A model structure-driven hierarchical decentralized stabilizing control structure for process networks

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Abstract

Based on the structure of process models a hierarchically structured state-space model has been proposed for process networks with controlled mass convection and constant physico-chemical properties. Using the theory of cascade-connected nonlinear systems and the properties of Metzler and Hurwitz matrices it is shown that process systems with controlled mass convection and without sources or with stabilizing linear source terms are globally asymptotically stable. The hierarchically structured model gives rise to a distributed controller structure that is in agreement with the traditional hierarchical process control system structure where local controllers are used for mass inventory control and coordinating controllers are used for optimizing the system dynamics. The proposed distributed controller is illustrated on a simple non-isotherm jacketed chemical reactor.

Keywords: process control, process modeling, stability, plant wide control

1. Introduction

It is widely known that process systems are highly nonlinear and form complex networks. The complex dynamics of a process network is caused partially by the complex dynamic behavior of the component subsystems, but also by the effect of complex interactions. In order to cope with this complex

nonlinear dynamics two principally different controller design approaches exist: the centralized and decentralized ones. The latter is most widely used in complex process plants because it offers the possibility to handle nonlinearities locally, i.e. controlling the operating units, for example, and then handle the interactions plant-wide. One of the key critical steps in this approach is to decompose the process plant and/or its control system into hierarchical and decentralized structures.

The plantwide control problem that deals with designing a complex distributed controller for a given complex process plant is widely investigated in process control and forms a traditional area of it. The first approaches were based on linear or linearized dynamic models and their properties (such as steady-state gains), see e.g. [1] or [2], where graph-theoretic approaches could be applied for efficient solution [3]. Applying the theory of linear systems, systematic approaches have been developed for complex large scale systems in general (see e.g. [4]), and for process plants in particular [5], [6]. The performance limitations in decentralized control were also investigated in the linear(ized) model case [7].

The above mentioned systematic methods include heuristic elements in determining the controller structure, i.e. the matching of controlled and manipulated variables in the plant ([5], [6]), and they have identified controller layers that should form a hierarchy. One of such heuristics is to regulate the inventories, most notably the masses in each operating unit using the lowest controller layer of the hierarchy [8].

Although the general modern theory of possibly nonlinear, hierarchical, multilevel and distributed systems and control is well developed (see e.g. [9] for an early, and [10] for a recent reference), there are powerful and specially developed techniques for nonlinear process systems [11], too.

More recently, modern robust control techniques have been proposed for distributed control of plantwide chemical processes [12], with an attempt to extend it to the nonlinear case [13] using the notion of dissipativity [14]. This approach was further extended to the decentralized case using a Hamilton-Jacobi equation approach [15]. Powerful distributed and hierarchical variants of the popular model predictive control (MPC) have also been developed and applied to complex process plants, see [10] for a recent review.

Utilizing the engineering insight into the physics and chemistry of the system, the thermodynamic passivity approach [16] as a special control approach has been proposed for nonlinear process systems that is based on controlling its inventories [17]. The controller design method has been combined with

passivity [18], too. In addition to the material and energy connections in the process network, information and communication interconnections of the system and its control system are also considered in a framework integrating physics communication and computation in [19]. Furthermore, the inventory control scheme was also extended with local nonlinear controllers (see [20] and [21]) to construct stabilizing controllers to arbitrary steady-state points. Further improvements of the physically motivated nonlinear controller design have been achieved by using passivity [22], control Lyapunov [23] and Hamiltonian approaches [24, 25, 26] to nonlinear process systems.

Although the above physically motivated nonlinear control approaches exploit successfully the properties of nonlinear process systems, but the hierarchical structure of process models has not been fully utilized in process control structure design. This inherent hierarchy of dynamic process models seems useful to apply, because powerful approaches in systems and control theory (for example the contraction theory approach [27] or the theory of interconnected nonlinear systems [28]) have been proposed for stability analysis for hierarchically decomposed systems.

A critical and still generally open problem in applying the powerful hierarchical decentralized control techniques is how to decompose a complex nonlinear plant into subsystems [10]. This is traditionally performed using the process layout, where the operating units form the subsystems, but then the complex interactions, the material and energy recycles, for example, are difficult to handle.

Aim and problem statement. The main aim of this paper is to propose a decomposition that is based on the hierarchical structure of dynamic process models based on first engineering principles and use this for designing decentralized control systems to stabilize the subsystems and maintain stable performance as these subsystems are integrated into the complex process system.

The first paper in this direction [29] investigated the simplest case of process systems with constant holdup in each balance volume to show that such systems with constant pressure and no source are structurally asymptotically stable. The restriction of constant mass holdup, however, is a severe limitation which does not hold in almost any practical situation.

The above results are extended in this paper for the case of process systems with time-varying regulated mass holdup and stabilizing sources. For analyzing the stability of process systems in this extended case, the dynamic

3

model of the system based on first engineering principles will be brought to a nonlinear cascade-connected state-space model form [28].

The usual hierarchical structure of process models and that of process control systems is considered in this paper, where low level controllers provide regulated mass holdup in each balance volume and the high level controller(s) are used for controlling the other process variables, such as temperatures and concentrations. This structure enables to partition the system model into a controlled mass subsystem that acts as a "driving subsystem" to the other part that is the "driven subsystem" [28].

With the above model structure, the stabilizing controller design will be performed by using local distributed controllers acting on the driven subsystem.

Basic assumptions. The starting point of the analysis is the general form of the state equation of a lumped process system originated from the differential conservation balances of the conserved extensive quantities over perfectly stirred regions or balance volumes. A perfectly stirred region is the smallest elementary part of the process system over which conservation balances are constructed. The following *assumptions* are made about the regions:

$\mathcal{A}1$ *Physico-chemical properties, like heat capacity, density, and heat transfer coefficients are constant.*

$\mathcal{A}2$ *The pressure is assumed to be constant.*

The above two assumptions imply that only incompressible liquid phases can be present in the regions.

The paper is organized as follows. We start with the lumped dynamic model of the mass subsystem of a process system in the next section. Thereafter we develop the model of the energy and component mass subsystems in section 3. The stability analysis of the hierarchically decomposed state-space model is given in section 4. The distributed controller structure driven by the hierachically decomposed model structure is described in section 5 illustrated by a simple case study of a jacketed CSTR. Finally conclusions are drawn.

2. The mass subsystem

Following the philosophy and the incremental approach of building a process model [31], we distinguish two subsystems in a process system. The

basic subsystem is the mass subsystem upon which the energy and component mass subsystem is built.

2.1. The mass conservation balance equations

The *overall mass balance* of the perfectly stirred region j is given by the equation

$$\frac{dm^{(j)}}{dt} = v_{in}^{(j)} - v_{out}^{(j)} \quad , \quad j = 1, \ldots, \mathcal{C} \tag{1}$$

where $v_{in}^{(j)}$ and $v_{out}^{(j)}$ are the *mass in- and outflow rates* respectively and $\mathcal{C}$ is the number of the regions.

Note that a definite flow direction (i.e. in- or out to/from a balance volume) is associated to any mass flow, i.e. $v_{in}^{(j)} \geq 0$ and $v_{out}^{(j)} \geq 0$. This implies, that two separate flows are defined to pipes where flow in either direction is allowed.

As the overall mass is conserved, the balance (1) has no source term. As we only consider process systems with incompressible fluid phases under assumptions $\mathcal{A}1$-$\mathcal{A}2$, only the convection of the overall mass is present in the conservation balance equations.

Convective flows. Like in any process network, the regions are connected by flows, that can be convective flows or transfer flows. In order to describe the general case let us assume that the outlet flow of region j is divided into parts described by ratios $\alpha_\ell^{(j)}$ satisfying the equation

$$\sum_{\ell=0}^{\mathcal{C}} \alpha_\ell^{(j)} = 1 \quad , \quad j = 0, \ldots, \mathcal{C} \tag{2}$$

where $\alpha_j^{(\ell)}$ is the ratio of the outlet flow $v^{(\ell)}$ of region ℓ flowing into region j. Fig. 1 illustrates the notation. By using flows to and from the environment which is described by defining a pseudo-region with index 0 we obtain

$$v_{in}^{(j)} = \sum_{\ell=0}^{\mathcal{C}} \alpha_j^{(\ell)} v_{out}^{(\ell)} \quad , \quad j = 0, \ldots, \mathcal{C} \tag{3}$$

