

# Consistency of Steady-State Models Using Insight about Extensive Variables\*

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Fundamental consistency relationships exist between the effect of changes in extensive variables under steady-state conditions. These relationships are derived using physical insight about scaling of extensive variables. The relationships may be used to obtain data for or to check consistency of linear steady-state models used in process control and design. The derivation and use of these relationships is very similar to that of the Gibbs-Duhem equation of thermodynamics. Surprisingly, these scaling consistency relationships seem to be unknown in the chemical engineering community and examples demonstrate inconsistency in some widely used published models.

Keywords: modelling, steady-state, control theory, process design, thermodynamics.

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# 1 Introduction

Intuitively, it is obvious that if we have some information or insight about a physical system, then this information should be used when deriving a model for the system. For example, we may easily distinguish between extensive and intensive variables. Under certain conditions this information may be used to derive what is here called the “scaling” consistency relationship. One might expect that the idea of using consistency relations is straightforward and in common use. However, this appears not to be the case. For example, although consistency relations based on material balance constraints have been reported for distillation column models, they do not seem to be in common use, and the scaling consistency relationship mentioned above does not even seem to have been published before.

This paper addresses linear steady-state models. The first step in deriving such models is to identify the set of independent variables. Next, the effect of small changes in these independent variables on the dependent variables is sought. An example of a steady-state model used for process control is

$$dy = g_{yu_1} du_1 + g_{yu_2} du_2 \quad (1)$$

where  $u_1$  and  $u_2$  are the independent variables, and  $y$  is some dependent variable. The differentials  $dy$ ,  $du_1$  and  $du_2$  denote small changes in these variables. The objective of this paper is to derive consistency relationships between the steady-state gains  $g_{yu}$ .

Models such as Eq.1 are also used in steady-state sensitivity analysis of processes. In this case the gain  $g_{yu}$  might express the sensitivity of  $y$  (eg., equipment size or investment) with respect to some design variable  $u$  (such as flow rate or product specification). Although it is often referred to process control in this paper, it is implicitly understood that the results apply to any steady-state model of the form in Eq.1.

*Previous work on consistency relationships.* Häggblom and Waller (1988) and Skogestad and Morari (1987) have independently published consistency relationships based on 1) Material balances, and 2) Variable transformations (change of independent variables). These relationships were derived for distillation column models, but the ideas may of course be applied more generally.

*Scaling consistency relationship.* This paper addresses a third and possibly even more fundamental consistency relationship which so far seems to have been overlooked. This relationship is derived using physical insight about the difference between extensive and intensive variables. Intensive variables, such as pressure and temperature, are point values independent of the size of the system. Extensive variables, such as volume and mass, depend on the size of the system in an additive way. This means that if two equal subsystems are combined to form a new system, that is, if the original system is “scaled” by a factor two, then the intensive variables are unchanged while the extensive variables are doubled. Using this insight combined with Euler’s Theorem of homogeneous functions one is “out of nothing” able to derive some quite interesting relationships. The derivation of these relationships is very similar to that of the Gibbs-Duhem equation of thermodynamics.

*Example 1.* Consider the flash tank with heater in Fig.1 with independent variables  $F$  (feed rate),  $z$  (feed composition) and  $Q$  (heat input). Pressure is assumed constant. Let  $y$

denote any dependent intensive variable, e.g., liquid composition, temperature or density. The linear steady-state model becomes

$$dy = g_{yF}dF + g_{yQ}dQ + g_{yz}dz \quad (2)$$

Imagine increasing the throughput (load) of the tank from 0 to its present steady-state value. Furthermore, assume that the intensive variables of the system are kept unchanged during this scaling of the extensive variables. Formally, we may integrate Eq.2 by increasing  $F$  and  $Q$  from 0 to  $F^*$  and  $Q^*$ , while keeping  $y$  and  $z$  constant. We obtain the following scaling consistency relationship between the gains,  $g_{yF}$  and  $g_{yQ}$ , for extensive variables

$$0 = g_{yF}F^* + g_{yQ}Q^* \quad (3)$$

The superscript  $*$  to denote the steady-state value is omitted in the rest of the paper. There are numerous applications of this relationship. For example, if we know the effect,  $g_{yF}$ , of a change in feed rate on  $y$ , then we may derive “for free” the effect,  $g_{yQ}$ , of a change in heat input.

The scaling assumption is very common within chemical engineering. For example, when establishing mass and energy balances for a flowsheet, one generally assumes that all streams may be scaled without affecting the stream properties (intensive variables).

In the paper we use Euler’s theorem of homogeneous functions to show rigorously how relationships such as (3) may be derived. We shall also review what consistency relationships may be derived from material balances and variable transformations. Applications include a mixer, a reactor and a distillation column.

