Hamiltonian View on Process Systems

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The thermodynamic approach of analyzing structural stability of process plants was extended to construct the simple Hamiltonian model of lumped process systems. This type of model enables us to design a nonlinear PD feedback controller for passivation and loop shaping. This approach is applicable for lumped process systems where Kirchhoff convective transport takes place together with the transfer and sources of various types, and the manipulable input variables are the flow rates. Systems with constant mass holdup and uniform pressure in every balance volume satisfy these conditions. General results are shown by simple examples of practical importance: on a bilinear heat exchanger cell and on an isotherm CSTR with nonlinear reaction.

Introduction

Passivity theory plays a key role in analyzing stability of nonlinear systems as it is shown that passive systems are asymptotically stable under mild conditions (Hill and Moylan, 1980). Furthermore, passivity analysis has become one of the most important approaches in a nonlinear system and control theory and the relationship of passivity to other system properties, like finite gain has also been investigated (Hill and Moylan, 1980).

Based on this understanding, a passivity based approach has been developed for passivation of nonlinear mechanical systems using the specialities of the system model originating from Newton's law (Slotine, 1988; Nijmejer and van der Schaft, 1990). This approach uses the Hamiltonian description of mechanical systems known from theoretical mechanics and derives stabilizing nonlinear state feedback controllers.

The passivity based stability analysis of process systems was invented based on the theory of passive systems (Desoer and Vidyasagar, 1975) by Ydstie and Alonso (1997). A thermodynamic approach of analyzing structural stability of process systems was then developed (Hangos et al., 1999) which uses an entropy-based storage function together with the nonlinear state space model originating from conservation balances.

The final aim of passivity analysis is to achieve passivity by suitable feedback. Farschman et al. (1998) have developed nonlinear control strategies for process systems based on passivity.

The aim of this article is to construct the Hamiltonian description of process systems using the analogue of mechanical systems based on a thermodynamical approach. Such a description would allow the performance of passivity (stability) analysis of nonlinear process systems and construct nonlinear feedback controllers for passivation (stabilization) and loop-shaping.

The definition of simple Hamiltonian system models is provided. Then, nonlinear state equations of lumped process systems are derived and analyzed together with the system variables and the decomposition of the state equations driven by the mechanisms (convection, transfer, and sources). This leads to the simple Hamiltonian system model of process systems. The way of passivation and loop-shaping is described next based on previously introduced concepts. Two case studies, a nonlinear heat exchanger cell and an isothermal CSTR with an autocatalytic reaction, illustrate the use of the proposed approach. Finally, conclusions are drawn.

Simple Hamiltonian System Models

The notion of simple Hamiltonian systems originates from the classical theoretical mechanics. In contrast to the description based on forces and accelerations using Newton's law, this description uses the general energy function of mass point systems to describe their motions based on the generalized positions and momenta as well as on the momentum conservation.

Therefore, the definition of simple Hamiltonian systems is given in this section based on the mechanical analogue (Nijmejer and van der Schaft, 1990).

Mechanical analogue

The idea of the Hamiltonian description of systems originates from theoretical mechanics. A mass point system con-

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sisting of n mass points is described by its

- vector of generalized co-ordinates $q = [q_1, \ldots, q_n]^T$,
- vector of generalized momenta $p = [p_1, \ldots, p_n]^T$

where q can be regarded as the state and p as the co-state variable both needed to describe the state of the system uniquely. Because of the physical interpretation, a simple relationship holds between the state and co-state variables

$$p = M(q)\dot{q} \tag{1}$$

where $M(q)$ is a positive definite symmetric matrix. It is important to note that only the co-state variable p is a conserved extensive quantity.

The generalized energy of a mechanical system driven by the external forces u_i, $i = 1, \ldots, m$ is given by the Hamiltonian function

$$H(q, p, u) = H_0(q, p) - \sum_{i=1}^{m} q_i u_i$$

where the internal Hamiltonian $H_0(q, p)$ is in the form

$$H_0(q,p) = \frac{1}{2} p^T M^{-1}(q) p + V(q)$$

with $V(q)$ being the potential energy and $1/2 p^T M^{-1}(q) p$ being the kinetic energy.

Simple Hamiltonian systems

The prior mechanical concepts can be generalized to a wide class of systems enabling Hamiltonian description. In some of the cases the Hamiltonian function is in the special, *input affine form*

$$H(q, p, u) = H_0(q, p) - \sum_{j=1}^{m} H_j(q, p) u_j \tag{2}$$

where H_0 is the *internal Hamiltonian* and $H_j(q, p)$, $j = 1, \ldots, m$ are the *interaction or coupling Hamiltonians*, q is the state and p is the co-state variable.

Furthermore, we may associate *natural (or artificial) outputs* to the system as follows

$$y_j = -\frac{\partial H}{\partial u_j}(q,p,u) = H_j(q,p), \qquad j = 1, \ldots, m. \tag{3}$$

Notice that the natural (artificial) outputs have nothing to do with the real outputs of the system; rather, we define an artificial output variable to each of the input variables as a usually nonlinear function of the state and co-state variables.

With the above definitions, *the nonlinear state-space model of an affine Hamiltonian input-output system* is in the form

$$\dot{q}_i = \frac{\partial H_0}{\partial p_i}(q, p) - \sum_{j=1}^{m} \frac{\partial H_j}{\partial p_i}(q, p) u_j, \qquad i = 1, \ldots, n \tag{4}$$

$$\dot{p}_i = -\frac{\partial H_0}{\partial q_i}(q, p) + \sum_{j=1}^{m} \frac{\partial H_j}{\partial q_i}(q, p) u_j, \qquad i = 1, \ldots, n \tag{5}$$

$$y_j = H_j(q, p), \qquad j = 1, \ldots, m \tag{6}$$

Note, that the state variable of the system in system theoretical sense is the vector $x = [q, p]^T$ composed of the state and co-state variables respectively.

We may further specialize in the prior definition to obtain the notion of simple Hamiltonian systems.

Definition 1 (Simple Hamiltonian System). *A simple Hamiltonian system is an affine Hamiltonian system where the functions H_0, H_1, $\ldots$, H_m are of the following special form*

$$H_0(q, p) = \frac{1}{2} p^T G(q) p + V(q) \tag{7}$$

with $G(q)$ a positive definite symmetric $n \times n$ matrix for every q, and

$$H_j(q, p) = H_j(q), \qquad j = 1, \ldots, m \tag{8}$$

With the above requirements on the internal and coupling Hamiltonians, *the nonlinear state-space model of an affine Hamiltonian input-output system* specializes to the form

$$\dot{q}_i = \frac{\partial H_0}{\partial p_i}(q, p) = G(q) p, \qquad i = 1, \ldots, n \tag{9}$$

$$\dot{p}_i = -\frac{\partial H_0}{\partial q_i}(q, p) + \sum_{j=1}^{m} \frac{\partial H_j}{\partial q_i}(q)\, u_j \tag{10}$$

$$y_j = H_j(q), \qquad j = 1, \ldots, m \tag{11}$$

The following important result shows the role of the internal Hamiltonian (Van der Schaft, 2000).

Lemma 1. *The internal Hamiltonian $H_0(q, p)$ is a storage function of the simple Hamiltonian system with respect to the supply rate $\sum_j H_j(q) u_j$.*

Nonlinear State Equation of Process Systems

The starting point of the construction of a simple Hamiltonian model of lumped process systems is the general form of their state equation. As we shall see later, the differential conservation balance equations for the conserved extensive quantities will form Eq. 10 in the simple Hamiltonian model. This equation will be in a standard input-affine form of a nonlinear concentrated parameter system model

$$\dot{p} = f(q) + \sum_{i=1}^{m} g_i(q) u_i \qquad u \in \boldsymbol{R}^m, \quad f(0) = 0 \tag{12}$$

with u being the vector of input variables, p the vector of conserved extensive quantities, and q the vector of related thermodynamical driving force variables.

