords: lumped process systems, differential algebraic equations, stability analysis, local linearization

1. INTRODUCTION

Lumped dynamic process systems are known to be modelled by differential and algebraic equations (DAEs). The differential equations originate from conservation balances for the extensive conserved quantities while the algebraic constitutive equations describing physico-chemical properties, equations of state, reaction rates and intensive-extensive relationships complete the model as described by Hangos and Cameron (2001). The general form of DAE process models consists of an input-affine differential part, and the algebraic equations are given in an implicit form:

$$\frac{dx}{dt} = f(x,z) + \sum_{i=1}^{p} g_i(x,z)u_i \tag{1}$$

$$0 = h(x,z) \tag{2}$$

where x is the state vector, $u = [u_1 \dots u_p]^T$ is the vector of manipulable control inputs u_i and z is the vector of algebraic variables. Note that control inputs only occur in the differential part of the model.

Dynamic nonlinear analysis techniques like in the book of Isidori (1995) are not directly applicable to DAE models but they should be transformed into nonlinear input-affine state-space model form by possibly substituting the algebraic equations into the differential ones. There are two possible approaches for nonlinear stability analysis: Lyapunov's direct method (using an appropriate Lyapunov-function candidate) or local asymptotic stability analysis using the linearized system model.

In this paper, only the latter will be considered for the purpose of showing the influence of algebraic equations on open loop stability of process systems using illustrative examples of a continuous fermentation process model and a countercurrent heat exchanger. Special emphasis is put into the effect of different mechanisms, such as convection, transfer and reaction, occurring in lumped parameter process systems on local stability.

2. LOCAL STABILITY OF LUMPED PROCESS MODELS

This section contains the basic notions and techniques which are used for local stability analysis of lumped process models.

2.1. The structure of nonlinear DAE process models

The structure of lumped process models depend on both the mechanisms taking place in the system and on the choice of input variables. Two practically important different cases are considered.

1. *Inlet intensive potential variables as inputs*
   Hangos *et al.* (1999) showed that if the control inputs are chosen to be the intensive potential variables at the inlets then the differential equations (1) of the above general DAE process models are in the following special form:

$$\dot{x} = A_{trans}x + Q_{\Phi}(x,z) + B_{outconv}x + B_{inconv}u \tag{3}$$

   where the coefficient matrices A_{trans}, B_{oconv} and B_{inconv} are constant matrices originating from the convective terms, while Q_{ϕ} is a smooth nonlinear function representing the transfer and source terms, respectively.

2. *Flowrates as input variables*
   If the flowrates of the convective flows are chosen to be the input variables, then the differential (conservation) equations take the following special form:

$$\dot{x} = A_{trans}x + Q_{\Phi}(x,z) + \sum_{i=1}^{p} g_{conv_i}(x,z)u_i \tag{4}$$

   where A_{trans} is a constant matrix term, while the nonlinear smooth functions g_{conv} and Q_{ϕ} originate from the convective terms and source terms, respectively.

Under the assumption that physico-chemical properties are constant and specifications result in an index 1 model, the algebraic equations are always substitutable into (1).

2.2. Open loop local stability analysis of DAE models

For the purpose of stability analysis, we need to linearize the DAE model around a steady state operating point $[x^* \; z^*]^T$, which is in the following form in the case of the general model (1-2):

$$\dot{\overline{x}} = \left.\frac{\partial f}{\partial x}\right|_{(x^*,z^*)} \overline{x} + \left.\frac{\partial f}{\partial z}\right|_{(x^*,z^*)} \overline{z} + \Big(g_1(x^*,z^*) \;\; g_2(x^*,z^*) \;\; \ldots \;\; g_p(x^*,z^*) \Big)\, \overline{u} \tag{5}$$

$$0 = \left.\frac{\partial h}{\partial x}\right|_{(x^*,z^*)} \overline{x} + \left.\frac{\partial h}{\partial z}\right|_{(x^*,z^*)} \overline{z} \tag{6}$$

for given operating point values of the input variables u_i^* $(i = 1, \ldots, p)$, and with the centered variables $\overline{x} = x - x^*$, $\overline{z} = z - z^*$ and $\overline{u} = u - u^*$.

