The effect of algebraic equations on the stability of process systems modelled by differential algebraic equations

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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 different continuous fermentation process models, a simple evaporator system, a two-stage fruit condenser and a countercurrent heat exchanger.

Bifurcation analysis is used to investigate the effect of the steady-state values on the stability of DAE model for a simple single input continuous fermentation.

1 Introduction

Lumped dynamic process systems are known to be modelled by differential and algebraic equations (DAEs) [1]. The differential equations originate from conservation balances for the extensive conserved quantities while the algebraic constitutive equations complete the model.

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 [2] 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. Similarly to the standard purely differential nonlinear state-space model case, 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.

In this paper, we systematically show the influence of algebraic equations on open loop stability of process systems using illustrative examples of different continuous fermentation process models, a simple two-phase evaporator system, a two-stage fruit condenser 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 Stability of dynamical systems in DAE form

In this section, we summarize the results available in the literature about the stability of DAE systems. For first, general descriptions will be considered, while the second part concerns with the stability of process systems. Since we discuss lumped parameter models, only DAE systems with finite dimensional state space models will be considered.

2.1 Stability of linear and nonlinear DAEs

The *state equation* of the most commonly used, "generalized" form of linear DAE systems is the following:

$$E\begin{pmatrix} \dot{x} \\ \dot{z} \end{pmatrix} = A\begin{pmatrix} x \\ z \end{pmatrix} + Bu, \qquad \begin{pmatrix} x(t_0) \\ z(t_0) \end{pmatrix} = \begin{pmatrix} x_0 \\ z_0 \end{pmatrix} \tag{3}$$

where x, z and u denote the differential, algebraic and control input vectors, E, A, B are constant coefficient matrices of appropriate dimensions and E is *singular* [3]. Note that process models used in this work are with $\dot{z} = 0$ and therefore the singular matrix E can be written in the following form:

$$E = \left[\begin{array}{c|c} I_{n\times n} & 0_{n\times m} \\ \hline 0_{m\times n} & 0_{m\times m} \end{array}\right]$$

where $I_{n\times n}$ is an identity matrix. There were several attempts to extend the dynamical properties of ordinary state space representations into DAE models (see e.g. [4] and [5]). For asymptotic stability the results of standard state space theory have been generalized successfully. Lyapunov's theorem has a form which is very similar to the original one, stating internal stability for a DAE system in the form of (3) if for any positive definite symmetric matrix Q there is a positive definite symmetric matrix P that fulfills Lyapunov's equation [6]:

$$A^T PE + E^T PA = -Q$$

The method of eigenvalue checking also exists: asymptotic stability is proved if and only if the poles of the system (roots of matrix pencil $\mathcal{P} = det(sE - A)$) have negative real parts [7]. Note that the presented results allows us to investigate the stability of nonlinear input-affine DAE models by local linearization, if it can be performed. As a main difference to the standard state space models, linearization is not possible in general [6]. A sufficient condition is that the differential index of the model equals to one at the operating point. (The differential index shows how many times a DAE model has to be differentiated to get a standard (purely differential) state space model [3]). There are various representations of nonlinear DAE systems.

We do not aim to study them but consider one having a special case of interest in stability investigation: the semiexplicit representation. Its state equation is in the following form:

$$\dot{x}(t) = f(x(t), z(t)) \quad (4)$$
$$0 = g(x(t), z(t)) \quad (5)$$

where initial conditions (x_0, z_0) satisfying (5) are given, functions f and g are nonlinear smooth functions, x and z are the vectors of differential and algebraic variables. This kind of description can be used for representing nonlinear process models, though this class of DAE models is much wider than the class will be used in the following. For systems given in (4)-(5), the method of stability analysis has been presented in [6], with the help of implicit function theorem, using an appropriate Lyapunov function. A considerable result of this work is that algebraic variables are not negligible in stability analysis, they take part in the Lyapunov function.

2.2 Stability of lumped parameter process systems

Lumped parameter process systems can be described by nonlinear DAEs with input affine differential parts. The differential (balance) equations describe the change of extensive quantities such as mass and energy, while the algebraic (constitutive) equations describe the temperature and pressure dependence of physico-chemical properties, equations of state and intensive-extensive relationships [1]. Since process systems are usually made of more processing units, the emphasis is usually put on the stability of interconnected subsystems.

Two main different approaches are used for stability analysis: local analysis using linearization, and Lyapunov-like analysis.

The former method has been applied for distillation columns which can be regarded as networks being a sequence of distillation trays [8]. Homogeneous non-reactive distillation columns with two components, constant component flows and constant (or fast change of) total mass and energy in every

plate (constant molar overflow (CMO) model) proved to be asymptotically stable. Global asymptotic stability of a similar, but multicomponent and one-stage distillation process is also proved in this work.

Asymptotic stability of the former binary distillation columns has also been investigated by Lyapunov technique [9]. The drawback of this method is that the choice of an appropriate Lyapunov-function is intuitive in general, and can be hard-to-applicable for systems with large dimension state space representations. Note that multicomponent multi-stage separation processes are NOT stable in general, and systems can be reported stable mistakenly by the neglection of algebraic equations (see an example in [10]).

In [11], stability of chemical process plants is considered. This work addresses a *class* of processes, which is, however, not a wide one: constant holdups, molar flow rates, physico-chemical properties and pressure are assumed and the dynamics of inteconnections is neglected. The *structural* stability of binary exchange-equilibrium plants (process networks with only convective transport and binary transfer with binary equilibrium) is proved by means of linearization, with the help of conservation matrices. The idea of treating different mechanisms occuring in lumped parameter models of chemical processes (convection, transfer, reaction) separately (as additive terms) proved to be useful.

Passivity theory [12] is used in [13] to prove that interconnected systems with Kirchoff convection and without source term is structurally asymptotically stable. For indicating stability, a thermodynamic storage function (as Lyapunov function) is used. Another work discusses networks of interconnected systems being asymptotically stable with controlled mass holdups [14].

3 Local stability analysis of lumped process models

This section contains the basic notions and techniques which are used for local stability analysis of lumped process models. Both the process engineering and the system engineering material is briefly summarized.

3.1 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*
   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 [15]:
   $$\dot{x} = \Psi_{trans}(x, z) + Q_{\Phi}(x, z) + B_{outconv}x + B_{inconv}u \tag{6}$$
   where the coefficient matrices B_{oconv} and B_{inconv} are constant matrices originating from the convective terms, while Ψ_{trans} and Q_{ϕ} are smooth nonlinear vector fields representing the transfer and source terms, respectively. If constant transfer coefficients and a linear $x = \Lambda y$ relationship with the constant matrix Λ and y being the vector of intensive potential variables, are assumed, then by substituting the algebraic transfer rate equations into the balance equations the transfer term becomes a linear function of the state variables:
   $$\Psi_{trans} = A_{trans}x \tag{7}$$
   where A_{trans} is a constant coefficient matrix.

   Reaction rates, equations of state (if pressures are not constants) and extensive-intensive relationships appear in the algebraic constitutive equations (2). In the general case, these equations also describe the physico-chemical properties related to the transfer [1].

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:

$$\dot{x} = \Psi_{trans}(x,z) + Q_{\Phi}(x,z) + \sum_{i=1}^{p} g_{conv_i}(x,z)u_i \tag{8}$$

   where the nonlinear smooth function g_{conv} originates from the convective terms, while Q_{ϕ} and Ψ_{trans} are smooth nonlinear functions representing the source and transfer terms, respectively. If constant transfer coefficients and a linear relationship between the state and potential variables are assumed, the transfer term will be in the form of (7).

Under the assumption that the physico-chemical properties are constant and the specifications result in an index 1 model, the algebraic equations are always substitutable into (1). In this case, the algebraic dependence can be written as $z = \widetilde{h}(x,z)$, where the variable coincidence matrix (structure matrix) of $\mathrm{J}_{\widetilde{h},z} = \left[\frac{\partial \widetilde{h}}{\partial z}\right]$ can be written in an upper or lower triangular form.

3.2 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):

$$\dot{\overline{x}} = \left.\frac{\partial f}{\partial x}\right|_{(x^*,z^*)} \overline{x} + \left.\frac{\partial f}{\partial z}\right|_{(x^*,z^*)} \overline{z} + \Big(g_1(x^*,z^*) \;\; g_2(x^*,z^*) \;\; \ldots \;\; g_p(x^*,z^*)\Big)\,\overline{u} \tag{9}$$

$$0 = \left.\frac{\partial h}{\partial x}\right|_{(x^*,z^*)} \overline{x} + \left.\frac{\partial h}{\partial z}\right|_{(x^*,z^*)} \overline{z} \tag{10}$$

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:

$$\overline{z} = -\left.\left(\frac{\partial f}{\partial z}\left(\frac{\partial h}{\partial z}\right)^{-1}\frac{\partial h}{\partial x}\right)\right|_{(x^*,z^*)} \overline{x} \tag{11}$$

This yields to a purely differential representation:

$$\dot{\overline{x}} = \left.\left(\frac{\partial f}{\partial x} - \frac{\partial f}{\partial z}\left(\frac{\partial h}{\partial z}\right)^{-1}\frac{\partial h}{\partial x}\right)\right|_{(x^*,z^*)} \overline{x} + \Big(g_1(x^*,z^*) \;\; \ldots \;\; g_p(x^*,z^*)\Big)\,\overline{u} \tag{12}$$

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

$$0 = f(x^*,z^*) + \sum_{i=1}^{p} g_i(x^*,z^*)u_i^* \tag{13}$$

$$0 = h(x^*,z^*) \tag{14}$$

A necessary condition on the solvability of the system of equation 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. Note that if this system of equations is nonsingular, there is a finite (or farthest countably infinite) number of solutions of (13)-(14).