## 2 Notation

Assume that the values of the independent variables,  $u_i$ , uniquely determine the value of the dependent variable  $y$ . Then

$$y = y(u_1, u_2, \dots, u_i, \dots) \quad (4)$$

We consider steady-state only, that is, time is not an independent variable. A small change in the independent variables yield a new steady-state, and the change in the dependent variable,  $dy$ , may be obtained as the total differential of  $y$  with respect to the independent variables.

$$dy = \left( \frac{\partial y}{\partial u_1} \right)_{u_{j,j \neq 1}} du_1 + \left( \frac{\partial y}{\partial u_2} \right)_{u_{j,j \neq 2}} du_2 + \dots \quad (5)$$

In process control, the term “gains” is usually used to denote the partial derivatives in this equation and we write

$$dy = g_{yu_1}du_1 + g_{yu_2}du_2 + \dots \quad (6)$$

where

$$g_{yu_1} = \left( \frac{\partial y}{\partial u_1} \right)_{u_2} \quad (7)$$

In process control the independent variables are usually denoted inputs and the dependent variables are denoted outputs. Furthermore, the inputs  $u$  are usually divided into two classes, namely manipulated inputs  $m$  and disturbances  $d$ . Note that the set of disturbances is often fixed, while the set of manipulated inputs may vary depending on the control configuration. When there are several inputs and outputs ( $u$  and  $y$  are vectors) the equations are more compactly written on matrix form

$$dy = [G \ G_d]du = Gdm + G_d dd \quad (8)$$

The matrix,  $G$ , belonging to the manipulated inputs, is denoted the gain matrix, and  $G_d$  is denoted the disturbance gain matrix. With the notation in equations 6 to 8 it may not be clear what independent variables ( $u$ 's) were used when evaluating the gain. In some cases we shall use a superscript on the gain to show explicitly the independent variables

$$g_{yu_1}^{u_1 u_2} \equiv g_{yu_1} \quad (9)$$

### 3 Previous work on consistency relationships

#### 3.1 Consistency from variable transformations

The set of independent variables is not necessarily fixed, that is, the role of dependent and independent variables may change. For example, recall the flash tank in Fig.1. In Case 1 we have feed flow  $F$  and heat input  $Q$  as independent variables, and vapor composition  $y$  and liquid outflow  $F_L$  as dependent variables. Another possible choice of independent variables is  $F$  and  $F_L$  (Case 2), with  $y$  and  $Q$  as dependent variables. Physically, this change in independent variables may be realized by changing level control from  $F_L$  (Case 1) to  $Q$  (Case 2). The effect of a change in, for example,  $F$  on composition  $y$  will be entirely different in these two cases, but these gains are related through consistency relationships.

Let  $u_1$  and  $u_2$  be the independent variables, and assume that the effect of small changes in these on the dependent variables  $y_1$  and  $y_2$  is known. We have

$$dy_1 = \left( \frac{\partial y_1}{\partial u_1} \right)_{u_2} du_1 + \left( \frac{\partial y_1}{\partial u_2} \right)_{u_1} du_2 \quad (10)$$

$$dy_2 = \left( \frac{\partial y_2}{\partial u_1} \right)_{u_2} du_1 + \left( \frac{\partial y_2}{\partial u_2} \right)_{u_1} du_2 \quad (11)$$

or in process control notation

$$dy_1 = g_{11} du_1 + g_{12} du_2 \quad (12)$$

$$dy_2 = g_{21} du_1 + g_{22} du_2 \quad (13)$$

(In terms of the tank example above we have for Case 1  $u_1 = F$ ,  $u_2 = Q$ ,  $y_1 = y$  and  $y_2 = F_L$ .) Next, choose the independent variables to be  $u_1$  and  $y_2$  (Case 2). We then seek to find

$$dy_1 = \left( \frac{\partial y_1}{\partial u_1} \right)_{y_2} du_1 + \left( \frac{\partial y_1}{\partial y_2} \right)_{u_1} dy_2 \quad (14)$$

or

$$dy_1 = \hat{g}_{11} du_1 + \hat{g}_{12} dy_2 \quad (15)$$

How are these partial derivatives (gains) related to the ones in Eq. 12-13? Simple algebra shows that the answer is

$$\hat{g}_{11} = g_{11} - g_{12}g_{21}/g_{22} \quad (16)$$

$$\hat{g}_{12} = g_{12}/g_{22} \quad (17)$$

Such variable transformation consistency relationships may also be obtained from more systematic methods, for example, the Jacobian transformations used in thermodynamics (eg., Callen, 1960, p.128).

The issue of variable transformations arises frequently in cases with stream splitting or with control of levels (liquid holdup) and pressure (vapor holdup). The reason is that holdup must be constant at steady state (no accumulation of mass), that is, we have to implicitly assume that some variable is assigned to control the holdup. However, there may be several options on how to do this, and the set of independent variables left for other purposes may vary. This was illustrated in the tank example above where we in Case 1 assumed liquid level to be controlled by liquid outflow  $F_L$  (possibly self-regulation) leaving  $Q$  as an independent variable, and in Case 2 assumed level to be controlled by heat input  $Q$  leaving  $F_L$  as an independent variable. A similar situation occurs in distillation columns where there are five variables that may be manipulated ( $L, V, V_T, D, B$ , see Fig.2), but only two of these are independent, because pressure, condenser level and reboiler level have to be constant at steady-state.

