Process Systems and Inventory Control

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A framework for modeling constraints on the dynamic behavior of systems obeying the laws of thermodynamics is discussed. These constraints induce dissipativity and we call a system obeying such constraints a process system. Passivity theory then shows that low-dimensional macroscopic analysis can be used for control system design. The inputs and outputs converge to their set points and the state vector converges to a stationary passive state provided one exists. Several examples are developed to support the theory and an extension is proposed for systems with equipment constraints.

Introduction

In this article we provide two distinct contributions in the area of process control. First we establish a formal connection between thermodynamics and the passivity theory of nonlinear control. The theory is based on the observation that the availability/exergy forms a natural dissipation function for nonlinear stability analysis of chemical process systems (Ydstie and Alonso, 1997). In principle it should therefore be possible to derive control system structures directly from the thermodynamics. Some examples to illustrate this point are developed. The concepts of exergy loss and dissipation also play roles in process design so this link may lead to results in the emerging area of interaction between process design and control (Narraway et al., 1991).

Second, we develop further an approach to process control where the manipulated variables are chosen so that selected process inventories follow their respective set points (Ydstie and Viswanath, 1994). The inventory flows and their respective supply rates are normally linked to process measurements through nonlinear transformations and in this way the method provides a procedure for selecting process measurements and manipulated variables. In the transformed space we follow standard procedures and use Lyapunov theory to synthesize low-dimensional (PID type) controller structures. System stability follows via the thermodynamic connection, and the approach we develop, therefore, provides an entry point for the design of distributed control strategies for large-scale chemical production systems.

In this article, the notion of a process system is defined, and key relationships between thermodynamics and nonlinear control are discussed. The existence of a stationary passive state, which can be stabilized by external controls, is linked to the existence of a dissipation inequality. Inventory control with simple observers is described, as well as a flash application and a reactor separator problem. This example makes it clear that a successful implementation relies on a precise understanding of equipment and thermodynamic constraints. The theory is extended, therefore, to constrained systems, and inventory control of the flash problem in the light of equipment constraints is reexamined.

Dissipation and Passivity of Process Systems

We focus on finite-dimensional dynamical systems, $\mathcal{S}$, whose dynamics can be represented by the equations

$$\dot{x} = f(x) + g(d, x, u), \qquad x(0) = x_0$$
$$y = h(x) \tag{1}$$

The real variable $t \in [0, \infty)$ is time, $\mathcal{X}$ is the state space, $\mathcal{U}$ and $\mathcal{D}$ are the sets of input variables and disturbances, and $\mathcal{Y}$ is the set of output variables. We assume without further motivation that the vector functions f and g, the initial condition x_0, and the input functions u and d are sufficiently well behaved to ensure that the solution to the differential Eq. 1 exists and is unique for all $t > 0$. We assume furthermore that there exists a stationary point and that the coordinate system has been chosen so that at the stationary point we have $x = d = u = 0$ and $f(0) = h(0) = g(0,0,0) = 0$. We have abused notation in the sense that the dimension of x in general is much higher than that of d and u.

An inventory for system $\mathcal{S}$ is an additive continuous (C^1) function v: $\mathcal{X} \rightarrow \mathcal{R}^+$ so that if x_1 is the state of system $\mathcal{S}_1$

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and x_2 is the state of another system $\mathcal{S}_2$ then we have

$$v(x) = v(x_1) + v(x_2) \tag{2}$$

Or stated more concisely, the inventory of a system is equal to the sum of the inventories of its subsystems. One important distinction between an extensive variable and an inventory is that an inventory is non-negative, whereas an extensive variable may be negative. One example of an extensive variable, which is not an inventory, is the Helmholtz energy, which is not bounded from below.

From Eq. 1 and continuity, we write a differential equality for an arbitrary vector of inventories $v = (v_1, \ldots, v_n)^T$ so that

$$\frac{dv(x)}{dt} = \frac{\partial v(x)}{\partial x} f(x) + \frac{\partial v(x)}{\partial x} g(d,x,u)$$

In the following we will use the notation $L_f v = (\partial v/\partial x) f$ and $L_g v = (\partial v/\partial x) g$ for the directional derivatives. We can then write

$$\frac{dv(x)}{dt} = p(x) + \phi(d,y,u) \tag{3}$$

where

$$p(x) = L_f v(x) + p^*, \qquad p^* = p(0)$$

$$\phi(d,y,u) = L_g v(x) - p^*$$

p is called the rate of production and p^* the vector of steady-state production rates. ϕ, the rate of supply, admits the decomposition

$$\phi(d,y,u) = \sum_{i=1}^{m} J_i \tag{4}$$

The vectors J_i for $i = 1, \ldots, m$ are called boundary fluxes, and they describe the rate of addition/depletion of inventory (such as energy/material) at m distinct points in physical space. We use the convention $J > 0$ if inventory flows into the system.

The ith inventory is *conserved* if

$$p_i(x) = 0 \qquad \text{for all } x \in \mathfrak{X}$$

It satisfies the *Clausius-Planck property* if

$$p_i(x) \geq 0 \qquad \text{for all } x \in \mathfrak{X}$$

The first law of thermodynamics states that there exists an inventory E, called the energy function, which is conserved and the second law states that there exists an inventory S, called the entropy function, which satisfies the Clausius-Planck property. We write these properties as

$$\frac{dE(x)}{dt} = \phi_E(d,y,u) \tag{5}$$

and

$$\frac{dS(x)}{dt} = p_S(x) + \phi_S(d,y,u) \qquad p_S(x) \geq 0 \tag{6}$$

A system which has inventories E and S that obey Eqs. 5 and 6 is called a *process system*. The definitions above prompt us to the following definitions.

Definition 1: *The stationary state $x = 0$ is said to be a passive state if $L_f S(x) \geq 0$ with equality if and only if $x = 0$.* A passive state is a state of minimum entropy production since $p_S(x) \geq p_S^*$ with equality if and only if $x = 0$ (Kreuzer, 1981). A weakly passive state satisfies the same condition with $L_F S(x) = 0$ for $x \in O$, where O is an open neighborhood around 0. Similar notions have been developed in the area of mathematical systems theory (Hill and Moylan, 1980; Byrnes et al., 1991).

Definition 2: *A system $\mathcal{S}$ is dissipative if there exists an inventory $\Delta(x)$ so that $L_f \Delta(x) < 0$ for $x \neq 0$ and $L_f \Delta(x) = 0$ for $x = 0$.* A weakly dissipative system is defined in a similar way with $L_f \Delta(x) = 0$ if $x \in O$. Δ is called a storage function for S. A dissipative system is said to be *passive* if $\Delta(0) = 0$ and the supply rate ϕ_Δ can be written so that

$$\phi_\Delta = u^T y$$

where u is the manipulated input and y is the output in transformed coordinates. Since passive systems are easy to control, there is a significant interest in finding coordinate representations that render a system passive (Byrnes et al., 1991). Some such relationships are developed below.

Let v^* be an arbitrary vector of constant set points. From Eq. 3, it follows that we can write

$$(\phi + p)^T (v - v^*) = \dot{v}^T (v - v^*) = \frac{1}{2} \frac{d}{dt} (v - v^*)^T (v - v^*)$$

It follows that the mapping

$$(\phi + p) \rightarrow (v - v^*)$$

is passive with storage function $\Psi = 1/2 (v - v^*)^T (v - v^*)$. We show in the next section how this observation can lead to stabilizing control of process inventories using strictly passive feedback.

Result 1: *Let $\mathcal{S}$ be a dissipative system with storage function Δ and let E satisfy the conservation property. Suppose furthermore that there exists a constant A_0 so that*

$$\Delta \leq E + A_0 \qquad \text{for all } x \in \mathfrak{X}$$

It follows that there exists an entropy function. Moreover, $x = 0$ is a passive state.

Proof 1: Let $t_0 > 0$ be an arbitrary real number and define a new variable σ so that

$$t_0\sigma = E - \Delta + A_0, \qquad \text{with } t_0 > 0$$

It follows immediately that $\sigma: \mathcal{X} \to \mathcal{R}^+$ and that $\sigma \in C^1$. By differentiating and rearranging the terms, we can write

$$\frac{d\sigma}{dt} = p_\sigma(x) + \phi_\sigma(d,y,u)$$

where

$$p_\sigma(x) = -\frac{1}{t_0} L_f\Delta(x) + p_\sigma^*$$

$$\phi_\sigma(d,y,u) = \frac{1}{t_0}[\phi_E(d,y,u)_\sigma - \phi_\Delta(d,y,u)_\sigma] - p_\sigma^*$$

Thus, σ is an entropy function since $L_f\Delta(x) < 0$ for $x \neq 0$ and $L_f\Delta(x) = 0$ for $x = 0$.

This result shows that we can derive the second law of thermodynamics and minimum entropy production at $x = 0$ from the first law and the dissipation inequality. Result 2 achieves the opposite result since we derive the dissipation inequality from the first and second laws of thermodynamics and the existence of a passive state.

Result 2: *Let $\mathcal{S}$ be a process system and let $x = 0$ be a passive state. $\mathcal{S}$ is dissipative with supply rate*

$$\phi_A = \phi_E - T_0(\phi_S + p_S^*)$$

for any constant $T_0 > 0$. Conversely, suppose that a process system is dissipative with supply rate ϕ_A, then $x = 0$ is a passive state.

Proof 2: Define the following inventory [this function is related to the exergy (available work) $H - T_0S$ where $H = U + PV$ is the enthalpy (Bejan, 1982)]

$$A = E - T_0S + A_0 \tag{7}$$

where A_0 is a constant. Ydstie and Alonso (1997) show that for any $T_0 > 0$ there exists A_0 so that $A(x) \geq 0$ for all $x \in \mathcal{X}$. We can now write

$$\begin{aligned}\frac{dA}{dt} &= \phi_E - T_0(p_S + \phi_S)\\ &= \phi_E - T_0(p_S - p_S^*) - T_0(\phi_S + p_S^*)\\ &= -T_0L_fS(x) + \phi_E - T_0(\phi_S + p_S^*)\\ &= -T_0L_fS(x) + \phi_A\end{aligned}$$

The state $x = 0$ is a passive state. It follows that $-T_0L_fS(x) < 0$ for $x \neq 0$ and $L_fS(x) = 0$ if $x = 0$. The first part of the result then follows.

For the second part, we have $L_f\Delta(x) \leq 0$ for all x with equality if and only if $x = 0$. We then set $\Delta(x) = A(x)$ so that we get

$$L_fA(x) = -T_0L_fS(x)$$

and it follows from this definition that $x = 0$ is a passive state.

These results can be restated by saying that the following are equivalent.

(1) $\mathcal{S}$ is dissipative with storage function $\Delta \leq E + A_0$ for some constant A_0.

(2) $\mathcal{S}$ is a process system, and $x = 0$ is a passive state.

(3) $\mathcal{S}$ is a process system with dissipation function A.