The aim of this section is to develop the state equation of a lumped process system in the input-affine form above and to investigate its decomposition driven by the principal mechanisms.

General assumptions

The state equations originate from the differential conservation balances of the conserved extensive quantities over perfectly stirred balance volumes called regions. A perfectly stirred region is the smallest elementary part of the process system over which conservation balances are constructed. The following *general assumptions* are made about the regions: (1) *Constant mass holdup is assumed in every region,* (2) *Constant pressure is assumed in the system, and* (3) *Constant physico-chemical properties are assumed.*

Note that the first two assumptions are related, and they ensure a simple form of the convection term in the conservation balance equations. The third assumption is of technical nature only and it simplifies notation. With this assumption, the algebraic constitutive equations can always be substituted into the conservation balances.

The basic equation which drives all the other conservation balances is the *overall mass balance* of the perfectly stirred region j

$$\frac{dm^{(j)}}{dt} = v_{\text{in}}^{(j)} - v_{\text{out}}^{(j)} = 0 \tag{13}$$

where $v_{\text{in}}^{(j)}$ and $v_{\text{out}}^{(j)}$ are the mass in- and out-flow rates, respectively. The above equation implies that there is no difference between the in- and out-flows of any of the r regions, that is

$$v_{\text{in}}^{(j)} = v_{\text{out}}^{(j)} = v^{(j)}$$

Under the above conditions, the general form of a differential balance equation of a conserved extensive quantity $\phi^{(j)}$ for a perfectly stirred region j takes the form (Hangos and Cameron, 1997, 2001)

$$\frac{d\phi^{(j)}}{dt} = C_{\phi}^{(j)} v^{(j)} \Phi_{\text{in}}^{(j)} - C_{\phi}^{(j)} v^{(j)} \Phi^{(j)} + \psi_{\phi,\text{transfer}}^{(j)} + \psi_{\phi,\text{source}}^{(j)} \tag{14}$$

where $C_{\phi}^{(j)}$ is a constant composed of physico-chemical properties and depends on the type of $\phi^{(j)}$ and $\Phi^{(j)}$; $\Phi_{\text{in}}^{(j)}$ are the related engineering driving force variables in the region and at the inlet, respectively. The general terms $\psi_{\phi,\text{transfer}}^{(j)}$ and $\psi_{\phi,\text{source}}^{(j)}$ account for the transfer and the sources respectively and will be discussed in detail later.

Observe that the overall mass balance (Eq. 13) is a special case of the general balance Eq. 14 with

$$\psi_{m,\text{transfer}}^{(j)} = 0, \qquad \psi_{m,\text{source}}^{(j)} = 0, \qquad \frac{dm^{(j)}}{dt} = 0,$$
$$\Phi^{(j)} = \Phi_{\text{in}}^{(j)} = C_{\phi}^{(j)} = 1 \tag{15}$$

It is important to note that the relation $\psi_{m,\text{transfer}}^{(j)} = 0$ is a consequence of the constant pressure assumption.

Note that the *conserved extensive quantity* $\phi^{(j)}$ of region j can be any variable from the following set

$$\phi^{(j)} \in \left\{ \left(m_k^{(j)},\ k = 1, \ldots, K \right),\ E^{(j)} \right\} \tag{16}$$

where $E^{(j)}$ is the energy, and $m_k^{(j)}$ is the component mass of the kth component with K being the number of components in the region.

In order to simplify notation, then same number of components is assumed to be present in each region. This can be formally achieved by assuming every component in the system to be present in each region and assuming identically zero concentration for those which are actually not present.

The related *engineering driving force variables* being intensive variables are taken from the set

$$\mathbf{\Phi}^{(j)} \in \left\{ \left(c_k^{(j)},\ k = 1, \ldots, K \right),\ T^{(j)} \right\} \tag{17}$$

where $T^{(j)}$ is the temperature and $c_k^{(j)}$ is the concentration of the kth component in the region.

Finally, the constant $C_{\phi}^{(j)}$ is chosen as

$$C_{\phi}^{(j)} = \begin{cases} 1 & \text{if} \quad \phi^{(j)} = m_k^{(j)} \\ c_P^{(j)} & \text{if} \quad \phi^{(j)} = E^{(j)} \end{cases} \tag{18}$$

where $c_P^{(j)}$ is the specific heat of the material in region j.

System variables

A possible *state vector* $\hat{p}$ for the nonlinear state-space model is the vector

$$\hat{p} = \left\{ \left[\left(m_k^{(j)},\ k = 1, \ldots, K \right),\ E^{(j)} \right],\quad j = 1, \ldots, \mathcal{C} \right\}^T,$$
$$|\hat{p}| = n = (K+1) * \mathcal{C} \tag{19}$$

with K being the number of components and $\mathcal{C}$ being the number of regions. Note that the linear relationship

$$m^{(j)} = \sum_{k=1}^{K} m_k^{(j)} \tag{20}$$

enables us to choose the complete set of component masses to be present in the state vector.

The *potential input variables* (including both manipulable input variables and disturbances) are also fixed by the state Eq. 14 being time-dependent variables (signals) appearing on the righthand side of the equations and not being state variables, that is

$$\hat{u} = \left[\left(v^{(j)},\ \mathbf{\Phi}_{\text{in}}^{(j)} v^{(j)} \right),\quad j = 1, \ldots, \mathcal{C} \right]^T \tag{21}$$

Note that we have formed a composite input vector $(\mathbf{\Phi}_{\text{in}}^{(j)} v^{(j)})$ from two signals to have the corresponding term in the balance Eq. 14 in a homogeneous form.

Moreover, any external signal present in the source relations $\psi_{\phi,\text{source}}^{(j)}$ should also be included in the set of potential input variables.

Normalized system variables

In order to transform the general form of conservation balance equations into canonical nonlinear state equations, the state and input variables need to be normalized using a suitable steady state as reference. For the reference input-state pair (p^*, u^*), the lefthand sides of the balance Eq. 14 are zero.

A normalized variable is the difference between its actual and reference value, that is

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

The normalized state variables and the normalized input variables are then as follows

$$p = \left[(p^{(j)});\, j = 1, \dots, \mathfrak{C} \right]^T,$$

$$p^{(j)} = \left[\left(\overline{m}_k^{(j)},\, k = 1, \dots, K \right), \overline{E}^{(j)} \right]^T \; |p| = n = (K+1) * \mathfrak{C} \quad (22)$$

$$u_E = \left[\left(\bar{v}^{(j)}, \overline{\mathbf{\Phi}_{\text{in}}^{(j)} v^{(j)}} \right), j = 1, \dots, \mathfrak{C} \right]^T \quad (23)$$

We shall restrict ourselves to the case when only the mass-flow rates form the set of input variables with the inlet engineering driving force variables being constant. Then, the set of normalized input variables specializes to

$$u = \left[(\bar{v}^{(j)}), \quad j = 1, \dots, \mathfrak{C} \right]^T \quad (24)$$

It is important to note here that we essentially manipulate the residence times $v^{(j)}/m^{(j)}$ of the regions by manipulating the flow rates, because the overall mass in the regions is assumed to be constant.

Convective terms in the conservation balance equations

Until, now, we have assumed that the regions are only coupled by the transfer terms, but now we consider convective flows joining regions. In order to describe the general case let us assume that the outlet flow of the region j is divided into parts and fed into other regions giving rise to the equation

$$\sum_{\ell=0}^{\mathfrak{C}} \alpha_\ell^{(j)} = 1, \qquad j = 0, \dots, \mathfrak{C} \quad (25)$$

where $\alpha_j^{(\ell)}$ is the ratio of the outlet flow $v^{(\ell)}$ of region ℓ flowing into region j and $0 \le \alpha_j^{(\ell)} \le 1$.

