

CONSISTENCY RELATIONS IN PROCESS MODELING

Esref Eskinat

*Department of Mechanical Engineering, Bogazici University,
Istanbul, Turkey
E-mail : eskinat@boun.edu.tr*

Abstract: Fundamental mass and energy balances that exist in process systems can be used for modeling. Elements of transfer function matrices come out to be dependent when these balances are observed. Examples are given on two process system models. These relationships have the potential of application in modeling, identification and model reduction.

Keywords: Process control, Consistency relations, Modeling

1. INTRODUCTION

The consistency relations are derived from overall mass and energy balances of a process. They seem 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 all of the papers mentioned above note that these relations may be extended to dynamic case, no systematic approach that extends their work to dynamic case seems to have been published. This paper, motivated by the work of [Farschmann et.al. (1998)], tries to fill this gap by a general formulation of consistency relations of process systems.

Consistency relations are always satisfied for analytically derived models. Therefore, they do not contain any extra information if the mass and energy balances of the process are observed. 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 the model and/or parameters of the system are important for a selected control structure.

In the paper, consistency relations will be derived from the conserved inventories of a process for the linear(ized) models. They are applied on a heat exchanger and a distillation column model. Finally, potential applications of these relations will be pointed out.

2. CONSISTENCY RELATIONS

Notation and some of the ideas in this section are adopted from Farschmann et.al. (1998). Consider the following process system :

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

x_i are the internal states of the process and x_e are the states that constitute the output y . It is assumed that the output of the process y is equal to the 'external' states x_e . Since the output of most process systems can be expressed as a linear function of the states (i.e., $y = Cx$) and since the special form of \hat{C} in equation (1) can be obtained

by a state transformation, this assumption is not restrictive. Associated with the system (1), there are conserved inventories $v(x)$, such as component mass and energy. Consistency relations express the conservation property of $v(x)$ in differential form. The time derivative of an inventory $v(x)$ can be expressed as [Farschmann et.al. (1998)]:

$$\begin{aligned} \frac{dv}{dt} &= \frac{\partial v}{\partial x} \frac{dx}{dt} = \frac{\partial v}{\partial x} f(x) + \frac{\partial v}{\partial x} g(x, u, w) \\ &= p(x) + \phi(y, u, w) \end{aligned} \quad (2)$$

where $p(x)$ is the rate of production and $\phi(y, u, w)$ is the rate of supply of the inventory. If the inventory $v(x)$ is conserved, then, $p(x) = 0$.

2.1 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 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:

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

This equation can be used to relate input and disturbance gains of the process. If the output y is kept constant ($dy = 0$), and equation (3) is integrated, the form in which consistency relations are used in and Skogestad (1991) can be obtained. These relations which are 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 type 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. We are mainly concerned with these relations in this paper.

Since $dy = G_{yu}(0)du + G_{yw}(0)dw$, where $G_u(0)$ and $G_w(0)$ are the steady state gain matrices for inputs and disturbances, equation (3) can be expressed as:

$$\begin{aligned} dv &= \left(\frac{\partial \phi}{\partial u} + \frac{\partial \phi}{\partial y} G_{yu}(0) \right) du \\ &+ \left(\frac{\partial \phi}{\partial w} + \frac{\partial \phi}{\partial y} G_{yw}(0) \right) dw = 0 \end{aligned} \quad (4)$$

If du and dw are independent, equation (4) can be satisfied if both terms inside parentheses are zero. Therefore we obtain:

$$\gamma_u^T = \alpha_0^T G_{yu}(0) \quad (5)$$

$$\gamma_w^T = \alpha_0^T G_{yw}(0) \quad (6)$$

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 (5) may be compactly expressed as:

$$\begin{bmatrix} G_{yu}(0)^T \\ G_{yw}(0)^T \end{bmatrix} \alpha_0 = \begin{bmatrix} \gamma_u \\ \gamma_w \end{bmatrix} \quad (7)$$

This equation relates column elements of $G_{yu}(0)$ and $G_{yw}(0)$. However, it is possible to extend these relations to the dynamic case as well.