The laws of thermodynamics were first developed for systems at thermodynamic equilibrium. In this theory the state of system 1 is represented by

$$v(x) = [n_1(x), \ldots, n_{n_c}(x), E(x), V_t]^T \tag{8}$$

where n_i now denotes the number of moles of species i, n_c is the number of distinct chemical species, E denotes the energy, and V_t is the volume of the system. Equation 8 is also referred to as the microcanonical ensemble.

As an example, consider a constant volume closed system. The storage function A defined in Eq. 7 then satisfies

$$\frac{dA}{dt} \leq \dot{Q} - T_0\frac{\dot{Q}}{T} = \frac{\dot{Q}}{T}(T - T_0)$$

where T is the temperature of the system and T_0 is the temperature of the surroundings. Suppose now that we can manipulate the heating rate so that $\dot{Q} = -K(T - T_0)$ with $K > 0$. It then follows that $(T - T_0) \to 0$ as $t \to \infty$ since $T > 0$ and $A \geq 0$. Moreover, $x \to 0$ is a passive state which in this case corresponds to an equilibrium state.

Classical irreversible thermodynamics (CIT) extends the equilibrium theory to nonequilibrium systems by postulating that the relationship between thermal and mechanical properties of a physical system are the same as for a uniform system at equilibrium when we consider a unit cell with sufficiently small dimensions. Irreversibility is then due to chemical reaction within the cell and gradients established between local systems under shear conditions. Under this hypothesis, the macroscopic system defined by Eq. 1 is subdivided into unit cells, sufficiently large to be treated as macroscopic thermodynamic systems, but sufficiently small so that equilibrium is established in each cell. The microcanonical ensemble then represents the state of each unit cell and for each cell we can write

$$\dot{S} = w^T\dot{v} = w^Tp + w^T\phi$$

where

$$w(x) = \frac{\partial S}{\partial v}$$

are called intensive variables conjugate to v.

In the following we consider a unit cell (a cube) with constant volume and we decompose ϕ as described by Eq. 4. By combining the equations above and adding and subtracting w_iJ_i to each term in the summation, we can write

$$\dot{S} = \underbrace{w^T p + \sum_{i=1}^{6} (w - w_i)^T J_i}_{\text{entropy production} = p_S} + \underbrace{\sum_{i=1}^{6} w_i^T J_i}_{\text{entropy flux} = \phi_S} \tag{9}$$

We now introduce the following notation

$$Y = \begin{pmatrix} p \\ J_1 \\ \cdot \\ J_6 \end{pmatrix}, \quad X = \begin{pmatrix} w \\ w - w_1 \\ \cdot \\ w - w_6 \end{pmatrix}$$

where X is called the vector of thermodynamic forces and Y is a vector of thermodynamic fluxes. With these definitions

$$p_S = X^T Y \tag{10}$$

$$\frac{dv}{dt} = IY(d, y, u) \tag{11}$$

I is a matrix consisting of zeros and ones so that

$$I = [I_n, I_n, \ldots, I_n]$$

where I_n is the identity matrix. CIT now introduces constitutive equations and writes

$$Y = LX$$

where L is a positive definite matrix of phenomenological parameters. The symmetry of L was postulated for systems close to equilibrium by Onsager (1931). The classical examples in process systems of these constitutive equations are

$$\dot{Q} = -k(T_1 - T_2) \qquad \text{Fourier's law}$$

$$\dot{n} = -D(c_1 - c_2) \qquad \text{Fick's law}$$

where k is the coefficient of heat conduction and D is the diffusion coefficient.

In the example of heat conduction between cells 1 and 2 we can define the thermodynamic force as

$$X = w_1 - w_2 = \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

so that the heat flux is given by

$$\dot{Q} = \frac{L}{T_1 T_2}(T_2 - T_1)$$

and it follows that we can write the relationship between L and the coefficient of heat conduction so that

$$k = \frac{L}{T_1 T_2}$$

Since $L > 0$, it follows that the entropy production associated with an arbitrary interconnection

$$p_S = \left(\frac{1}{T_1} - \frac{1}{T_2} \right)^2 L$$

is positive.

Consider now a distributed system consisting of an arbitrary collection of N sub-systems $\mathcal{S}_i$, $i = 1, \ldots, N$ exchanging heat according to Fourier's Law. We can heat/cool at two distinct points indicated by subscripts 1 and 2 where the boundary temperatures are $T_{0,1}$ and $T_{0,2}$, respectively. The storage function described in Eq. 7 then satisfies

$$\frac{dA}{dt} \le \dot{\tilde{Q}}_1 + \dot{\tilde{Q}}_2 - T_{0,1}\frac{\dot{\tilde{Q}}_1}{T_1} - T_{0,2}\frac{\dot{\tilde{Q}}_2}{T_2}$$

$$= \frac{\dot{\tilde{Q}}_1}{T_1}(T_1 - T_{0,1}) + \frac{\dot{\tilde{Q}}_2}{T_2}(T_2 - T_{0,2})$$

where $\dot{\tilde{Q}}_i = \dot{Q}_i - \dot{Q}_i^*$, $i = 1, 2$. Q_i^* is the steady-state heating/cooling rate that corresponds to the stationary state $x = 0$ and $T_{0,1} \neq T_{0,2}$. Suppose now that we can manipulate $\dot{Q}_1$ and $\dot{Q}_2$ independently so that $\dot{\tilde{Q}}_i = -K_i(T_i - T_{0,i})$, where $K_i > 0$, $i = 1, 2$. We then get $(T_i - T_{0,i}) \to 0$ as $t \to \infty$ since $T_i > 0$ and $A \ge 0$. However, in this case the passive state is a nonequilibrium state. This example illustrates that we can achieve stability in a distributed system by using proportional control. Stability of the uncontrolled modes follows due to the dissipative nature of the system and the use of measurement and manipulated variable pairings that are physically close (colocated in space).

Similar relationships can be written for multicomponent diffusion and chemical reaction near equilibrium. Some progress has also been made in connecting thermodynamics with stability theory for systems with fluid flow (Kreuzer, 1981).

Another way to apply the result is to assume $E = E^*$, a constant, and that the boundary conditions are stationary so that by a proper change of reference frame we have $d = y = u = 0$. We can then conclude that the net entropy flux is constant at the boundary of the physical system so that

$$\phi_S(0,0,0) = \phi_S^*$$

By letting $x = 0$ correspond to a passive state we get

$$p_S(x) = L_f S(x) + p_S^* \ge p_S^* \qquad \text{for all } x \in \mathfrak{X}$$

Since we have $L_f S(x) = 0$ for $x = 0$ we get

$$\frac{dS}{dt} = p_S^* + \phi_S^*$$

We have

$$S \ge 0, \quad \text{and} \quad \limsup_{t \to \infty} S \le \frac{E^* - A_0}{T_0} < \infty$$

because $E = E^*$ is bounded and A_0 is defined in Eq. 7. We conclude that $p_S^* + \phi_S^* = 0$. Therefore, we get

$$\phi_A = \phi_E - T_0(\phi_S + p_S^*) = 0$$

since $\phi_S = \phi_S^* = -p_S^*$ and $\phi_E = 0$. It follows that the state converges to a passive state.

Corollary 1: *Consider a process system and assume that a passive state exists. The state converges to the passive state provided that the total energy and the boundary conditions are fixed.*

Process systems are interconnected in a natural manner. By letting N be the number of systems to be interconnected, we can write

$$\dot{x}_i = f_i(x) + g_i(d_i, x_i, u_i), \qquad i = 1, \ldots, N$$

The interconnected system is shown in Figure 1. Without further motivation, we assume that the composite system is well behaved so that solutions to all initial value problems exist. We now have the following results.

Result 3: *Consider a system $\mathcal{S}$ constructed by an arbitrary interconnection of N process systems. $\mathcal{S}$ is then a process system.*

Proof 3: This follows from additivity of the inventories since we can define the energy and entropy of the interconnected system so that

$$E(x) = \sum_{i=1}^{N} E_i(x) \geq 0, \qquad S(x) = \sum_{i=1}^{N} S_i(x) \geq 0$$

where E_i and S_i denote the energy and entropy of each subsystem. We choose a coordinate representation for the local systems so that $L_f E_i(x) = 0$ and $L_f S_i(x) \geq 0$ for $i = 1, \ldots, N$. We then have from Eq. 3 and additivity that

$$p_E = \sum_{i=1}^{N} p_{E_i} = 0, \qquad p_S = \sum_{i=1}^{N} p_{S_i} \geq 0$$

and the result then follows since the first and second laws now hold for $\mathcal{S}$.

Result 4: *Let $x_i = 0$, $i = 1, \ldots, N$ be a passive state for N process systems $\mathcal{S}_i$. The state $x = 0$ is then a passive state for the interconnected system provided that the entropy production associated with the interconnection is negligible.*

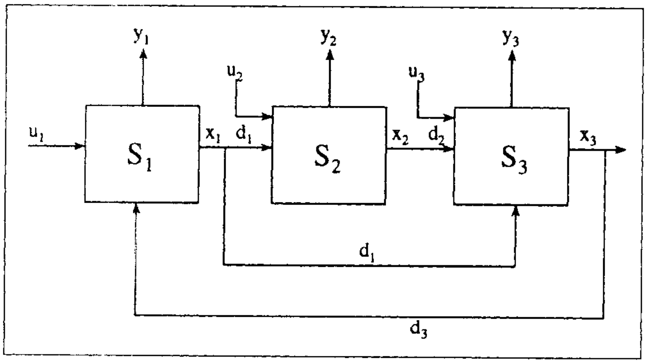

Figure 1. Block diagram for system.

Proof 4: This follows immediately since

$$L_f S(x) = \sum_{i=1}^{N} L_f S_i(x) \geq 0$$

with equality if and only if $x = 0$.

The extension to weakly passive states follows along the same lines.

We can now calculate the properties of the state of minimum entropy production for a nonequilibrium system consisting of N unit cells with inventories v_i by solving the following optimization problem

$$\min_{X_i} \frac{1}{2} \sum_{i=1}^{N} X_i^T L_i X_i, \qquad \text{Subject to: } \frac{dv}{dt} = 0$$

The Lagrange form of the optimization problem is

$$\mathcal{L} = \frac{1}{2} \sum_{i=1}^{N} X_i^T L_i X_i + \lambda^T I Y_i(d, y, u), \qquad \frac{\partial \mathcal{L}}{\partial X_i} = 0$$

where λ are the Lagrange multipliers. By furthermore assuming that the L_is are constant, we have

$$\frac{\partial \mathcal{L}}{\partial X_i} = L_i X_i + L_i I^T \lambda = 0$$

hence

$$X_i = -I^T \lambda, \qquad \text{a constant}$$

It follows that the forces satisfy the equipartition principle (Sauar et al., 1996) and that the forces are stationary at the passive state.

