Dynamic Consistency Relations for Process Modeling

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Consistency relations are derived from fundamental physical laws such as overall mass and energy balances of a process. They appear to have been first used by Skogestad and Morari (1987) and by Haggblom and Waller (1988) in the context of process control and later elaborated by Skogestad (1991). These relations provide means for establishing relationships between steady-state gains of multivariable processes. Although the articles mentioned above note that these relations may be extended to a dynamic case, no systematic approach appears to have been published that extends their work to a dynamic case. This article, motivated by the work of Farschmann et al. (1998), tries to fill this gap by a general formulation of consistency relations for process systems.

Consistency relations are always satisfied for analytically derived models. Therefore, they do not contain any additional information if the mass and energy balances of the process are observed by the model. However, for empirically derived and/or simplified models, they can bring extra information which may improve the model. Since the consistency relations can be derived without detailed knowledge of the system, their use might be worthwhile. In addition they may be used to check whether the uncertainty of certain parameters are important for a selected control structure.

In this article, dynamic consistency relations are derived from the conserved inventories of a process for the linear(ized) models. A heat exchanger and a distillation column model are used to illustrate their utility. Finally, potential applications of the dynamic consistency relations are pointed out.

Consistency Relations

Notation and some of the ideas in this section are adopted from Farschmann et al. (1998). It is assumed that the measured output y, input u, and the disturbances w of the process are made up of boundary fluxes to the process and can be expressed by the function $\phi(y,u,w)$. This assumption is satisfied for most process systems. Internal state description of the system can be expressed as

$$\begin{aligned}\dot{x} &= f(x) + g(x,u,w)\\ y &= \hat{C}x = [I \quad 0]\begin{bmatrix} x_e \\ x_i \end{bmatrix}\end{aligned} \tag{1}$$

x_i are the internal states of the process and x_e are the states that constitute the output y (it is possible to extend the results of this article to the case $y = h(x_e,u)$). Since the output of most process systems can be expressed as a linear function of the states (that is, $y = Cx$) and since the special form of $\hat{C}$ in Eq. 1 can be obtained by a state transformation, this assumption is not restrictive, but is used for brevity. It is further assumed that the number of outputs is at least equal to the number of inputs. Associated with the system (Eq. 1), there are conserved inventories $\upsilon(x)$, for example, component mass and energy. Consistency relations express the conservation property of $\upsilon(x)$ in differential form. The time derivative of an inventory $\upsilon(x)$ can be expressed as in Farschmann et al. (1998)

$$\begin{aligned}\frac{d\upsilon(x)}{dt} = \frac{\partial \upsilon}{\partial x}\frac{dx}{dt} = \frac{\partial \upsilon}{\partial x}f(x) + \frac{\partial \upsilon}{\partial x}g(x,u,w)\\ = p(x) + \phi(y,u,w)\end{aligned} \tag{2}$$

where $p(x) = (\partial \upsilon/\partial x)f(x) + p^*$ is the rate of production, $\phi(y,u,w) = (\partial \upsilon/\partial x)g(x) - p^*$ is the rate of supply of the inventory, and p^* is the steady-state production rate. Note that the rate of supply ϕ is a function of y rather than x because of the special form of y in Eq. 1. If i'th inventory $\upsilon_i(x)$ is conserved, then, $p_i(x) = 0$.

Steady-state relations

The conserved inventories of processes, such as component mass and energy, can be expressed at steady state with the function $\phi(y,u,w) = 0$ (Farschmann et al., 1998), which states that the difference between input and output fluxes of the inventories is zero at steady state. The consistency relationship at steady state simply expresses the following differential identity

$$d\phi = \frac{\partial \phi}{\partial y}dy + \frac{\partial \phi}{\partial u}du + \frac{\partial \phi}{\partial w}dw = 0 \tag{3}$$

This equation can be used to relate input and disturbance gains of the process. If the output y is kept constant ($dy = 0$), and Eq. 3 is integrated, the form consistency relations used in Skogestad (1991) can be obtained. These relations, called *consistency from variable transformations* in Skogestad (1991), are valid only for the steady state and result in relations between the *row* elements of the gain matrices. Other types of consistency relations which Skogestad (1991) calls *consistency from material balances* result in relations between the *column* elements of transfer function matrices. These relations are used to determine dependencies for one input (or disturbance) variable. Only the latter of the relations is dealt with in this article.