The ratios described above are now used to define a convection ratio matrix

$$C_{conv} = \begin{bmatrix} -(1 - \alpha_1^{(1)}) & \alpha_1^{(2)} & \ldots & \alpha_1^{(\mathcal{C})} \\ \ldots & \ldots & \ldots & \ldots \\ \alpha_{\mathcal{C}}^{(1)} & \alpha_{\mathcal{C}}^{(2)} & \ldots & -(1 - \alpha_{\mathcal{C}}^{(\mathcal{C})}) \end{bmatrix} \tag{4}$$
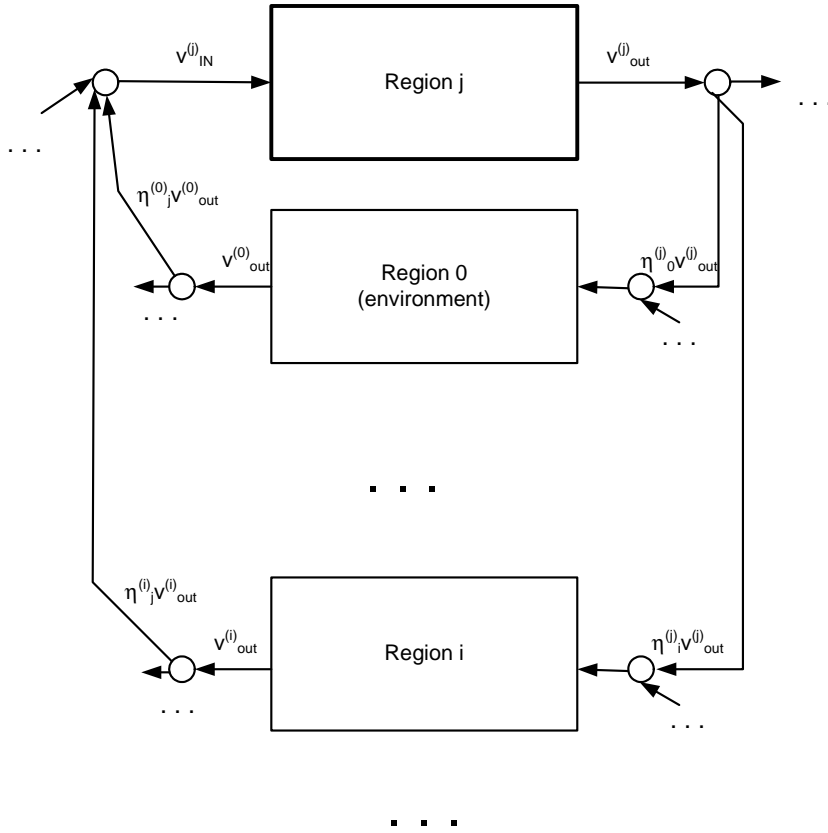
5

Figure 1: The convection network

Only the ratios belonging to the internal flows (that is *not* from the environment) are included.

Well-connected convection networks. In order to be able to ensure that one can regulate the overall mass $m^{(j)}$ of every region at a given strictly positive value by manipulating the flow rates, we assume that

$\mathcal{A}3$ *every region has at least one physical inflow and one outflow either from/to another region or the environment.*

Such a convection network will be called *well-connected.* This implies that there is no individual sink or source balance volume in the network.

It is important to note that Eq. (2) guarantees that C_{conv} is a so-called *compartmental matrix* (see the exact definition below). This fact allows

us to establish simple conditions for the asymptotic stability of the mass subsystem.

Definition 1. *A real square matrix* $F = \{f_{ij}\}_{i,j=1}^n \in \mathbb{R}^{n \times n}$ *is said to be a compartmental matrix if all of its off-diagonal elements are non-negative and all of its column-sums are non-positive, i.e.*

$$f_{ij} \geq 0 \quad i, j = 1, \ldots, n, \ i \neq j \tag{5}$$

$$\sum_{i=1}^{n} f_{ij} \leq 0, \quad j = 1, \ldots, n \tag{6}$$

We remark that a compartmental matrix is a special case of a *Metzler-matrix* having the property that its off-diagonal elements are non-negative. It is known that a linear autonomous system of the form $\dot{x} = Ax$ is *positive* (i.e. the non-negative orthant is invariant for the dynamics) if and only if A is a Metzler-matrix [32]. It is also clear that compartmental matrices belong to the set of *column diagonally dominant matrices* characterized by the property that the absolute value of the diagonal element in any column is larger than or equal to the sum of the absolute values of the off-diagonal elements in that column [33].

It is straightforward to associate a directed graph to the mass-convection subsystem in the following way: let the nodes (vertices) of the graph be the perfectly stirred regions (not including the environment). There is a directed edge from node i to node j if and only if there is a mass flow from region i to region j. A *strongly connected component* of a directed graph is a maximal set of vertices in which there is a directed path from any one vertex to any other vertex in the set [34]. (We remark that a strongly connected component may consist of only one vertex, since any vertex is trivially connected to itself.) A *trap* is a node or set of nodes in the directed graph from which there are no directed edges towards the environment nor to other nodes not in the set. A trap is called *simple* if it does not strictly contain a trap [35]. In other words, a simple trap is a strongly connected component from which there is no outgoing directed edge, i.e. no outflow. Physically, a trap means a sink subnetwork in the convection network from where there is no outflow. Under assumption $\mathcal{A}3$, only such convection networks are considered here that cannot contain any simple trap consisting of a single balance volume.

The eigenvalues and thus the (asymptotic) stability of the mass-convection system is strongly related to the directed graph structure of the convection

network. The following important properties of compartmental matrices are taken and adapted from [35, 36, 37], where more details can be found.

(C1) The eigenvalues of compartmental matrices are either zero or they have negative real parts. This trivially implies that compartmental matrices cannot have purely imaginary eigenvalues or eigenvalues with positive real parts.

(C2) Let us suppose that the mass-convection network is such that in its associated directed graph, there exists a directed path between any distinct pair of nodes (i.e. the directed graph of the network is *strongly connected*). Then 0 is an eigenvalue of C_{conv} if and only if $\sum_{i=1}^{n}[C_{conv}]_{ij} = 0$ for $j = 1, \ldots, n$.

(C3) Zero is an eigenvalue of C_{conv} of multiplicity m if and only if the associated directed graph contains m simple traps. In such a case, the eigenvectors corresponding to the zero eigenvalues are linearly independent.

2.2. Controlled mass convection network

In order to make the overall mass subsystem asymptotically stable, we firstly eliminate any traps in the mass convection subsystem as a part of the control structure. This is done by adding an outflow to the environment from at least one balance volume of each simple trap of the original convection network. (In practice a suitable outflow can be realized by allowing flows in either directions in the same pipe.) By doing this, from now on we can assume the following based on (C3):

$\mathcal{A}4$ Each eigenvalue of C_{conv} has strictly negative real part (i.e. C_{conv} is a *Hurwitz matrix*).

Moreover, let us apply a full state feedback controller in the form of

$$v_{out}^{(j)} = \kappa^{(j)} m^{(j)} + v_{ref}^{(j)} \quad , \quad \kappa^{(j)} > 0 \tag{7}$$

that is a set of local controllers that stabilize the mass inventory of each region using the manipulated variables $v_{out}^{(j)}$. This way of controlling the masses in each region can be regarded as a special version of mass inventory control (see e.g. [20]).

With these outlet mass flows the inlet flow to region j can be written as follows:

$$v_{in}^{(j)} = \sum_{\ell=1}^{\mathcal{C}} \alpha_j^{(\ell)} \left(\kappa^{(\ell)} m^{(\ell)} + v_{ref}^{(\ell)} \right) + \alpha_j^{(0)} v_{out}^{(0)} \quad , \quad j = 1, \ldots, \mathcal{C} \qquad (8)$$

where

$$\alpha_j^{(0)} v_{out}^{(0)} = v_{IN}^{(j)}$$

is the flow from the environment.

Considering Eq. (8) with Eq. (1) gives

$$\frac{dm^{(j)}}{dt} = \sum_{\ell=1}^{\mathcal{C}} \alpha_j^{(\ell)} \left(\kappa^{(\ell)} m^{(\ell)} + v_{ref}^{(\ell)} \right) - \kappa^{(j)} m^{(j)} - v_{ref}^{(j)} + v_{IN}^{(j)} \quad , \quad j = 1, \ldots, \mathcal{C} \quad (9)$$

that is the mass balance of the controlled mass subsystem.

We now define the mass, and the mass in- and out-flow vectors

$$M = [\, m^{(1)} \ \ldots \ m^{(\mathcal{C})}]^T \quad , \quad V_{IN} = [\, v_{IN}^{(1)} \ \ldots \ v_{IN}^{(\mathcal{C})}]^T \qquad (10)$$

$$V_{OUT} = [\, v_{out}^{(1)} \ \ldots \ v_{out}^{(\mathcal{C})} \,]^T$$

with $\mathcal{K} = diag\{\kappa^{(j)} \mid j = 1, \ldots, \mathcal{C}\}$ and with a reference signal vector for the overall masses $V_{ref} = [v_{ref}^{(j)} \ \ldots \ v_{ref}^{(\mathcal{C})}]^T$.

With the above vectors and matrices Eq. (7) can be written as

$$V_{OUT} = \mathcal{K}M + V_{ref} \qquad (11)$$

Using matrix-vector formulation we can transform the mass conservation equation (9) into a linear time-invariant state equation as follows:

$$\frac{dM}{dt} = C_{conv}\mathcal{K}M + C_{conv}V_{ref} + V_{IN} \qquad (12)$$

The usual way of controlling the mass holdups in every balance volume of a process system is to set suitable reference values for the system mass inlet flowrates V_{IN}^* and suitable setpoints V_{ref} for the controllers such that a *positive steady-state reference value* M^* is obtained. The reference values for the masses in each balance volume can be obtained by solving the steady-state version of Eq. (12) for $M^* > 0$:

$$0 = C_{conv}\mathcal{K}M^* + C_{conv}V_{ref} + V_{IN}^* \qquad (13)$$

This way one ensures $m^{(j)} > 0$, i.e. there is no empty holdup in the system. *This implies that $v_{out}^{(j)}$ is positive, as well.*

9

Definition 2. *A mass convection network with the linear time-invariant state equation (12) and with a positive definite, diagonal, state feedback matrix $\mathcal{K}$ is called a controlled mass convection network.*

As the coefficient matrices C_{conv} and $\mathcal{K}$ are constant matrices in the state equations (12), the overall mass subsystem of a process systems is a linear time-invariant (LTI) system.