As we will see later, non-monotonic algebraic equations may increase the number of operating points.

3.3 Local stability analysis of DAE process models

The general form of lumped conservation balance equations both in the case of manipulated inlet potential variables (Eq. (6)) and manipulated flowrates (Eq. (8)) are broken down into additive terms that correspond to mechanisms (transfer, convection and source).

Mechanism-wide stability analysis is applied to investigate the effect of mechanisms on local stability. Earlier results show that

(1) transfer is a stabilizing term, because (when relation (7) holds) the eigenvalues of the matrix A_{trans} are on the open left-half plane [11],

(2) 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 (6) with the algebraic dependence (2) is in the following form:

$$\begin{aligned}\dot{\overline{x}} &= \left(\left(\frac{\partial \Psi_{trans}}{\partial x} - \frac{\partial \Psi_{trans}}{\partial z}\left(\frac{\partial h}{\partial z}\right)^{-1}\frac{\partial h}{\partial x}\right)\Bigg|_{(x^*,z^*)} + \right. \\ &+ \left. B_{outconv} + \left(\frac{\partial Q_\Phi}{\partial x} - \frac{\partial Q_\Phi}{\partial z}\left(\frac{\partial h}{\partial z}\right)^{-1}\frac{\partial h}{\partial x}\right)\Bigg|_{(x^*,z^*)}\right)\overline{x} + B_{inconv}\overline{u} \qquad (15)\end{aligned}$$

   Since the coefficient matrices B_{inconv} and $B_{outconv}$ in Eq.(6) 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.

   If the transfer coefficients are considered constants and there is a linear relationship between the state and potential variables, then the transfer term is linear with a constant coefficient matrix A_{trans}. Therefore the above equation specializes to

$$\dot{\overline{x}} = \left(A_{trans} + B_{outconv} + \left(\frac{\partial Q_\Phi}{\partial x} - \frac{\partial Q_\Phi}{\partial z}\left(\frac{\partial h}{\partial z}\right)^{-1}\frac{\partial h}{\partial x}\right)\Bigg|_{(x^*,z^*)}\right)\overline{x} + B_{inconv}\overline{u} \qquad (16)$$

2. *Flowrates as input variables*
   The linearized model of (8) with the algebraic dependence (2) is similar to the former case:

$$\begin{aligned}\dot{\overline{x}} &= \left(\left(\frac{\partial \Psi_{trans}}{\partial x} - \frac{\partial \Psi_{trans}}{\partial z}\left(\frac{\partial h}{\partial z}\right)^{-1}\frac{\partial h}{\partial x}\right)\Bigg|_{(x^*,z^*)} + \right. \\ &+ \left.\left(\frac{\partial Q_\Phi}{\partial x} - \frac{\partial Q_\Phi}{\partial z}\left(\frac{\partial h}{\partial z}\right)^{-1}\frac{\partial h}{\partial x}\right)\Bigg|_{(x^*,z^*)}\right)\overline{x} + \left(g_{conv_1}(x^*,z^*)\ \ldots\ g_{conv_p}(x^*,z^*)\right)\overline{u} \qquad (17)\end{aligned}$$

   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.

If the transfer coefficients are considered constants and there is a linear relationship between the state and potential variables, then the transfer term is linear, and the equation above can be written as

$$\begin{aligned}\dot{\overline{x}} &= \left(A_{trans} + \left(\frac{\partial Q_\Phi}{\partial x} - \frac{\partial Q_\Phi}{\partial z}\left(\frac{\partial h}{\partial z}\right)^{-1}\frac{\partial h}{\partial x}\right)\Big|_{(x^*,z^*)}\right)\overline{x} + \\ &+ \left(g_{conv_1}(x^*,z^*) \ \ldots \ g_{conv_p}(x^*,z^*)\right)\overline{u} \end{aligned} \tag{18}$$

4 Case study 1: fermentation process models

In the following examples, local stability of continuous fermentation processes will be considered. The control inputs are the intensive potentials at the inlets as described in (6) but without transfer term. The effect of algebraic equations on the local stability of the fermentation system will be investigated using different reaction kinetic schemes (given by algebraic equations) from the simplest to the more complex cases. Moreover, general stability conditions will be given for determining the possible regions of stability.

4.1 Case study 1A: a simple fermentation process

A simple continuous fermentation process (for example in [16]) 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) which the biomass consumes. The control input of the system is the substrate feed concentration S_F. The reaction rate is determined by the function r given by an algebraic equation.

$$\dot{X} = -\frac{F}{V}X + r \tag{19}$$

$$\dot{S} = -\frac{F}{V}S - \frac{1}{Y}r + \frac{F}{V}S_F \tag{20}$$

$$0 = \mu(X,S) - r \tag{21}$$

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 (15) with no transfer effect ($\Phi_{trans} = 0$). We also have to note that $\frac{\partial h}{\partial r} = -I$ in this case. The reaction term depends on the algebraic variable only, therefore $\frac{\partial Q_\Phi}{\partial X} = \frac{\partial Q_\Phi}{\partial S} = 0$. Using these properties, we determine the linearized model of the simple fermenter:

$$\begin{bmatrix} \dot{\overline{X}} \\ \dot{\overline{S}} \end{bmatrix} = \left(\begin{bmatrix} -\frac{F}{V} & 0 \\ 0 & -\frac{F}{V} \end{bmatrix} - \begin{bmatrix} 1 \\ -\frac{1}{Y} \end{bmatrix}\begin{bmatrix} -1 \end{bmatrix}^{-1}\begin{bmatrix} \frac{\partial r}{\partial X}\big|_* & \frac{\partial r}{\partial S}\big|_* \end{bmatrix}\right)\begin{bmatrix} \overline{X} \\ \overline{S} \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{F}{V} \end{bmatrix}\overline{S}_F \tag{22}$$

Finally, we get the following linearized model:

$$\begin{bmatrix} \dot{\overline{X}} \\ \dot{\overline{S}} \end{bmatrix} = \left(\begin{bmatrix} -\frac{F}{V} & 0 \\ 0 & -\frac{F}{V} \end{bmatrix} + \begin{bmatrix} \frac{\partial r}{\partial X}\big|_* & \frac{\partial r}{\partial S}\big|_* \\ -\frac{1}{Y}\frac{\partial r}{\partial X}\big|_* & -\frac{1}{Y}\frac{\partial r}{\partial S}\big|_* \end{bmatrix}\right)\begin{bmatrix} \overline{X} \\ \overline{S} \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{F}{V} \end{bmatrix}\overline{S}_F \tag{23}$$

As it seems, the state matrix of the linearized model consists of two terms: the output convection term ($B_{outconv}$) and the reaction term (A_{source}), where

$$A_{source} = \begin{bmatrix} -\frac{F}{V} & 0 \\ 0 & -\frac{F}{V} \end{bmatrix}, \ B_{outconv} = \begin{bmatrix} \frac{\partial r}{\partial X}\big|_* & \frac{\partial r}{\partial S}\big|_* \\ -\frac{1}{Y}\frac{\partial r}{\partial X}\big|_* & -\frac{1}{Y}\frac{\partial r}{\partial S}\big|_* \end{bmatrix}.$$

It is important to note that $A_{source} = A_{source}(X^*, S^*)$ i.e. the source term depends on the steady state.