Then, the mass in-flow of region j is put together from the out-flows of all the other regions including the region itself and also the environment which is described as a pseudo-region with index 0

$$v^{(j)} = \sum_{\ell=1}^{\mathfrak{C}} \alpha_j^{(\ell)} v^{(\ell)}, \qquad j = 0, \dots, \mathfrak{C} \quad (26)$$

Because constant holdup is assumed in every region, the sum of convective in-flows is equal to the sum of the convective out-flows of the process system

$$v^{(0)} = \sum_{\ell=1}^{\mathfrak{C}} \alpha_0^{(\ell)} v^{(\ell)} \quad (27)$$

It is important to note that the composite system consisting of the original process system and its environment is closed with $\mathfrak{C} + 1$ *regions each of constant holdup.*

The above described convection is termed *Kirchhoff convection* network because of its analogous properties to the Kirchhoff laws for electrical circuits (Hangos et al., 1999).

Under these conditions, both the input and output convection terms in the general conservation balance Eqs. 14 ($v^{(j)}\mathbf{\Phi}_{\text{in}}^{(j)}$ and $v^{(j)}\mathbf{\Phi}^{(j)}$, respectively) contain the input variable $u_j = v^{(j)}$ in a linear way in case of the input convective term and in a bilinear way (with $u_j p_k$ type bilinearity) for the output convective term. It is important to observe that the presence of an output convective term makes the state equations nonlinear, as bilinearity is the most mild type of nonlinearity.

Transfer term in the conservation balance equations

In thermodynamics one associates *thermodynamical driving forces* as being intensive variables to each of the conserved extensive quantities

$$P^{(j)} = \left[-\frac{\mu_1^{(j)}}{T^{(j)}} \cdots - \frac{\mu_K^{(j)}}{T^{(j)}} \frac{1}{T^{(j)}} \right]^T \quad (28)$$

where $\mu_k^{(j)}$ is the chemical potential for the component k and $T^{(j)}$ is the temperature in region j.

The difference of these driving force variables induces transfer flows between regions in mutual contact. It is assumed that the transfer term of any of the regions can be decomposed into pair-wise transfer which are additive

$$\psi_{\phi,\text{transfer}}^{(j)} = \sum_{\ell=1}^{\mathfrak{C}} \psi_{\phi,\text{transfer}}^{(j,\ell)}$$

The celebrated *Onsager relationship* of the irreversible thermodynamics connects the transfer fluxes $\psi_{\phi,\text{transfer}}^{(j,\ell)}$ with the thermodynamical driving force variables in the form

$$\phi_{\phi,\text{transfer}}^{(j,\ell)} = L^{(j,\ell)} (P^{(j)} - P^{(\ell)}) \quad (29)$$

where the matrix $L^{(j,\ell)}$ is positive definite and symmetric (Glansdorf and Prigogine, 1971; Kreutzer, 1983).

If we further *choose the thermodynamical equilibrium point as reference value for the thermodynamical driving force vari-*

ables where

$$P^{*(j)} = P^{*(\ell)} \tag{30}$$

then we can develop the normalized version of the Onsager relation in the form of

$$\psi_{\phi,\text{transfer}}^{(j,\ell)} = L^{(j,\ell)}\left(\bar{P}^{(j)} - \bar{P}^{(\ell)}\right), \quad L^{(j,\ell)} > 0,$$

$$\left(L^{(j,\ell)}\right)^T = L^{(j,\ell)} \tag{31}$$

The normalized thermodynamical driving force variables can be collected to a vector

$$q = \left[\left(\left(-\frac{\overline{\mu_k^{(j)}}}{T^{(j)}},\ k = 1, \ldots, K\right), \frac{\bar{1}}{T^{(j)}}\right); \quad j = 1, \ldots, \mathcal{C}\right]^T,$$

$$|q| = n = (K+1) * \mathcal{C} \tag{32}$$

where $q = [\bar{P}^{(1)}, \ldots, \bar{P}^{(\mathcal{C})}]^T$. Then, the general transfer term of all of the regions can be written in the form of

$$\psi_{\phi,\text{transfer}} = \frac{1}{2} \sum_{j=1}^{\mathcal{C}} \sum_{\ell=1}^{\mathcal{C}} \left(I^{(j,\ell)} \otimes L^{(j,\ell)}\right) q \tag{33}$$

where $\otimes$ represents Kronecker product and $I^{(j,\ell)}$ is a $\mathcal{C} \times \mathcal{C}$ dimension matrix where

$$I_{jj}^{(j,\ell)} = I_{\ell\ell}^{(j,\ell)} = 1, \quad I_{j\ell}^{(j,\ell)} = I_{\ell j}^{(j,\ell)} = -1$$

and zero otherwise (Hangos et al., 1999).

It is important to observe that every matrix $(I^{(j,\ell)} \otimes L^{(j,\ell)})$ in the sum above is positive semi-definite and symmetric therefore their sum is also positive semi-definite and symmetric.

It is important to note that the reference point for the conserved extensive quantities should be a thermodynamical equilibrium point which is selected taking into account the desired set point value(s) for control. This implies that the reference point for the input variables should be chosen in such a way that the righthand side of the general conservation balances (Eq. 14) gives zero.

There are a number of consequences of the prior requirement on the selection of the reference points:

(1) If there is *no source term* in the general conservation balances, then the requirement specializes to

$$u^* = 0.$$

(2) If we have *no transfer term*, we can select u^* arbitrarily. It is therefore reasonable to choose q^* such that it is equal to its set point value for control and then choose u^* to satisfy the requirement.

(3) In the general case we find a thermodynamical equilibrium point close to the reference points and therefore choose u^*.

Source term in the conservation balances

The choice of input variables being the mass-flow rates implies that the source term in any of the lumped balance equations (Eq. 14) depends only on the engineering driving force variables, as it is formulated in the equation below

$$\psi_{\phi,\text{source}}^{(j)} = \Psi_{\phi}^{(j)}\left(T^{(j)}, c_1^{(j)}, \ldots, c_{K-1}^{(j)}\right) \tag{34}$$

where $\Psi_{\phi}^{(j)}$ is a given nonlinear function.

We also notice from Eq. 28 that the vector of the thermodynamic driving force variables $P^{(j)}$ in any of the regions is also the function of the engineering driving force variables. Therefore, the source term can also be written in the form

$$\psi_{\phi,\text{source}}^{(j)} = \hat{Q}_{\phi}^{(j)}\left(P^{(j)}\right) = Q_{\phi}^{(j)}\left(q^{(j)}\right) \tag{35}$$

Decomposition of the state equation driven by mechanisms

Now, we can assemble the various terms in the general conservation balance equations to form the general state space model of a process system with the normalized conserved extensive variables as state variables as in Eq. 22 and the normalized mass-flow rates in Eq. 24 as input variables. Under the above conditions on the form of the terms and on the state and input variables, one can decompose the lumped balance equations (Eq. 14) into structurally different additive parts with clear engineering meaning as follows

$$\dot{p} = A_{\text{transfer}} q + Q_{\phi}(q) + \sum_{i=1}^{\mathcal{C}} N_i p u_i + B_{\text{conv}} u \tag{36}$$

where the coefficient matrices A_{transfer}, B_{conv} and $(N_i,\ i = 1, \ldots, \mathcal{C})$ are constant matrices originating from the transfer and convective terms, respectively. It is important to remember that the coefficient matrix A_{transfer} is positive semi-definite and symmetric. The generally nonlinear source term $Q_{\phi}(q)$ is a vector-valued nonlinear function containing the partial source functions $Q_{\phi}^{(j)}$ in each region in its blocks.