Possible input variables. Eq. (12) has only one set of possible input variables V_{IN}, because V_{ref} is used to set a positive reference value for each mass holdup. These variables, however, act usually as disturbances, but they can also be manipulated as, for example, external cooling mass flow rates (see later in subsection 5.2).

2.3. Stability of the controlled mass convection network

Using the above dynamic model and algebraic results, the following statement about the stability of controlled mass convection network can be stated.

Lemma 1. *The unique positive steady-state point M^* of a well-connected controlled mass convection network described by the dynamic model (12) is asymptotically stable. Moreover, the solutions of the state equation (12) remain positive and bounded for any positive initial condition.*

Proof. It is easy to see that the state matrix $C_{conv}\mathcal{K}$ in Eq. (12) is also a compartmental matrix, since the columns of C_{conv} are scaled by positive constants. Moreover, the unweighted directed graph structures corresponding to C_{conv} and $C_{conv}\mathcal{K}$ are identical. Thus, it follows from property (C3) and $\mathcal{A}_4$ that the controlled mass convection network is asymptotically stable.

Finally, using known results from the theory of positive systems [32, 38], the positivity of the solutions of (12) can be guaranteed if the elements of $C_{conv}V_{ref} + V_{IN}$ are nonnegative. ∎

3. The energy and component mass subsystems

Under the assumptions stated in the Introduction, the differential balance equation of a conserved, extensive quantity ϕ for a perfectly stirred region j takes the form [31]:

$$\frac{d\phi^{(j)}}{dt} = \phi_{in}^{(j)} - \phi_{out}^{(j)} + q_{\phi,transfer}^{(j)} + q_{\phi,source}^{(j)} \tag{14}$$

10

The first two terms account for the in- and outflow respectively, $q^{(j)}_{\phi,transfer}$ is the transfer and $q^{(j)}_{\phi,source}$ is the source term. The transfer term is used to describe heat transfer or a lumped version of diffusion [31], for example, while the source term can refer to e.g. the chemical reactions.

3.1. Process variables

The conserved extensive quantities $\phi^{(j)}$ of region j are given by the vector

$$\phi^{(j)} = [\ E^{(j)},\ (m^{(j)}_k, k = 1, \dots, K - 1)\ ]^T \tag{15}$$

where $E^{(j)}$ is the internal energy and $m^{(j)}_k$ is the component mass of the kth component with K being the number of components in the region. The related *engineering driving force variables or potentials are*

$$P^{(j)} = [\ T^{(j)},\ (c^{(j)}_k,\ k = 1, \dots, K - 1)\ ]^T \tag{16}$$

where $T^{(j)}$ is the temperature and $c^{(j)}_k$ is the concentration of the kth component.

Now we combine the vectors of the conserved extensive quantities (15) and the corresponding potentials (16) so that

$$\phi = [(\phi^{(1)})^T \ \dots \ (\phi^{(\mathcal{C})})^T]^T \quad , \quad P = [(P^{(1)})^T \ \dots \ (P^{(\mathcal{C})})^T]^T$$

With these definitions and Assumption $\mathcal{A}$1. we find that the relationship between conserved extensive quantities and the potentials is linear [29], so that

$$\phi^{(j)} = Q^{(j)} P^{(j)} \tag{17}$$

where $Q^{(j)}$ is a positive definite diagonal matrix, i.e. $Q^{(j)} > 0$ in the form

$$Q^{(j)} = \begin{bmatrix} c^{(j)}_P m^{(j)} & 0 & \dots & 0 \\ 0 & m^{(j)} & 0 \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & m^{(j)} \end{bmatrix} = m^{(j)} \theta^{(j)} \tag{18}$$

$$\theta^{(j)} = \begin{bmatrix} c^{(j)}_P & 0 & \dots & 0 \\ 0 & 1 & 0 \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 1 \end{bmatrix} \tag{19}$$

11

where $c_P^{(j)}$ is the specific heat of the material in region j and $\theta^{(j)}$ is a *constant coefficient matrix*.

Let us define a *positive definite diagonal matrix* Q block-diagonally from the individual matrices $Q^{(j)}$ and similarly a *positive definite constant matrix* θ from the $\theta^{(j)}$-s so that

$$Q = \begin{bmatrix} Q^{(1)} & 0 & \ldots & 0 \\ 0 & Q^{(2)} & 0 \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & Q^{(\mathcal{C})} \end{bmatrix} , \quad \theta = \begin{bmatrix} \theta^{(1)} & 0 & \ldots & 0 \\ 0 & \theta^{(2)} & 0 \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & \theta^{(\mathcal{C})} \end{bmatrix} \quad (20)$$

The *positive definiteness of $Q(M)$ holds under the condition, that $M > 0$ is assumed (element-wise)*, as it is seen from the definition of the mass vector M in (10) and that of the matrix Q in (20) and (18). This follows since we assume positive mass holdup in each balance volume.

Using the above matrices we can write Eq. (17) in vector form:

$$\phi = Q(M) \cdot P = \left(diag\{E^{(K)} \otimes M\} \right) \theta \cdot P \quad (21)$$

where $\otimes$ represents the Kronecker product and $E^{(K)}$ is a K-dimensional vector with all of its entries being 1. We recall that the Kronecker product of two matrices A and B is given by

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \ldots & a_{1n}B \\ a_{21}B & a_{22}B & \ldots & a_{2n}B \\ \ldots & \ldots & \ldots & \ldots \\ a_{m1}B & a_{m2}B & \ldots & a_{mn}B \end{bmatrix}$$

3.2. The intensive variable form of the balance equations

The transfer and the source terms in the conservation balance equations depend on the *driving force variables*. Therefore the intensive variable form of the conservation balance equations will be used for the analysis and controller design. This form is obtained by using Eqs. (17) and (18) in Eq. (14) and substituting the right-hand side of Eq. (9) for the term $\frac{dm^{(j)}}{dt}$. Thus the following intensive variable form is obtained:

$$m^{(j)}\theta^{(j)}\frac{dP^{(j)}}{dt} = q_{conv}^{(j)} + q_{transfer}^{(j)} + q_{source}^{(j)} \quad , \quad j = 1, \ldots, \mathcal{C} \quad (22)$$

12

The transfer term. The transfer term $q_{\phi,transfer}^{(j)}$ in the balance equations (14) has the following general linear form:

$$q_{transfer}^{(j)} = \sum_{\ell=1}^{\mathcal{C}} q_{transfer}^{(j,\ell)} = \sum_{\ell=1}^{\mathcal{C}} L^{(j,\ell)} \left(P^{(\ell)} - P^{(j)} \right) \tag{23}$$

The transfer coefficient matrices $L^{(j,\ell)} \in \mathbb{R}^{K \times K}$ are constant under Assumption 1. The driving force is given by the difference between $P^{(j)}$ and $P^{(\ell)}$ [31]. Examples include the Fourier and Fick laws for heat conduction and diffusion.

The transfer term (23) is a special case of the Onsager relationship in irreversible thermodynamics when one neglects the cross-effects, and assumes an ideal, monotonous dependence of the thermodynamic driving force variables on the potentials [29]. This theory shows that the matrices $L^{(j,\ell)}$ *are positive definite and symmetric.*

Collecting all the transfer terms in the conservation balances into a single vector

$$q_{transfer} = [\ (q_{transfer}^{(1)})^T \ \cdots \ (q_{transfer}^{(\mathcal{C})})^T\ ]^T$$

we can write the overall transfer rate relation

$$q_{transfer} = \mathcal{L}\ P \quad , \quad \mathcal{L} < 0 \ , \ \mathcal{L}^T = \mathcal{L} \tag{24}$$

where the transfer matrix $\mathcal{L}$ is negative definite and symmetric in the following form:

$$\mathcal{L} = \frac{1}{2} \sum_{j=1}^{\mathcal{C}} \sum_{\ell=1}^{\mathcal{C}} \left(I^{(j,\ell)} \otimes L^{(j,\ell)} \right), \quad j \neq \ell \tag{25}$$

In the above equation $I^{(j,\ell)}$ is a negative semi-definite $\mathcal{C} \times \mathcal{C}$ dimensional matrix where

$$I_{jj}^{(j,\ell)} = I_{\ell\ell}^{(j,\ell)} = -1 \ , \ \left(I_{j\ell}^{(j,\ell)} = I_{\ell j}^{(j,\ell)} = +1, \ell \neq j \right) \tag{26}$$

and zero otherwise. Here we used the property that each matrix $\left(I^{(j,\ell)} \otimes L^{(j,\ell)} \right)$ in the sum (25) is negative semi-definite and symmetric therefore their sum $\mathcal{L}$ is also *negative semi-definite and symmetric.* Moreover, it is easy to see that $\mathcal{L}$ is such a compartmental matrix where both the column-sums and row-sums are zero.

The convective term. The intensive form of the convective term $q_{k,conv}^{(j,\ell)}$ for component k entering region j from region ℓ is

$$\alpha_j^{(\ell)} v_{out}^{(\ell)} \left(\theta_{kk}^{(\ell)} P_k^{(\ell)} - \theta_{kk}^{(j)} P_k^{(j)} \right)$$

where this form is a consequence of substituting the right-hand side of Eq. (9) for the term $\frac{dm^{(j)}}{dt}$ into the conservation balance equations when forming their intensive variable form (see [31] Chapter 5. for details).