We finish the section by relating the definitions above to physical variables that can be measured. The energy can be decomposed into the internal, kinetic, and potential energies so that

$$E = U + KE + PE$$

In the following we will ignore the kinetic and potential energy so that E corresponds to the internal energy U. Thus, we can write using standard notation

$$\frac{dE}{dt} = \sum_{i=1}^{m} J_{E,i}(d, y, u)$$

$$J_{E,i}(d, y, u) = \dot{m}(PV + U) + \dot{Q} + \dot{W}$$

where P is the pressure, V is the specific volume (m^3), $\dot{m}$ is the mass or molar flow rate, $\dot{Q}$ is the heat input, and $\dot{W}$ is the work. Furthermore, the Gibbs relation allows us to express the relationship between entropy and other state variables as

$$TdS = dU + PdV - \sum_{i=1}^{n_c} \mu_i dn_i$$

This defines a one-to-one map from the extensive variables S, U, and n_i to the so-called intensive variables T, P, V, and μ_i. T is called the temperature, and μ_i the chemical potential of species i. These relationships can now be used to define more explicitly how to implement control systems as demonstrated in the examples in the sections that follow.

Inventory Control for Conserved Properties

An inventory control system controls process inventories v to their set points v^* by choosing the manipulated input variable so that the candidate Lyapunov function decreases. A particularly useful candidate for our purposes is the following function

$$\Psi = \frac{1}{2}(v - v^*)^T K_c^{-1}(v - v^*)$$

where K_c is a diagonal matrix of controller gains. From the inventory balance, we then get

$$\frac{d\Psi}{dt} = (v - v^*)^T K_c^{-1}[p(x) + \phi(d,y,u) - \dot{v}^*]$$

We now can implement the following PF-F (Proportional Feedback-Feedforward) control

$$\text{Choose } u \text{ so that:} \quad \phi(d,y,u) = -p(x) - K_c(v - v^*) + \dot{v}^* \tag{12}$$

This law is well defined provided $\phi(d,y,u)$ is invertible with respect to u. Assuming this to be the case we get,

$$\frac{d\Psi}{dt} = -(v - v^*)^T(v - v^*) \le -2\bar{k}_c\Psi$$

where $\bar{K}_c$ is the smallest gain. The solution to this differential inequality is given by

$$\Psi(t) \le \Psi(0)\exp(-2\bar{k}_c t)$$

From this equation, we see that the speed of response of the unconstrained system is governed by the magnitude of K_c. Furthermore, since K_c is diagonal we find that the error in each inventory satisfies the equation

$$v_i(t) - v_i^*(t) = \exp(-K_{c_i}t)[v_i(0) - v_i(0)^*], \qquad i = 1,\ldots,n \tag{13}$$

and it follows that v converges to the set point v^* as required. The decay rate is exponential and there is no overshoot or oscillation.

It is possible to use nonlinear feedback control. The only requirement is that the feedback gain $K_c(t)$ should be positive and piecewise continuous. Shinskey (1967), for example, suggests setting

$$K_c = K_{c_0} + K_{c_1}|e|$$

where K_{c_0} and K_{c_1} are positive constants and e is the error $(v - v^*)$. This approach makes it possible to have large gains when the error is large and small gains when the error is small. This can give good performance for loops that have low-level noise. Gain scheduling and interpolation using fuzzy logic and/or neural networks can be used as well.

The controller described in Eq. 12 can be solved for a unique u if and only if the function $\phi(d,y,u)$ is invertible with respect to u for a given x and d. The following assumption is therefore critical for the application of inventory control as stated above.

Assumption 1: *The mapping $\phi(d,y,u)$ is one-to-one with respect to the vector u for all $x \in \mathfrak{X}$ and $d \in \mathfrak{D}$.* What the assumption asks for is that for all x and d control variables u exist to assign the flux vector ϕ to arbitrary values in $\Re^n$. In other words, we require that

$$\text{rank}\left(\frac{\partial\phi}{\partial u}\right) = n \quad \text{for all } x \in \mathfrak{X} \text{ and } d \in \mathfrak{D}$$

The assumption imposes design constraints on the process. These design constraints can be used to verify the feasibility of a given design. The assumption can be used to determine which variables should be measured and manipulated and how these variables should be coupled. Some of these properties will be illustrated in the examples described below.

Example 1: *Control of a drum boiler.* In the drum boiler, the water is circulated through the furnace tubes where it vaporizes partially. The rest of the feedwater returns through the cooler downcomers to begin another pass through the furnace tubes. The steam leaving the boiler is saturated.

A simplified nonlinear model of a ship boiler shown in Figure 2 was developed and verified by Tyssø (1981). The differential-algebraic equations of this model are presented in Appendix 1. The version we use has six state variables and a number of algebraic constraints which make it difficult to apply nonlinear geometric control or even nonlinear predictive control to achieve stabilization of typical output variables. Below, we show how we can use inventory control to redefine control objectives and define a simple nonlinear control structure which achieves stabilization of the system.

We now develop the inventory balance for the boiler. By neglecting friction losses and gravitational terms, the mass and energy balances for the boiler are simply written as [A discussion on how friction losses and gravitational terms can be estimated for a wide variety of fluid-flow systems and dif-

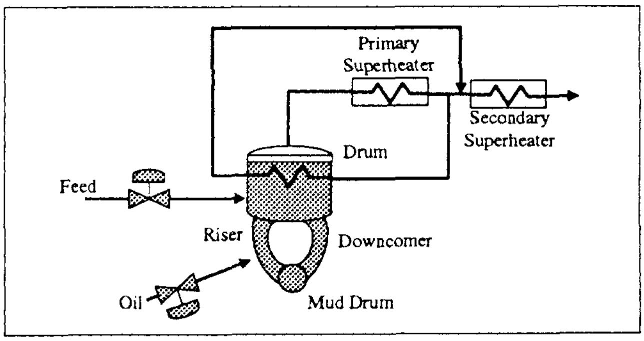

Figure 2. Drum boiler.

ferent geometries is given in the classic book by Bird et al. (1960). In a normal boiler example it is not necessary to include such terms to obtain stable control.]

$$\frac{dM}{dt} = \dot{m}_F - \dot{m}_V$$

$$\frac{dU}{dt} = \dot{Q} + \dot{m}_F h_F - \dot{m}_V h_V$$

where h_i is the enthalpy of steam i. These equations can be written in the form of Eq. 3

$$\frac{dv}{dt} = \phi(d,y,u) = \begin{pmatrix} L_{g_M} \\ L_{g_U} \end{pmatrix} \omega = G(y)\omega \tag{14}$$

where

$$\omega = \begin{pmatrix} \dot{m}_F \\ \dot{m}_V \\ \dot{Q} \end{pmatrix}, \quad G = \begin{pmatrix} 1 & -1 & 0 \\ h_F & -h_V & 1 \end{pmatrix}$$

The term $L_f v(x) = 0$ since mass and energy are conserved. In this case $\operatorname{rank}[G(y)] = 2$ for all x and it follows that we can specify at most two objectives independently.

In an equilibrium system we relate the maximum number of independent objectives to the phase rule. In general, the number of degrees of freedom of an equilibrium system is governed by the Gibbs phase rule

$$f = n_c - p - r - s + 2$$

In this expression $f = 1$ denotes the degrees of freedom, which are the number of intensive properties that need to be specified, $p = 2$ the number of phases, $n_c = 1$ the number of components, $s = 0$ the number of special conditions, and $r = 0$ the number of chemical reactions. In order to specify the system, we also need to specify one total extensive property to determine the size of the system, for example, total mass. This then gives the number of control objectives that can be specified for this problem as $\min\{f, \dim(\omega) - 1\}$, which, of course, coincides with the rank condition given in Assumption 1.

Since $\dim(\omega) = 3 > f$, as given by the phase rule, we need to choose a subset for manipulated variables u and the remaining variables are disturbance variables d. In the case that we want to deliver steam at a variable demand we have to set

$$u = \begin{pmatrix} \dot{m}_F \\ \dot{Q} \end{pmatrix}, \qquad d = \dot{m}_V$$

where $\dot{m}_V$ is the demand rate, which is set by downstream equipment. (If we want to evaporate a variable amount of liquid, the roles of $\dot{m}_V$ and $\dot{m}_F$ are interchanged.) The inventory controller can now be expressed as

$$\begin{pmatrix} 1 & 0 \\ h_F & 1 \end{pmatrix} \begin{pmatrix} \dot{m}_F \\ \dot{Q} \end{pmatrix} = \left[\begin{pmatrix} \dot{m}_V \\ \dot{m}_V h_V \end{pmatrix} - \begin{pmatrix} K_{c_1}(M - M^*) \\ K_{c_2}(U - U^*) \end{pmatrix} \right]$$

where M^* and U^* are set points for the total mass and energy.

In the implementation it is necessary to develop a measurement system to estimate the total mass holdup and the total internal energy of the system. Suppose we choose

$$M = V_{dw}\rho_{dw} + V_s\rho_s; \quad dU = (V_{dw}\rho_{dw}c_{vw} + V_s\rho_s c_{vs})dT$$

This can further be simplified by using the fact that $V_t = V_{dw} + V_s$ is a constant. We can also assume $\rho_s \ll \rho_{dw}$. Mass-flow rates can be estimated by using a pressure-drop calculation

$$\dot{m} = \rho f = a_i\sqrt{\Delta P}$$

where a_i can either be determined from correlations or can be estimated adaptively. For gases, the gauge pressure also is needed to estimate the mass flow. Hence, the control equation takes the form

$$\dot{m}_F = a_1\sqrt{P_{\text{out}}\Delta P_{\text{out}}} - K_{c_1}(M - M^*)$$

$$\dot{Q} = -a_1\sqrt{P_{\text{out}}\Delta P_{\text{out}}}\,c_{vl}T_{in} + K_{c_1}(M - M^*)c_{vl}T_{in} + a_1\sqrt{P_{\text{out}}\Delta P_{\text{out}}}\,c_{vv}T_{\text{out}} - K_{c_2}(U - U^*)$$

The controller design that we obtain from the equations above is as shown in Figure 3. The mass balance part of this control structure is equivalent to Figure 7.2 in Shinskey (1967). However, the liquid level measurement in this scheme may give false estimates due to a well documented inverse response problem. The inverse response is due to a problem with the observer for M and not with the controller *per se*.