2.2 Dynamic Relations

The consistency relations derived from conserved inventories of the process can be extended to the dynamic case as well. In this case equation (2) can be written as:

$$\frac{dv(x)}{dt} = \frac{\partial v}{\partial y} \frac{dy}{dt} + \frac{\partial v}{\partial x_i} \frac{dx_i}{dt} = p(x) + \phi(y, u, w) \quad (8)$$

Linearizing equation (8) about an equilibrium point, we can obtain:

$$\begin{aligned} \frac{\partial v}{\partial y} \delta y - \frac{\partial \phi}{\partial y} \delta y = \\ \frac{\partial \phi}{\partial u} \delta u + \frac{\partial \phi}{\partial w} \delta w + \frac{\partial p}{\partial x} \delta x - \frac{\partial v}{\partial x_i} \delta x_i \end{aligned} \quad (9)$$

Note that all partial derivative terms are row vectors and that the δ terms before the variables indicate small deviations. Since $\frac{\partial p}{\partial x} \delta x = \frac{\partial p}{\partial y} \delta y + \frac{\partial p}{\partial x_i} \delta x_i$, equation (9) may be written as:

$$\begin{aligned} \left(\frac{\partial v}{\partial y} \delta y - \frac{\partial p}{\partial y} \delta y - \frac{\partial \phi}{\partial y} \delta y \right) = \\ \left(\frac{\partial \phi}{\partial u} \delta u + \frac{\partial \phi}{\partial w} \delta w - \frac{\partial v}{\partial x_i} \delta x_i + \frac{\partial p}{\partial x_i} \delta x_i \right) \end{aligned} \quad (10)$$

Defining:

$$\delta y = G_{yu}(s)\delta u + G_{yw}(s)\delta w \quad (11)$$

$$\delta x_i = H_u(s)\delta u + H_w(s)\delta w \quad (12)$$

$$\alpha^T = s \frac{\partial v}{\partial y} - \frac{\partial p}{\partial y} - \frac{\partial \phi}{\partial y} \quad (13)$$

$$\beta^T = s \frac{\partial v}{\partial x_i} - \frac{\partial p}{\partial x_i} \quad (14)$$

$$\gamma_u^T = \frac{\partial \phi}{\partial u} \quad (15)$$

$$\gamma_w^T = \frac{\partial \phi}{\partial w} \quad (16)$$

and after taking its Laplace transform, equation (10) leads to:

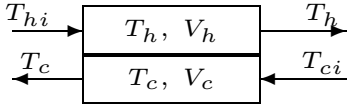


Fig. 1. Simplified heat exchanger process

$$\begin{aligned} & (\alpha^T(s)G_{yu}(s) + \beta^T(s)H_u(s) - \gamma_u^T) \delta u + \\ & (\alpha^T(s)G_{yw}(s) + \beta^T(s)H_w(s) - \gamma_w^T) \delta w = 0 \end{aligned} \quad (17)$$

Since δu and δw are independent, equation (17) can be satisfied only if both terms inside the parentheses are zero. Therefore, equation (17) can be compactly expressed as:

$$\begin{bmatrix} G_{yu}(s) & G_{yw}(s) \\ H_u(s) & H_w(s) \end{bmatrix}^T \begin{bmatrix} \alpha(s) \\ \beta(s) \end{bmatrix} = \begin{bmatrix} \gamma_u \\ \gamma_w \end{bmatrix} \quad (18)$$

Note that for $s = 0$, and no internal generation ($p(x) = 0$) we get the steady-state consistency relationship given in equation (7).

For a general non-reacting 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 (17) 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 equation (17) have dimensions $N \times (N - 1) = (n_c + 1) \times n_c$. The dimension of $\beta(s)$ in this equation is $n_{x_i} \times (N - 1)$ where n_{x_i} is the dimension of x_i .