As we have seen in section 2.1 before, the inlet of any of the regions is composed of the outlet of all the other regions as described in Eq. (3). Therefore, the inlet mass flow of region j can be computed by Eq. (8) in case of a controlled mass convection network. Similarly, the convective term $q_{k,conv}^{(j)}$ of a conserved extensive quantity $\phi_k^{(j)}$ in region j can also be written as a sum using the intensive form of the partial inlet convective flows $q_{k,conv}^{(j,\ell)}$ above so that

$$q_{k,conv}^{(j)} = \sum_{\ell=1}^{C} \alpha_j^{(\ell)} v_{out}^{(\ell)} \left(\theta_{kk}^{(\ell)} P_k^{(\ell)} - \theta_{kk}^{(j)} P_k^{(j)} \right) + v_{IN}^{(j)} \left(\theta_{IN,kk}^{(j)} P_{IN,k}^{(j)} - \theta_{kk}^{(j)} P_k^{(j)} \right) =$$

$$= \sum_{\ell=1}^{C} \alpha_j^{(\ell)} \left(\kappa^{(\ell)} m^{(\ell)} + v_{ref}^{(\ell)} \right) \left(\theta_{kk}^{(\ell)} P_k^{(\ell)} - \theta_{kk}^{(j)} P_k^{(j)} \right) + v_{IN}^{(j)} \left(\theta_{IN,kk}^{(j)} P_{IN,k}^{(j)} - \theta_{kk}^{(j)} P_k^{(j)} \right)$$

where $\theta_{IN,kk}^{(j)}$ is the coefficient for the driving force variable $P_{IN,k}^{(j)}$ at the inlet from the environment to region j.

In order to develop a compact matrix-vector form of the convective term suitable for stability analysis, we introduce the vector variables describing the conditions at the inlet of each of the regions

$$P_{IN} = [\ P_{IN,1}^{(1)} \dots P_{IN,K}^{(1)}; \dots; P_{IN,1}^{(C)} \dots P_{IN,K}^{(C)}\ ]^T$$

and

$$\theta_{IN} = diag\{\ \theta_{IN,11}^{(1)} \dots \theta_{IN,KK}^{(1)}; \dots; \theta_{IN,11}^{(C)} \dots \theta_{IN,KK}^{(C)}\ \}$$

With these vectors and matrices we arrive at the following form of the convective term:

$$q_{conv} = q_{convt} + \mathcal{V}_{IN} \cdot (\theta_{IN} P_{IN} - \theta P)$$

where

$$\mathcal{V}_{IN} = diag\{E^{(K)} \otimes V_{IN}\}$$

14

is a diagonal matrix with positive elements, and

$$q_{conv}^{(j)} = [\; q_{1,conv}^{(j)} \;\; \cdots \;\; q_{K,conv}^{(j)} \;]^T \;\;,\;\; q_{conv} = [\; (q_{conv}^{(1)})^T \;\; \cdots \;\; (q_{conv}^{(\mathcal{C})})^T \;]^T$$

$$q_{convt}^{(j)} = [\; q_{convt,1}^{(j)} \;\; \cdots \;\; q_{convt,K}^{(j)} \;]^T \;\;,\;\; q_{convt} = [\; (q_{convt}^{(1)})^T \;\; \cdots \;\; (q_{convt}^{(\mathcal{C})})^T \;]^T$$

with

$$q_{convt,k}^{(j)} = \sum_{\ell=1}^{\mathcal{C}} \alpha_j^{(\ell)} v_{out}^{(\ell)} \left(\theta_{kk}^{(\ell)} P_k^{(\ell)} - \theta_{kk}^{(j)} P_k^{(j)} \right) \tag{27}$$

being the *convective term that is in a similar form to the transfer terms.*

The next step is to observe the similarity of Eq. (27) above with the transfer rate equation (23). In the case of $q_{convt}^{(j)}$ the driving force becomes $\left(\theta^{(\ell)} P^{(\ell)} - \theta^{(j)} P^{(j)} \right)$ and the coefficient values are now dependent on the masses $m^{(\ell)}$ in the regions through $v_{out}^{(\ell)}$. These coefficients can be arranged to a diagonal positive semi-definite matrix:

$$N^{(\ell,j)}(M) = \alpha_j^{(\ell)} v_{out}^{(\ell)} \cdot I^{(K)}$$

where $I^{(K)}$ is a unit matrix of dimension $K \times K$.

The overall transfer-analog convective term for the whole system is now in the form:

$$q_{convt} = \mathcal{N}(M)\, \theta P \;\;,\;\; \mathcal{N} \leq 0 \tag{28}$$

where the convection matrix $\mathcal{N}(M)$ is negative semi-definite:

$$\mathcal{N}(M) = \sum_{j=1}^{\mathcal{C}} \sum_{\ell=1}^{\mathcal{C}} \left(U^{(\ell,j)} \otimes N^{(\ell,j)} \right), \;\; j \neq \ell \tag{29}$$

with $U^{(\ell,j)}$ being a negative semi-definite $\mathcal{C} \times \mathcal{C}$ dimensional matrix where

$$U_{jj}^{(\ell,j)} = -1 \;,\;\; \left(U_{j\ell}^{(\ell,j)} = +1,\; j \neq \ell \right) \tag{30}$$

and zero otherwise. For $j \neq \ell$, each Kronecker product in the sum (29), is a Metzler matrix with zero row sums. Therefore, $\mathcal{N}^T(M)$ is a compartmental matrix for any elementwise positive M.

With the above notations the convection term takes the following compact matrix-vector form:

$$q_{conv} = \mathcal{N}(M) \cdot \theta P + \mathcal{V}_{IN} \cdot (\theta_{IN} P_{IN} - \theta P) \tag{31}$$

Now we can put together the compact matrix-vector form of the conservation balances for energy and component masses in intensive form, where all the terms depend explicitly on the driving force variables P:

$$Q(M)\frac{dP}{dt} = \mathcal{N}(M) \cdot \theta P + \mathcal{V}_{IN} \cdot (\theta_{IN} P_{IN} - \theta P) + \mathcal{L} \cdot P + q_{source}(P) \quad (32)$$

4. Stability of the hierarchically decomposed state-space model

In this section we show that the centered conservation balances together with the centered mass balance equations form a hierarchical combination of a linear time-invariant and a nonlinear set of state equations. The asymptotic stability analysis uses this hierarchy to demonstrate the stability of the system with controlled mass convection network.

For this purpose we unite all the conservation balance equations for overall masses and the other conserved quantities and form a hierarchically arranged cascade-connected set of nonlinear state equations [28].

4.1. The compact centered conservation balance equations

A *deviation variable* $\overline{Y}$ with its steady-state (constant) reference value Y^* is defined as follows:

$$\overline{Y} = Y - Y^*$$

Centered mass conservation balances. The centered version of the mass balance equation (12) is obtained by substituting the deviation system variables, i.e. the deviation masses and mass flow rates into the balance to obtain:

$$\frac{d\overline{M}}{dt} = C_{conv}\mathcal{K}\overline{M} + \overline{V}_{IN} \quad (33)$$

where the steady-state reference values are obtained by solving Eq. (13).

Centered energy and component mass conservation balances. The steady-state reference value P^* of the driving force variables is determined by choosing a reference value P_{IN}^* for them at the inlet, and the reference value of the inlet mass flowrates $\mathcal{V}_{IN}^*$ used for the centered version of the mass balances by solving

$$0 = \mathcal{N}(M) \cdot \theta P^* + \mathcal{V}_{IN}^* \cdot (\theta_{IN} P_{IN}^* - \theta P^*) + \mathcal{L} \cdot P^* + q_{source}(P^*)$$

for P^*.

It is important to note that the solution of the above equation may not be unique caused by the nonlinearity in the source term $q_{source}(P^*)$, so more than one steady-state reference value P^* can be obtained.

Then the centered compact intensive form of the conservation balance equations is as follows:

$$
\begin{aligned}
Q(M)\frac{d\overline{P}}{dt} = {} & \mathcal{N}(M) \cdot \theta\overline{P} + \mathcal{V}_{IN} \cdot \theta_{IN}\overline{P}_{IN} - \overline{\mathcal{V}}_{IN} \cdot \theta_{IN}P_{IN}^* - \mathcal{V}_{IN} \cdot \theta\overline{P} + \overline{\mathcal{V}}_{IN} \cdot \theta P^* \\
& + \mathcal{L} \cdot \overline{P} + \overline{q}_{source}(\overline{P})
\end{aligned}
\tag{34}
$$

4.2. The hierarchically decomposed state-space equations

Here we explore the special structure of the compact centered conservation balance equations (33) and (34) and show that they form a special hierarchy.

Lemma 2. *Assume zero deviation inputs*

$$
\overline{\mathcal{V}}_{IN} = 0 \quad , \quad \overline{P}_{IN} = 0
\tag{35}
$$

for the centered conservation balance equations (33) and (34). Then these equations form a cascade-connected nonlinear system [28] with the equilibrium point $(0,0)$, i.e. with $M = M^*$ and $P = P^*$.

Proof. By assuming zero deviation inputs in (35), we set the variables $\mathcal{V}_{IN}$ and P_{IN} to their reference values, i.e. $\mathcal{V}_{IN} = \mathcal{V}_{IN}^*$ and P_{IN}^*.