Therefore, the decomposed state equation contains a linear state term for the transfer originating from Eq. 33, a general nonlinear state term for the sources as in Eq. 35, a bilinear input term for the output convection, and a linear input term for the input convection respectively.

This way, we obtained that the above state equation in Eq. 36 with the normalized state (Eq. 22) and input vectors (Eq. 24) is a special case of the *standard input-affine form of nonlinear concentrated parameter state-space equations.* It is important to emphasize that the state equation of process systems is always in an input-affine form of Eq. 12 because of the structure of the general state Eq. 14.

Supply Rate

In the theoretical framework of system theory, systems are described in terms of their input-output behavior. A system is then represented by an abstract operator S mapping the inputs $u(.)$ of the system into its outputs $y(.)$ where both the inputs and outputs are signals, that is, time-dependent functions from a given signal space

$$y = S[u]$$

In order to characterize the system the input and output signal spaces and the system operator should be given.

The state-space representation of a system is a way to represent its behavior by introducing an internal signal, the so-called state. The state-space representation of a concentrated parameter nonlinear system is *not unique*, and consists of two equations: the so-called state equation, like Eq. 12, and an output equation being a nonlinear algebraic equation in the form

$$y = h(p)$$

The notion of the supply rate is based on the input-output description of the system and used for its input-output stability analysis. It characterizes the net supply provided to the system by its environment in the form of

$$\int_{t_0}^{t} a(\tau)\,d\tau \tag{37}$$

where $a(.)$ is the supply rate.

There are two forms of supply rate that are used in analyzing stability of nonlinear systems:

- *Work by External Forces*. If the input variables describe the effect of external forces acting on the system and the output describes the position of the system in a space, then the supply rate is described as

$$a(\tau) = y(\tau)^T u(\tau) \tag{38}$$

- *Net Energy*. When both of the input and the output variables carry energy with them, then the net supply rate is the difference between the energy fed into the system and that emitted by it

$$a(\tau) = u^T(\tau) R_u u(\tau) - y^T(\tau) R_y y(\tau)$$

with suitably chosen positive definite input and output weighting matrices R_u and R_y.

It should be noted that passivity is defined for the "work by external forces" type supply rate, Eq. 38.

Supply rate of process systems

In order to find the natural supply rate of process systems the set of input and output variables should be defined for which passivity is defined (Nijmejer and van der Schaft, 1990). Therefore, we clearly have a different supply rate for a different input variable selection.

Simple Hamiltonian System Model of Process Systems

Here we construct the simple Hamiltonian model of process systems using the properties of their state equations.

State and co-state variables for process systems

Following the mechanical analogue, the following state and co-state variables are identified for the Hamiltonian description of process systems

$$p = \left[\overline{\phi}^{T(1)} \cdots \overline{\phi}^{T(\mathfrak{C})} \right]^T \tag{39}$$

$$q = \left[\overline{P}^{T(1)} \cdots \overline{P}^{T(\mathfrak{C})} \right]^T \tag{40}$$

Observe that the above variables are exactly the same as before in Eqs. 22 and 32, that is, the generalized momenta are the normalized conserved extensive variables and the generalized co-ordinates are the normalized thermodynamical driving forces.

In addition to the state-space model equations, there is a linear static (that is, time invariant) relationship between the state and co-state variables of a process system in the form

$$q = Qp \tag{41}$$

where Q is a negative definite symmetric block-diagonal matrix of the form

$$Q = \begin{bmatrix} Q^{(1)} & 0 & \cdots & 0 \\ 0 & Q^{(2)} & 0 \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & Q^{(\mathfrak{C})} \end{bmatrix} \tag{42}$$

The above equations are the consequences of the definitions of the state and co-state variables in Eqs. 39 and 40, and of the concavity of the entropy function (Alonso et al., 2000, Lemma A1 in the Appendix).

There is another relationship between the state and co-state variables of a process system which is an analogue of the mechanical relationship Eq. 1. This can be derived from the form of the Onsager relationship in Eq. 33, which gives an expression for the transfer rate of conserved extensive quantities as a function of the related thermodynamical driving forces

$$\dot{p}_{\text{transfer}} = \psi_{\phi,\text{transfer}} = \mathfrak{L} q, \quad \mathfrak{L} > 0, \ \mathfrak{L}^T = \mathfrak{L} \tag{43}$$

where the matrix $\mathfrak{L}$ is positive definite and symmetric in the following form

$$\mathfrak{L} = \frac{1}{2} \sum_{j=1}^{\mathfrak{C}} \sum_{\ell=1}^{\mathfrak{C}} \left(I^{(j,\ell)} \otimes L^{(j,\ell)} \right)$$

Observe, that the matrix $\mathfrak{L}$ in Eq. 43 is the same as the transfer matrix A_{transfer} in the decomposed state Eq. 36.

Input variables for the Hamiltonian description

In order to have a Hamiltonian description of process systems we have to assume that only the mass-flow rates form the set of input variables with the inlet engineering driving force variables being constant. Then, the set of normalized input variables is the same as in Eq. 24

$$u = \left[(\bar{v}^{(j)}),\ j = 1, \ldots, \mathcal{C} \right]^T.$$

Hamiltonian function of process systems

Following the mechanical analogue, the Hamiltonian function of process systems describes the direction of changes taking place in an open-loop system. The mechanical analogue and the general defining properties (Eqs. 7–11) of simple Hamiltonian systems will be used for the construction of the simple Hamiltonian model of process systems using the Onsager relationship (Eq. 43) and the conservation balances (Eq. 14) together with the relationships between the state and co-state variables (Eq. 41).

The Hamiltonian function is then constructed in two sequential steps as follows.

(1) *The Kinetic Term*. The kinetic term is constructed from the Onsager relationship (Eq. 43) by transforming it to the form of Eq. 9 using the relationship between the state and co-state variables (Eq. 41) to obtain

$$\dot{q} = (Q\,\mathcal{L}\,Q)p = \mathcal{G}p \qquad (44)$$

where $\mathcal{G}$ is a positive semi-definite symmetric matrix not depending on q. Symmetricity follows from the identity

$$(Q\,\mathcal{L}\,Q)^T = Q\,\mathcal{L}\,Q \quad \text{with} \quad Q^T = Q,\ \mathcal{L}^T = \mathcal{L}$$

and positive semi-definiteness is a simple consequence of the positive semi-definiteness of $\mathcal{L}$

$$x^T(Q\,\mathcal{L}\,Q)x = (Qx)^T\,\mathcal{L}\,(Qx) = y^T\mathcal{L}\,y \geq 0 \forall x$$

The kinetic term $T(p)$ in the Hamiltonian function will be constructed to satisfy Eq. 9, that is

$$T(p) = \frac{1}{2}p^T\mathcal{G}p \qquad (45)$$

(2) *The Potential Term and the Coupling Hamiltonians*. The potential term and the coupling Hamiltonians are derived by matching the terms in the special form of the defining Hamiltonian property (Eq. 10) taking into account that now $\mathcal{G}$ does not depend on q

$$\dot{p}_i = -\frac{\partial H_0}{\partial q_i}(q,p) + \sum_{j=1}^{m} \frac{\partial H_j}{\partial q_i}(q)u_j = -\frac{\partial V(q)}{\partial q_i} + \sum_{j=1}^{m} \frac{\partial H_j}{\partial q_i}(q)u_j \qquad (46)$$

and that of the decomposed general conservation balances Eq. 36 with the flow-rates as input variables

$$\dot{p} = \left[\, \mathcal{L}q + Q_\phi(q) \right] + \sum_{j=1}^{m} \left(N_j Q^{-1} q u_j + B_{j,\mathrm{conv}} u_j \right) = f(q) + \sum_{j=1}^{m} g_j(q) u_j \qquad (47)$$

where $B_{j,\mathrm{conv}}$ is the jth column of the input convection matrix B_{conv} in the decomposed state equation (Eq. 36).