If $\left.\frac{\partial h}{\partial z}\right|_{(x^*,z^*)}$ is invertible (which is equivalent with that the model has a differential index equal to one), the vector of centered algebraic variables $\overline{z}$ can be explicitly expressed in terms of state variables $\overline{x}$ yielding to a purely differential representation:

$$\dot{\overline{x}} = \left.\left(\frac{\partial f}{\partial x} - \frac{\partial f}{\partial z}\left(\frac{\partial h}{\partial z}\right)^{-1}\frac{\partial h}{\partial x}\right)\right|_{(x^*,z^*)} \overline{x} + \Big(g_1(x^*,z^*) \;\; \ldots \;\; g_p(x^*,z^*) \Big)\, \overline{u} \tag{7}$$

The operating point(s) $[x^* \quad z^*]^T$ can be determined for prescribed input values u^* by solving (1-2) with $\dot{x} = 0$ which means the solution of an algebraic system of equations.

A necessary condition on the solvability of the system of equations above is that the number of differential (algebraic) equations equals to the number of differential (algebraic) variables (degree of freedom equals to zero), and the original DAE system has differential index 1.

2.3. Mechanism-wide local stability analysis of DAE process models

We investigate the effect of mechanisms (transfer, convection, reaction) on local stability using that both (3) and (4) are broken down into additive terms of these mechanisms. Earlier results of Hangos and Perkins (1997) show that transfer is a stabilizing term, because the eigenvalues of the matrix A_{trans} are on the open left-half plane, and in case of constant mass holdups in each balance volume, Kirchoff convection matrices ensure that convection may also be a stabilizing term.

Further mechanism-wide stability considerations of the locally linearized models in the above two input variable cases are as follows.

1. *Inlet intensive potential variables as inputs*
   The linearized model of (3) with the algebraic dependence (2) is in the following form:

$$\dot{\overline{x}} = \left(A_{trans} + B_{outconv} + \left(\frac{\partial Q_\Phi}{\partial x} - \frac{\partial Q_\Phi}{\partial z} \left(\frac{\partial h}{\partial z} \right)^{-1} \frac{\partial h}{\partial x} \right) \Bigg|_{(x^*, z^*)} \right) \overline{x} + B_{inconv} \overline{u} \tag{8}$$

   Since the coefficient matrices A_{trans}, B_{inconv} and $B_{outconv}$ in Eq.(3) are constant matrices, the algebraic dependence (2) only affects the transfer and source terms in the model and thus has a major effect on the open loop stability of the system.

2. *Flowrates as input variables*
   The linearized model of (4) with the algebraic dependence (2) is similar to the former case:

$$\begin{aligned} \dot{\overline{x}} &= \left(A_{trans} + \left(\frac{\partial Q_\Phi}{\partial x} - \frac{\partial Q_\Phi}{\partial z} \left(\frac{\partial h}{\partial z} \right)^{-1} \frac{\partial h}{\partial x} \right) \Bigg|_{(x^*, z^*)} \right) \overline{x} + \\ &+ \left(g_{conv_1}(x^*, z^*) \ \ldots \ g_{conv_p}(x^*, z^*) \right) \overline{u} \end{aligned} \tag{9}$$

   The main difference is that convection is affected by the inputs therefore the state matrix of the linearized model contains the transfer and source terms only.

3. CASE STUDY 1: A CONTINUOUS FERMENTATION PROCESS

A simple continuous fermentation process (for example in Takamatsu *et al.* (1975)) is used as a case study with constant liquid volume V. The liquid feed (F), the temperature and all physico-chemical properties are assumed constant. The state variables are the concentration of biomass (X) and of that the substrate (S).

The control input of the system is the substrate feed concentration S_F which is an intensive potential at the inlet as described in (3) and there is no transfer term. The reaction rate expression is given by an algebraic equation for the reaction rate r.

$$\dot{X} = -\frac{F}{V} X + r \tag{10}$$

$$\dot{S} = -\frac{F}{V} S - \frac{1}{Y} r + \frac{F}{V} S_F \tag{11}$$

$$0 = \mu(X, S) - r \tag{12}$$

3.1. Stability of the simple fermenter

We will show that the stability of the model depends on the reaction kinetics only.