3. EXAMPLES

3.1 Simplified Heat Exchanger Model

Consider the simplified model of counterflow heat exchanger in Figure 1. 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, the overall energy balance gives:

$$\begin{aligned} & V_c \frac{dT_c}{dt} + V_h \frac{dT_h}{dt} = \\ & q_c(T_{ci} - T_c) + q_h(T_{hi} - T_h) \end{aligned} \quad (19)$$

linearizing equation (19) about a steady state operating point, we obtain :

$$\begin{aligned} & V_c \frac{d\delta T_c}{dt} + V_h \frac{d\delta T_h}{dt} = \delta q_c(\bar{T}_{ci} - \bar{T}_c) \\ & + \delta q_h(\bar{T}_{hi} - \bar{T}_h) - \bar{q}_c \delta T_c - \bar{q}_h \delta T_h \end{aligned} \quad (20)$$

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 above section, and defining $\tau_h = V_h/\bar{q}_h$ and $\tau_c = V_c/\bar{q}_c$ equation (20) leads to:

$$\begin{bmatrix} g_{hh}(s) & g_{hc}(s) \\ g_{ch}(s) & g_{cc}(s) \end{bmatrix}^T \begin{bmatrix} \bar{q}_h(1 + \tau_h s) \\ \bar{q}_c(1 + \tau_c s) \end{bmatrix} = \begin{bmatrix} (\bar{T}_{hi} - \bar{T}_h) \\ (\bar{T}_{ci} - \bar{T}_c) \end{bmatrix} \quad (21)$$

which is of the same form with the upper part of equation (18). The expression for the consistency relations in equation (21) 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]:

$$\begin{aligned} G(s) &= \frac{\gamma}{(\tau s + 1)(\tau s + 1 + 2a)} \\ & \begin{bmatrix} \tau s + 1 + a & -a \\ a & -(\tau s + 1 + a) \end{bmatrix} \end{aligned} \quad (22)$$

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

Note that equation (21) is obeyed by the model in (22), regardless of the parameter a . This should have been obvious, since the parameter a relates to the heat transfer inside the heat exchanger whereas equation (21) is obtained from an 'exterior' energy balance.

3.2 Distillation Column Model

As a second and a more complicated example, consider the model of the binary distillation process in Figure 2 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 . Equimolar 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:

$$\begin{aligned} & \frac{d}{dt}(M_B x_B + \sum_{j=2}^N M_j x_j + M_D x_D) = \\ & F z_F - D x_D - B x_B \end{aligned} \quad (23)$$

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,

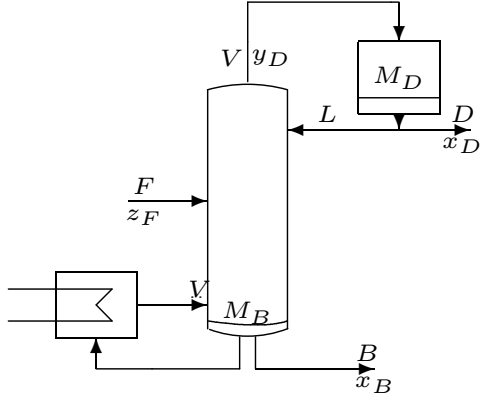


Fig. 2. Binary distillation process

starting from column bottoms (counted as tray number 1) and ending at condenser drum (tray number $N + 1$). Linear flow dynamics for each tray is assumed, that is:

$$\frac{L_j(s)}{L_{j+1}(s)} = \frac{1}{\tau_t s + 1} \quad (24)$$

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, and linearizing and taking Laplace transform, equation (23) leads to:

$$\begin{aligned} & (\bar{M}_B s + \bar{B}) \delta x_B + (\bar{M}_D s + \bar{D}) \delta x_D + \\ & s \left(\sum_{j=2}^N \bar{M}_j \delta x_j + \bar{x}_j \delta M_j \right) = \\ & \bar{x}_D (\delta L - \delta V) - \bar{x}_B (\delta V - g_L(s) \delta L) \end{aligned} \quad (25)$$