Now we need to relate the mass holdup and internal energy of the control model to variables in the boiler model. If we choose the mass of the water in the drum ($V_{dw}\rho_{dw}$) and enthalpy in the risers (H_{ro}) as the inventories to be stabilized, the choice of manipulated variables would be the feedwater flow rate ($\dot{m}_w$) and the heat input ($\dot{Q}_{rw}$), which can be adjusted by varying the fuel flow rate ($\dot{m}_{\text{oil}}$). The control objectives of drum pressure or temperature and steam flow rate are then translated to their corresponding set points in the extensive variables chosen. From the dynamic equations for

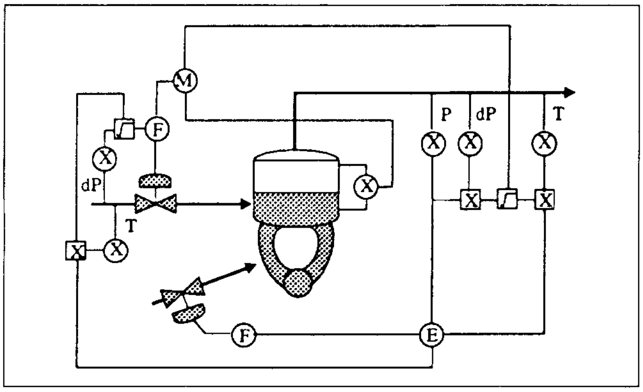

Figure 3. Feedback-feedforward control scheme for drum boiler.

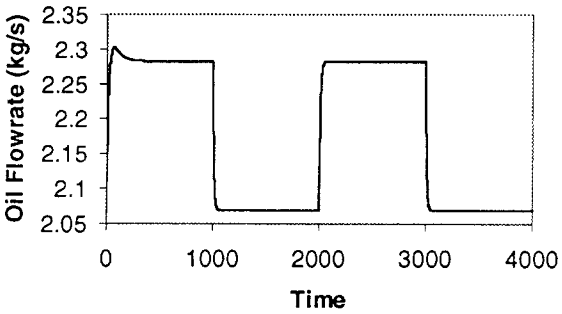

Figure 4. Oil flow rate to boiler.

the model listed above, $\phi(d, y, u)$ becomes apparent from the expressions for dH_{ro}/dt and dV_{dw}/dt. The control expressions therefore become

$$\dot{Q}_{rw} = - K_1(H_{ro} - H_{ro}^*) + \dot{m}_{\text{dow}}(H_{ro} - H_{\text{dow}}) + \dot{m}_o \lambda \frac{X_0}{2}$$

$$\dot{m}_w = - K_2[V_{dw}\rho_{dw} - (V_{dw}\rho_{dw})^*] + \dot{m}_{\text{dow}} - (1 - X_0)\dot{m}_0$$

where $K_1 = K_{c_1} V_r \rho_{ro}$ and $K_2 = K_{c_2}\rho_{dw}$. We can see that these control expressions are analogous to those previously derived. The production rate of the steam was varied between 29.2 kg/s and 32.2 kg/s for a given mass and energy set point. The control objectives were maintained for the entire time. The resulting manipulated variable profiles are shown in Figures 4 and 5.

From Eq. 13, we now conclude that the total mass and the internal energy of the boiler system converge to their respective set points, as shown in the simulations. We assume furthermore that all the boundary conditions (feedwater temperature and pressure, demand rate, and downstream pressure) are fixed. The corollary developed in the previous section now applies since the model is based on vapor liquid equilibrium, and we conclude that the state converges to a passive state, which in this case is a stationary state.

Inventory Control via Observers

The Lyapunov type analysis leads to a fairly general set of conditions for stability which can include robust and adaptive control as special cases. We will not strive for this level of generality and focus instead on a class of controllers which can be classified as decoupling PID design with nonlinear feedforward.

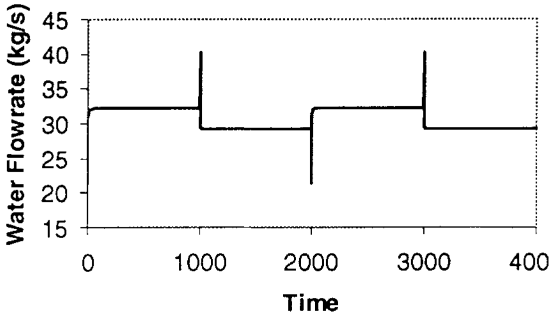

Figure 5. Feed flow rate to boiler.

We propose the following control structure

$$\phi(d, y, u) = - \Pi(x) - K_c\tilde{\upsilon} - \tau_D\dot{\tilde{\upsilon}} + \dot{\upsilon}^* \tag{15}$$

where $\tilde{\upsilon} = \upsilon - \upsilon^*$ is the error and

$$\Pi(x) = \hat{p}(x) + \tau_I^{-1}\int_0^t \tilde{\upsilon}\, d\xi + \hat{p}(0)$$

$\hat{p}(x)$ is an estimate of the production vector $p(x)$, which may be generated by an extended Kalman filter or a nonlinear observer. The feedback part of the controller (the right side of Eq. 15) is referred to as PID control without reset windup and $K_c > 0$, $\tau_I > 0$, and $\tau_D \geq 0$ are the diagonal matrices of proportional gains, integral times, and derivative times, respectively. The structure of the feedback-feedforward system is shown in Figure 6.

In this figure, available process measurements y are used to reconstruct estimates of the signals needed for feedback, namely the inventory vector υ with its set points and the signals needed for feedforward, which include the part of the state vector x and the disturbance vector d needed to calculate the flux vector $\phi(d, y, u)$ so that it can be inverted with respect to u.

Solving ϕ with respect to u with the PID terms set to zero gives a feedforward control structure

$$\phi(d, y, u) = 0$$

This corresponds to the feedforward design for the material balance as discussed by Buckley (1964), and the energy balance as discussed by Shinskey (1967). We also note that the extensive variable control approach by Georgakis (1986) can be related to our approach by noting that in Figure 6, the observer can correspond to the extensive variable synthesizer (EvS) and the inversion block ϕ to the extensive variable analyzer (EvA).

Equations 3 and 15 together give the closed loop for the controlled inventory

$$(1 + \tau_D)\dot{\tilde{\upsilon}} = p - \hat{p} - K_c\tilde{\upsilon} - \tau_I^{-1}\int_0^t \tilde{\upsilon}\, d\xi - \hat{p}(0) \tag{16}$$

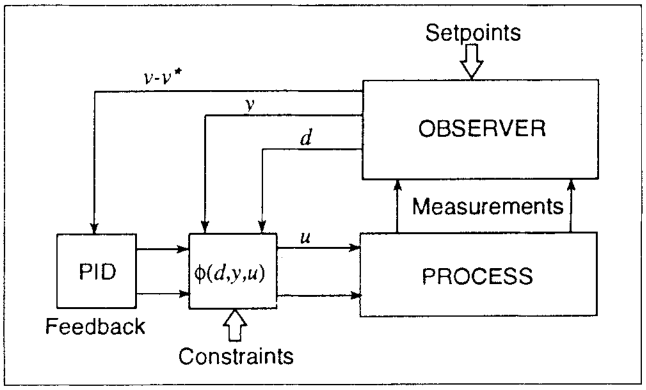

Figure 6. Feedback-feedforward structure for PID inventory control.

The response of the inventory is linearized if $p - \hat{p} = 0$ and the results developed in the previous section apply directly. Thus, the controller is an example of output linearization. In the case that there is an observer error this result no longer applies since there is a mismatch. We now want to analyze the effect of such a mismatch. Motivated by adaptive control theory, we introduce the following assumptions concerning the estimation error $p - \hat{p}$.

Assumption 2: *The estimation error vector satisfies*

$$p - \hat{p} = p^* + \Pi_0 \tilde{v} + \Pi_1 \int_0^t e^{-\int_\xi^t \gamma^2 d\xi} \Pi_2^T \tilde{v} d\xi$$

where p^* is an arbitrary constant and Π_0, Π_i $(i = 1, 2)$, and γ are bounded and uniformly continuous matrix, vector, and scalar functions in t.

Assumption 2 states that the magnitude of the estimation error $p - \hat{p}$ should depend in a continuous manner on the inventory error vector $\tilde{v}$, through a direct term and a memory term, with the exception of a steady-state offset p^*. Such conditions are generally satisfied by a Kalman filter in a linear case and a nonlinear observer in a nonlinear case.

Result 5: *Suppose that the two previous assumptions are satisfied and the proportional gain is sufficiently large so that*

$$K_c - \Pi_0 - \epsilon_0 \epsilon_0^T \geq \epsilon I > 0$$

for some $\epsilon > 0$ and for all t. Where $\epsilon_0 = (\Pi_1 + \Pi_2)/2\gamma$. It follows that $\lim_{t \to \infty} \tilde{v} = 0$.

Proof 5: Define the deviation variables

$$\tilde{p} = p^* - \hat{p}$$

where $\dot{\hat{p}} = \tau_I^{-1} v$ with $\hat{p}(0) = p_0$. It then follows that

$$(I + \tau_D)\dot{\tilde{v}} = \tilde{p} - (K_c - \Pi_0)\tilde{v} + \Pi_1 \beta \tag{17a}$$

$$\dot{\tilde{p}} = -\tau_I^{-1}\tilde{v} \tag{17b}$$

$$\dot{\beta} = -\gamma^2 \beta + \Pi_2^T \tilde{v} \tag{17c}$$

We now define the storage function

$$\Psi(t) = \frac{1}{2}\tilde{v}^T(I + \tau_D)\tilde{v} + \frac{1}{2}\tilde{p}^T \tau_I \tilde{p} + \frac{1}{2}\beta^2 \geq 0 \tag{18}$$

so that from Eqs. 17a–17c

$$\dot{\Psi}(t) = -\tilde{v}^T(K_c - \Pi_0)\tilde{v} + \tilde{v}^T(\Pi_1 + \Pi_2)\beta$$
$$- \gamma^2 \beta^2 + \tilde{v}^T(\epsilon_0 \epsilon_0^T)\tilde{v} - \tilde{v}^T(\epsilon_0 \epsilon_0^T)\tilde{v}$$

Hence,

$$\dot{\Psi}(t) = -\tilde{v}^T(K_c - \Pi_0 - \epsilon_0 \epsilon_0^T)\tilde{v} - (\gamma\beta - \epsilon_0^T \tilde{v})^2 \leq -\epsilon \tilde{v}^T \tilde{v} < 0$$

by integration we have

$$\Psi(t) \leq \Psi(0) - \epsilon \int_0^t \|\tilde{v}(s)\|^2 d\xi \tag{19}$$

From Eqs. 18 and 19, we have a constant c_0 such that

$$\|\tilde{v}\| + \|\tilde{p}\| + |\beta| \leq c_0$$

It is now easy to show that $\ddot{\Psi}$ is bounded so that $\dot{\Psi}$ is uniformly continuous. The result follows from Eq. 19 by application of Barbalat's lemma (Slotine and Li, 1991).

Example 2: *Control of a Ternary Flash.* In this example, we consider the control of a ternary flash vessel. The feed stream is separated into a vapor and a liquid stream. The compositions of the vapor and liquid streams are different since the vapor pressures of the components are not the same at the specified temperature. The degree of separation can be adjusted by manipulating the flow rates, as well as the heat input to the vessel.

We must first write the macroscopic component, mass, and energy balances for the flash. In practice we only need to write as many equations as there are independent control objectives. It will be shown that the maximum number of control objectives for a two-phase flash is three, which is less than the number of possible control objectives in a ternary system.