The linearized model of the fermenter is a special case of (8) with no transfer effect ($A_{trans} = 0$) in the following form:

$$\begin{bmatrix} \dot{\overline{X}} \\ \dot{\overline{S}} \end{bmatrix} = \left(\begin{bmatrix} -\frac{F}{V} & 0 \\ 0 & -\frac{F}{V} \end{bmatrix} + \begin{bmatrix} \frac{\partial r}{\partial X}\Big|_* & \frac{\partial r}{\partial S}\Big|_* \\ -\frac{1}{Y}\frac{\partial r}{\partial X}\Big|_* & -\frac{1}{Y}\frac{\partial r}{\partial S}\Big|_* \end{bmatrix} \right) \begin{bmatrix} \overline{X} \\ \overline{S} \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{F}{V} \end{bmatrix} \overline{S}_F \tag{13}$$

The state matrix A of the linearized model consists of the sum of the diagonal output convection term ($B_{outconv}$) and the reaction term (A_{source}), where only the source term depends on the steady state. Since A is a matrix polynomial of the source term ($A = -\frac{F}{V}(A_{source})^0 + (A_{source})^1$) and the linearized reaction term is *singular* because there is a single reaction term, then - according to Gantmacher (1959) - the eigenvalues of A can be computed easily:

$$\lambda(A)_1 = -\frac{F}{V} + 0 = -\frac{F}{V}, \quad \lambda(A)_2 = -\frac{F}{V} + trace(A_{source})|_* = \frac{\partial r}{\partial X}\Big|_* - \frac{1}{Y}\frac{\partial r}{\partial S}\Big|_* - \frac{F}{V} \tag{14}$$

It leads to the stability condition

$$\frac{\partial r}{\partial X}\Big|_* - \frac{1}{Y}\frac{\partial r}{\partial S}\Big|_* < \frac{F}{V} \tag{15}$$

3.2. Stability of the simple fermenter with different reaction kinetics

With five different reaction kinetic expressions (μ functions), the model exhibits different stability properties. Investigation is performed by eigenvalue checking of the linearized models at the operating point(s) in the following cases.

1. Constant characteristics $\mu = K$ results in a linear time invariant (LTI) model which is globally asymptotically stable. This case is the basis of all the following models, containing only the effect of the differential variables.

2. The linear reaction rate $\mu = Kx$ gives also an LTI model with the operating point of biomass wash-out, which is stable if $K < \frac{F}{V}$.

3. The simplest nonlinear, a bi-linear reaction rate $\mu = KSX$ causes two operating points: a wash-out point and an other one.

4. With the monotonous nonlinear characteristics $\mu = \frac{\mu_{max}S}{k_s+S}X$ we similarly get to two operating points.

5. A qualitatively different nonlinear non-monotonous reaction rate function is $\mu = \frac{\mu_{max}S}{k_1+S+k_2S^2}X$, which induces two real operating points (apart from the wash-out point). These three points have the usual stability property pattern (two stable and the other unstable). *This case indicates that the lack of monotonicity is the one which drives the stability pattern and can result in multiple real operating points.*

Local stability properties of the models with different reaction kinetics are summarized in Table 1.

As an important conclusion, *the convective term alone is stable independently of the steady state, moreover it may stabilize the effect of the source term.*

Table 1. The effect of reaction kinetics

Reaction kinetics	**Model type**	**Eigenvalues***	**Stable if**
$r = K$	linear time invariant	$-\frac{F}{V},\ -\frac{F}{V}$	unconditionally
$r = KX$	linear time invariant	$-\frac{F}{V},\ K-\frac{F}{V}$	$K < \frac{F}{V}$
$r = KSX$	nonlinear input affine	(1) $-\frac{F}{V},\ S_F^*K-\frac{F}{V}$	(1) $S_F^*K < \frac{F}{V}$
	with operating points (1),(2)	(2) $-\frac{F}{V},\ -S_F^*K+\frac{F}{V}$	(2) $S_F^*K > \frac{F}{V}$
$r = \frac{\mu_{max}S}{k_s+S}X$	nonlinear input affine	(1) $-\frac{F}{V},\ \frac{S_F^*\mu_{max}}{ks+S_F^*}-\frac{F}{V}$	(1) $\frac{S_F^*\mu_{max}}{k_s+S_F^*} < \frac{F}{V}$
	with operating points (1),(2)	(2) $-\frac{F}{V},\ \lambda_M$	(2) $\lambda_M < 0$
$r = \frac{\mu_{max}S}{k_1+S+k_2S^2}X$	nonlinear input affine	(1) $-\frac{F}{V},\ \lambda_{L1}$	(1) $\lambda_{L1} < 0$
	with operating points (1),(2),(3)	(2) $-\frac{F}{V},\ \lambda_{L2}$	(2) $\lambda_{L2} < 0$
		(3) $-\frac{F}{V},\ \lambda_{L3}$	(3) $\lambda_{L3} < 0$