Notice the advantage that the dependence of A_{source} on the algebraic variable r is *linear*. This is the reason of the singularity of the linearized reaction matrix term. Also note that this simple model has only one balance volume, therefore it is a Kirchoff convection network with only one region [13], therefore $B_{outconv}$ is negative definite. Moreover, $B_{outconv}$ is a unit matrix multiplied by a negative constant. The latter property has two consequences:

1. The convective term is always stable, moreover it may stabilize the effect of the source term.
2. The negative definiteness (which implies stability) of the state matrix $A = B_{outconv} + A_{source}$ can be investigated in a simpler way, because of the strict connection between the eigenvalues of A_{source} and A:

$$\lambda_A I - A = \lambda_A I - B_{outconv} - A_{source} = (\lambda_A + \frac{F}{V})I - A_{source} \tag{24}$$

Therefore the connection between the eigenvalues of the state matrix and the source term matrix is the following:

$$(\lambda_A)_i = (\lambda_{Asource})_i - \frac{F}{V} \tag{25}$$

As we mentioned above, A_{source} is a singular matrix. Thus, A_{source} has a zero eigenvalue [17]:

$$(\lambda_{Asource})_1 = 0 \tag{26}$$

The trace of A_{source} equals to the sum of its eigenvalues [17]: $trace(A_{source}) = (\lambda_{Asource})_1 + (\lambda_{Asource})_2$. From this we can determine the other eigenvalue:

$$(\lambda_{Asource})_2 = trace(A_{source})|_* = \left.\frac{\partial r}{\partial X}\right|_* - \frac{1}{Y}\left.\frac{\partial r}{\partial S}\right|_* \tag{27}$$

Using Eq.(25), we get the eigenvalues of the linearized model:

$$(\lambda_A)_1 = -\frac{F}{V} \tag{28}$$

$$(\lambda_A)_2 = \left.\frac{\partial r}{\partial X}\right|_* - \frac{1}{Y}\left.\frac{\partial r}{\partial S}\right|_* - \frac{F}{V} \tag{29}$$

For a negative definite A, both of its eigenvalues must be negative. It leads to the stability condition

$$\left.\frac{\partial r}{\partial X}\right|_* - \frac{1}{Y}\left.\frac{\partial r}{\partial S}\right|_* < \frac{F}{V} \tag{30}$$

Now let us see the operating point stability of the simple fermenter model with five different reaction kinetics r. The stability investigation is performed by eigenvalue checking of the linearized models at the operating point(s). The determination of the operating points is performed by solving the DAE model equations of the fermenter with $\dot{(X)} = \dot{(S)} = 0$ for a given general steady state input parameter S_F^*. The system of equations has to be solved for X^* and S^*:

$$0 = -\frac{F}{V}X^* + r^* \tag{31}$$

$$0 = -\frac{F}{V}S^* - \frac{1}{Y}r^* + \frac{F}{V}S_F^* \tag{32}$$

$$0 = \mu(X^*, S^*) - r^* \tag{33}$$

Local stability has been investigated for five different reaction kinetic terms. Table 1. shows the number of operating points and the eigenvalues at these points. As this Table shows well, $\lambda_1 = -\frac{F}{V}$ in all cases. Stability condition (30) which is equivalent with $\lambda_2 < 0$ is also given for these steady states.

1. Constant characteristics $r = K$ results in a linear time invariant (LTI) model which is globally asymptotically stable with the unique steady state $(X^*, S^*) = (\frac{KV}{F}, -\frac{KV}{FY} + S_F^*)$. This case is the basis of all the following models, containing only the effect of the differential variables.

2. The linear reaction rate $r = Kx$ gives also an LTI model with the operating point of biomass wash-out $(X^*, S^*) = (0, S_F^*)$, which is stable if $K < \frac{F}{V}$.

3. The simplest nonlinear, a bi-linear reaction rate $r = KSX$ causes two operating points: a wash-out point and an other one. The wash-out point $(X^*, S^*) = (0, S_F^*)$ is stable if $S_F^* K < \frac{F}{V}$, while the real operating point $(X^*, S^*) = (YS_F^* - \frac{YF}{KV}, \frac{F}{KV})$ is stable if $S_F^* K > \frac{F}{V}$.

4. With the monotonous nonlinear characteristics $r = \frac{\mu_{max} S}{k_s + S} X$ we similarly get to two operating points. The stability of conditions on the wash-out point $(X^*, S^*) = (0, S_F^*)$ and the real operating point $(X^*, S^*) = (YS_F^* - \frac{YFk_S}{\mu_{max} V - F}, \frac{Fk_S}{\mu_{max} V - F})$ can be found in Table 1.

5. A qualitatively different nonlinear non-monotonous reaction rate function is $r = \frac{\mu_{max} S}{k_1 + S + k_2 S^2} X$, which induces two real operating points (apart from the wash-out point):

$$X_{2,3}^* = YS_F^* - \frac{Y}{2k_2 F}(\mu_{max} V - F \pm \sqrt{\mu_{max}^2 V^2 - 2\mu_{max} VF + F^2(1 - 4k_1 k_2)}) \quad (34)$$

$$S_{2,3}^* = \frac{1}{2k_2 F}(\mu_{max} V - F \pm \sqrt{\mu_{max}^2 V^2 - 2\mu_{max} VF + F^2(1 - 4k_1 k_2)}) \quad (35)$$

   These three points have the usual stability property pattern of reactive systems (two stable and one unstable). Stability conditions are also given for these three operating points in Table 1. Note that the duplication of real operating points comes from the non-monotonic characteristics of the reaction rate which means that that for given rate $r^* = const. > 0$ there exist *two pairs* of (X^*, S^*) which fulfills (31)-(32). The trivial case when $r^* = 0$ gives the wash-out point. 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 characteristics are summarized in Table 1. As it shows, the algebraic variable r has an important effect both on stability and the number of operating points of the system.

Bifurcation analysis of the fermenter models In this section, we investigate the impact of the positive real parameter S_F^* on the number of operating points and their stability with different reaction characteristics. Namely, we consider the eigenvalues of the system as functions of the steady-state value of control input. This steady-state value determines the steady-state value of the state variables thus this analysis shows the effect of steady-state values on local stability.

Since $\lambda_1 = -\frac{F}{V} < 0$ independently of the reaction kinetics, we only have to take the other eigenvalue into account as a function of the steady state value of control input parameter: $\lambda_2 = \lambda_2(S_F^*)$. Using stability investigation, Fold bifurcation points will be determined for the five models with different reaction kinetics. A Fold bifurcation point occurs when an eigenvalue of the system crosses the imaginary axis in the complex plane, and therefore corresponds to the boundary of stability). Results are summarized in Table 2. and discussed briefly in the following.

1. For the constant rate $r = K$ the operating point is globally stable, and the asymptotic behaviour of the system does not depend on the control input parameter S_F^*. Note that the steady state point depends on the control input.

2. For linear characteristics $r = KX$, the single wash-out steady state shows global stability for feasible system parameter values ($K < \frac{F}{V}$). Global stability is ensured by that the Jacobian is constant (does not depend on the value of the operating point). In this case λ_2 is also independent from the control input.

Reaction kinetics	**Model type**	**Eigenvalues***	**Stable if**
$r = K$	linear time invariant	$-\frac{F}{V}, \quad -\frac{F}{V}$	unconditionally
$r = KX$	linear time invariant	$-\frac{F}{V}, \quad K - \frac{F}{V}$	$K < \frac{F}{V}$
$r = KSX$	nonlinear input affine	(1) $-\frac{F}{V}, \quad S_F^* K - \frac{F}{V}$	(1) $S_F^* K < \frac{F}{V}$
	with operating points (1),(2)	(2) $-\frac{F}{V}, \quad -S_F^* K + \frac{F}{V}$	(2) $S_F^* K > \frac{F}{V}$
$r = \frac{\mu_{max} S}{k_s + S} X$	nonlinear input affine	(1) $-\frac{F}{V}, \quad \frac{S_F^* \mu_{max}}{ks + S_F^*} - \frac{F}{V}$	(1) $\frac{S_F^* \mu_{max}}{k_s + S_F^*} < \frac{F}{V}$
	with operating points (1),(2)	(2) $-\frac{F}{V}, \quad \lambda_M$	(2) $\lambda_M < 0$
$r = \frac{\mu_{max} S}{k_1 + S + k_2 S^2} X$	nonlinear input affine	(1) $-\frac{F}{V}, \quad \lambda_{L1}$	(1) $\lambda_{L1} < 0$
	with operating points (1),(2),(3)	(2) $-\frac{F}{V}, \quad \lambda_{L2}$	(2) $\lambda_{L2} < 0$
		(3) $-\frac{F}{V}, \quad \lambda_{L3}$	(3) $\lambda_{L3} < 0$

Table 1: The effect of reaction kinetics

*where S_F^* is the value of S_F at the operating point,
$\lambda_M = -\frac{\mu_{max}(\mu_{max} V^2 S_F^* - 2VFS_F^* - Fk_sV) + F^2(k_s + S_F^*)}{k_s \mu_{max} V^2}$,
$\lambda_{L1} = \frac{\mu_{max} S_F^*}{k_1 + S_F^* + k_2 S_F^{*2}} - \frac{F}{V}, \quad \lambda_{L2,L3} = \frac{(R - S_F^*)(k_2 F(F - \mu_{max} V) R + \mu_{max}^2 V^2 - 2F^2 k_1 k_2 - 2\mu_{max} VF + F^2)}{\mu_{max} k_1 V^2}$
with $R = \frac{\mu_{max} V - F \pm \sqrt{(F - \mu_{max} V)^2 - 4k_1 k_2 F^2}}{2k_2 F}$.

3. For the bilinear model with $r = KSX$, Fold bifurcation point is at $S_F^* = \frac{F}{KV}$ for both steady states, but they show stability in a contrary manner: The wash-out point is stable in the region where $S_F^* < \frac{F}{KV}$ and the real operating point is unstable here, while the real point is stable and the wash-out point is unstable if $S_F^* > \frac{F}{KV}$. Therefore the system shows local stability with switching the steady state at the bifurcation point. At this point, both points are on the boundary of stability. We have to note that only local stability occurs in this model because the general Jacobian matrix depends on the values of the state variables. The bifurcation curve is linear for both operating points as depicted in Fig. 1.