Joining the centered overall mass balance equations (33) and that of the conservation balances (34) with *assuming zero deviation input* results in the coupled dynamical system

$$
\begin{aligned}
\dot{\overline{M}} &= C_{conv}\mathcal{K}\overline{M} \tag{36} \\
\dot{\overline{P}} &= Q^{-1}(M)\left(\mathcal{N}(M) \cdot \theta\overline{P} - \mathcal{V}_{IN}^* \cdot \theta\overline{P} + \mathcal{L}\overline{P} + \overline{q}_{source}(\overline{P})\right) \tag{37}
\end{aligned}
$$

The overall mass balance equations do not depend on the other conservation balance equations so the equation above clearly forms a *cascade-connected hierarchy*

$$
\begin{aligned}
\frac{dz}{dt} &= g(z) \\
\frac{dx}{dt} &= f(x, z)
\end{aligned}
\tag{38}
$$

with $z = \overline{M}$ and $x = \overline{P}$. ∎

17

4.3. Stability analysis of the hierarchical system equations

In this sub-section, the stability of the cascade system (36)-(37) will be studied using the properties of stable Metzler matrices and the theory of linear time-varying systems.

4.3.1. The source-free case

Let us first consider the case when no source term is present, i.e. $\overline{q}_{source}(\overline{P}) = 0$ in (37). This corresponds to the case where there are no chemical reactions in the system. It is clear from (36)-(37) and (38) that $(x, z) = (0, 0)$ is an equilibrium point of the source-free system. For examining the stability of this equilibrium point, we will use the following relevant results from [28].

Theorem 1 (Corollary 10.3.2 in [28]). *Consider the system* (38). *Suppose the equilibrium $x = 0$ of $\dot{x} = f(x, 0)$ is locally asymptotically stable and the equilibrium $z = 0$ of $\dot{z} = g(z)$ is locally asymptotically stable. Then, the equilibrium $(x, z) = (0, 0)$ of* (38) *is locally asymptotically stable.*

Theorem 2 (Corollary 10.3.3 in [28]). *Consider the system* (38). *Suppose the equilibrium $x = 0$ of $\dot{x} = f(x, 0)$ is globally asymptotically stable and the equilibrium $z = 0$ of $\dot{z} = g(z)$ is globally asymptotically stable. Suppose the integral curves of the composite system are defined for all $t \geq 0$ and bounded. Then, the equilibrium $(x, z) = (0, 0)$ of* (38) *is globally asymptotically stable.*

It was shown previously that $C_{conv}\mathcal{K}$ is a Hurwitz matrix, therefore (36) is a globally asymptotically stable linear time-invariant system. For $M = M^*$ and zero source term, (37) can be written as

$$\dot{\overline{P}} = Q^{-1}(M^*)(A_1 + A_2)\overline{P} \tag{39}$$

where

$$A_1 = \mathcal{N}(M^*) \cdot \theta - \gamma \mathcal{V}_{IN}^* \cdot \theta \tag{40}$$
$$A_2 = \mathcal{L} - (1 - \gamma)\mathcal{V}_{IN}^* \cdot \theta \tag{41}$$

with $0 < \gamma < 1$.

We will use the following additional notions. A quadratic matrix $A \in \mathbb{R}^{n \times n}$ is called *diagonally stable* if there exists a *positive definite diagonal* solution R for the corresponding Lyapunov equation, i.e. $A^T R + RA$ is

negative definite for a positive definite diagonal R matrix. A matrix $A \in \mathbb{R}^{n \times n}$ is called *D-stable* if the product DA is Hurwitz stable for any $n \times n$ *positive definite diagonal* matrix D. The following properties of the above mentioned matrices will be used.

(P1) Hurwitz stable Metzler matrices are diagonally stable [39].

(P2) Diagonally stable matrices are D-stable [40].

(P3) Let $H_1, H_2 \in \mathbb{R}^{n \times n}$ be Metzler and Hurwitz. Then $H_1 + \delta H_2$ is Hurwitz for all $\delta > 0$ if and only if $H_1 + \delta H_2$ is non-singular for all $\delta > 0$ [41].

Now we are ready to state the results on the local asymptotic stability of the source-free case.

Theorem 3. *Consider a hierarchically decomposed state-space model of a process system with no source term that obeys assumptions $\mathcal{A}_1$-$\mathcal{A}_4$. Further assume that there exists $0 < \gamma < 1$ such that A_1 and A_2 in (40)-(41) are of full rank, and $A_1 + A_2$ is of full rank, too. Then, the equilibrium point $\overline{M} = 0$, $\overline{P} = 0$ of the system (37)-(36) with $\overline{q}_{source}(\overline{P}) = 0$ is locally asymptotically stable.*

Proof. $\mathcal{N}^T(M^*)$ is compartmental matrix with zero column sums, therefore, $(\mathcal{N}(M^*) - \gamma \mathcal{V}_{IN}^*)^T$ is a compartmental matrix, too, that is of full rank. Consequently, $\mathcal{N}(M^*) - \gamma \mathcal{V}_{IN}^*$ is a Hurwitz Metzler matrix (see property (C1) in sub-section 2.1) that is D-stable by (P1) and (P2) (and it's transpose is D-stable, too). Therefore, A_1 is also a Hurwitz Metzler matrix. A similar argument applies to A_2: $\mathcal{L}$ is both row and column conservation compartmental matrix and therefore A_2 is a Hurwitz-stable Metzler matrix, since it is of full rank. Using (P3), we can conclude that $A_1 + A_2$ is a Hurwitz Metzler matrix if $A_1 + A_2$ is of full rank. In this case, $A_1 + A_2$ is D-stable by (P2) and thus $Q^{-1}(M^*)(A_1 + A_2)$ in (39) is Hurwitz for any elementwise positive M^*. $\blacksquare$

Remark 1. *It is important to note that the structure of the input convection matrix $\mathcal{V}_{IN}^*$ plays a crucial role in showing the asymptotic stability of a hierachically decomposed process system. Earlier in proving the asymptotic stability of the mass convection subsystem we saw, that the output convective flows to the environment had to be chosen appropriately (see subsection 2.2), while the placing of the inlet mass flows to the system affect the asymptotic stability of the driving force variable subsystem.*

19

For examining global asymptotic stability of (39) with (40)-(41) in the source-free case, we will treat (41) as a linear time-varying system, where the time-dependence is present through the change of M. Let us define

$$A_1'(M(t)) = \mathcal{N}(M(t)) \cdot \theta - \gamma \mathcal{V}_{IN}^* \cdot \theta \qquad (42)$$

Then,

$$\dot{\overline{P}} = A(t)\overline{P} \qquad (43)$$

where

$$A(t) = Q^{-1}(M(t)) \left(A_1'(M(t)) + A_2 \right). \qquad (44)$$

Repeating the reasoning for Theorem 3, it is easy to see that $A(t)$ is a Hurwitz matrix for all $t \geq 0$ if $A_1'(M(t))$, A_2 and $(A_1'(M(t)) + A_2)$ are of full rank for $t \geq 0$. However, it is known that the Hurwitz property of $A(t)$ for any $t \geq 0$ does not generally guarantee the exponential stability of the dynamics (39). But if the change of M is 'sufficiently slow', then stability follows as the following theorem says.

Theorem 4 (Theorem 8.7 in [42]). *Suppose for the linear state equation (43) with $A(t)$ continuously differentiable there exist finite positive constants α, μ such that, for all t, $\|A(t)\| \leq \alpha$ and every pointwise eigenvalue of $A(t)$ satisfies $Re[\lambda(t)] \leq -\mu$. Then there exists a positive constant β such that if the time-derivative of $A(t)$ satisfies $\|\dot{A}(t)\| \leq \beta$ for all t, the state equation (39) is uniformly exponentially stable.*

We remark that the proof of Theorem 4 shows how to compute an appropriate β from the system model.

Corollary 1. *Consider a hierarchically decomposed state-space model (36)-(37) of a process system with no source term that obeys assumptions $\mathcal{A}_1$-$\mathcal{A}_4$. Assume that there exists $0 < \gamma < 1$ such that $A_1'(M(t))$, A_2 and $(A_1'(M(t)) + A_2)$ are of full rank for $t \geq 0$. Then, the controller gain $\mathcal{K}$ in (11) can always be chosen such that the zero equilibrium of (36)-(37) is globally asymptotically stable.*

Proof. Clearly, by the global asymptotic stability of the mass subsystem (40), $\|A(t)\|$ will be bounded for all t. Moreover, $\|\dot{A}(t)\|$ can be set arbitrarily small using the control gain $\mathcal{K}$ in (11), since it is known that $\|C_{conv}\mathcal{K}\| \leq \|C_{conv}\| \cdot \|\mathcal{K}\|$, and for any eigenvalue λ of $C_{conv}\mathcal{K}$ it is true that $|\lambda| \leq \|C_{conv}\mathcal{K}\|$. Therefore, the boundedness of the integral curves of (39) can be assured by proper mass control applying Theorem 4, and finally, global asymptotic stability of the source-free dynamics can be assured by Theorem 2.

4.3.2. Stabilizing linear sources

Now we consider a special class of source terms that do not destabilize the network when they are present. In process systems, chemical reactions are the most characteristic and common source terms, therefore these will be considered here. The analysis of the general case of nonlinear chemical reactions as sources, however, is a challenging task that requires individual analysis. This is seen in [30] where a feedforward output-feedback controller is designed for a simple CSTR with exothermic isotonic kinetics. Therefore, we restrict our study to a simple case here.