For this system, we write n_c mass balance equations and one energy balance equation. Here n_c is the number of components in the system. This gives the differential algebraic equations as shown below

$$\frac{dM}{dt} = \dot{m}_F - \dot{m}_L - \dot{m}_V$$

$$\frac{dM_i}{dt} = \dot{m}_F z_i - \dot{m}_L x_i - \dot{m}_V y_i \qquad i = 2..n_c$$

$$\frac{dU}{dt} = \dot{m}_F h_F - \dot{m}_L h_L - \dot{m}_V h_V + \dot{Q}$$

$$\sum_{i=1}^{n_c} z_i = 1$$

$$\sum_{i=1}^{n_c} x_i = 1$$

$$\sum_{i=1}^{n_c} y_i = 1$$

$$y_i = K(x_i, T)x_i \qquad i = 2..n_c$$

Here M is the total molar holdup, M_i is the total molar holdup of species i, K is the equilibrium function, and x_i, y_i, and z_i are mole fractions. The steady-state operating conditions for the flash are shown in Table 1. It is difficult to apply nonlinear control to control the flash temperature and pressure directly since these are calculated via the equilibrium relationships. These cannot normally be written in an explicit

Table 1. Steady-State Flash Data

$\dot{m}_{F_{\text{benzene}}}$	5 mol/s	$m_{F_{o\text{-dichlorobenzene}}}$	5 mol/s
$\dot{m}_{F_{\text{toluene}}}$	5 mol/s	$\dot{m}_V$	7.5 mol/s
T	393 K	P	1 bar

form. Below, we show how the control problem is made simple by considering the inventories.

Writing the differential equations in vector form gives the following

$$
v = \begin{bmatrix} M \\ M_2 \\ M_3 \\ U \end{bmatrix}
$$

$$
\phi(d,y,u) = \begin{bmatrix} \dot{m}_F - \dot{m}_L - \dot{m}_V \\ \dot{m}_F z_2 - \dot{m}_L x_2 - \dot{m}_V y_2 \\ \dot{m}_F z_3 - \dot{m}_L x_3 - \dot{m}_V y_3 \\ \dot{m}_F h_F - \dot{m}_L h_L - \dot{m}_V h_V + \dot{Q} \end{bmatrix}
$$

In this case the conservation property holds, so $p(x) = 0$ in Eq. 3. We can further decompose ϕ into a product of a convection vector of disturbances and a state dependent matrix of densities and mole fractions so that

$$
\phi = G(y)\,\omega
$$

where

$$
\omega(u,d) = \begin{bmatrix} \dot{m}_F \\ \dot{m}_L \\ \dot{m}_V \\ \dot{Q} \end{bmatrix}
$$

$$
\phi(d,y,u) = \begin{bmatrix} 1 & -1 & -1 & 0 \\ z_2 & -x_2 & -y_2 & 0 \\ z_3 & -x_3 & -y_3 & 0 \\ h_F & -h_L & -h_V & 1 \end{bmatrix} \begin{bmatrix} \dot{m}_F \\ \dot{m}_L \\ \dot{m}_V \\ \dot{Q} \end{bmatrix}
$$

Here, we see that the $\operatorname{rank}(G(y)) = 4$, which is greater than the maximum number of possible control objectives. Thus, we must pick a subset of inventories to control. For this example, we assume that the feedrate is a disturbance. Therefore, it is natural to decompose the convection vector into a vector of control variables and a vector of disturbance variables so that

$$
\omega = (u', d')^T
$$

where $u = (\dot{m}_L, \dot{m}_V, \dot{Q})^T$ and $d = \dot{m}_F$. In this expression, u is the vector of manipulated variables and d is a convection term which is specified externally and is treated as a disturbance. We have now reduced the number of objectives that can be specified by one, and we, therefore, define the function $\phi(d,y,u)$ as

$$
\phi(d,y,u) = G_u u + G_d d
$$

where

$$
G_u = \begin{bmatrix} -1 & -1 & 0 \\ -x_3 & -y_3 & 0 \\ -h_L & -h_V & 1 \end{bmatrix}
$$

$$
G_d = \begin{bmatrix} 1 \\ z_3 \\ h_F \end{bmatrix}
$$

Assumption 1 applies to this expression as G_u is invertible for all $i \in [1, n_c]$ except in the case of an azeotrope. For an azeotrope, G_u becomes singular. The matrix G_u will also become singular when there is a loss of a phase. For instance, if a two-phase flash system moves out of the phase envelope, the matrix will become singular and one less objective can be maintained. Assuming there are no azeotropes to cross and we are operating in the two-phase region, we can use the following proportional feedback-feedforward law to control the system

$$
\begin{bmatrix} \dot{m}_V \\ \dot{m}_L \\ \dot{Q} \end{bmatrix} = \frac{1}{y_3 - x_3} \begin{bmatrix} -y_3 & 1 & 0 \\ x_3 & -1 & 0 \\ h_V x_3 - h_L y_3 & -h_V + h_L & y_3 - x_3 \end{bmatrix} \times \begin{bmatrix} -\dot{m}_F z_3 - K_{c_1}(M_3 - M_3^*) \\ -\dot{m}_F - K_{c_2}(M - M^*) \\ -\dot{m}_F h_F - K_{c_3}(U - U^*) \end{bmatrix}
$$

In order to implement this control structure, the state variables must be defined with physical quantities and estimates from the measured system properties. It is assumed that the flash drum is of uniform cross-sectional area A_{cs} and volume V_t. The inventories can then be written as

$$
M = lA_{cs}(\rho_L - \rho_V) + V_t \rho_V
$$

$$
M_3 = lA_{cs}\rho_L x_3 + V_t \rho_V K x_3 - lA_{cs}\rho_V K x_3
$$

$$
U = lA_{cs}\rho_L h_L + (V_t - lA_{cs})\rho_V h_V
$$

Rewriting these equations in vector notation, we get

$$
\begin{bmatrix} M \\ M_3 \\ U \end{bmatrix} = \begin{bmatrix} A_{cs} & V_t & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & A_{cs} & V_t & -A_{cs} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & A_{cs} & V_t & -A_{cs} \end{bmatrix} \times \begin{bmatrix} l(\rho_L - \rho_V) \\ \rho_V \\ l x_3 \rho_L \\ K x_3 \rho_V \\ K l x_3 \rho_V \\ l \rho_L h_L \\ \rho_V h_V \\ l \rho_V h_V \end{bmatrix}
$$

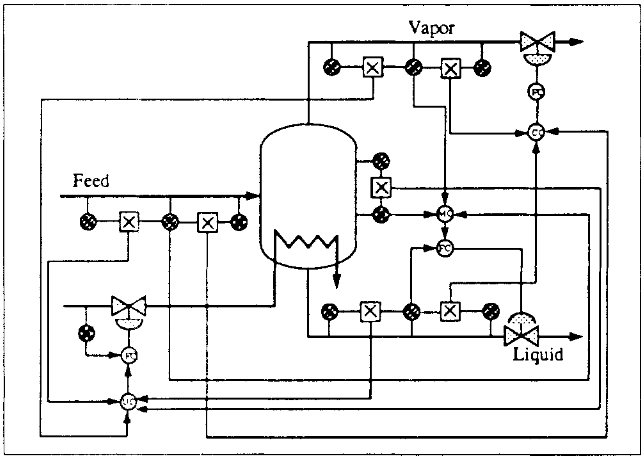

Figure 7. Feedback-feedforward control scheme for flash vessel.

Although the measurement vector contains many components, it is only necessary to measure the level l, the composition x_3, and the temperature T to obtain all of the components in the vector. Since compositions are not normally available, they can be estimated from the temperature and pressure of the system. The other variables can be calculated using an appropriate thermodynamics package. In this example, UNIFAC was used to model the behavior of the liquid phase and Pitzer was used to model the behavior of the vapor phase.

In order to test this control strategy, we have applied it to a flash model for the separation of benzene, o-dichlorobenzene, and toluene. We now need to relate the macroscopic variables for control. This step is easy to carry out and we get the control system shown in Figure 7.

The system was subjected to a change in the feed composition, as well as the feed flow rate. As can be seen in Figure 8, the energy objective of the control system is achieved. The mole and component objectives were also maintained.

Example 3: *Control of a Reactor Flowsheet.* The flowsheet contains a continuous stirred-tank reactor and a flash vessel. The vapor stream from the flash unit is being recycled back to the reactor. Pure components A and B are also being fed to the reactor. The objectives of the control system are the total number of moles, as well as the total number of moles of one of the components in the reactor with competing reactions and the total number of moles, as well as the total number of moles of one of the components in the flash. The reactions are described as follows

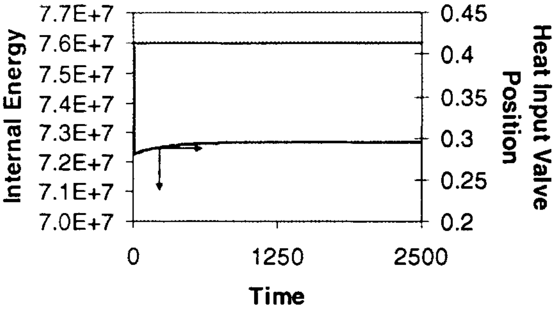

Figure 8. Energy controller for flash.

$$A + B \xrightarrow{k_1} C$$

$$A + C \xrightarrow{k_2} D$$

The reactions are both second-order elementary reactions. The reaction expressions represent a typical alkylation type reaction. The differential algebraic equations for the reactions are described by the following set of equations

$$\frac{dM}{dt} = \dot{m}_F - \dot{m}_L + p_{\text{net}}$$

$$\frac{dM_i}{dt} = \dot{m}_F z_i - \dot{m}_L x_i + p_i \qquad i = 2..n_c$$

$$p_A = -V_t k_1 c_A c_B - V k_2 c_A c_C$$

$$p_B = -V_t k_1 c_A c_B$$

$$p_C = V_t k_1 c_A c_B - V k_2 c_A c_C$$

$$p_D = V_t k_2 c_A c_C$$

$$\sum_{i=1}^{n_c} z_i = 1$$

$$\sum_{i=1}^{n_c} x_i = 1$$

where p_{net} is the net production rate in mol/s, c_i is the concentration of species i, and p_i is the production rate of species i.

The flash is assumed to be a constant relative volatility flash and has the following differential algebraic equations

$$\frac{dM}{dt} = \dot{m}_F - \dot{m}_L - \dot{m}_V$$

$$\frac{dM_i}{dt} = \dot{m}_F z_i - \dot{m}_L x_i - \dot{m}_V y_i \qquad i = 2..n_c$$

$$\sum_{i=1}^{n_c} z_i = 1$$

$$\sum_{i=1}^{n_c} x_i = 1$$

$$\sum_{i=1}^{n_c} y_i = 1$$

$$y_i = K(x_i) x_i \qquad i = 2..n_c$$

The initial steady-state operating conditions for the process are shown in Table 2.