From this correspondence, the potential energy term $V(q)$ and the coupling Hamiltonian $H_j(q)$ should satisfy

$$f_i(q) = -\frac{\partial V(q)}{\partial q_i}, \quad g_{ij}(q) = \frac{\partial H_j}{\partial q_i}(q) \qquad (48)$$

With the above ingredients, the Hamiltonian function of a process systems is written in the form

$$H(p,q,u) = T(p) + V(q) - \sum_{j=1}^{m} H_j(q)u_j \qquad (49)$$

satisfying all the required properties (Eqs. 9–11).

We may further specialize the form of the Hamiltonian function using the decomposition of the state function $f(q)$ in Eq. 47 according to the mechanisms (transfer and source) to get a decomposition of the potential term $V(q)$ to satisfy Eq. 48

$$V(q) = V_{\mathrm{transfer}}(q) + V_Q(q), \quad V_{\mathrm{transfer}}(q) = -\frac{1}{2}q^T\mathcal{L}q, \quad \frac{\partial V_Q(q)}{\partial q} = -Q_\phi(q) \qquad (50)$$

Substituting the above decomposed potential term to the Hamiltonian function (Eq. 49), above, we obtain

$$H(p,q,u) = V_Q(q) - \sum_{j=1}^{m} H_j(q)u_j \qquad (51)$$

It can be seen that *there is no kinetic term in the equation above because*

$$T(p) = -V_{\mathrm{transfer}}(q)$$

but the internal Hamiltonian does only contain the potential term originating from the sources.

This constructive derivation gives rise to the following theorem which summarizes the main result.

Theorem 1. *A process system with the input variables (Eq. 24) being the flow rates, the state and co-state variables (Eqs. 39 and 40) enable us to construct a simple Hamiltonian system model with the Hamiltonian function (Eq. 51) and with the underlying relationships (Eqs. 44, 47, 41, and 48).*

Remarks

There are important remarks in regard to the previous discussion.

- *Supply rate.* As already mentioned, the internal Hamiltonian function is a storage function of the system with respect to the supply rate $\Sigma_{j=1}^{m} H_j(q)u_j$. Recall that the artificial output variables have been defined to be equal to the coupling Hamiltonians, that is, $y_j = H_j(q)$. Therefore, the supply rate of the system can be written in the form of

$$a = y^T u$$

which is exactly in the form of Eq. 38.

- *Internal Hamiltonian.* It is important to note that the internal Hamiltonian is a storage function for process systems which gives the total entropy power (entropy produced in unit time). This can be checked by computing the units in the Hamiltonian function. It is very interesting that an early intuition of Slotine (1988) also suggests a Hamiltonian function being the entropy production for systems governed by the laws of thermodynamics. *Therefore, the storage function derived from the simple Hamiltonian description is entirely different from the entropy-based storage function proposed before* (Hangos et al., 1999). This is explained by the known fact that the storage function of a nonlinear system in *not unique*.
- *Time Derivative of the Hamiltonian Storage Function.* For stability analysis, the time derivative of the storage function is important which is in a special form in this case

$$\frac{dH_0(q,\,p)}{dt} = \sum_{i=1}^{n} \left(\frac{\partial H_0}{\partial p_i} \frac{dp_i}{dt} + \frac{\partial H_0}{\partial q_i} \frac{dq_i}{dt} \right) =$$

$$= \sum_{i=1}^{n} \left(\frac{\partial H_0}{\partial p_i} \frac{\partial H_0}{\partial q_i} - \frac{\partial H_0}{\partial q_i} \frac{\partial H_0}{\partial p_i} \right) = 0 \quad (52)$$

where the defining Eqs. 9 and 10 have been used for the derivation with $u = 0$. The above equality shows that the total entropy production is constant in time, that is, entropy is produced in the open process system. This is in good agreement with our engineering expectations.

Passivation and Loop-Shaping Based on the Hamiltonian Description

In order to stabilize simple Hamiltonian systems which are not open-loop stable because of not being passive, we should again recall that the internal Hamiltonian $H_0(q,\,p)$ is a storage function for the system with the supply rate $\Sigma_j H_j(q)u_j$. The construction of the simple Hamiltonian system models also ensures that in any equilibrium point $p = 0$. Moreover, the passivity in the neighborhood does only depend on the potential energy $V(q)$, because the kinetic energy term $T(p)$ in itself is always positive semi-definite with negative semi-definite time derivative.

Passivation and loop-shaping is then directed towards modifying the potential energy part $V(q)$ of the Hamiltonian description by a suitable state feedback in such a way that the modified potential energy $\overline{V}(q)$ is positive definite with its time derivative being negative definite.

The first result (Nijmejer and van der Schaft, 1990; Theorem 12.27) shows that a stable equilibrium point $(q_0,\,0)$ is not necessarily asymptotically stable.

Lemma 2. *Let $(q_0,\,0)$ be an equilibrium point of the simple Hamiltonian system given by Eqs. 7–8. Suppose that $V(q) - V(q_0)$ is a positive definite function on some neighborhood of q_0. Then, the system for $u = 0$ is stable but not asymptotically stable.*

We can improve the situation, that is, to make this stable equilibrium point asymptotically stable by introducing a derivative output feedback to every input-output pair as follows

$$u_i = -k_i^D \dot{y}_i = -k_i^D \frac{dH_i}{dt}, \quad i = 1, \ldots, m \qquad (53)$$

which physically means adding damping to the system with a positive damping factor k_i^D. Observe that here we use the time derivative of the artificial (natural) output to the system which is a nonlinear function of the co-state variables in the general case.

It can be shown that the above derivative feedback makes the time derivative of the closed-loop Hamiltonian negative definite with arbitrary positive gain k_i^D such that

$$\frac{dH_0(q,p)}{dt} = -\sum_{i\text{-}1}^{m} k_i^D (\dot{y})^2 < 0$$

Recall that the time derivative of the open-loop internal Hamiltonian is equal to zero, as shown by Eq. 52.

The main assumption in Lemma 2 was the positive definiteness of the difference $V(q) - V(q_0)$ near an equilibrium point q_0. If this assumption does not hold, then let us apply a linear proportional static output feedback

$$u_i = -k_i y_i + v_i, \quad i = 1, \ldots, m \qquad (54)$$

with v_i being the new controls to the simple Hamiltonian system Eqs. 7–8.

The resulting system is again a simple Hamiltonian system with the internal Hamiltonian

$$\overline{H}_0(q,p) = \frac{1}{2} p^T G(q) p + \overline{V}(q) \qquad (55)$$

where $\overline{V}(q)$ is the new potential energy

$$\overline{V}(q) = V(q) + \frac{1}{2} \sum_{i=1}^{m} k_i y_i^2 \qquad (56)$$

and with the state-space model

$$\dot{q}_i = \frac{\partial \overline{H}_0}{\partial p_i}(q,p), \quad i=1, \ldots, n$$

$$\dot{p}_i = -\frac{\partial \overline{H}_0}{\partial q_i}(q,p) + \sum_{j=1}^{m} \frac{\partial H_j}{\partial q_i}(q) v_j, \quad i=1, \ldots, n$$

$$y_j = H_j(q), \quad j=1, \ldots, m$$

Equation 56 shows that we have added a positive term to the "old" potential energy. *By choosing the feedback gains $k_i > 0$ sufficiently large, we may shape the potential energy in such a way that it becomes positive definite.*

The concrete form of the potential energy $V(q)$ together with Eq. 56 gives a guideline for tuning the nonlinear proportional controllers. *We should choose k_i, $i = 1, \ldots, m$ large enough to get a positive definite $\overline{V}(q)$ in the entire region of interest around the equilibrium set point q_0.* Observe that we have as many "independent" single-input single-output proportional controllers as the number of input variables, and their effect is summed up to make the potential energy positive definite. This whole set of controllers can be seen as a special version of nonlinear static state feedback with a diagonal gain matrix where the nonlinearity is present in the artificial output values $j_j = H_j(q)$, $j = 1, \ldots, m$.