In order to find the simplest case when the sources do not destabilize the system, we consider *isotherm linear chemical reactions with mass action law* as sources that have a positive equilibrium point. When only such reactions are present, then the vector of driving force variables consists of only the component concentrations, and the source vector $q_{source}^{(j)}$ in region j depends only on the driving force variables $P^{(j)}$ of the same region in a linear way

$$q_{source}^{(j)} = \overline{\mathcal{A}}_k P^{(j)} \tag{45}$$

where $\overline{\mathcal{A}}_k$ is obtained from the Kirchhoff (or Laplace) matrix of the reaction graph (usually denoted by A_k) by removing its k-th row and column where k is the number of an arbitrary reference chemical complex (see [43]). If all graph components of the reaction system are strong components (in other words, the reaction network is *weakly reversible*), then it is easy to prove that $\overline{\mathcal{A}}_k$ is a Hurwitz compartmental matrix.

Definition 3. *A source term $\overline{q}_{source}$ is called stabilizing linear, if*

(i) *it has a block structure, i.e. $\overline{q}_{source}^{(j)}(P^{(j)})$,*

(ii) *$\overline{q}_{source,k}^{(j)}$ depends linearly on $P_k^{(j)}$,*

(iii) the coefficient matrix $\overline{\mathcal{A}}_k$ is a Hurwitz-stable Metzler matrix.

Corollary 2. *Assume that a process system obeys the conditions in Corollary 1 with a stabilizing linear source $\overline{\mathcal{A}}_k$ such that $A_1'(M(t)) + A_2 + \overline{\mathcal{A}}_k$ is of full rank. Then, the controller gain $\mathcal{K}$ in (11) can always be selected such that the zero equilibrium of (36)-(37) is globally asymptotically stable.*

Proof. The result directly follows from the proof of Theorem 3 if one augments the matrices A_1 and A_2 with the third term $\overline{\mathcal{A}}_k$ such that the coefficient matrix of Eq. (39) becomes $A_1 + A_2 + \overline{\mathcal{A}}_k$. ∎

Note that a similar result has recently been published for lumped process systems composed of incompressible fluid phases [44] and having an equilibrium point using dissipativity analysis. Under these conditions - that form a special case of our analysis - it has been shown that the system is asymptotically stable if it has only dissipative production (source) terms.

4.4. A simple example without source term

Consider a simple process system consisting of two regions identified by the upper indexes (h) and (c) as it is depicted in Fig. 2. The system can be regarded as a simple perfectly stirred but unusual heat exchanger where we feed back the hot side at the inlet of the cold side and consider controlled mass holdups. The figure shows that we have both convection and transfer joining the two regions but there is *no source term*.

The *centered mass balances* for the system are in the form:

$$\frac{d\overline{m^{(h)}}}{dt} = \overline{v}^{(h,in)} - \kappa^{(h)}\overline{m^{(h)}} \tag{46}$$

$$\frac{d\overline{m^{(c)}}}{dt} = \kappa^{(h)}\overline{m^{(h)}} - \kappa^{(c)}\overline{m^{(c)}} \tag{47}$$

The above equations give rise to Eq. (33) with

$$\overline{M} = \begin{bmatrix} \overline{m^{(h)}} \\ \overline{m^{(c)}} \end{bmatrix} \quad , \quad \overline{V}_{IN} = \begin{bmatrix} \overline{v^{(h,in)}} \\ 0 \end{bmatrix}$$

$$C_{conv} = \begin{bmatrix} -1 & 0 \\ 1 & -1 \end{bmatrix} \quad , \quad \mathcal{K} = \begin{bmatrix} -\kappa^{(h)} & 0 \\ 0 & -\kappa^{(c)} \end{bmatrix}$$
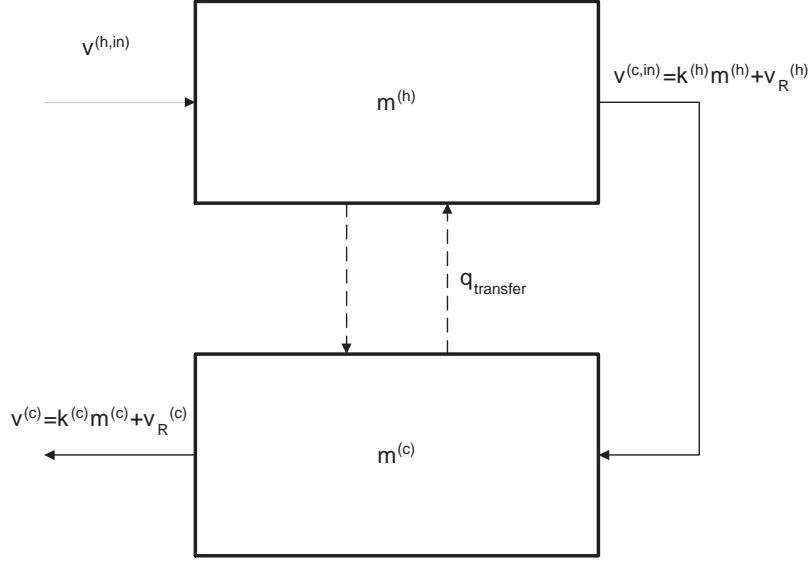
Figure 2: A simple process system

The *conservation balances for energy* are considered in their intensive variable form as

$$c_P^{(h)} m^{(h)} \frac{dT^{(h)}}{dt} = v^{(h,in)} \left(c_P^{(h,in)} T^{(h,in)} - c_P^{(h)} T^{(h)} \right) + K_T \left(T^{(c)} - T^{(h)} \right) \tag{48}$$

$$c_P^{(c)} m^{(c)} \frac{dT^{(c)}}{dt} = \left(\kappa^{(h)} m^{(h)} + v_{ref}^{(h)} \right) \left(c_P^{(h)} T^{(h)} - c_P^{(c)} T^{(c)} \right) + K_T \left(T^{(h)} - T^{(c)} \right) \tag{49}$$

This implies the following particular form of the additional matrices in the model:

$$Q = \begin{bmatrix} c_P^{(h)} m^{(h)} & 0 \\ 0 & c_P^{(c)} m^{(c)} \end{bmatrix} \quad , \quad \theta = \begin{bmatrix} c_P^{(h)} & 0 \\ 0 & c_P^{(c)} \end{bmatrix} \quad , \quad \mathcal{L} = \begin{bmatrix} -K_T & K_T \\ K_T & -K_T \end{bmatrix}$$

Moreover, we now have only two energy balances and $K = 1$. Thus the transfer term in the model is indeed

$$q_{transfer} = \mathcal{L}P = \begin{bmatrix} -K_T T^{(h)} + K_T T^{(c)} \\ K_T T^{(h)} - K_T T^{(c)} \end{bmatrix}$$

The overall convection matrix $\mathcal{N}$ is simple in this case, because

$$N^{(h,c)} = v_{out}^{(h)} = \kappa^{(h)} m^{(h)} \quad , \quad N^{(c,h)} = 0 \quad , \quad U^{(h,c)} = \begin{bmatrix} 0 & 0 \\ 1 & -1 \end{bmatrix}$$

23

and then

$$\mathcal{N} = \begin{bmatrix} 0 & 0 \\ v_{out}^{(h)} & -v_{out}^{(h)} \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ \kappa^{(h)} m^{(h)} & -\kappa^{(h)} m^{(h)} \end{bmatrix}$$

Furthermore, we can easily construct the variables characterizing the inlet of the system:

$$\theta_{IN} = \begin{bmatrix} c_P^{(h,in)} & 0 \\ 0 & 0 \end{bmatrix} \quad , \quad P_{IN} = \begin{bmatrix} T^{(h,in)} \\ 0 \end{bmatrix} \quad , \quad \mathcal{V}_{IN} = \begin{bmatrix} v^{(h,in)} & 0 \\ 0 & 0 \end{bmatrix}$$

If we finally take into account that we do not have any source term, i.e. $q_{source(P)} = 0$, then our energy balance equations (46) and (47) can be written exactly in the form of Eq. (34).

It is easy to see that the matrix $(\mathcal{N}(M) - \mathcal{V}_{IN}^*)\theta + \mathcal{L}$ is generally of full rank here. Corollary 1 then implies that this simple process system is globally uniformly exponentially stable provided that the derivative of M is appropriately bounded at any time instant.

It should be emphasized that only the mass is controlled in the system that implies the stability of both the mass and the energy subsystem in this case. Therefore, we could achieve total inventory control by controlling only the mass inventories, i.e. by less control loops than the usual inventory control [17].

5. Distributed controller structure driven by the model hierarchy

In this section we show that the hierarchically decomposed state-space model enables us to design a simple yet powerful distributed controller structure, with two layers.

A simple case study is used to illustrate how one can design a hierarchically decomposed distributed controller using the above principles.

5.1. The two control layers

Overall mass control layer. Driven by the hierarchical structure of dynamic process model, the local controllers that keep constant mass holdup in each of the balance volumes form the lower, mass control layer. These local controllers operate independently of each other and ensure the stability of the energy and component mass subsystems in their intensive variable form as long as their source terms fulfill the condition of Corollaries 1 or 2.

Note that the simplest proportional controller manipulating the outlet mass flow rate was assumed in this paper to regulate the mass in a balance volume, but more sophisticated controller types can also be used.

24

Selective stabilizing and coordinating layer. These local controllers are dedicated to stabilize or regulate intensive variables, such as temperature or concentrations in a balance volume if the corresponding conservation balance equation has a non-stabilizing source term. The manipulable input variables that are most suitable for this purpose are the corresponding intensive variables at the inlet of the balance volume, such as the inlet temperature(s) for the temperature as intensive variable, and the inlet concentrations for the corresponding concentration variables, respectively.