The flowsheet with the basic control structure is shown in Figure 9.

Writing the differential equations in the form of Eq. 3 for the reactor, we have

Table 2. Steady-State Flowsheet Data

$\dot{m}_{F_A}$	142.61 mol/s	$\dot{m}_{F_B}$	188.637 mol/s
V_t	0.05 m^3	$\dot{m}_{F_V}/\dot{m}_{F_{\text{flash}}}$	0.5
α_A	4	α_B	3
α_C	2	α_D	1
k_1	0.005 m^3/mol/s	k_2	0.002 m^3/mol/s

$$v = \begin{bmatrix} M \\ M_C \end{bmatrix}$$

$$p(x) = \begin{bmatrix} p_{\text{net}} \\ p_C \end{bmatrix}$$

$$\phi(d,y,u) = \begin{bmatrix} \dot{m}_{F_A} + \dot{m}_{F_B} - \dot{m}_L + \dot{m}_{\text{recycle}} \\ \dot{m}_{F_{\text{recycle},C}} - \dot{m}_L x_C \end{bmatrix}$$

where the feed flow rate to the reactor has been decomposed into the feed flow rate of component A, the feed flow rate of component B, and the recycle flow rate. We can further decompose the flux vector into a control part and a disturbance part. This results in the following decomposition

$$\phi(d,y,u) = \begin{bmatrix} 1 & -1 \\ 0 & -x_C \end{bmatrix} \begin{bmatrix} \dot{m}_{F_B} \\ \dot{m}_L \end{bmatrix} + \begin{bmatrix} \dot{m}_{F_A} + \dot{m}_{\text{recycle}} \\ \dot{m}_{F_{\text{recycle},C}} \end{bmatrix}$$

We see here that the feed flow rate of component A and the recycle stream is treated as the disturbance, and the control vector is the feed flow rate of component B and the total liquid product flow rate. For this example, a PI controller was used to control the reactor. The closed-loop control law then has the following form

$$\begin{bmatrix} \dot{m}_{F_B} \\ \dot{m}_L \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ 0 & -x_C \end{bmatrix}^{-1}$$
$$\times \begin{bmatrix} -\dot{m}_{F_A} - \dot{m}_{\text{recycle}} - p_{\text{net}} - K_{c_1}\left[e_1 + \tau_{I_1}^{-1}\int e_2 dt\right] \\ -\dot{m}_{F_{\text{recycle},C}} - p_C - K_{c_2}\left[e_2 + \tau_{I_2}^{-1}\int e_2 dt\right] \end{bmatrix}$$

$$e_1 = M - M^*$$
$$e_2 = M_C - M_C^*$$

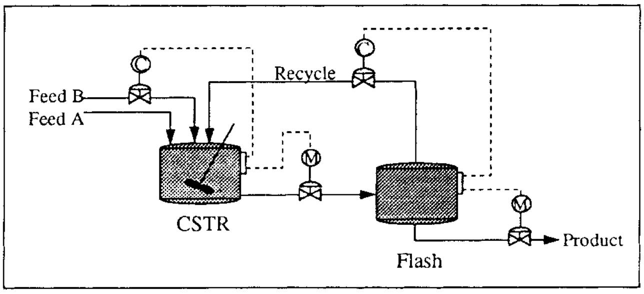

Figure 9. Flowsheet.

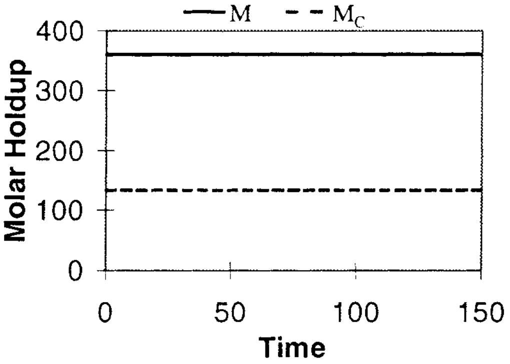

Figure 10. Control objectives for reactor.

Similar equations can be derived for the flash unit as well. These equations are the same as those used in Example 2 without the energy controller. The set points for the process inventories were initially taken as those values obtained from the steady-state operating conditions. The system was initially integrated at steady state for fifty time steps. The feed of component A was then increased from 142 mol/s to 160 mol/s, and the system was integrated for another hundred time steps. Figures 10 and 11 show the control objectives and the manipulated variables for the reactor. We see that the control objectives are maintained at their set points for all time. Figures 12 and 13 show the control objectives and manipulated variables for the flash. Again, we see that the control objectives are maintained at their set point for all time. In this example it was assumed that we could directly measure all necessary process variables.

Inventory Control with Equipment Constraints

Consider the system in Figure 14, where $\dot{m}_1$ is the mass-flow rate into the tank and $\dot{m}_2$ is the mass-flow rate out of the tank.

The net flux

$$\phi_M(d,y,u) = \dot{m}_1(x) - \dot{m}_2(x)$$

is clearly a function of the power of the pump, as well as the head pressure, and there exist states so that Assumption 1 is not satisfied. For example, Assumption 1 breaks down if the

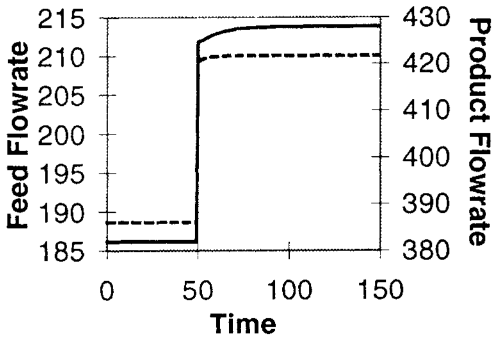

Figure 11. Manipulated variables for reactor.

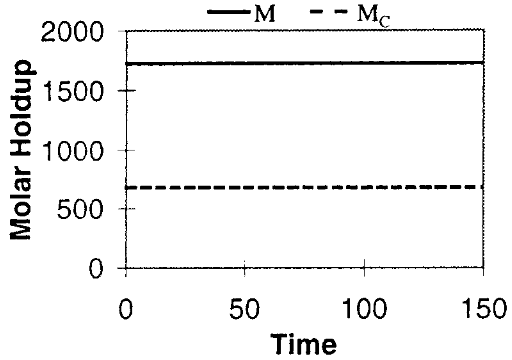

Figure 12. Control objectives for flash.

head pressure is large and the pumping capacity is insufficient to balance $\dot{m}_2$. The purpose of this section is to investigate this issue and thereby lay down the foundation for a theory to study the steady-state feasibility of a given design.

Definition 3: *Let $\epsilon > 0$ be a real number. An inventory $v(x)$ is said to be ϵ-controllable if there exists a $u \in \mathcal{U}$ such that for all $x \in \mathcal{X}$ and all $d \in \mathcal{D}$ the following is true*

$$\min_{u\in\mathcal{U}} \phi(d,y,u)+\epsilon \le -p(x) \le \max_{u\in\mathcal{U}} \phi(d,y,u)-\epsilon \qquad (20)$$

From Eq. 3, we see that if an inventory is ϵ-controllable then it is possible to choose u so that $\dot{v}$ is either positive or negative. It follows that the inventory can be controlled since it can be increased or decreased for every $x \in \mathcal{X}$ and $d \in \mathcal{D}$ by an appropriate choice of $u \in \mathcal{U}$.

The PID controller with antireset windup is somewhat more complicated to state since it includes switching logic. First, we define an auxiliary variable

$$\phi_c(d,y,u) = -\Pi(x) - K_c\tilde{v} - \tau_D\dot{\tilde{v}} + \dot{v}^*$$

where

$$\Pi(x) = \hat{p}(x) + \tau_I^{-1}\int_0^t \tilde{v} b\, d\xi + \hat{p}(0) \qquad \Pi[x(0)] = \hat{p}[x(0)]$$

The binary variable b turns the integrator on and off depending on when a constraint is active.

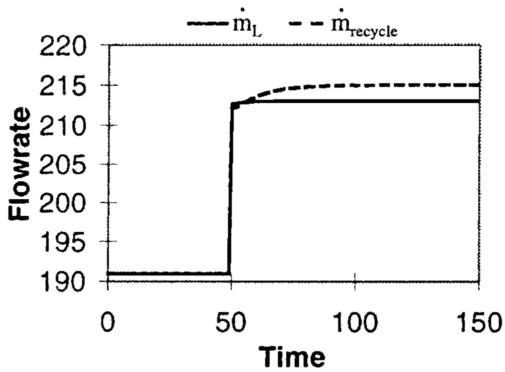

Figure 13. Manipulated variables for flash.

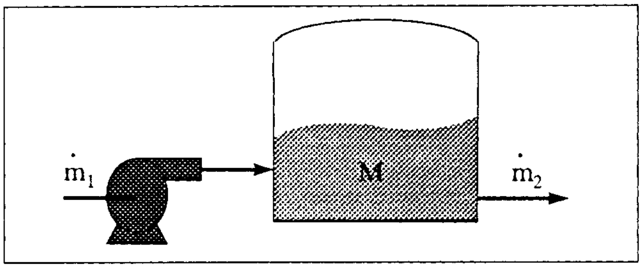

Figure 14. Tank system.

$$b = \begin{cases} 0 & \text{if } \phi = \max\limits_{u\in\mathcal{U}} \phi(d,y,u) \text{ or } \phi = \min\limits_{u\in\mathcal{U}} \phi(d,y,u) \\ 1 & \text{otherwise} \end{cases}$$

The function $\Pi(x)$ is an estimate of $p(x)$ so we constrain this such that

$$\min_{u\in\mathcal{U}} \phi(d,y,u)+\epsilon \le -\Pi(x) \le \max_{u\in\mathcal{U}} \phi(d,y,u)-\epsilon \qquad (21)$$

The switching function is designed so that $\Pi(x)$ lies between the bounds in Eq. 20 and that the integrator is turned off if the flux variable ϕ is constrained. The constrained PID controller can be described by the following

$$\phi(d,y,u) = \begin{cases} \phi_c(d,y,c) & \text{if } \phi_{\min} < \phi_c < \phi_{\max} \\ \phi_{\min} & \text{if } \phi_c \le \phi_{\min} \\ \phi_{\max} & \text{if } \phi_c \ge \phi_{\max} \end{cases}$$

Assumption 3: *The inventory v is ϵ-controllable.*

Result 6: *Suppose that assumptions 3 and 2 are satisfied. The PID controller with antireset windup gives $\lim_{t\to\infty} \|v - v^*\| = 0$ provided $\tau_I > 0$, $\tau_D \ge 0$, $K_c > 0$, and*

$$\begin{array}{lll} \text{i)} & \dot{v}^* \le \frac{1}{2}\epsilon & \text{if } \phi(d,y,u) = \max\limits_{u\in\mathcal{U}} \phi(d,y,u) \\ \text{ii)} & \dot{v}^* \ge -\frac{1}{2}\epsilon & \text{if } \phi(d,y,u) = \min\limits_{u\in\mathcal{U}} \phi(d,y,u) \\ \text{iii)} & |\dot{v}^*| \le K_c \le \infty & \text{otherwise} \end{array}$$