Moreover, we can achieve passivity even by a single PD controller if we can realize a large enough gain k_{j^*} to make the modified potential energy $\overline{V}(q)$ positive definite.

It is important to note that *passivation is only needed when we have a source term making the system not passive.* In the case of a passive system, the proportional nonlinear state feedback controllers above will shape the dynamic response of the system similarly to the way pole-placement controllers act on the dynamics of a stable linear time-invariant system (Kailath, 1980).

Case Study: A Nonlinear Heat Exchanger Cell

Consider the simplest possible model of a heat exchanger consisting of only two perfectly stirred regions or lumps for the hot and cold sides, respectively. We shall call one of the lumps the hot ($j = h$) and the other one the cold ($j = c$) side. The lumps with their variables are depicted in Figure 1.

Conservation balances and system variables

The continuous-time state equations of the heat exchanger cell above will be derived from the following energy conservation balances

$$\frac{dE^{(c)}(t)}{dt} = v_c(t) c_P^{(c)} \left(T_{ci}(t) - T^{(c)}(t)\right) + UA\left(T^{(h)}(t) - T^{(c)}(t)\right) \quad (57)$$

$$\frac{dE^{(h)}(t)}{dt} = v_h(t) c_P^{(h)} \left(T_{hi}(t) - T^{(h)}(t)\right) + UA\left(T^{(c)}(t) - T^{(h)}(t)\right) \quad (58)$$

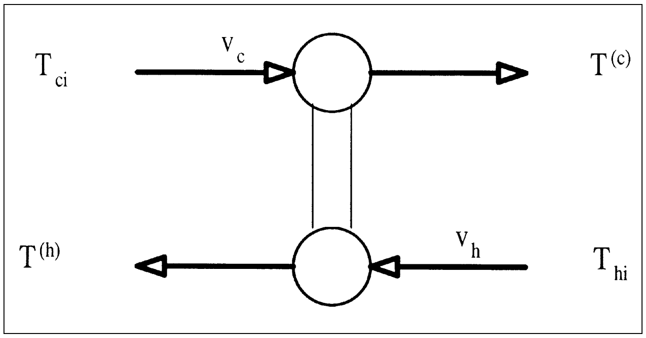

Figure 1. Heat exchanger cell and its variables.

where T_{ji} and $T^{(j)}$ are the inlet and outlet temperature and v_j is the mass flow rate of the two sides ($j = c, h$), respectively. Note that we now have two regions, that is, $\mathfrak{C} = 2$. Observe that these model equations contain an input and output convection and a transfer term expressed in engineering driving forces, but there is no source term.

The vector of conserved extensive quantities consists of the internal energies for the two regions

$$\phi = [E^{(h)}, E^{(c)}]^T, \quad n = 2 \quad (59)$$

Let us choose the volumetric flow rates v_c and v_h as input variables.

Extensive-intensive relationships

Let us choose a reference thermodynamical equilibrium state for the heat exchanger cell such that

$$T^{*(h)} = T^{*(c)} = T^{*}. \quad (60)$$

The energy-temperature relations are known from elementary thermodynamics

$$E^{(j)} = c_P^{(j)} m^{(j)} T^{(j)} + E_0, \quad \overline{E}^{(j)} = E^{(j)} - E^{*(j)} \quad (61)$$

where $m^{(j)}$ is the constant overall mass of region j. From Eq. 61, expanding $1/T^{(j)}$ into Taylor series we obtain

$$\overline{T}^{(j)} = -(T^*)^2 \overline{\frac{1}{T^{(j)}}}$$

$$\overline{\frac{1}{T^{(j)}}} = Q^{(j)} \overline{E}^{(j)}, \qquad Q^{(j)} = -\frac{1}{c_P^{(j)} m^{(j)} (T^*)^2} \quad (62)$$

with $Q^{(j)} < 0$ being a constant in this case. Therefore,

$$Q = \begin{bmatrix} -\frac{1}{c_P^{(h)} m^{(h)} (T^*)^2} & 0 \\ 0 & -\frac{1}{c_P^{(c)} m^{(c)} (T^*)^2} \end{bmatrix}.$$

Normalized system variables

With the reference equilibrium state (Eq. 60), we can easily define the normalized state and thermodynamical driving force variables as

$$q = \left[\frac{\overline{1}}{T^{(h)}}, \frac{\overline{1}}{T^{(c)}} \right]^T$$

$$p = \left[\overline{E^{(h)}}, \overline{E^{(c)}} \right]^T$$

From the conservation balance equations (Eqs. 57 and 58), it follows that now the reference point for the input variables is the zero vector; therefore

$$u = [v_h, v_c]^T.$$

Decomposed state equation in input affine form

With the defined normalized system variables, the conservation balance equations (Eqs. 57 and 58) can be written in the following canonical form

$$\frac{dp}{dt} = \mathfrak{A}_{\text{transfer}} q + B_{1c} u + \sum_{i=1}^{2} N_i u_i \tag{63}$$

with

$$\mathfrak{A}_{\text{transfer}} = (T^*)^2 \begin{bmatrix} UA & -UA \\ -UA & UA \end{bmatrix},$$

$$B_{1c} = \begin{bmatrix} c_P^{(h)} \overline{T}_{hi} & 0 \\ 0 & c_P^{(c)} \overline{T}_{ci} \end{bmatrix} \tag{64}$$

$$N_1(\overline{T}^{(h)}) = \begin{bmatrix} -c_P^{(h)} \overline{T}^{(h)} \\ 0 \end{bmatrix}, \quad N_2(\overline{T}^{(c)}) = \begin{bmatrix} 0 \\ -c_P^{(c)} \overline{T}^{(c)} \end{bmatrix}$$

where $\mathfrak{A}_{\text{transfer}}$ and B_{1c} are constant matrices and N_1 and N_2 are linear functions of the normalized engineering driving force variables. Observe that now the transfer function matrix $L^{(c,h)}$ is just a constant UA (an 1×1 matrix) and

$$I^{(c,h)} = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}.$$

Hamiltonian description of the heat exchanger cell

Let us now develop the Hamiltonian description of the nonlinear heat exchanger cell model. The internal Hamiltonian of the heat exchanger cell system is easily constructed from the special form of the Hamiltonian developed for process systems in Eq. 51 taking into account that there is no source term in the conservation balance equations, such as $V_Q(q) = 0$

$$H_0(q, p) = 0 \tag{65}$$

Now, we need to identify the coupling Hamiltonian $H_1(q)$ and $H_2(q)$ from the co-state Eq. 63 for the input variables

$$u = [v_h, v_c]^T$$

The coupling Hamiltonians can be reconstructed from the vector functions $g_1(q)$ and $g_2(q)$, respectively, which are the gradient vectors of the corresponding coupling Hamiltonians

$$\frac{\partial H_1}{\partial q} = g_1(q), \quad \frac{\partial H_2}{\partial q} = g_2(q)$$