where:

$$g_L(s) = \frac{1}{(\tau_t s + 1)^N} \quad (26)$$

Expressing δx_D and δx_B in terms of inputs δL and δV :

$$\begin{bmatrix} \delta x_D \\ \delta x_B \end{bmatrix} = \begin{bmatrix} g_{x_D L}(s) & g_{x_D V}(s) \\ g_{x_B L}(s) & g_{x_B V}(s) \end{bmatrix} \begin{bmatrix} \delta L \\ \delta V \end{bmatrix} \quad (27)$$

equation (25) may be written as:

$$\begin{aligned} & \begin{bmatrix} g_{x_D L}(s) & g_{x_B L}(s) \\ g_{x_D V}(s) & g_{x_B V}(s) \end{bmatrix} \begin{bmatrix} \bar{M}_D s + \bar{D} \\ \bar{M}_B s + \bar{B} \end{bmatrix} \\ & + \begin{bmatrix} s \sum_{j=2}^N (\bar{M}_j g_{x_j L}(s) + \bar{x}_j g_{M_j L}(s)) \\ s \sum_{j=2}^N \bar{M}_j g_{x_j V}(s) \end{bmatrix} \\ & = \begin{bmatrix} (\bar{x}_D - g_L(s) \bar{x}_B) \\ -(\bar{x}_D - \bar{x}_B) \end{bmatrix} \end{aligned} \quad (28)$$

Equation (28) for binary distillation is again of the same form as equation (18). This equation is more complex than the corresponding equation for the heat exchanger model (21), because distillation contains multiple stages which are internal to the process. Some of the terms in (28) 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 j^{th} 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. More will be said about this in the next section. Another interesting fact is that the level control gains K_D and K_B do not influence the consistency relation (28). 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 equation (28) (setting $s = 0$) as:

$$\begin{bmatrix} k_{x_D L} & k_{x_B L} \\ k_{x_D V} & k_{x_B V} \end{bmatrix} \begin{bmatrix} \bar{D} \\ \bar{B} \end{bmatrix} = \begin{bmatrix} (\bar{x}_D - \bar{x}_B) \\ -(\bar{x}_D - \bar{x}_B) \end{bmatrix} \quad (29)$$

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

4. APPLICATIONS

The consistency relations have the potential of application in:

- Steady state and dynamic gain reconciliation.
- Deriving reduced order models.
- Model uncertainty description for 'internal' parameter changes.

Each of these cases shall be briefly reviewed in this section:

4.1 Steady state and dynamic gain reconciliation

Analytically derived transfer functions always obey the consistency relations in equation (18). 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 the gains transfer function elements can be done, as described in [Eskinat(1995)], by expressing the steady-state consistency relations as constraint equations on the system parameters and then solving a constrained minimization problem to obtain the system parameters.

Suppose the system transfer function is linearly parameterized in terms of the system parameters θ as $G(s) = B^T(s)\theta$. The consistency relations at

steady state may be expressed as in equation (7). With some manipulation, upper part of equation (7) can be expressed as a linear function of parameters θ :

$$\Lambda\theta = \gamma_u \quad (30)$$

Then, the linear equations in (30) can be enforced in parameter estimation, using constrained least squares. The constrained estimates obeying (30) are given by:

$$\bar{\theta} = \hat{\theta} - R^{-1}\Lambda^T(\Lambda R^{-1}\Lambda^T)^{-1}(\Lambda\hat{\theta} - \gamma_u) \quad (31)$$

where $\hat{\theta}$ is the unconstrained solution and R is the covariance matrix of $\hat{\theta}$. Variance of the estimated parameters $\bar{\theta}$ are also reduced in this approach. See Eskinat (1995) for more details.

Reconciling dynamic transfer function elements is more problematic since the consistency relations may contain many unknown terms, as in equation (28). 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.

4.2 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 paper notes that ‘‘Obtaining consistent low order dynamic models of high purity distillation columns is (...) an open research problem’’ (The term ‘consistent’ is used in the sense 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 as 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 plant data and/or optimization techniques. In addition the parameters obtained will be more reliable.