Since $dy = G_u(0)du + G_w(0)dw$, where $G_u(0)$ and $G_w(0)$ are the steady-state gain matrices for inputs and disturbances, Eq. 3 can be expressed as

$$d\phi = \left(\frac{\partial \phi}{\partial u} + \frac{\partial \phi}{\partial y} G_u(0) \right) du + \left(\frac{\partial \phi}{\partial w} + \frac{\partial \phi}{\partial y} G_w(0) \right) dw = 0$$

If du and dw are independent, Eq. 4 can be satisfied when both terms inside parentheses are zero. Therefore, we obtain

$$\gamma_u^T = \alpha_0^T G_u(0) \tag{4}$$

$$\gamma_w^T = \alpha_0^T G_w(0) \tag{5}$$

where $\alpha_0^T = -\,\partial\phi/\partial y$, $\gamma_u^T = \partial\phi/\partial u$ and $\gamma_w^T = \partial\phi/\partial w$ are constant row vectors. Equations 4 and 5 may be compactly expressed as

$$\begin{bmatrix} G_u(0)^T \\ G_w(0)^T \end{bmatrix} \alpha_0 = \begin{bmatrix} \gamma_u \\ \gamma_w \end{bmatrix} \tag{6}$$

Column elements of $G_u(0)$ and $G_w(0)$ are related within themselves with Eq. 6.

Dynamic relations

Consistency relations derived from the conserved inventories of a process can be extended to the dynamic case. For this purpose, Eq. 2 can be written as

$$\frac{dv(x)}{dt} = \frac{\partial v}{\partial y}\frac{dy}{dt} + \frac{\partial v}{\partial x_i}\frac{dx_i}{dt} = p(x) + \phi(y,u,w) \tag{7}$$

Linearizing Eq. 7 about an equilibrium point, we can obtain

$$\frac{\partial v}{\partial y}\delta \dot{y} - \frac{\partial \phi}{\partial y}\delta y = \frac{\partial \phi}{\partial u}\delta u + \frac{\partial \phi}{\partial w}\delta w + \frac{\partial p}{\partial x}\delta x - \frac{\partial v}{\partial x_i}\delta \dot{x}_i \tag{8}$$

Note that all partial derivative terms are row vectors. Since $(\partial p/\partial x)\delta x = (\partial p/\partial y)\delta y + (\partial p/\partial x_i)\delta x_i$, Eq. 8 may be expressed as

$$\left(\frac{\partial v}{\partial y}\delta \dot{y} - \frac{\partial p}{\partial y}\delta y - \frac{\partial \phi}{\partial y}\delta y \right) = \left(\frac{\partial \phi}{\partial u}\delta u + \frac{\partial \phi}{\partial w}\delta w - \frac{\partial v}{\partial x_i}\delta \dot{x}_i + \frac{\partial p}{\partial x_i}\delta x_i \right) \tag{9}$$