*where S_F^* is the value of S_F at the operating point,

$R = \frac{\mu_{max}V-F\pm\sqrt{(F-\mu_{max}V)^2-4k_1k_2F^2}}{2k_2F}$, $\lambda_M = -\frac{\mu_{max}(\mu_{max}V^2S_F^*-2VFS_F^*-Fk_sV)+F^2(k_s+S_F^*)}{k_s\mu_{max}V^2}$,

$\lambda_{L1} = \frac{\mu_{max}S_F^*}{k_1+S_F^*+k_2{S_F^*}^2}-\frac{F}{V}$, $\lambda_{L2,L3} = \frac{(R-S_F^*)(k_2F(F-\mu_{max}V)R+\mu_{max}^2V^2-2F^2k_1k_2-2\mu_{max}VF+F^2)}{\mu_{max}k_1V^2}$.

4. CASE STUDY 2: A CASCADE OF HEAT EXCHANGERS

A countercurrent heat exchanger will be considered in this section, which is modelled as a cascade of K simple heat exchanger cells leading to a lumped parameter system. Constant volumes and physico-chemical properties are assumed in every balance volume. The volumetric flowrates of hot and cold liquid streams are v_h and v_c. The dynamics of the system is described by the intensive form of the energy balance equations of both sides for every cell (T_{h_k} and $T_{c_k},\ k = 1 \dots K$), and the algebraic variables ($Z_k,\ k = 1 \dots K$) describe the transfer effect:

$$\dot{T}_{c_k} = \frac{v_c}{V_c}(T_{c_{k+1}} - T_{c_k}) + \frac{1}{c_{pc}\rho_c V_c}\, Z_k \tag{16}$$

$$\dot{T}_{h_k} = \frac{v_h}{V_h}(T_{h_{k-1}} - T_{h_k}) - \frac{1}{c_{ph}\rho_h V_h}\, Z_k \tag{17}$$

$$0 = UA(T_{h_k} - T_{c_k}) - Z_k \tag{18}$$

The potential input variables of the system are the volumetric flowrates (v_h and v_c) and the inlet temperatures (T_{h_0} and $T_{c_{K+1}}$).

4.1. Stability of the heat exchanger model

It is proved by Hangos and Perkins (1997) that in case of constant physico-chemical properties, pressure and mass holdups in each balance volumes, the convection term is stable in asymptotic sense, and the transfer is also stable in Lyapunov sense.

Two cases will be considered according to the input specifications.

1. If the *input specification contains the flowrates* $u = [v_c\ \ v_h]^T$ and the inlet temperatures are constants then the resulted model is bilinear in the input term. The state term is $linear$, and contains the effect of the transfer only, therefore $A = A_{trans}$. This matrix is block diagonal consisting of identical 2×2 diagonal blocks A_{Dk}. These blocks are singular with $rank(A_{Dk}) = 1$ determining the eigenvalues of A:

$$\lambda(A_{Dk})_1 = 0,\ \lambda(A_{Dk})_2 = trace(A_{Dk}) = -(\frac{UA}{c_{pc}\rho_c V_c} + \frac{UA}{c_{ph}\rho_h V_h}) < 0 \tag{19}$$

therefore the system is globally on the boundary of stability.

2. With *input specification containing the inlet temperatures* $u = [T_{c_{K+1}} \; T_{h_0}]^T$ and constant flowrates the state space model of the system is linear. The state matrix is in the form of $A = A_{conv} + A_{trans}$ with A_{trans} being the same as in the first case. $A = A_{conv}$ is a Kirchoff convection matrix (see Hangos and Perkins (1997)) with its eigenvalues being negative, thus $A = A_{conv}$ is a negative definite matrix. Since A_{trans} is negative semi-definite, $A = A_{trans} + A_{conv}$ is negative definite therefore the system is globally asymptotically stable. In conclusion: *convection has a globally stabilizing effect on the system*.

5. CONCLUSION

Local asymptotic stability of lumped process systems modelled by DAE models is investigated in this paper using local linearization and eigenvalue checking. The effect of algebraic constitutive equations influencing the source as well as the transfer term in the differential conservation balances is considered. Case studies are used to systematically show the influence of algebraic equations on the open loop local stability of process systems using illustrative examples of a continuous fermentation process model and a countercurrent heat exchanger.

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