If the conservation balance equations in a balance volume have a well-identifiable non-stabilizing part (i.e. the source term of a region that does not fulfill the properties of a stabilizing source in Definition 3), such as an exothermic chemical reaction, then it is enough to control only the affected intensive variable. In this case an input-output linearization-based nonlinear controller [45] can be a reasonable option (provided that the nonlinear model is accurate enough), because - assuming the corresponding inlet intensive variable as the input - the relative degree of this input-output pair is one. An example of such a controller choice is given in the following section.

5.2. A simple chemical reactor example

The chemical reactor example in [20] has been chosen here that allows us to compare our approach to the one based on inventory control and thermodynamics. A simple process system of a jacketed chemical reactor is considered that consists of two regions identified by the upper indexes (r) and (j). An exothermic irreversible first order $A \to B$ exothermic chemical reaction is taking place in the reactor with the reaction rate $\rho = k_R exp(\frac{E}{RT^{(r)}})c_A^{(r)}$ and reaction enthalpy H. The flowsheet of the system and the connections between the two regions are shown in Fig. 3.

Model equations. The *centered mass balances* for the system are in the form:

$$\frac{d\overline{m^{(r)}}}{dt} = \overline{v^{(r,in)}} - k^{(r)}\overline{m^{(r)}} \tag{50}$$

$$\frac{d\overline{m^{(j)}}}{dt} = \overline{v^{(j,in)}} - k^{(j)}\overline{m^{(j)}} \tag{51}$$

The above equations correspond to Eq. (33) with

$$\overline{M} = \left[\begin{array}{c} \overline{m^{(r)}} \\ \hline \overline{m^{(j)}} \end{array} \right] \quad , \quad \overline{V_{IN}} = \left[\begin{array}{c} \overline{v^{(r,in)}} \\ \hline \overline{v^{(j,in)}} \end{array} \right]$$
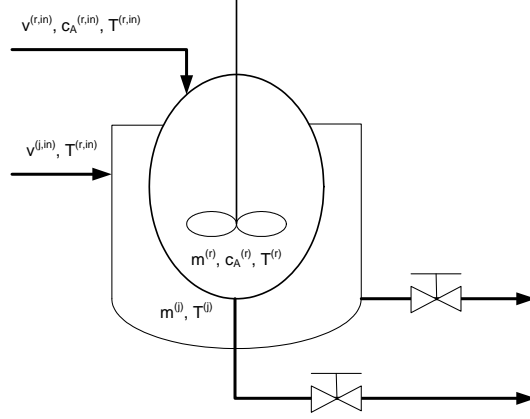
25

Figure 3: A simple process system

$$C_{conv} = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \quad , \quad \mathcal{K} = \begin{bmatrix} -k^{(r)} & 0 \\ 0 & -k^{(j)} \end{bmatrix}$$

The intensive form of the component mass balance for component A and for the two energy balances are

$$m^{(r)}\frac{dc_A^{(r)}}{dt} = v^{(r,in)}\left(c_A^{(r,in)} - c_A^{(r)}\right) - k_R \exp(\frac{E}{RT^{(r)}})c_A^{(r)}m^{(r)} \tag{52}$$

$$c_P^{(r)}m^{(r)}\frac{dT^{(r)}}{dt} = v^{(r,in)}\left(c_P^{(r,in)}T^{(r,in)} - c_P^{(r)}T^{(r)}\right) + K_T\left(T^{(j)} - T^{(r)}\right) +$$

$$+ Hk_R \exp(\frac{E}{RT^{(r)}})c_A^{(r)}m^{(r)} \tag{53}$$

$$c_P^{(j)}m^{(j)}\frac{dT^{(j)}}{dt} = v^{(j,in)}\left(c_P^{(j,in)}T^{(j,in)} - c_P^{(j)}T^{(j)}\right) + K_T\left(T^{(r)} - T^{(j)}\right) \tag{54}$$

The vector of intensive variables in the regions and in the inlet are

$$P = [\ c_A^{(r)}\ ,\ T^{(r)}\ ,\ T^{(j)}]^T \quad , \quad P_{IN} = [\ c_A^{(r,in)}\ ,\ T^{(r,in)}\ ,\ T^{(j,in)}]^T \tag{55}$$

Assuming the same coefficient matrix for the inlet and the regions, i.e. $\theta_{IN} = \theta$, the following matrices and vectors in the compact model equation (32) are obtained

$$Q = \begin{bmatrix} m^{(r)} & 0 & 0 \\ 0 & c_P^{(r)}m^{(r)} & 0 \\ 0 & 0 & c_P^{(j)}m^{(j)} \end{bmatrix} \quad , \quad \theta = \begin{bmatrix} 1 & 0 & 0 \\ 0 & c_P^{(r)} & 0 \\ 0 & 0 & c_P^{(j)} \end{bmatrix}$$

26

$$
\mathcal{L} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & -K_T & K_T \\ 0 & K_T & -K_T \end{bmatrix} \quad , \quad \mathcal{N} = 0 \quad , \quad \mathcal{V}_{IN} = \begin{bmatrix} v^{(r,in)} & 0 & 0 \\ 0 & v^{(r,in)} & 0 \\ 0 & 0 & v^{(j,in)} \end{bmatrix}
$$

Note that the overall convection matrix is a zero matrix, because the two regions are not connected by convection, but only by energy transfer.

In this case we have a non-zero source term

$$
q_{source(P)} = [\; -k_R \exp(\frac{E}{RT^{(r)}})c_A^{(r)}m^{(r)} \; , \; Hk_R \exp(\frac{E}{RT^{(r)}})c_A^{(r)}m^{(r)} \; , \; 0 \;]^T \quad (56)
$$

with

$$
\mathrm{sign}(\frac{\partial q_{source(P)}}{\partial P}) = \begin{bmatrix} - & - & 0 \\ + & + & 0 \\ 0 & 0 & 0 \end{bmatrix}
$$

Model parameters. Based on the model parameters in ([20]), the model parameters and reference values collected in Table 1 were used for the controller design.

Steady states. The steady states under controlled mass holdups can be calculated by solving the nonlinear equations that is obtained from Eqs. (52-54) by setting their left hand sides equal to zero. Fig. 4 shows the phase plane $c_A^{(r)} - T^{(r)}$ where the red curve with star markers corresponds to the stationary balance for $c_A^{(r)}$, and the black one composed of '+' signs to $T^{(r)}$. The intersections of these curves are the steady states of the reactor model. Three steady states are present under the parameter set in Table 1 (two of them are visible in Fig. 4.), the middle unstable one at $c_A^{(r*)} = 0.7768 \; mol/kg$, $T^{(r*)} = 380.9906 \; K$ and $T^{(j*)} = 372.71876 \; K$ is chosen as the set-point for the stabilizing controller design.

Note that with the same parameters but the inventory controllers as the lower controller layer, three different set-points have been found in [20], where the middle unstable one at $c_A^{(r*)} = 0.5 \; mol/kg$, $T^{(r*)} = 400 \; K$ was used there as the set-point.

Potential input variables. The variables at the inlet of the reactor ($v^{(r,in)}$, $c_A^{(r,in)}$ and $T^{(r,in)}$) and that of the jacket ($v^{(j,in)}$ and $T^{(j,in)}$) are the potential input variables for the selective stabilizing controller layer.

Note that the stabilizing controller in [20] that is used to keep the unstable steady state of the reactor, used the jacket temperature $T^{(j)}$ as a manipulable variable, that can only be manipulated indirectly through either the jacket inlet flow rate $v^{(j,in)}$ or inlet temperature $T^{(j,in)}$.

Ident.	unit	Definition	value
$k^{(r)}$	$[s^{-1}]$	reactor controller gain	100
$k^{(r)}$	$[s^{-1}]$	jacket controller gain	100
k_{lin}	$[s^{-1}]$	linearizing controller gain	0.4
$c_P^{(*)}$	$[\frac{J}{kg \cdot K}]$	water specific heat ($* \in \{r,j\}$)	$4.187 \cdot 10^3$
$c_P^{(*,in)}$	$[\frac{J}{kg \cdot K}]$	inlet water specific heat ($* \in \{r,j\}$)	$4.187 \cdot 10^3$
k_R	$[s^{-1}]$	pre-exponential factor	e^{25}
$\frac{E}{R}$	$[s^{-1}]$	activation energy (normalized)	-10^4
$\frac{H}{c_P^{(r)}}$	$[-]$	reaction enthalpy (normalized)	400
$\frac{v^{(r,in)}}{m^{(r)}}$	$[s^{-1}]$	residence time in reactor	1
$\frac{v^{(j,in)}}{m^{(j)}}$	$[s^{-1}]$	residence time in jacket	0.1
$\frac{K_T}{c_P^{(r)} m^{(j)}}$	$[s^{-1}]$	heat transfer coefficient (normalized)	1
$\overline{m^{(r)}}$	$[kg]$	reactor overall mass (reference)	100
$\overline{m^{(j)}}$	$[kg]$	jacket overall mass (reference)	100
$v_{ref}^{(r,in)}$	$[\frac{kg}{s}]$	reactor inlet mass flow rate (reference)	100
$v_{ref}^{(j,in)}$	$[\frac{kg}{s}]$	jacket inlet mass flow rate (reference)	10
$c_A^{(r,in)}$	$[mol/kg]$	inlet component concentration (reactor)	1
$T^{(r,in)}$	$[K]$	inlet temperature (reactor)	300
$T^{(j,in)}$	$[K]$	inlet temperature (jacket)	290

Table 1: Model parameters

The mass control layer. Here we use two independent P-controllers that manipulate the outlet mass flow rates $v_{out}^{(r)}$ and $v_{out}^{(j)}$ to keep the masses $m^{(r)}$ and $m^{(j)}$, respectively, at their reference values. Their operation is already taken into account in the model equations (50) and (51).