Observe that the gradients are naturally given in terms of the engineering driving force variables Φ, but we need to transform them into the form depending on the co-state variables q. In the heat exchanger cell case we have

$$g_1(\overline{T}^{(h)}) = \begin{bmatrix} -c_P^{(h)} \overline{T}^{(h)} + c_P^{(h)} \overline{T}_{hi} \\ 0 \end{bmatrix} = \begin{bmatrix} c_P^{(h)} (T^*)^2 q_1 + c_P^{(h)} \overline{T}_{hi} \\ 0 \end{bmatrix} = g_1(q)$$

$$g_2(\overline{T}^{(h)}) = \begin{bmatrix} 0 \\ c_P^{(c)} \overline{T}^{(c)} + c_P^{(c)} \overline{T}_{ci} \end{bmatrix} = \begin{bmatrix} 0 \\ -c_P^{(c)} (T^*)^2 q_2 + c_P^{(c)} \overline{T}_{ci} \end{bmatrix} = g_2(q)$$

By partial integration, we get that

$$H_1(q) = \frac{1}{2} c_P^{(h)} (T^*)^2 q_1^2 + c_P^{(h)} \overline{T}_{hi} q_1 \tag{66}$$

$$H_2(q) = \frac{1}{2} c_P^{(c)} (T^*)^2 q_2^2 + c_P^{(c)} \overline{T}_{ci} q_2 \tag{67}$$

From the passivity analysis, we know that the system is inherently passive but it has a pole at the stability boundary, because there is no source term and $V_Q(q) = 0$. Therefore, we can perform stabilization by a derivative feedback and loop shaping by a static feedback using PD controllers.

Simple Unstable CSTR Example

Let us have an isotherm CSTR with fixed mass holdup m and constant physico-chemical properties. A second-order

$$2A + S \rightarrow T + 3A$$

autocatalytic reaction takes place in the reactor where the substrate S is present in a great excess. Assume that the inlet concentration of component A (c_{Ain}) is constant and the inlet mass-flow rate v is used as input variable. We develop the Hamiltonian description of the system around its steady-state point determined as the set point for passivation and loop shaping. This description is then used for a nonlinear proportional feedback controller to stabilize the system.

Conservation balance equation and system variables

The state equation is a single component mass conservation balance equation for component A in the form

$$\frac{dm_A}{dt} = \frac{d(m \cdot c_A)}{dt} = vc_{Ain} - vc_A + k \cdot m \cdot c_A^2 \qquad (68)$$

where k is the reaction rate constant. Note that we only have a single region, therefore, $\mathfrak{C} = 1$.

The given steady-state concentration c_A^* with a nominal mass-flow rate v^* satisfies

$$0 = v^*(c_{Ain} - c_A^*) + k \cdot m(c_A^*)^2$$

From this, we can determine v^* as

$$v^* = -\frac{k \cdot m(c_A^*)^2}{c_{Ain} - c_A^*}$$

which should be non-negative; therefore, $c_{Ain} \le c_A^*$ should hold. The given steady-state concentration c_A^* also determines the nominal value of the conserved extensive quantity m_A being the component mass in this case

$$m_A^* = m \cdot c_A^*$$

The engineering driving force variable to the component mass m_A is the concentration c_A and the thermodynamical driving force is

$$\bar{P} = -R'\bar{\mu}_A = -R''\overline{\ln c_A} \cong -R\bar{c}_A$$

with R being a constant under isotherm conditions and assuming ideal mixtures.

Hamiltonian description

It follows from the above that the normalized system variables for the Hamiltonian description of the simple unstable CSTR are as follows

$$p = \bar{m}_A = m_A - m_A^*, \quad q = -(c_A - c_A^*), \quad u = v - v^* \qquad (69)$$

Observe that the constant R has been omitted from the definition of the co-state variable q as compared to the thermodynamical driving force P above. From the variable definitions above, we see that the matrix Q specializes to

$$Q = -\frac{1}{m}$$

From the conservation balance (Eq. 68), it is seen that there is only a single region present in the system and there is no transfer term. Therefore, the transfer coefficient matrix $\mathcal{L} = 0$. This implies that now the reference point for the state and co-state variables can be chosen arbitrarily. However, the source term Q_ϕ is now present as a second-order term originating from the autocatalytic second-order reaction.

If we substitute the normalized variables (Eq. 69) to the conservation balance (Eq. 68), the following normalized state equation is obtained

$$\frac{dp}{dt} = \left(k \cdot m \cdot q^2 - (2k \cdot m \cdot c_A^* + v^*) \cdot q\right) + (\bar{c}_{Ain} + q)u \qquad (70)$$

From this equation, we can identify the elements of the Hamiltonian description to be

$$\frac{\partial V_Q}{\partial q}(q) = -\left(k \cdot m \cdot q^2 - (2k \cdot m \cdot c_A^* + v^*) \cdot q\right),$$

$$\frac{\partial H_1}{\partial q}(q) = (\bar{c}_{Ain} + q)$$

By partial integration, we get

$$V_Q(q) = -\frac{1}{3}k \cdot m \cdot q^3 + \frac{1}{2}(v^* + 2k \cdot m \cdot c_A^*) \cdot q^2 \qquad (71)$$

$$H_1(q) = \frac{1}{2}q^2 + \bar{c}_{Ain}q \qquad (72)$$

Passivity analysis of the unstable CSTR

The passivity analysis is performed using the internal Hamiltonian of the system

$$H_0(q,p) = V_Q(q) = -\frac{1}{3}k \cdot m \cdot q^3 + \frac{1}{2}(v^* + 2k \cdot m \cdot c_A^*) \cdot q^2.$$

We can see that this function is of no definite sign because of the presence of the second- and third-order terms of different constant coefficients. This means that the system fails to be passive in the general case.

Passivation and loop-shaping of the unstable CSTR

System Parameters and Open-Loop Response. Let us introduce the normalized concentration variables $\bar{c}_A = c_A - c_A^*$ and $\bar{c}_{Ain} = c_{Ain} - c_A^*$. The conservation balance (Eq. 68) then takes

Table 1. Parameter Values of the Simulated CSTR

m	1,800	kg
k	5×10^{-4}	m^3/kmol · s
c_{Ain}	0.4	kmol/m^3
c_A^*	2.3	kmol/m^3
v^*	2.5058	kg/s
k_c	10	—

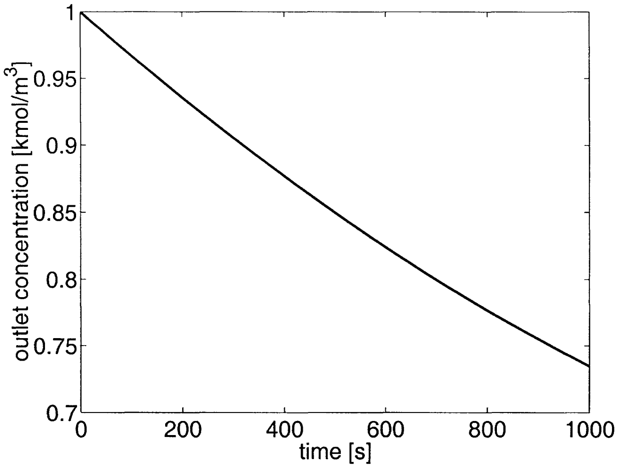

Figure 2. Open-loop simulation with $c_A(0) = 1$ kmol/m^3.

the form

$$\frac{d\bar{c}_A}{dt} = k\cdot\bar{c}_A^2 + \left(2k\cdot c_A^* - \frac{v^*}{m}\right)\cdot\bar{c}_A + \frac{\bar{c}_{Ain}-\bar{c}_A-c_A^*}{m}\cdot u \qquad (73)$$

The parameter values used in the simulations are shown in Table 1. There were two initial concentration values ($c_A(0)$) given for the simulations:

- 1 kmol/m^3 and
- 2.8 kmol/m^3

respectively.

It is easily seen from the data that c_A^* is an unstable equilibrium for the system, as illustrated in Figures 2 and 3.