4. The system with the nonlinear yield function $r = \frac{\mu_{max} S}{k_S + S} X$ has also a real and a wash-out steady state. If $\mu_{max} < \frac{F}{V}$, the local stability of the wash-out point is provided. If the opposite of the condition is fulfilled, the stability of this point coincides with of the real steady state point. For both cases and both steady states the bifurcation point is at $S_F^* = \frac{k_s F}{\mu_{max} V - F}$. The bifurcation diagram of the real operating point is depicted in Fig. 2. showing that this model is always stable. For the values of S_F^* less than the bifurcation point value there is no steady state.

5. For the nonlinear non-monotonous reaction rate $r = \frac{\mu_{max} S}{k_1 + S + k_2 S^2} X$ there are three operating points, one of them is the wash-out point. For this point, if $\frac{\mu_{max} S_F^*}{k_1 + S_F^* + k_2 S_F^{*2}} < \frac{F}{V}$ is fulfilled, then local stability is proved. The two real points coincide if $S_F^* = \sqrt{\frac{k_1}{k_2}}$. It is the optimal production case when the reaction rate is at its peak. Note that in this point can be either stable or unstable according to the system parameter values.

4.2 Case study 1B: Fermentation process with two substrates

This subsection describes the case when two substrates are needed simultaneously for the growth of the biomass. Extending the former model with another substrate concentration as described in [18] we get to the following system model:

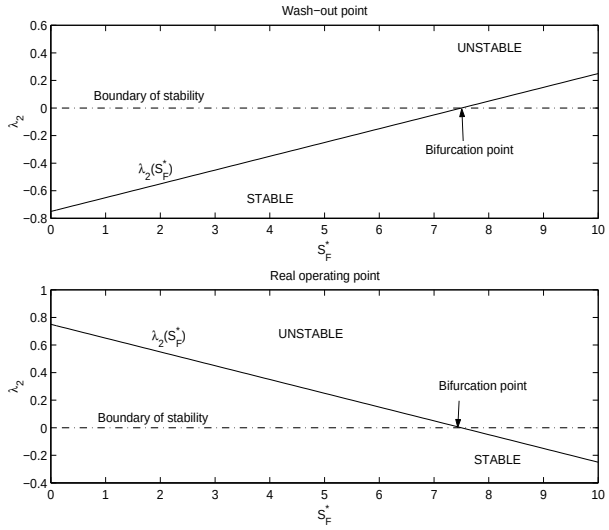

Figure 1: Bifurcation diagram of the bilinear rate case

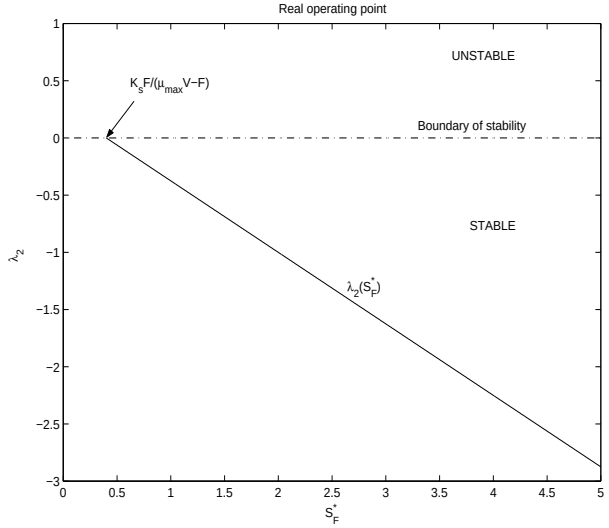

Figure 2: Bifurcation diagram of the Monod characteristics case

Reaction kinetics	**Operating point eigenvalues**	**Conditions**	**Stable if**
$r = K$	$-\frac{F}{V}, \quad -\frac{F}{V}$	-	unconditionally
$r = KX$	$-\frac{F}{V}, \quad K - \frac{F}{V}$	$K < \frac{F}{V}$	unconditionally
$r = KSX$	(1) $-\frac{F}{V}, \quad S_F^* K - \frac{F}{V}$	-	(1) $S_F^* < \frac{F}{KV}$
	(2) $-\frac{F}{V}, \quad -S_F^* K + \frac{F}{V}$	-	(2) $S_F^* > \frac{F}{KV}$
$r = \frac{\mu_{max} S}{k_s + S} X$	(1) $-\frac{F}{V}, \quad \frac{\mu_{max} S_F^*}{ks + S_F^*} - \frac{F}{V}$	$\mu_{max} < \frac{F}{V}$	unconditionally
		$\mu_{max} > \frac{F}{V}$	$S_F^* > \frac{k_s F}{\mu_{max} V - F}$
	(2) $-\frac{F}{V}, \quad -\frac{(S_F^*(\mu_{max} V - F) - k_s F)(\mu_{max} V - F)}{k_s \mu_{max} V^2}$	$S_F^* > \frac{k_s F}{\mu_{max} V - F}$	unconditionally

Table 2: Stability conditions for different reaction kinetics

$$\dot{X} = -\frac{F}{V}X + r \tag{36}$$

$$\dot{S}_1 = -\frac{F}{V}S_1 - \frac{1}{Y_1}r + \frac{F}{V}S_{F1} \tag{37}$$

$$\dot{S}_2 = -\frac{F}{V}S_2 - \frac{1}{Y_2}r + \frac{F}{V}S_{F2} \tag{38}$$

$$0 = \mu(X, S_1, S_2) - r \tag{39}$$

where the two substrate concentrations are S_1 and S_2. The physico-chemical properties, liquid volume and liquid feed are considered constant. There is only one reaction rate r in the model. The two system inputs (substrate inflow) are denoted by S_{F1} and S_{F2}. Note that the differential part of the model is in the form of (6).

Stability of the fermentation process with two substrates In order to perform stability investigation, we linearize the model according to (15):

$$\begin{bmatrix} \dot{\overline{X}} \\ \dot{\overline{S}}_1 \\ \dot{\overline{S}}_2 \end{bmatrix} = \left(\begin{bmatrix} -\frac{F}{V} & 0 & 0 \\ 0 & -\frac{F}{V} & 0 \\ 0 & 0 & -\frac{F}{V} \end{bmatrix} + \begin{bmatrix} \frac{\partial r}{\partial X}\big|_* & \frac{\partial r}{\partial S_1}\Big|_* & \frac{\partial r}{\partial S_2}\Big|_* \\ -\frac{1}{Y_1}\frac{\partial r}{\partial X}\Big|_* & -\frac{1}{Y_1}\frac{\partial r}{\partial S_1}\Big|_* & -\frac{1}{Y_1}\frac{\partial r}{\partial S_2}\Big|_* \\ -\frac{1}{Y_2}\frac{\partial r}{\partial X}\Big|_* & -\frac{1}{Y_2}\frac{\partial r}{\partial S_1}\Big|_* & -\frac{1}{Y_2}\frac{\partial r}{\partial S_2}\Big|_* \end{bmatrix} \right) \begin{bmatrix} \overline{X} \\ \overline{S}_1 \\ \overline{S}_2 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ \frac{F}{V} & 0 \\ 0 & \frac{F}{V} \end{bmatrix} \begin{bmatrix} \overline{S}_{F1} \\ \overline{S}_{F2} \end{bmatrix}$$

We met the same properties as in the one substrate case: $B_{outconv} = -\frac{F}{V}I$, and A_{source} is singular, with $rank_{max}(B_{outconv}) = 1$. Because of this, the eigenvalues of the model are:

$$(\lambda_A)_{1,2} = -\frac{F}{V}, \quad (\lambda_A)_3 = trace(A_{source})|_* - \frac{F}{V} = \frac{\partial r}{\partial X}\Big|_* - \frac{1}{Y_1}\frac{\partial r}{\partial S_1}\Big|_* - \frac{1}{Y_2}\frac{\partial r}{\partial S_2}\Big|_* - \frac{F}{V} \tag{40}$$

And the stability condition is:

$$\frac{\partial r}{\partial X}\Big|_* - \frac{1}{Y_1}\frac{\partial r}{\partial S_1}\Big|_* - \frac{1}{Y_2}\frac{\partial r}{\partial S_2}\Big|_* < \frac{F}{V} \tag{41}$$

As an important conclusion, if there is only one reaction kinetics in the model (with constant multipliers), then the source term will have only one eigenvalue different from zero independently of the number of substrates. This property remains unchanged even in the case when there is an energy balance in the model, i.e. the temperature is not constant.