The selective stabilizing controller. As the non-stabilizing terms in the conservation balances in intensive form (52)-(53) are related (while Eq. (54) is stable), an input-output nonlinear linearizing controller (see in [45]) was designed using $T^{(r,in)}$ as manipulable input variable, and $T^{(r)}$ as the output variable. The feedback law is given by

$$T^{(r,in)} = \frac{1}{b_{lin}} \left(-k_{lin}(T^{(r)} - T^{(r*)}) - f_{2,lin} \right), \qquad (57)$$
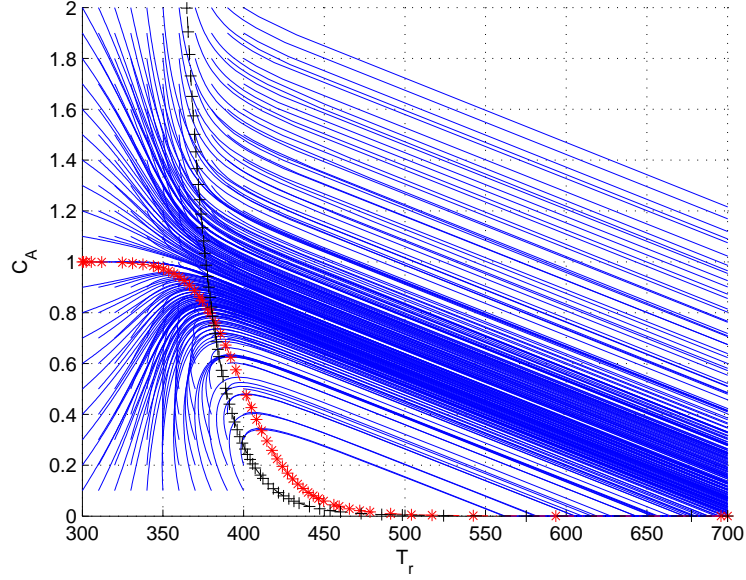
Figure 4: The phase plot of the reactor model with two of the the possible steady states

where

$$b_{lin} = \frac{v_{ref}^{(r,in)} c_P^{(r,in)}}{c_P^{(r)} \overline{m^{(r)}}} \tag{58}$$

$$f_{2,lin} = -\frac{v_{ref}^{(r,in)} T^{(r)}}{\overline{m^{(r)}}} + \frac{K_T(T^{(j)} - T^{(r)})}{c_P^{(r)} \overline{m^{(r)}}} + \frac{H k_R c_A^{(r)} \exp\left(\frac{E}{RT^{(r)}}\right)}{c_P^{(r)}}, \tag{59}$$

and the controller gain value $k_{lin} = 0.4$ was chosen. Note that any positive k_{lin} stabilizes the system, but its actual value determines the time-domain behavior of the controlled system.

The phase plane $c_A^{(r)} - T^{(r)}$ of the closed loop system depicted in Fig. 5 shows that the desired setpoint (marked with a red circle) is now a stable steady state point of the system. The time-domain operation of the controlled system can be seen in Fig. 6. The initial conditions used for the
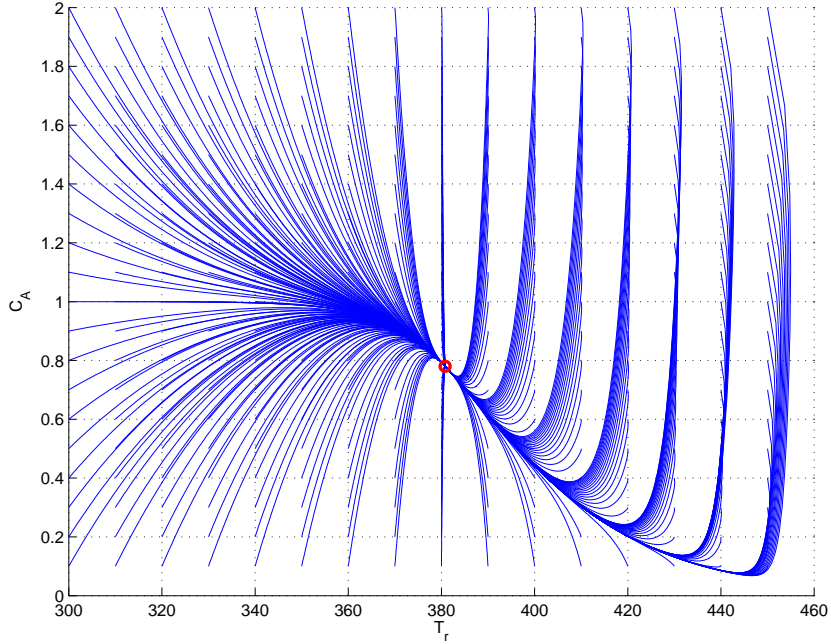
Figure 5: The phase plot of the controlled reactor model

simulation were the following:

$$m^{(r)}(0) = 105 \ kg, \quad m^{(r)}(0) = 95 \ kg, \quad c_A^{(r)}(0) = 0.8 \ \frac{mol}{kg} \qquad (60)$$

$$T^{(r)}(0) = 300 \ K, \quad T^{(j)}(0) = 290 \ K \qquad (61)$$

It is visible from the figure that $T^{(r)}$ indeed gives the desired linear response where the time constant is determined by the controller parameter k_{lin}. Moreover, the input temperature $T^{(r,in)}$ is within acceptable limits during the operation.

5.3. Discussion

It should be emphasized that the proposed model structure-driven hierarchical decentralized stabilizing controller structure is determined based on the model structure of process networks derived from first engineering principles. Therefore, this approach is highly similar to the one used for designing inventory control [17], as both approaches build on the principles of thermodynamics.
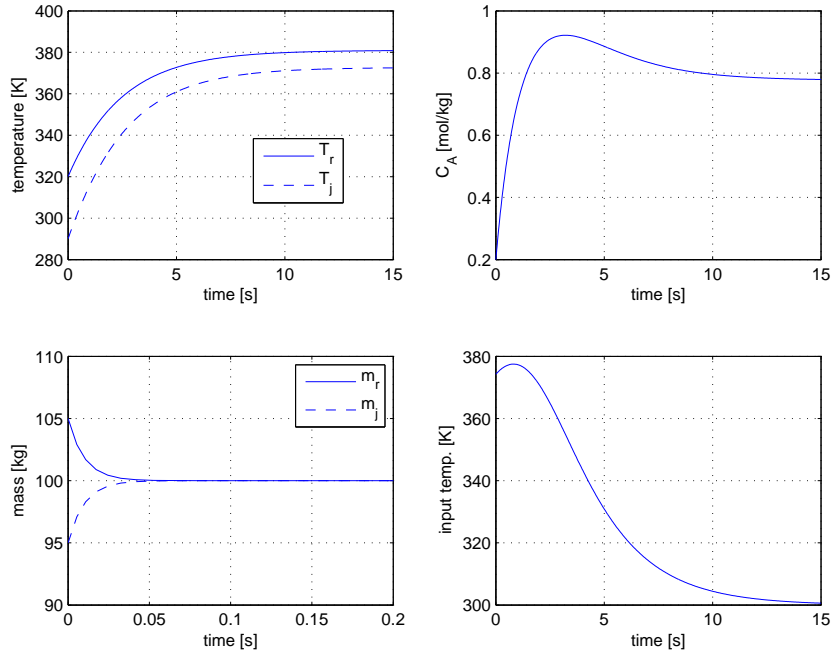
30

Figure 6: Time-domain behavior of the controlled reactor model

However, only the overall mass as inventory is controlled in each balance volume according to our approach, that implies the stability of all the mass, component masses and the energy subsystem in the stabilizig source term case. The selective stabilizing controllers acting on the other conservation balances (i.e. inventories) are needed only for some of the balances in their intensive form, that have non-stabilizing source terms. Therefore, we could achieve stabilizing control by less control loops and with generally less interactions among them, than the design that is based on inventory control [20].

Both the simple source-free example in subsection 4.4 and the simple jacketed chemical reactor example in subsection 5.2 illustrate the simplicity and the power of the proposed model structure-driven hierarchical decentralized stabilizing controller.

6. Conclusions

The asymptotic stability of process models consisting of lumped interconnected balance volumes and controlled mass holdups in each balance volumes

31

is investigated in this paper. The basic assumptions used on the constant physico-chemical properties and constant pressure ensure that the algebraic constitutive equations can all be substituted into the dynamic balance equations, that is, a purely ordinary differential equation model is resulted.

The dynamic behavior of the process model is investigated by using the results available for cascade-connected nonlinear systems and the properties of Metzler and Hurwitz matrices. It was shown that the system is globally asymptotically stable with no source term, and also with stabilizing linear source terms.

Based on the structure of the dynamic model, a hierarchically decomposed distributed controller structure is proposed, that consists of an overall mass control layer regulating the mass holdups at local set-points, and a selective stabilizing and coordinating layer for conservation balances with non-stabilizing source terms. This structure coincides well with the usual hierarchical process control system structure where local, distributed controllers take care of the level control and the coordinating controllers are used for optimizing the dynamics of the system.

The concepts and tools are illustrated on the example of a jacketed continuous stirred tank reactor, and compared to the physically-motivated inventory control scheme [20] developed for the same example.

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