Nonlinear Proportional Feedback Controller. Let us apply the following feedback controller

$$u = k_c y_1 + w = k_c\cdot\left[\frac{1}{2}\bar{c}_A^2 - (\bar{c}_{Ain}+c_A^*)\cdot\bar{c}_A\right] + w \qquad (74)$$

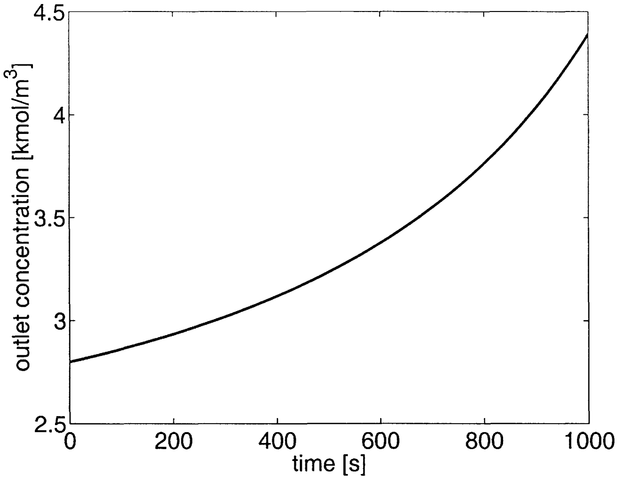

Figure 3. Open-loop simulation with $c_A(0) = 2.8$ kmol/m^3.

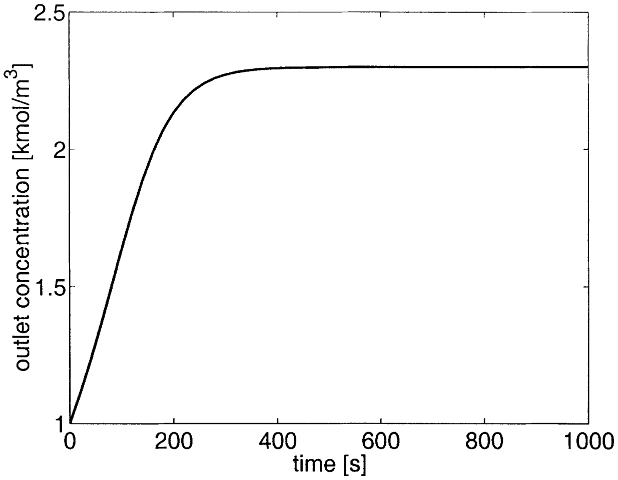

Figure 4. Closed-loop simulation with $c_A(0) = 1$ kmol/m^3.

where k_c is an appropriately chosen controller gain and w is the new reference signal. The new reference, w was set to 0 for the simulations. The chosen value of the controller gain is shown in Table 1.

The closed-loop simulation results in Figures 4 and 5 show that the proposed control method indeed stabilizes the equilibrium $c_A^* = 2.3$ kmol/m^3. Here again, the simulation was performed using two different initial conditions as above.

Stability Region. It is an important question for a nonlinear controller to determine its stability region as a function of the state variables with its parameter(s) fixed. For this very simple case, this problem can be solved analytically.

Let us consider the nonlinear proportional feedback controller above with its gain fixed at $k_c = 10$. In fact, it is easy to show that the resulting closed-loop system with the parameters described above is passive with respect to the supply rate $w\cdot y$ if

$$\bar{c}_A > -1.902 \text{ kmol/m}^3 \quad \text{and} \quad \bar{c}_A < 5.22 \text{ kmol/m}^3$$

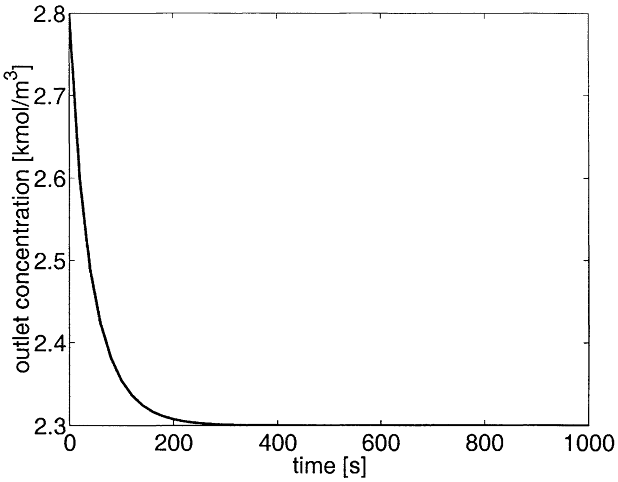

Figure 5. Closed-loop simulation with $c_A(0) = 2.8$ kmol/m^3.

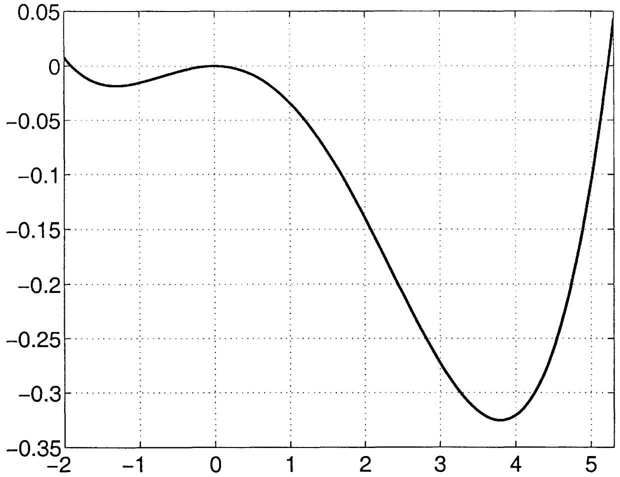

Figure 6. Time derivative of the storage function as a function of $\bar{c}_A$.

where $y = \bar{c}_A$.

In order to show this, let us take the simple storage function $V(\bar{c}_A) = 1/2\bar{c}_A^2$. It can be calculated that

$$\frac{\partial V}{\partial \bar{c}_A} \cdot \dot{\bar{c}}_A = \frac{\partial V}{\partial \bar{c}_A} \cdot f(\bar{c}_A) \le 0 \quad \text{if} \quad \bar{c}_A > -1.906 \quad \text{and} \quad \bar{c}_A < 5.22 \tag{75}$$

and equality holds within this interval only if $\bar{c}_A = 0$. Since $g(\bar{c}_A) = 1$ in the closed-loop state space model, we can deduce that

$$y = L_g V(\bar{c}_A) = \frac{\partial V}{\partial \bar{c}_A} \cdot g(\bar{c}_A) = \bar{c}_A \tag{76}$$

where L_g is the Lie-derivative of the simple storage function with respect to the function g. Therefore, it follows that the closed-loop system is passive in the given interval.

The time derivative of the storage function (as a function of $\bar{c}_A$) is depicted in Figure 6.

Conclusion

Using a thermodynamic approach of constructing and analyzing dynamic models of process plants, the simple Hamiltonian model of lumped process systems has been constructed based on mechanical analogue. The conserved extensive quantities form the set of state variables and the input variables are chosen to be the flow rates in the system.

The approach is applicable for systems where Kirchhoff convective transport takes place together with transfer and sources of various type. Systems with constant mass holdup and uniform pressure in every balance volume satisfy these conditions.

The resulting simple Hamiltonian model can be used for passivity analysis, because it contains a storage function together with the nonlinear state space model of the system in a special canonical form. This type of model enables us to design a nonlinear PD feedback controller for passivation and loop shaping.

The general results are illustrated in simple examples of practical importance: on a bilinear heat exchanger cell and in an isotherm CSTR with nonlinear reaction.

Further work will be directed towards designing and tuning nonlinear controllers for passivation and loop-shaping based on the Hamiltonian view on process systems. The determination of the stability region of these controllers also needs further study for realistic cases.

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