4.3 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

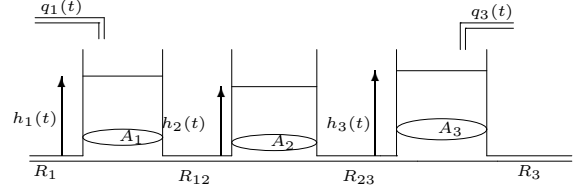


Fig. 3. Simple three-tank process.

α, β and γ terms in equation (18). For example, in the heat exchanger model, the term a in equation (22) is not seen in the consistency relation (21). 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 (28). Therefore, use of consistency relations clarify which parameters might be important for a selected control structure.

As an example, consider the heat exchanger model. Suppose the internal parameter a in equation (22) changes as $a = a_0 + w\delta_a$ where δ_a ($|\delta_a| < 1$) and w are scalars. Since the parametric uncertainty is linear fractional in terms of $G(s)$ and $w\delta_a$, after some calculation, the uncertain plant $G_p(s)$ with perturbation δ_a can be expressed as:

$$G_p(s) = G(s) + \frac{\gamma}{(\tau s + 1 + 2a_0)^2} \begin{bmatrix} -1 & -1 \\ 1 & 1 \end{bmatrix} w\delta_a \left(1 + \frac{2w\delta_a}{(\tau s + 1 + 2a_0)} \right)^{-1} \quad (32)$$

where $G(s)$ is defined in equation (22). Defining:

$$\zeta = w\delta_a \left(1 + \frac{2w\delta_a}{(\tau s + 1 + 2a_0)} \right)^{-1} \quad (33)$$

$$\Psi = \frac{\gamma}{(\tau s + 1 + 2a_0)^2} \begin{bmatrix} -1 & -1 \\ 1 & 1 \end{bmatrix} \quad (34)$$

Equation (32) can be expressed as:

$$G_p(s) = G(s) + \Psi(s)\zeta \quad (35)$$

where $\Psi(s)$ obeys:

$$\alpha^T(s)\Psi(s) = 0 \quad (36)$$

and $\alpha(s)$ is defined in equations (13) and (21). Therefore, $\alpha(s)$ is in the null space of $\Psi^T(s)$. This insight may be generalized to processes with multiple parameter variations.

As another example, consider the three-tank process shown in Figure 3. Considering h_1 and h_3 as outputs and q_1 and q_3 as inputs, the consistency equation for this process can be derived as:

$$\begin{bmatrix} g_{11}(s) & g_{31}(s) \\ g_{13}(s) & g_{33}(s) \end{bmatrix} \begin{bmatrix} A_1 s + 1/R_1 \\ A_2 s + 1/R_2 \end{bmatrix} + \begin{bmatrix} sA_2 g_{21}(s) \\ sA_2 g_{23}(s) \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad (37)$$

where $g_{ij}(s)$ is defined as the transfer function between i 'th tank height and j 'th flow. Since the parameters R_{21} and R_{23} do not appear in the consistency equation (37), consistency equations are not affected by the changes in these parameters. When R_{21} and R_{23} change, the individual transfer function elements $g_{ij}(s)$ change in such a way that the equation (37) holds. However, changes in other parameters of the process do affect the consistency equation (37). It can be seen that changes in R_1 and R_3 affect low frequencies in equation (37), whereas changes in A_1 , A_2 and A_3 only affect high frequencies. Although intuitively obvious for this example, these results show that consistency relations can be used to elucidate the effect of parameter changes.

5. CONCLUSIONS

The main contributions of the present paper can be summarized as follows:

- A general framework in which the consistency relations may be derived for general process systems.
- Extension of consistency relations to dynamic case, thus expressing dependencies amongst column elements of transfer function matrices.
- Application to two common process models.
- Indicating future directions in which the present work may be extended, specifically model reconciliation, physical model reduction and uncertainty modeling.

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