Proof 6: From ϵ-controllability and constraint control we have

$$\left.\begin{array}{r} \dot{v} = p + \phi_{\max} \ge \epsilon \\ \Pi + \phi_{\max} \ge \epsilon \\ \phi_c = -\Pi - K_c\tilde{v} - \tau_D\dot{\tilde{v}} + \dot{v}^* \ge \phi_{\max} \end{array}\right\} \text{ if } \phi = \phi_{\max} \qquad (22)$$

It follows that

$$-K_c\tilde{v} - \tau_D\dot{\tilde{v}} + \dot{v}^* \ge \Pi + \phi_{\max} \ge \epsilon \qquad (23)$$

Now, using Eqs. 22 and 23 this gives

$$-K_c\tilde{v} \ge \epsilon + \tau_D\dot{v} - (1+\tau_D)\dot{v}^* \ge (1+\tau_D)\epsilon - (1+\tau_D)\dot{v}^* \qquad (24)$$

We have $\dot{v}^* \le 1/2\,\epsilon$ and $\tau_D \ge 0$, so that from Eq. 24

$$-K_c\tilde{v} \ge (1+\tau_D)\frac{1}{2}\epsilon \ge \frac{1}{2}\epsilon > 0$$

Hence, since $\epsilon > 0$ and $K_c > 0$,

$$\tilde{v} \le \frac{-\epsilon}{2K_c} < 0 \quad \text{for } \phi = \phi_{\max} \tag{25}$$

Using Eqs. 3 and 20 again, we have

$$\dot{v} = p + \phi$$

$$\dot{\tilde{v}} + \dot{v}^* = p + \phi \ge \epsilon \quad \phi = \phi_{\max}$$

hence

$$\left.\begin{array}{l} \tilde{v} \le \dfrac{-\epsilon}{2K_c} < 0 \\ \dot{\tilde{v}} \ge \dfrac{1}{2}\epsilon > 0 \end{array}\right\} \text{for } \phi = \phi_{\max} \tag{26}$$

Through a similar analysis when $\phi = \phi_{\min}$, we get the following result

$$\left.\begin{array}{l} \tilde{v} \ge \dfrac{\epsilon}{2K_c} > 0 \\ \dot{\tilde{v}} \le -\dfrac{1}{2}\epsilon < 0 \end{array}\right\} \text{for } \phi = \phi_{\min} \tag{27}$$

By combining Eqs. 26 and 27, we then conclude that

$$\dot{\tilde{v}}\tilde{v} \le -\frac{1}{2}\epsilon|\tilde{v}| \quad \text{for } \phi = \phi_{\min} \text{ or } \phi = \phi_{\max} \tag{28}$$

We now define a storage function

$$\Psi = \frac{1}{2}(1+\tau_D)\tilde{v}^2 + \frac{1}{2}\tilde{p}^2\tau_I + \frac{1}{2}\delta\beta^2 \ge 0 \tag{29}$$

where δ is chosen so that

$$\delta = 2\frac{(1+\tau_D)K_c\gamma^2}{|\Pi_2|_\infty^2} > 0 \tag{30}$$

where $|\Pi_2|_\infty = \max_t|\Pi_2(t)|$. It will become evident why this particular form of δ was chosen later in the proof. We then have

$$\dot{\Psi} = b\dot{\Psi} + (1-b)\dot{\Psi}$$

Here the derivative of the storage function has been divided into two parts, one for the constrained case and one for the unconstrained case. By a similar development to that used earlier, we find there exists $\delta_1 > 0$, so that

$$b\dot{\Psi} \le -\delta_1 a\tilde{v}^2 \tag{31}$$

By using Eqs. 28 and 29, we get a PID controller with antireset windup, which gives

$$(1-b)\dot{\tilde{p}} = 0$$

$$(1-b)\dot{\Psi} \le (1-b)\left[(1+\tau_D)\dot{\tilde{v}}\tilde{v} + \delta\beta\dot{\beta}\right]$$

$$\le -(1-b)\left[(1+\tau_D)\frac{1}{2}\epsilon|\tilde{v}| + \delta\gamma^2\beta^2 - \delta\beta\Pi_2\tilde{v}\right]$$

Now from Eq. 28 we have

$$|\tilde{v}| \ge \frac{\epsilon}{2K_c}$$

so that

$$(1-b)\dot{\Psi} \le -(1-b)[(1+\tau_D)K_c\tilde{v}^2 - \delta|\Pi_2|_\infty|\beta\tilde{v}| + \delta\gamma^2\beta^2]$$

$$\le -(1-b)\delta_0\tilde{v}^2, \qquad \delta_0 = \frac{1}{2}(1+\tau_D)K_c > 0 \tag{32}$$

This result comes about by adding and subtracting $-(1-b)\mu_0\tilde{v}^2$ from the righthand side and completing the square. By combining Eqs. 31 and 32 we have

$$\dot{\Psi} \le -(1-b)\delta_0\tilde{v}^2 - b\delta_1\tilde{v}^2$$

$$\le -\delta_2\tilde{v}^2, \quad \delta_2 = \min_{i=0,1}\delta_i$$

The constraints give $\phi_{\min} \le \dot{v} \le \phi_{\max}$ and the result follows.

We will now return to the flash example and observe the stability of the system when one of the control valves is against a constraint. In this example, the energy set point was increased to the point where the steam flow rate could not be increased sufficiently to maintain the internal energy of the flash at its set point. The operating conditions of the flash are the same as those given in Table 1. The theory tells us that this system is not ϵ-controllable at the desired operating condition and that the control objective should be offset from its set point. Figure 15 shows that the control valve for the steam is against its upper bound and that the control objective (internal energy) is offset from its desired set point.

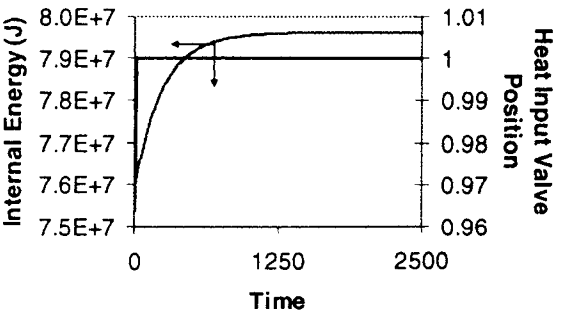

Figure 15. Energy controller for constrained system.

However, we are still able to control for the overall mass and component mass while stabilizing the energy of the system. We cannot guarantee convergence of the error to zero, however, as there will be an offset. This example leads directly into the issue of design feasibility. In order to control all of the objectives of the control system, the equipment must be redesigned. For instance, the heat-transfer area of the heating tubes could be increased to allow for faster transfer rates. Another possibility is to increase the capacity of the steam compressor. This will allow greater flow rates and hence faster heat transfer. At any rate, the system is obviously underdesigned for the given disturbance.

Conclusions

We have linked process thermodynamics and nonlinear control theory by introducing a new class of storage functions based on the first and second laws of thermodynamics. We then used these storage functions to show that:

(1) A passive stationary state is a state of minimum entropy production.

(2) Dissipativity is equivalent to the existence of an entropy function.

(3) A state is passive if and only if the system is dissipative with storage function $A = E - T_0 S + A_0$.

(4) A system with constant states at the boundary converges to a stationary passive state if one exists.

We developed the inventory control method further. A new stability result for inventory control is presented, and examples have been developed to support the theory. These include a ship boiler, a ternary flash, and a continuous stirred-tank reactor with multiple reaction paths. We provided results for inventory control of constrained systems. In this case controllability reduces to a steady-state feasibility problem. In the constrained flash example we expose a direct link between process control and process design.

Acknowledgment

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Notation

α = relative volatility
A = cross-sectional area, m^2
c = specific heat, J/g/°C
e = error
g = acceleration due to gravity, m/s^2
H = enthalpy, kcal/kg
k = proportionality constant
K_E = kinetic energy
λ = latent heat, kcal/kg
L = average height of risers, m
$L_f v$ = Lie derivative of inventory v wrt f
$L_g v$ = Lie derivative of inventory v wrt g
$\dot{m}$ = mass-flow rate, kg/s (boiler example)
$\dot{n}$ = molar flow rate, mol/s (flash and flowsheet examples)
ρ = density, kg/m^3
p = pressure, kp/cm^2
$\dot{Q}$ = heating rate, kcal/s
τ = time constant
t_0 = constant
T = temperature
w = intensive variables conjugate to v
X_0 = steam quality
z = level in the drum, m
$\Re$ = real space

Subscripts

ao = leaving attemperator
d = drum
dow = water entering downcomers
ds = steam in drum
dw = water in drum
eow = feed water leaving economizer
F = feed
F_A = feed of species A
F_B = feed of species B
I = integral
L = liquid product
o = steam water mixture leaving risers
oil = oil rate to burners
ps = primary superheater
psi = entering primary superheater
psm = metal in primary superheater
pso = leaving primary superheater
r = risers
recycle = recycle from flash to reactor
rm = riser metal
ro = steam water mixture in risers
rs = steam in risers
rw = water in risers
s = steam leaving drum
ss = secondary superheater
ssi = entering secondary superheater
ssm = metal in secondary superheater
sso = leaving secondary superheater
V = vapor product
w = water entering drum

Literature Cited

Bejan, A., *Entropy Generation Through Heat and Fluid Flow*, Wiley, New York (1982).

Bird, R., W. Stewart, and E. Lightfoot, *Transport Phenomena*, Wiley, New York (1960).

Buckley, P. S., *Techniques of Process Control*, Wiley, New York (1964).

Byrnes, C. I., A. Isidori, and J. C. Willems, "Passivity, Feedback Equivalence, and the Global Stabilization of Minimum Phases Nonlinear Systems," *IEEE Trans. on Automatic Control*, **36** (1991).

Georgakis, C., "On the Use of Extensive Variables in Process Dynamics and Control," *Chem. E. Sci.*, **41**, 1471 (1986).

Hill, D. J., and P. J. Moylan, "Dissipative Dynamical Systems: Basic Input-Output and State Properties," *J. Franklin Inst.*, **309**, 327 (1980).

Kreuzer, H. J., *Non-equilibrium Thermodynamics and Its Statistical Foundations*, Oxford University Press (1981).

Narraway, L. T., J. D. Perkins, and G. W. Barton, "Interaction Between Process Design and Process Control: Economic Analysis of Process Dynamics," *J. Proc. Cont.*, **1**, 243 (1991).

Onsager, L., *Physical Review*, Vol. 37 (1931).