4.3 Case study 1C: Fermenter with two biomasses consuming the same substrate

This model is the extension of the simple fermenter by an other biomass consuming the same substrate. All the model assumptions are the same as in the former case, except that there are two reaction kinetic terms r_1 and r_2 in the system, therefore the differential equation of the model is in the form of (6). The model equations of the system are:

$$\dot{X}_1 = -\frac{F}{V}X_1 + r_1 \tag{42}$$

$$\dot{X}_2 = -\frac{F}{V}X_2 + r_2 \tag{43}$$

$$\dot{S} = -\frac{F}{V}S - \frac{1}{Y_1}r_1 - \frac{1}{Y_2}r_2 + \frac{F}{V}S_F \tag{44}$$

$$0 = \mu_1(X_1, X_2, S) - r_1 \tag{45}$$

$$0 = \mu_2(X_1, X_2, S) - r_2 \tag{46}$$

Stability of the fermenter with two biomasses consuming the same substrate

In order to perform stability investigation, we linearize the model using (15):

$$\begin{bmatrix} \dot{\overline{X}}_1 \\ \dot{\overline{X}}_2 \\ \dot{\overline{S}} \end{bmatrix} = \left(\begin{bmatrix} -\frac{F}{V} & 0 & 0 \\ 0 & -\frac{F}{V} & 0 \\ 0 & 0 & -\frac{F}{V} \end{bmatrix} + \begin{bmatrix} \frac{\partial r_1}{\partial X_1}\Big|_* & 0 & \frac{\partial r_1}{\partial S}\Big|_* \\ 0 & \frac{\partial r_2}{\partial X_2}\Big|_* & \frac{\partial r_2}{\partial S}\Big|_* \\ -\frac{1}{Y_1}\frac{\partial r_1}{\partial X_1}\Big|_* & -\frac{1}{Y_2}\frac{\partial r_2}{\partial X_2}\Big|_* & -\frac{\partial(\frac{1}{Y_1}r_1+\frac{1}{Y_2}r_2)}{\partial S}\Big|_* \end{bmatrix} \right) \begin{bmatrix} \overline{X}_1 \\ \overline{X}_2 \\ \overline{S} \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \frac{F}{V} \end{bmatrix} \overline{S}_F$$

With two reactions, we have $rank(A_{source}) = 2$ (structurally), therefore it will have only one zero eigenvalue in general, which leads to $(\lambda_A)_1 = -\frac{F}{V}$. Therefore a necessary condition on stability is $(\lambda_A)_2 + (\lambda_A)_3 = trace(A) - (\lambda_A)_1 = trace(A_{source})|_* - 2\frac{F}{V} < 0$, which means

$$\frac{\partial r_1}{\partial X_1}\Big|_* + \frac{\partial r_2}{\partial X_2}\Big|_* - \frac{1}{Y_1}\frac{\partial r_1}{\partial S}\Big|_* - \frac{1}{Y_2}\frac{\partial r_2}{\partial S}\Big|_* < 2\frac{F}{V} \tag{47}$$

Note that it is a necessary, but *not sufficient* condition for stability. Computing the eigenvalues of the source term and using the condition (25), the eigenvalues of the system will be the following:

$$(\lambda_A)_1 = -\frac{F}{V}, \quad (\lambda_A)_{2,3} = \frac{1}{2}trace(A_{source})\Big|_* - \frac{F}{V} \pm \sqrt{expr1} \tag{48}$$

where

$$\begin{aligned} expr1 &= \left(\frac{1}{2}trace(A_{source})\Big|_* - \frac{F}{V}\right)^2 - \left(\frac{F}{V}\right)^2 + \left(\frac{\partial r_1}{\partial X_1}\Big|_* + \frac{\partial r_2}{\partial X_2}\Big|_* - \frac{1}{Y_1}\frac{\partial r_1}{\partial S}\Big|_* - \frac{1}{Y_2}\frac{\partial r_2}{\partial S}\Big|_*\right)\frac{F}{V} + \\ &+ \left(\frac{1}{Y_1}\frac{\partial r_1}{\partial S}\Big|_* - \frac{\partial r_1}{\partial X_1}\Big|_*\right)\frac{\partial r_2}{\partial X_2}\Big|_* + \frac{1}{Y_2}\frac{\partial r_1}{\partial X_1}\Big|_*\frac{\partial r_2}{\partial S}\Big|_* \end{aligned} \tag{49}$$

and the stability of the system fulfilling (47) depends on $expr1$.
If $expr1 < 0$, then the system is stable and exhibits some oscillating behaviour.
If $expr1 > 0$ and $(expr1)^2 > \left|\frac{1}{2}\,trace(A_{source})|_* - \frac{F}{V}\right|$ one of the eigenvalues will be positive, which leads to an unstable system.

5 Case study 2: Evaporator models

In these examples simple two-phase evaporator systems will be considered. These models contain convective flowrates as control inputs. There is no source term ($Q_\Phi = 0$) and transfer coefficients are NOT assumed constant, therefore the differential part of the DAE model is described by (8). The algebraic equations describe the effect of the transfer mechanism.

5.1 Case study 2A: A simple evaporator system with mass balances only

In the former examples we have only considered systems, when the structure matrix of $\frac{\partial \widetilde{h}}{\partial z}$ was diagonal. In the following example we show a model which does not fulfill this property, but the set of algebraic equations is substitutable into the differential ones (the structure matrix can be written in a triangular form).

Fig. 3. depicts a simple evaporator system with one liquid and one vapour phase. The mass of liquid and vapour are denoted by M_L and M_V, respectively. Let the control variables be the liquid feed F and liquid and vapour outflows L and V. The liquid evaporates with the transfer rate E. Constant temperature is assumed (no heating in the vessel), therefore we only need mass balances for

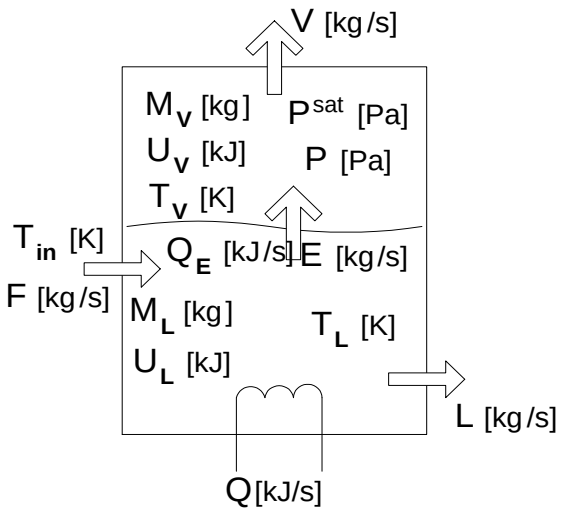

Figure 3: Two-phase evaporator system

both phases. The dynamic behaviour of the system is described by the following set of differential and algebraic equations:

$$\frac{dM_L}{dt} = F - L - E \tag{50}$$

$$\frac{dM_V}{dt} = E - V \tag{51}$$

$$0 = K_M(P^{sat} - P) - E \tag{52}$$

$$0 = \frac{1}{V_v - \frac{M_L}{\rho_L}} \frac{M_V}{m_\omega} RT_V - P \tag{53}$$

where V_v is the volume of the vessel, ρ_L is assumed constant, P^{sat} is also constant because of the constant temperature.

Consider the case where the value of control variables are chosen $F = L + E$ (the liquid mass is constant) and $V = 0$ (the ceiling of the vessel is closed)! If the transfer rate E is considered constant the mass of the vapour phase would continuously increase. This is the same case when the vapour pressure P is considered constant, because the magnitude of E is proportional to $P^{sat} - P$. In spite of that, in the real case the system arrives to the equilibrium when $P^{sat} = P$ and consequently E equals to zero.

Let us see the case when $F = L = V = 0$! If E is considered constant, the liquid phase would continuously decrease, and the vapour phase would increase. Neglecting the effect of P results in unstable phases object to the unique equilibrium of the real system. The former examples showed that possibly stable models can be reported unstable by neglecting the time-dependence of algebraic variables.

These examples show that considering the algebraic variables constant would leave to models reporting the stability of the systems in a totally incorrect manner.

Stability investigation of the evaporator system Now let's construct the linearized model of

the system according to (17)! Note that the matrix $\frac{\partial \widetilde{h}}{\partial z}$ is upper triangular in this case!

$$\begin{bmatrix} \dot{\overline{M_L}} \\ \dot{\overline{M_V}} \end{bmatrix} = \left(\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} - \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -1 & -K_M \\ 0 & -1 \end{bmatrix}^{-1} \begin{bmatrix} 0 & 0 \\ \frac{\rho_L R T_V}{m_\omega} \frac{M_V^*}{(\rho_L V_v - M_L^*)^2} & \frac{\rho_L R T_V}{m_\omega} \frac{1}{\rho_L V_v - M_L^*} \end{bmatrix} \right) \begin{bmatrix} \overline{M_L} \\ \overline{M_V} \end{bmatrix} + + \begin{bmatrix} 1 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} F \\ L \\ V \end{bmatrix} \tag{54}$$

Finally, we get the following linearized model:

$$\begin{bmatrix} \dot{\overline{M_L}} \\ \dot{\overline{M_V}} \end{bmatrix} = \begin{bmatrix} K_M \frac{\rho_L R T_V}{m_\omega} \frac{M_V^*}{(\rho_L V_v - M_L^*)^2} & K_M \frac{\rho_L R T_V}{m_\omega} \frac{1}{\rho_L V_v - M_L^*} \\ -K_M \frac{\rho_L R T_V}{m_\omega} \frac{M_V^*}{(\rho_L V_v - M_L^*)^2} & -K_M \frac{\rho_L R T_V}{m_\omega} \frac{1}{\rho_L V_v - M_L^*} \end{bmatrix} \begin{bmatrix} \overline{M_L} \\ \overline{M_V} \end{bmatrix} + \begin{bmatrix} 1 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} F \\ L \\ V \end{bmatrix} \tag{55}$$

where M_L^* and M_V^* denote the steady state values of the differential variables. As the linearized model shows, the state matrix is singular. It is caused by the singularity of the matrix $\frac{\partial f}{\partial z}$ (the dependence of the differential equations on the algebraic variable P is *indirect*: affects only through the algebraic variable E). Because of singularity, there is an eigenvalue equals to zero, and therefore the other one equals to the trace of the state matrix:

$$\lambda_1 = 0, \quad \lambda_2 = trace(A)|_* = K_M \frac{\rho_L R T_V}{m_\omega} \frac{M_V^*}{(\rho_L V_v - M_L^*)^2} - K_M \frac{\rho_L R T_V}{m_\omega} \frac{1}{\rho_L V_v - M_L^*} \tag{56}$$