Defining

$$\delta y = G_u(s)\,\delta u + G_w(s)\,\delta w \tag{10}$$

$$\delta x_i = H_u(s)\,\delta u + H_w(s)\,\delta w \tag{11}$$

$$\alpha^T = s\frac{\partial v}{\partial y} - \frac{\partial p}{\partial y} - \frac{\partial \phi}{\partial y} \tag{12}$$

$$\beta^T = s\frac{\partial v}{\partial x_i} - \frac{\partial p}{\partial x_i} \tag{13}$$

$$\gamma_u^T = \frac{\partial \phi}{\partial u} \tag{14}$$

$$\gamma_w^T = \frac{\partial \phi}{\partial w} \tag{15}$$

and after taking its Laplace transform, Eq. 9 leads to

$$\left(\alpha^T(s)G_u(s) + \beta^T(s)H_u(s) - \gamma_u^T \right)\delta u + \left(\alpha^T(s)G_w(s) + \beta^T(s)H_w(s) - \gamma_w^T \right)\delta w = 0 \tag{16}$$

Since δu and δw are independent, Eq. 16 can be satisfied only if both terms inside the parentheses are zero. Therefore, Eq. 16 can be compactly expressed as

$$\begin{bmatrix} G_u(s) & G_w(s) \\ H_u(s) & H_w(s) \end{bmatrix}^T \begin{bmatrix} \alpha(s) \\ \beta(s) \end{bmatrix} = \begin{bmatrix} \gamma_u \\ \gamma_w \end{bmatrix} \tag{17}$$

Equation 17 relates the column elements of transfer function matrices $G_u(s)$ and $G_w(s)$. Note that for $s = 0$, and no internal generation ($p(x) = 0$), we get the steady-state consistency relationships given in Eq. 6.

For a general nonreacting process, we have $n_c - 1$ independent component and mass balances and one energy balance, where n_c is the number of components. For each of these balances, an equation such as Eq. 16 can be written. Since a process can have $n_c + 1$ independent variables (plus the local inventories such as levels, which can be controlled by extra flows), the number of outputs y is $N = n_c + 1$. Therefore, the terms $\alpha(s)$ and $\gamma(s)$ in Eq. 16 have dimensions $N \times (N-1) = (n_c + 1) \times n_c$. The dimension of $\beta(s)$ in this equation is $N \times n_{x_i}$ where n_{x_i} is the dimension of x_i.

Examples

Simplified heat exchanger model

Consider the simplified model of a counterflow heat exchanger. Suppose the outputs of the system are exit temperatures of the hot and cold fluids T_h and T_c, and the inputs are flow rates of the two streams q_h and q_c. The system is modeled using a mixing tank assumption for the hot and cold fluid sides. Assuming that the input temperatures T_{hi} and T_{ci} remain constant and the densities and the specific heats of both streams are the same and no heat is lost to the environment, the overall energy balance gives

$$V_c\frac{dT_c}{dt} + V_h\frac{dT_h}{dt} = q_c(T_{ci} - T_c) + q_h(T_{hi} - T_h) \tag{18}$$

Linearizing Eq. 18 about a steady-state operating point, we obtain

$$V_c \frac{d\delta T_c}{dt} + V_h \frac{d\delta T_h}{dt} = \delta q_c\left(\overline{T}_{ci} - \overline{T}_c\right) + \delta q_h\left(\overline{T}_{hi} - \overline{T}_h\right) - \bar{q}_c \delta T_c - \bar{q}_h \delta T_h \tag{19}$$

The overbar denotes the steady-state values and the δ terms before the variables show small changes about the operating point. Following the procedure outlined in the previous section, and defining $\tau_h = V_h/\bar{q}_h$ and $\tau_c = V_c/\bar{q}_c$ (Eq. 19) leads to

$$\begin{bmatrix} g_{hh}(s) & g_{hc}(s) \\ g_{ch}(s) & g_{cc}(s) \end{bmatrix}^T \begin{bmatrix} \bar{q}_h(1+\tau_h s) \\ \bar{q}_c(1+\tau_c s) \end{bmatrix} = \begin{bmatrix} \left(\overline{T}_{hi} - \overline{T}_h\right) \\ \left(\overline{T}_{ci} - \overline{T}_c\right) \end{bmatrix} \tag{20}$$