Sauar, E., S. K. Ratkje, and K. Lien, "Equipartition of Forces—A New Principle for Process Design and Optimization," *Ind. Eng. Chem. Res.*, **35**, 4147 (1996).

Shinskey, F. B., *Process-Control Systems: Application, Design, Adjustment*, McGraw-Hill, New York (1967).

Slotine, J.-J. E., and W. Li, *Applied Nonlinear Control*, Prentice Hall, Englewood Cliffs, NJ (1991).

Tyssφ, A., "Modeling and Parameter Estimation of a Ship Boiler," *Automatica*, 157 (1981).

Ydstie, B., and K. Viswanath, "From Thermodynamics to Process Control," *Symp. on Process Systems Eng.* (1994).

Ydstie, B. E., and A. A. Alonso, "Process Systems and Passivity via the Clausius-Planck Inequality," *Syst. and Cont. Lett.*, **30**, 253 (1997).

Appendix

The following are the equations used to model the ship boiler as developed by Tyssø (1981). The equations are divided up according to the section of the boiler they appear in. The constants for the model are provided in Table A1.

Oil-air flue gas

$$\dot{Q}_{rm} = 6{,}425\dot{m}_{\text{oil}}$$

$$\dot{Q}_{psm} = 1{,}400\dot{m}_{\text{oil}}$$

$$\dot{Q}_{ssm} = 775\dot{m}_{\text{oil}}$$

Water-steam system

$$\frac{dV_{dw}}{dt} = \frac{1}{\rho_{dw}}[(1 - X_0)\dot{m}_o + \dot{m}_w - \dot{m}_{dow}]$$

$$\frac{d\rho_{ds}}{dt} = \frac{1}{V_t - V_{dw}}\left[\dot{m}_o + \dot{m}_w - \dot{m}_{dow} - \dot{m}_s + (\rho_{ds} + \rho_{dw})\frac{dV_{dw}}{dt}\right]$$

$$\frac{dH_{dw}}{dt} = \frac{1}{\rho_{dw}V_{dw}}[\dot{m}_o(1 - X_0)(H_{rw} - H_{dw}) + \dot{m}_w(H_{ewo} - H_{dw}) + \dot{m}_{ws}(H_{ss} - H_{dw}) + \dot{Q}_{aw}]$$

$$\frac{dH_{ro}}{dt} = \frac{1}{V_r\rho_{ro}}\left[\dot{Q}_{rw} - \dot{m}_{dow}(H_{ro} - H_{dow}) - \dot{m}_o\lambda\frac{X_0}{2}\right]$$

$$\frac{T_{rm}}{dt} = \frac{1}{4{,}785}\left(\dot{Q}_{rm} - \dot{Q}_{rw}\right)$$

$$H_{ro} = H_{rw} + X_0\frac{\lambda}{2}$$

$$\rho_{ro} = \rho_{rw} - \alpha(\rho_{rw} - \rho_{rs})$$

$$\alpha = \frac{\frac{X_0}{2}\rho_{rw}}{\rho_{rs} + \frac{X_0}{2}(\rho_{rw} + \rho_{rs})}$$

$$\dot{m}_{ws} = 0.81(H_{ws} - H_{dw})$$

$$\dot{m}_{dow}^2 = \frac{\rho_{dw}Lg - \rho_{ro}Lg}{\frac{k_3 + 1}{2A^2\rho_{ro}} + \frac{k_5}{\rho_{ro}} + \frac{k_4}{\rho_{dw}} + \frac{k_1 + 1}{2A^2\rho_{dw}} + 0.045\left(\frac{X_0\rho_{dw}}{\rho_{dw}} + 1\right)}$$

Table A1. Boiler Design Data

k_1	1.454	$\dot{m}_{\text{oil}}$	1.95 kg/s
k_4	0.01 l/m^4	$\dot{m}_w$	29.2 kg/s
k_5	0.25 l/m^4	T_{ewo}	200°C
k_C	30	k_{rw}	6,425 kcal/kg
g	9.8 m/s^2	L	11.7 m
A	1.7 m^2	k_{ss}	1.283 kcal/kg/°C
V_{dw}	8.2 m^3	V_t	13.3 m^3
V_d	8.2 m^3	V_r	9.8 m^3
Valve	0.19	P_d	73.2 N/cm^2

$$f_1 = \frac{0.5X_0\rho_{rw}^2}{[\rho_{rs} + 0.5X_0(\rho_{rw} - \rho_{rs})]^2}$$

$$f_2 = \frac{\rho_{rs}\rho_{rw}(\rho_{rs} - \rho_{rw})}{[\rho_{rs} + 0.5X_0(\rho_{rw} - \rho_{rs})]^2}$$

$$f_3 = 5.37\exp(-0.026\rho_{ds})$$

$$f_4 = \frac{1}{V_t - V_{dw}}$$

$$f_5 = \frac{\rho_{ds} - \rho_{dw}}{\rho_{dw}}$$

$$f_6 = \frac{1}{\rho_{ro}V_r}$$

$$f_7 = V_rf_1 - \frac{V_rf_2f_3}{\lambda}$$

$$k_3 = 3.62\left[1 + 2{,}400\left(\frac{0.5X_0}{P_d}\right)^{0.96}\right]$$

$$V_{dw} = A_dz + V_d$$

$$V_t = V_{ds} + V_{dw}$$

Super heater

$$P_{pso} = P_d - 0.0023\dot{m}_s^2$$

$$T_{psi} = T_s$$

$$T_{ps} = 0.5(T_{psi} + T_{psm})$$

$$\frac{dT_{psm}}{dt} = \frac{1}{0.11 * 8{,}450}\left(\dot{Q}_{psm} + \dot{m}_sc_{ps}(T_{psi} - T_{pso})\right)$$

$$\dot{m}_o = \frac{\dot{m}_{dow} - \frac{V_rf_2f_6}{\lambda}\left[\dot{Q}_{rw} - \dot{m}_{dow}(H_{ro} - H_{dow})\right] + f_4f_7(\dot{m}_{dow} + \dot{m}_s - \dot{m}_w) + f_4f_5f_7(\dot{m}_{dow} - \dot{m}_w - \dot{m}_{ws})}{1 + f_4f_7 + f_4f_5f_7(1 - X_0) - V_rf_2f_6\frac{X_0}{2}}$$

$$T_{pso}=\frac{-\left(\dot{m}_s^{0.8}k_{ps}\right)^2(T_{psm}-T_{psi})-2(\dot{m}_sc_{ps})^2T_{psi}}{2(\dot{m}_sc_{ps})^2}$$

$$+\frac{\sqrt{\left(\left(\dot{m}_s^{0.8}k_{ps}\right)^2(T_{psm}-T_{psi})-2(\dot{m}_sc_{ps})^2T_{psi}\right)^2-4(\dot{m}_sc_{ps})^2\left(\left(\dot{m}_s^{0.8}k_{ps}\right)^2\left(T_{psi}T_{psm}-T_{psm}^2\right)+(\dot{m}_sc_{ps})^2T_{pso}^2\right)}}{2(\dot{m}_sc_{ps})^2}$$

Attemporator

$$T_{dw}=\frac{H_{dw}+7.42}{1.063}$$

$$\dot{m}_a=0.3\dot{m}_s\,\text{valve}$$

$$\dot{Q}_{aw}=\dot{m}_ac_a(T_{pso}-T_{ao})$$

$$\dot{Q}_{rw}=0.6201(T_{rm}-T_s)^3$$

$$T_{ao}=\frac{-\left((\dot{m}_a^{0.8}k_{as})^2(T_{dw}-T_{pso})-2(\dot{m}_ac_a)^2T_{pso}\right)}{2(\dot{m}_ac_a)^2}$$

$$-\frac{\sqrt{\left((\dot{m}_a^{0.8}k_{as})^2(T_{dw}-T_{pso})-2(\dot{m}_ac_a)^2T_{pso}\right)^2-4(\dot{m}_ac_a)^2\left((\dot{m}_a^{0.8}k_{as})^2\left(T_{pso}T_{dw}-T_{dw}^2\right)+(\dot{m}_ac_a)^2T_{pso}^2\right)}}{2(\dot{m}_ac_a)^2}$$

Heat capacities

$$c_{ps}=31.94+0.001924(T_{ps}+273)+0.00001055(T_{ps}+273)^2-0.000000003596(T_{ps}+273)^3$$

$$c_a=31.94+0.001924(T_{pso}+273)+0.00001055(T_{pso}+273)^2-0.000000003596(T_{pso}+273)^3$$

$$c_{ss}=31.94+0.001924(T_{ss}+273)+0.00001055(T_{ss}+273)^2-0.000000003596(T_{ss}+273)^3$$

Secondary super heater

$$T_{ssi}=\frac{\dot{m}_aT_{ao}+(\dot{m}_s-\dot{m}_a)T_{pso}}{\dot{m}_s}$$

$$\frac{dT_{ssm}}{dt}=\frac{1}{0.11*8{,}450}\left(\dot{Q}_{ssm}+\dot{m}_sc_{ss}(T_{ssi}-T_{sso})\right)$$

$$T_{ss}=0.5(T_{ssm}+T_{ssi})$$

$$P_{ssi}=P_{pso}-0.0057(\dot{m}_s-\dot{m}_a)^2$$

$$P_{sso}=P_{ssi}-0.0023\dot{m}_s^2$$

$$T_{sso}=\frac{-\left((\dot{m}_s^{0.8}k_{ss})^2(T_{ssm}-T_{ssi})-2(\dot{m}_sc_{ss})^2\right)T_{ssi}}{2(\dot{m}_sc_{ss})^2}$$

$$+\frac{\sqrt{\left((\dot{m}_s^{0.8}k_{ss})^2(T_{ssm}-T_{ssi})-2(\dot{m}_sc_{ss})^2T_{ssi}\right)^2-4(\dot{m}_sc_{ss})^2\left((\dot{m}_s^{0.8}k_{ss})^2(T_{ssi}T_{ssm}-T_{ssm}^2)+(\dot{m}_sc_{ss})^2T_{ssm}^2\right)}}{2(\dot{m}_sc_{ss})^2}$$

Pressure dependencies

$$P_d=-1.64+2.263\rho_{ds}-0.007876\rho_{ds}^2+0.000013701\rho_{ds}^3$$

$$\rho_{dw}=902.4-3.062P_d+0.014663P_d^2-0.00005037P_d^3$$

$$\lambda=499.74-2.650P_d+0.0127685P_d^2-0.0000449558P_d^3$$

$$H_{rw}=165.373+3.0991P_d-0.0210698P_d^2+0.0000758123P_d^3$$

$$H_{ss}=665.132+0.391242P_d-0.00834955P_d^2+0.0000311942P_d^3$$

$$T_s=165.26+2.8289P_d-0.021351P_d^2+0.000075372P_d^3$$

Feed conditions

$$H_{ewo}=T_{ewo}1.063-7.42$$

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