Since $\lambda_1 = 0$, if $\lambda_2 < 0$ the system will be on the boundary of stability.
The condition $\lambda_2 < 0$ is equivalent to

$$\frac{M_L^* + M_V^*}{\rho_L} < V_v \tag{57}$$

which is a trivial, since vapour density is less than the liquid density (V_v denotes the volume of the vessel). We can conclude that the system is on the boundary of stability. Note that asymptotic stability can be provided by exchanging an input variable with a (possibly) stabilizing term of the differential variables (e.g. free outflow of liquid or a valve for the vapour phase). Also note that the singularity of the state matrix (and therefore that the system is on the boundary of stability) is a common consequence of the singularity of $\frac{\partial f}{\partial z}$ and that of $\frac{\partial f}{\partial x} = 0$.

5.2 Case study 2B: A simple evaporator system with mass and energy balances

Let us see what happens when temperature can also change. The system is depicted in Fig. 3. where the phase temperatures are denoted by T_L and T_V, while Q_E is the energy transfer between the two phases and T_{in} is the inlet temperature (disturbance). The specific heat capacities cp_L and cp_V are assumed constant. Note that intensive variables T_L and T_V are used in the balance equations instead of their extensive pairs U_L and U_V. Q denotes the heating of the liquid as an additional input variable.

The extended set of model equations will be the following:

$$\begin{aligned}
\dot{M}_L &= F - L - E && (58)\\
\dot{M}_V &= E - V && (59)\\
\dot{T}_L &= \frac{1}{cp_L M_L}((cp_L T_{in} - cp_L T_L)F - Q_E + Q) && (60)\\
\dot{T_V} &= \frac{1}{cp_V M_V}((cp_L T_L - cp_V T_V)E + Q_E) && (61)\\
0 &= K_M(P^{sat} - P) - E && (62)\\
0 &= K_{sa} e^{-\frac{K_{sb}}{T_L}} - P^{sat} && (63)\\
0 &= \frac{1}{V_v - \frac{M_L}{\rho_L}} \frac{M_V}{m_\omega} R T_V - P && (64)\\
0 &= K_U(T_V - T_L) - Q_E && (65)
\end{aligned}$$

Note that this model also belongs to (8) as the former one. As we will see later, the structure matrix of $\frac{\partial \widetilde{h}}{\partial z}$ is not diagonal, but it can be written in a triangular form, therefore the algebraic variables are substitutable.

Stability investigation of the evaporator system For being short, consider the linearized state space model of the evaporator system (according to (17)) with only the centered state variables (input variables don't play any role on the asymptotic stability of the system):

$$\begin{bmatrix} \overline{\dot{M}_L} \\ \overline{\dot{M}_V} \\ \overline{\dot{T}_L} \\ \overline{\dot{T}_V} \end{bmatrix} = \left(\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -\frac{(cp_L T_{in} - cp_L T_L^*)F^* - Q_E^* + Q^*}{cp_L (M_L^*)^2} & 0 & -\frac{F^*}{M_L^*} & 0 \\ 0 & -\frac{e_4 E^* + Q_E^*}{cp_V (M_V^*)^2} & \frac{cp_L E^*}{cp_V M_V^*} & -\frac{E^*}{M_V^*} \end{bmatrix} + \begin{bmatrix} e_2 M_V^* T_V^* & e_1 T_V^* & -e_3 & e_1 M_V^* \\ -e_2 M_V^* T_V^* & -e_1 T_V^* & e_3 & -e_1 M_V^* \\ 0 & 0 & \frac{K_U}{M_L^* cp_L} & -\frac{K_U}{M_L^* cp_L} \\ -e_2 e_4 \frac{T_V^*}{cp_V} & -e_1 e_4 \frac{T_V^*}{cp_V M_V^*} & \frac{e_3 e_4 - K_U}{cp_V M_V^*} & -\frac{e_1 e_4 M_V^* - K_U}{cp_V M_V^*} \end{bmatrix} \right) \begin{bmatrix} \overline{M_L} \\ \overline{M_V} \\ \overline{T_L} \\ \overline{T_V} \end{bmatrix} \quad (66)$$

where $e_1 = \frac{K_M \rho_L R}{(V_v \rho_L - M_L^*) m\omega}$, $e_2 = \frac{K_M \rho_L R}{(V_v \rho_L - M_L^*)^2 m\omega}$, $e_3 = \frac{K_M K_{sa} K_{sb}}{(T_L^*)^2} e^{-\frac{K_{sb}}{T_L^*}}$ and $e_4 = cp_L T_L^* - cp_V T_V^*$.

The first matrix contains the effect of the differential, the second contains the effect the algebraic part of the equations. (They will be denoted by A_{diff} and A_{alg} later on.) We will perform the eigenvalue check separately, because the eigenvalues of $A = A_{diff} + A_{alg}$ cannot be given in a closed form. By this way we will conclude in stronger (sufficient but possibly not necessary) conditions and a thinner stability region than we would get by considering the eigenvalues of A. Both of the matrices have rank equal to 2, i.e. $rank(A_{diff}) = 2$ and $rank(A_{alg}) = 2$. The eigenvalues of A_{diff} are negative or zero ($\lambda(A_{diff}) = 0,\ 0,\ -\frac{F^*}{M_L^*},\ -\frac{E^*}{M_V^*}$) therefore A_{diff} is negative semi-definite and with only the differential part the model would be on the boundary of stability. A_{alg} has two zero and two non-zero eigenvalues:

$$\lambda(A_{alg})_{1,2} = 0,\ \lambda(A_{alg})_{3,4} = \frac{1}{2}\, trace(A_{alg})|_* \pm \frac{\sqrt{expr}}{m_\omega cp_L cp_V M_L^* M_V^* (V_v rho_L - M_L^*)^2 T_L^*}$$

where $expr$ is an algebraic expression and $trace(A_{alg})|_*$ denotes the trace of A_{alg} at the operating point.

From its eigenvalues it seems that for ensuring the negative semi-definiteness of A_{alg}, its trace must be negative or zero:

$$trace(A_{alg})|_* = -K_M R\rho_L cp_L M_L^* M_V^* ((V_v\rho_L - M_L^*)T_L^* cp_L - M_V^* T_V^* cp_V) + \\ +m_\omega K_U (V_v\rho_L - M_L^*)^2 (cp_V M_V^* + cp_L M_L^*) \leq 0 \quad (67)$$

This is a necessary, but not sufficient condition.

Another condition can be derived using the eigenvalues of A_{alg}. It can be shown that if

$$T_V^* M_V^* (cp_L M_L^* + cp_V M_V^*) - cp_L (T_L^* M_V^* + T_V^* M_L^*)(V_v\rho_L - M_L^*) \geq 0 \quad (68)$$

then $\lambda(A_{alg})_{3,4} \leq 0$ and therefore A_{alg} is negative semi-definite. Note that this condition is sufficient, but *not necessary*. This example shows well that only considering the effect of the differential part one mistakenly reports the system being globally stable in Lyapunov sense, while it does not even fulfill the necessary stability condition (67).

6 Case study 3: A fruit condenser with only mass balances

A two-stage fruit condenser will be regarded in the following as an example for interconnected systems. The block diagram of the system is depicted in Fig. 4. Every stages contain a liquid and a vapour phase with masses M_{L_i}, M_{V_i}. Liquid phases contain two components (water and fruit), the masses of fruit are denoted by M_{F_i}. Evaporation is performed at every stage resulting a bigger fruit concentration c_i at every stage. Only water evaporates, therefore there is no fruit component at the vapour phases. The fruit juice inflow is controlled by the pump pressures P_{P_i}, which will be the input variables of the state space representation.