which is of the same form with the upper part of Eq. 17. The expression for the consistency relations in Eq. 20 is particularly simple because of the simplifying assumptions (mixing tank) made in modeling. Assuming $\tau_c = \tau_h = \tau$ and $\bar{q}_c = \bar{q}_h = \bar{q}$, the linearized model for this heat exchanger is (Jacobsen and Skogestad, 1994)

$$G(s) = \frac{\gamma}{(\tau s + 1)(\tau s + 1 + 2a)} \begin{bmatrix} \tau s + 1 + a & -a \\ a & -(\tau s + 1 + a) \end{bmatrix} \tag{21}$$

where $a = UA/\rho \bar{q} c_p$ and $\gamma = (\overline{T}_{hi} - \overline{T}_h)/\bar{q}_h = -(\overline{T}_{ci} - \overline{T}_c)/\bar{q}_c$.

Note that Eq. 20 is obeyed by the model in Eq. 21, regardless of the parameter a. This should have been obvious, since the parameter a relates to the heat transfer inside the heat exchanger, whereas Eq. 20 is obtained from an "exterior" energy balance.

Distillation Column Model

As a second and a more complicated example, consider the model of the binary distillation process with linear liquid dynamics in each tray. Suppose the conventional $L - V$ (reflux-boilup) structure is selected for the control of the compositions x_D and x_B. Equimolal overflow assumption renders vapor flow V up the column equal on all trays and makes the energy balance equation superfluous. An overall material balance for a component of the binary distillation column gives the following equation

$$\frac{d}{dt}\left(M_B x_B + \sum_{j=2}^{N} M_j x_j + M_D x_D \right) = F z_F - D x_D - B x_B \tag{22}$$

where F is the feed rate, D and B are the distillate and bottoms flow rates, x_D and x_B are the top and bottom compositions, and z_F is the feed composition and j is the index for the trays, starting from column bottoms (counted as tray number 1) and ending at a condenser drum (tray number $N + 1$). Linear flow dynamics for each tray is assumed, that is

$$\frac{L_j(s)}{L_{j+1}(s)} = \frac{1}{\tau_t s + 1} \tag{23}$$

with τ_t being the tray time constant and the reflux is $L = L_{N+1}$. Proportional level control on bottoms and condenser is also assumed ($\delta D = K_D \delta M_D$ and $\delta B = K_B \delta M_B$). Using these relations, and linearizing and taking Laplace transform, Eq. 22 leads to

$$\left(\overline{M}_B s + \overline{B}\right)\delta x_B + \left(\overline{M}_D s + \overline{D}\right)\delta x_D + s\left(\sum_{j=2}^{N} \overline{M}_j \delta x_j + \bar{x}_j \delta M_j \right) = \bar{x}_D(\delta L - \delta V) - \bar{x}_B\left[\delta V - g_L(s)\delta L\right] \tag{24}$$

where

$$g_L(s) = \frac{1}{(\tau_t s + 1)^N} \tag{25}$$

Expressing δx_D and δx_B in terms of inputs δL and δV

$$\begin{bmatrix} \delta x_D \\ \delta x_B \end{bmatrix} = \begin{bmatrix} g_{x_D L}(s) & g_{x_D V}(s) \\ g_{x_B L}(s) & g_{x_B V}(s) \end{bmatrix} \begin{bmatrix} \delta L \\ \delta V \end{bmatrix} \tag{26}$$

Equation 24 may be written as

$$\begin{bmatrix} g_{x_D L}(s) & g_{x_B L}(s) \\ g_{x_D V}(s) & g_{x_B V}(s) \end{bmatrix} \begin{bmatrix} \overline{M}_D s + \overline{D} \\ \overline{M}_B s + \overline{B} \end{bmatrix} + \left\{ \begin{matrix} \left[s \sum_{j=2}^{N} \overline{M}_j g_{x_j L}(s) + \bar{x}_j g_{M_j L}(s) \right] \\ \left(s \sum_{j=2}^{N} \overline{M}_j g_{x_j V}(s) \right) \end{matrix} \right\} = \left\{ \begin{matrix} \left[\bar{x}_D - g_L(s)\bar{x}_B\right] \\ -(\bar{x}_D - \bar{x}_B) \end{matrix} \right\} \tag{27}$$