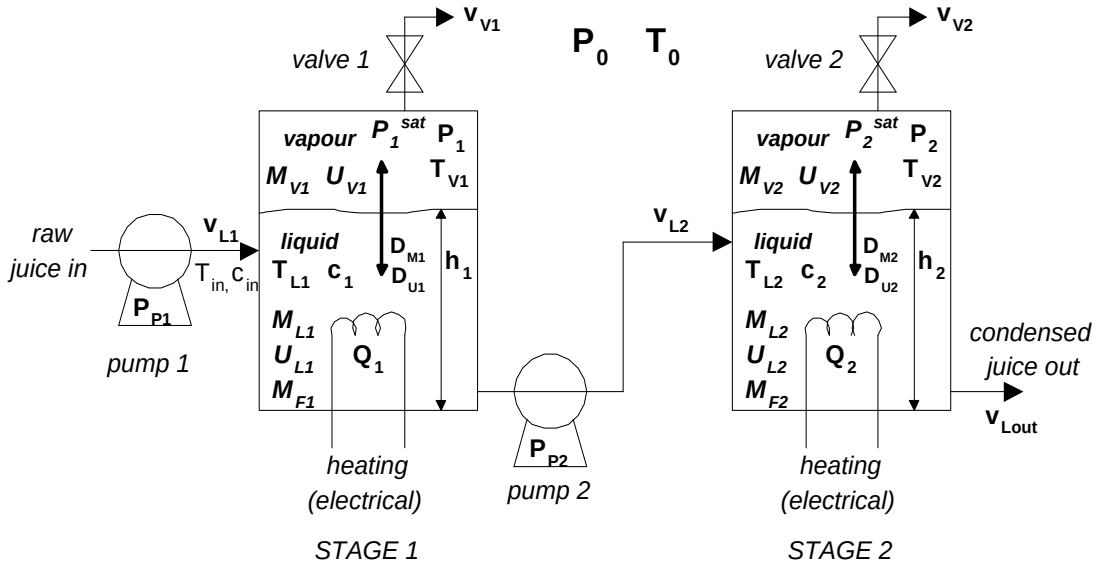

Figure 4: Two-stage fruit condenser

The state space model of the fruit condenser consists of 3 differential and 2 algebraic equations for

both stages:

$$\begin{aligned}
\dot{M}_{L_1} &= K_{P_1}(P_{P_1} - P_1) - K_{P_2}(P_{P_2} - P_2) - K_{M_1}(P_1 - P_1) && (69)\\
\dot{M}_{V_1} &= K_{M_1}(P_1^{sat} - P_1) - K_{V_1}(P_1 - P_0) && (70)\\
\dot{M}_{L_2} &= K_{P_2}(P_{P_2} - P_2) - K_{Lout}M_{L_2} - K_{M_2}(P_2^{sat} - P_2) && (71)\\
\dot{M}_{V_2} &= K_{M_2}(P_2^{sat} - P_2) - K_{V_2}(P_2 - P_0) && (72)\\
\dot{M}_{F_1} &= c_{in}K_{P_1}(P_{P_1} - P_1) - c_1K_{P_2}(P_{P_2} - P_2) && (73)\\
\dot{M}_{F_2} &= c_1K_{P_2}(P_{P_2} - P_2) - c_2K_{Lout}M_{L_2} && (74)\\
0 &= \frac{1}{V_{v_1} - \frac{M_{L_1}}{\rho_{L_1}}}\frac{M_{V_1}}{m_\omega}RT_{V_1} - P_1 && (75)\\
0 &= \frac{1}{V_{v_2} - \frac{M_{L_2}}{\rho_{L_2}}}\frac{M_{V_2}}{m_\omega}RT_{V_2} - P_2 && (76)\\
0 &= \frac{M_{F_1}}{M_{L_1}} - c_1 && (77)\\
0 &= \frac{M_{F_2}}{M_{L_2}} - c_2 && (78)
\end{aligned}$$

where P_i and P_i^{sat} denote the vapour pressure and the system pressure at stage i. This state space description belongs to models in the form of (6).

Stability investigation of the fruit condenser The structure matrix of $\frac{\partial \widetilde{h}}{\partial z}$ of the DAE system above is diagonal, therefore the algebraic variables are substitutable into the differential equations. According to (15) linearized state space model of the fruit condenser system can be written in the following form:

$$\dot{\overline{x}} = (A_{diff} + A_{alg})\,\overline{x} + B\overline{u} \qquad (79)$$

where $\overline{x} = \begin{bmatrix} \overline{M_{L_1}} & \overline{M_{V_1}} & \overline{M_{L_2}} & \overline{M_{V_2}} & \overline{M_{F_1}} & \overline{M_{F_2}} \end{bmatrix}^T$, $\overline{u} = \begin{bmatrix} \overline{P_{P_1}} & \overline{P_{P_2}} \end{bmatrix}^T$,

$$A_{diff} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & -K_{Lout} & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & -c_2^*K_{Lout} & 0 & 0 & 0 \end{bmatrix},$$

$$A_{alg} = \begin{bmatrix} -(K_{P_1} - K_{M_1})e_1 & -(K_{P_1} - K_{M_1})e_2 & K_{P_2}e_3 & K_{P_2}e_4 & 0 & 0\\ -(K_{M_1} + K_{V_1})e_1 & -(K_{M_1} + K_{V_1})e_2 & 0 & 0 & 0 & 0\\ 0 & 0 & -(K_{P_2} - K_{M_2})e_3 & -(K_{P_2} - K_{M_2})e_4 & 0 & 0\\ 0 & 0 & -(K_{M_2} + K_{V_2})e_3 & -(K_{M_2} + K_{V_2})e_4 & 0 & 0\\ M_{51} & -c_{in}K_{P_1}e_2 & c_1^*K_{P_2}e_3 & c_1^*K_{P_2}e_4 & -\frac{K_{P_2}(P_{P_2}^* - P_2^*)}{M_{L_1}^*} & 0\\ -\frac{K_{P_2}(P_{P_2}^* - P_2^*)M_{F_1}^*}{(M_{L_1}^*)^2} & 0 & M_{63} & -c_1^*K_{P_2}e_4 & \frac{K_{P_2}(P_{P_2}^* - P_2^*)}{M_{L_1}^*} & -K_{Lout} \end{bmatrix}$$

with $M_{51} = -c_{in}K_{P_1}e_1 + \frac{K_{P_2}(P_{P_2}^* - P_2^*)M_{F_1}^*}{(M_{L_1}^*)^2}$, $M_{63} = -c_1^*K_{P_2}e_3 + \frac{K_{Lout}M_{F_2}^*}{(M_{L_2}^*)^2}$, $e_1 = -\frac{\rho_{L_1}RM_{V_1}^*T_{V_1}^*}{(V_{v_1}\rho_{L_1} - M_{L_1}^*)^2m_\omega}$,
$e_2 = -\frac{\rho_{L_1}RT_{V_1}^*}{(V_{v_1}\rho_{L_1} - M_{L_1}^*)m_\omega}$, $e_3 = -\frac{\rho_{L_2}RM_{V_2}^*T_{V_2}^*}{(V_{v_2}\rho_{L_2} - M_{L_2}^*)^2m_\omega}$ and $e_4 = -\frac{\rho_{L_2}RT_{V_2}^*}{(V_{v_2}\rho_{L_2} - M_{L_2}^*)m_\omega}$.

We perform the check of eigenvalues of A_{diff} and A_{alg} separately, and show that the system is globally stable in Lyapunov sense (exactly say, it is at least globally on the boundary of asymptotic

stability). Taking a look at the matrices above, we can recognize that both A_{diff} and A_{alg} are lower block-triangular matrices:

$$A = A_{diff} + A_{alg} = \left[\begin{array}{c|c} A_{11} & 0 \\ \hline A_{21} & A_{22} \end{array}\right]$$

where A_{11} is a 4×4, while A_{21} and is A_{22} are 4×2 and 2×2 matrices.

Applying contraction theory [19], stability investigation falls out into two parts. Assuming that the elements of A_{21} are bounded in a neighbourhood of the operating point (i.e. $\exists \varepsilon_1, \varepsilon_2, \varepsilon_3 > 0 : V_{v_1}\rho_{L_1} - M_{L_1} > \varepsilon_1, V_{v_2}\rho_{L_2} - M_{L_2} > \varepsilon_2, M_{L_1} > \varepsilon_3$), the stability of the system can be investigated by checking the eigenvalues of A_{11} and A_{22} separately. These bounds have well defined physical meanings: the first and second means that the vessels must not be full of water, while the third assures that there is always a minimal amount of water at vessel 1.

The eigenvalues of the second diagonal block are the following:

$$\lambda(A_{diff_{22}}) = -\frac{K_{P_2}(P^*_{P_2} - P^*_2)}{M^*_{L_1}}, -K_{Lout}\ , \quad \lambda(A_{alg_{22}}) = 0, 0$$

Near feasible operating point values ($P^*_{P_2} > P^*_2$), negative semi-definiteness of $A_{alg_{22}}$ and therefore stability is provided.

Both $A_{diff_{11}}$ and $A_{alg_{11}}$ can be written in an upper-triangular form:

$$A_{11} = A_{diff_{11}} + A_{alg_{11}} = \left[\begin{array}{c|c} M_{11} & M_{12} \\ \hline 0 & M_{22} \end{array}\right]$$

where all block matrices are of size 2×2.

If M_{12} is bounded, eigenvalue check can be performed on the diagonal elements M_{11} and M_{22} separately. Boundedness of M_{12} is provided by the second condition above ($V_{v_2}\rho_{L_2} - M^*_{L_2} > \varepsilon_2$). Since $rank(M_{alg_{11}}) = rank(M_{alg_{22}}) = 1$, they both have one zero and an other eigenvalue which equals to the trace of the corresponding matrix. The eigenvalues of $M_{diff_{ii}}$ is much simpler: there is only one non-zero between them. The eigenvalues of the differential and algebraic components of M_{11} and M_{22} are the following:

$$\begin{aligned}
\lambda(M_{diff_{11}}) &= 0, 0 \\
\lambda(M_{alg_{11}}) &= 0, -\frac{K_{P_1}M^*_{V_1} + (V_{v_1}\rho_{L_1} - M^*_{L_1} - M^*_{V_1})K_{M_1} + (V_{v_1}\rho_{L_1} - M^*_{L_1})K_{V_1})}{(V_{v_1}\rho_{L_1} - M^*_{L_1})^2 m_\omega} \\
\lambda(M_{diff_{22}}) &= -K_{Lout}, 0 \\
\lambda(M_{alg_{22}}) &= 0, -\frac{K_{P_2}M^*_{V_2} + (V_{v_2}\rho_{L_2} - M^*_{L_2} - M^*_{V_2})K_{M_2} + (V_{v_2}\rho_{L_2} - M^*_{L_2})K_{V_2})}{(V_{v_2}\rho_{L_2} - M^*_{L_2})^2 m_\omega}
\end{aligned}$$

which are non-positive if the conditions $V_{v_1}\rho_{L_1} - M^*_{L_1} - M^*_{V_1} \geq 0$ and $V_{v_2}\rho_{L_2} - M^*_{L_2} - M^*_{V_2} \geq 0$ are fulfilled. Notice that if $\rho_{L_1} \geq \rho_{vapour_1}\ \rho_{L_2} \geq \rho_{vapour_2}$ then these conditions are automatically fulfilled by the physical boundaries of the system (maximal value of the mass of the liquid phase i is $max(M_{L_i}) = \frac{V_{v_i}}{\rho_i}$).

Near feasible parameter and operating point values all the investigated matrices are negative semi-definite, proving that A_{11} is stable in Lyapunov sense. As it has been shown A_{21} is bounded and A_{22} is also negative semi-definite, therefore the stability of the two-stage fruit condenser system is proved. These results can be easily extended for arbitrary number of stages.

7 Case study 4: A cascade of heat exchangers

Let us see a class of lumped parameter models with convection and transfer only! In this example we will compare two models that belong to different model classes according to their input specifications!

A countercurrent heat exchanger will be considered in this section. The system consists of two tubes with heat conducting walls encompassing a hot and a cold liquid stream. Heat transfer occurs between the two streams which are called the hot and the cold side. The accurate model contains distributed parameters since the temperature of the tubes changes continuously (the temperature of the cold (hot) stream increases (decreases) along the transfer area). Another approximation is modelling the long pipe with a cascade of K simple heat exchanger cells which leads to a lumped parameter system as shown in Fig. 5. Constant volumes are assumed in both tubes. The hot and cold liquid streams enter

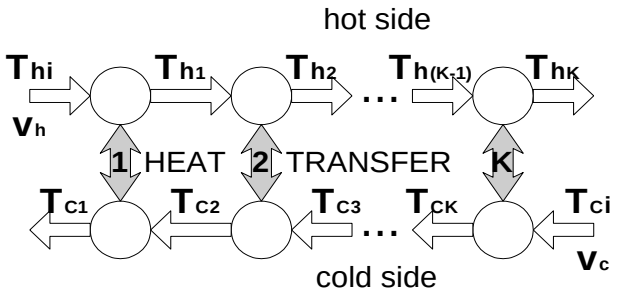

Figure 5: The cascade model of heat exchanger

the k-th cell with constant volumetric flowrates v_h and v_c. The dynamics of the system is described by the change of temperatures of both sides for every cell (T_{h_k} and T_{c_k}, $k = 1 \dots K$), and the algebraic variable describes the transfer effect:

$$\dot{T}_{c_k} = \frac{v_c}{V_c}(T_{c_{k+1}} - T_{c_k}) + \frac{1}{c_{pc}\rho_c V_c}\, Z \tag{80}$$

$$\dot{T}_{h_k} = \frac{v_h}{V_h}(T_{h_{k-1}} - T_{h_k}) - \frac{1}{c_{ph}\rho_h V_h}\, Z \tag{81}$$

$$0 = UA(T_{h_k} - T_{c_k}) - Z \tag{82}$$

$$x = [\dots T_{c_k}, T_{h_k} \dots]^T,\ k = 1 \dots K \tag{83}$$

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

Stability of the heat exchanger model It is well-known that in case of constant physico-chemical properties, pressure, masses and constant convective flows the convection term is stable in asymptotic sense, and the transfer is also stable in Lyapunov sense [11].

Two cases will be considered according to the input specifications, and showing the effect of choice on the type of stability.

For first, if the input specification contains the flowrates $u = [v_c \;\; v_h]^T$ and the inlet temperatures are considered constant then the resulted model is bilinear in the input term. According to (17), the

linearized model is in the following form:

$$\begin{bmatrix} \dot{\overline{T_{c_1}}} \\ \dot{\overline{T_{h_1}}} \\ \dot{\overline{T_{c_2}}} \\ \dot{\overline{T_{h_2}}} \\ \vdots \end{bmatrix} = \begin{bmatrix} -c_1 & c_1 & 0 & 0 & \dots \\ c_2 & -c_2 & 0 & 0 & \dots \\ 0 & 0 & -c_1 & c_1 & \dots \\ 0 & 0 & c_2 & -c_2 & \dots \\ \vdots & \vdots & \vdots & \vdots & \end{bmatrix} \begin{bmatrix} \overline{T_{c_1}} \\ \overline{T_{h_1}} \\ \overline{T_{c_2}} \\ \overline{T_{h_2}} \\ \vdots \end{bmatrix} + \begin{bmatrix} \frac{T^*_{c_2}-T^*_{c_1}}{V_c} & 0 \\ 0 & \frac{T^*_{h_0}-T^*_{h_1}}{V_h} \\ \frac{T^*_{c_3}-T^*_{c_2}}{V_c} & 0 \\ 0 & \frac{T^*_{h_1}-T^*_{h_2}}{V_h} \\ \vdots & \vdots \end{bmatrix} \begin{bmatrix} \overline{v_c} \\ \overline{v_h} \end{bmatrix} \tag{84}$$

with the constants $c_1 = \frac{UA}{c_{pc}\rho_c V_c}$, $c_2 = \frac{UA}{c_{ph}\rho_h V_h}$ and the operating point values $T^*_{c_k}$, $T^*_{h_k}$. The state term is *linear*, and contains the effect of the transfer only which is described by the algebraic term, therefore $A_{diff} = 0$ and $A = A_{alg} = A_{trans}$ - the state matrix contains only the effect of heat transfer. This matrix is block diagonal consisting of identical 2×2 diagonal blocks A_{Dk}. These blocks are singular with $rank(A_{Dk}) = 1$ because of the single transfer term. Thus, global stability results can be deduced by checking the eigenvalues of A:

$$\lambda(A_{Dk})_1 = 0,\ \lambda(A_{Dk})_2 = trace(A_{Dk}) = -(c_1 + c_2)$$

Since c_1 and c_2 are positive constants $\lambda(A_{Dk})_2$ is negative, global Lyapunov stability is proved. Moreover, the system is globally on the boundary of stability.

For second, consider the system with constant flowrates v_c, v_h and input specification $u = [T_{c_{K+1}}\ T_{h_0}]^T$. The state space model of the system will be linear in this case, and the state matrix will be in the following form:

$$A = A_{conv} + A_{trans}$$

The transfer matrix term A_{trans} is the same as in the first case (i.e. a negative semi-definite matrix). The convection matrix term will be in the following special form:

$$A_{conv} = \begin{bmatrix} -\frac{v_c}{V_c} & 0 & \frac{v_c}{V_c} & 0 & 0 & 0 & \dots \\ 0 & -\frac{v_h}{V_h} & 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & -\frac{v_c}{V_c} & 0 & \frac{v_c}{V_c} & 0 & \dots \\ 0 & \frac{v_h}{V_h} & 0 & -\frac{v_h}{V_h} & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & -\frac{v_c}{V_c} & 0 & \dots \\ 0 & 0 & 0 & \frac{v_h}{V_h} & 0 & -\frac{v_h}{V_h} & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \end{bmatrix}$$

The eigenvalues of this matrix are at its diagonal, however A_{conv} is *not* a diagonal matrix. This interesting property might be because the convection has only one inflow and one outflow point. Because the eigenvalues of A_{conv} are negative, it is a negative definite matrix. We know that the sum of a negative semi-definite and a negative definite matrix is negative definite, therefore $A = A_{trans} + A_{conv}$ is negative definite. This proves global asymptotic stability for the second case.

Considering the two cases investigated, we can observe that the convection term appeared in the input term choosing flowrate inputs, and turned in the state term when inlet temperatures were specified. By comparison, we can conclude that convection globally stabilizes the system.

8 Conclusion and future work

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 different continuous fermentation process models, a simple evaporator system, a two-stage fruit condenser and a countercurrent heat exchanger.

For a single input continuous fermentation process, bifurcation analysis is used to investigate the effect of the steady-state values on the stability of DAE systems.

Further work is directed towards a systematic mechanism-wide local stability analysis of DAE process models. A further aim is to extend the local stability investigations into global ones using Lyapunov technique.

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