Equation 27 for binary distillation is again of the same form as Eq. 17. This equation is more complex than the corresponding equation for the heat exchanger model (Eq. 20), because distillation contains multiple stages which are internal to the process. Some of the terms in Eq. 27 such as $g_{x_j L}(s)$, $g_{x_j V}(s)$ and $g_{M_j L}(s)$ are the transfer functions that relate composition and the holdup at jth tray to the input variables L and V. If a detailed first principle dynamic model of the system is available, these terms in the above equation can be computed from it. Otherwise, they have to be estimated from simple models. An interesting fact is that the level control gains K_D and K_B do not influence the consistency relation (Eq. 27). This is also expected; it is well-known that the L-V distillation control structure is not affected by the tuning of the level controllers. The steady-state consistency relation for distillation can be obtained from Eq. 27 setting $s = 0$ as

$$\begin{bmatrix} g_{x_D L}(0) & g_{x_B L}(0) \\ g_{x_D V}(0) & g_{x_B V}(0) \end{bmatrix} \begin{bmatrix} \overline{D} \\ \overline{B} \end{bmatrix} = \begin{bmatrix} (\bar{x}_D - \bar{x}_B) \\ -(\bar{x}_D - \bar{x}_B) \end{bmatrix} \tag{28}$$

This equation was given both in Haggblom and Waller (1988) and Skogestad and Morari (1987).

Discussion and Conclusions

The dynamic consistency relations that relate the transfer function matrix elements of a process have the potential of application in the following areas.

Steady state and dynamic gain reconciliation

Analytically derived transfer functions always obey the consistency relations in Eq. 17. For empirical and/or simplified models, consistency equations are not automatically satisfied, unless we reconcile them with the data and/or with the model in hand. Reconciliation of steady-state gains of transfer function elements can be done by expressing the steady-state consistency relations as constraint equations on the system parameters and then solving a constrained minimization problem.

Reconciling dynamic transfer function elements is more problematic since the consistency relations may contain many unknown terms, as in Eq. 27. However, if the internal stages of the process are made up of identical subsystems (as identical trays in the case of distillation), then estimating a model for a single subsystem can give us information about the rest. It might then be possible to reconcile the dynamics of the process as well as the steady state.

Reduced order models

As noted by Jacobsen and Skogestad (1994), there is a need for developing low order models, whose parameters have physical significance. For example, the above mentioned article notes that obtaining consistent low order dynamic models of high purity distillation columns is an open research problem. (The term "consistency" in this statement is not in this article's sense, rather that the number of slow poles of the model should be the same with the real process.) Consistency relations in conjunction with some physical insight about the process can help us derive realistic lower order models. Lower order models may not satisfy the consistency relations exactly, but these relations can be used to define a criterion to be minimized while obtaining the parameters of reduced models. In this case, parameters will have more physical significance compared to the ones estimated purely using data. In addition, the estimated parameters will be more reliable.

Model uncertainty

Consistency relations help us determine the effect of variation of certain parameters on the overall mass and energy balances. The parameters that do not affect the overall balances do not appear in α, β, and γ terms in Eq. 17. For example, in the heat exchanger model, the term a in Eq. 21 is not seen in the consistency relation 20. Similarly, for the distillation column model, the relative volatility and level control gains K_D and K_B have no effect on the consistency relation 27. Therefore, use of consistency relations can clarify which parameters might be important for a selected control structure. It might also be possible to reduce conservatism in "black-box" uncertainty modeling by expressing the portion of the uncertainty that does not violate the mass and energy balances in structured form.

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