Several authors have recently applied variable transformations to derive consistent models for distillation columns. For example, Häggblom and Waller (1988), Skogestad and Morari (1987) and Takamatsu et al. (1987) show how gains for one distillation configuration (selecting two independent variables from the set  $L, V, D$  and  $B$ , see Fig. 2) may be derived when data for another configuration are known. Mijares et al. (1985) applied the method of Jacobian transformations to compute the Relative Gain Array for various configurations. The use of variable transformations is also implicit in the RGA-calculations of Shinskey (1967, 1984).

### 3.2 Consistency from material balances

One fundamental relationship which often applies is the steady-state material balance. For example, the steady-state overall material balance for the flash tank in Fig.1 is

$$F_L + F_V = F \quad (18)$$

and we have  $dF_L + dF_V = dF$ . This exact equation may be used to derive consistency relations between the gain elements for the independent variables  $F_L$  and  $F_V$ . For example,

partial differentiation with respect to  $F$  yields  $\partial F_L/\partial F + \partial F_V/\partial F = 1$ , or

$$g_{F_L F} + g_{F_V F} = 1 \quad (19)$$

and differentiating (18) with respect to  $Q$  yields

$$g_{F_L Q} + g_{F_V Q} = 0 \quad (20)$$

(here we have assumed that two independent variables,  $F$  and  $Q$ , do not affect each other; mathematically  $\partial F/\partial Q = g_{FQ} = 0$ ). We may also use the component material balance

$$F_L x + F_V y = F z. \quad (21)$$

and we have  $F_L dx + F_V dy = -x dF_L - y dF_V + d(Fz)$ . This exact equation may be used to derive consistency relations involving the gain elements for  $x$  and  $y$ . For example, partial differentiation with respect to  $Q$  gives (assuming  $F$ ,  $z$  and  $Q$  are independent variables)

$$F_L g_{xQ} + F_V g_{yQ} = -x g_{F_L Q} - y g_{F_V Q} \quad (22)$$

Skogestad and Morari (1987) and Häggblom and Waller (1988) have used component material balances to derive similar consistency relationships for distillation column models.

Note that these material balance relationships involve only one *input* variable, and yield consistency relationships between column elements of the gain matrices in Eq.(8). This is fundamentally different from the scaling relationship derived in Eq.(3) which involves only one *output* variable, resulting in consistency relationship between row elements in the gain matrices. The consistency relationships based on variable transformations in Eq.(16) yield relationships between gain matrices corresponding to different choices of independent variables.

## 4 The Scaling Consistency Relationship

### 4.1 Euler's Theorem of homogeneous functions

To understand the limitations of the scaling consistency relationships it is instructive to study the derivation of Euler's theorem. The derivation given here is taken from the book on thermodynamics by Modell and Reid (1983). Consider a variable  $y$  which is a function of the independent variables  $a, b, c, d$ .

$$y = y(a, b, c, d) \quad (23)$$

Differentiating yields the linear relationship

$$dy = \left(\frac{\partial y}{\partial a}\right)_{b,c,d} da + \left(\frac{\partial y}{\partial b}\right)_{a,c,d} db + \left(\frac{\partial y}{\partial c}\right)_{d,a,b} dc + \left(\frac{\partial y}{\partial d}\right)_{c,a,b} dd \quad (24)$$

$a, b$  are intensive variables and  $c, d$  are extensive variables. Assume that scaling the extensive variables,  $c$  and  $d$ , by a factor  $k$ , with  $a$  and  $b$  constant, results in an increase in  $y$  by a factor  $k^h$  (we see that  $h = 0$  if  $y$  is an intensive variable and  $h = 1$  if  $y$  is an extensive variable). Mathematically,  $y$  is assumed to be homogeneous to the degree  $h$  in  $c$  and  $d$ , that is

$$y(a, b, kc, kd) = k^h y(a, b, c, d) \quad (25)$$

Differentiating this expression and collecting terms making use of the fact that  $c, d$  and  $k$  are *independent* variables yields Euler's theorem (Modell and Reid, 1983):

$$h \cdot y = \left( \frac{\partial y}{\partial c} \right)_{d,a,b} c + \left( \frac{\partial y}{\partial d} \right)_{c,a,b} d \quad (26)$$

Note that Eq.26 may be obtained directly from Eq.24 by formally integrating Eq.24 from zero to actual conditions with the intensive variables  $a, b$  constant (and also  $y$  constant if  $h = 0$ ). In terms of process control notation Eq.26 becomes

$$h \cdot y = \sum_{u_e} g_{yu_e} u_e \quad (27)$$

where  $u_e$  denotes the independent extensive variables. This equation will be referred to as the scaling consistency relationship in the following. The implications of Eq.27 may be easier to understand if relative changes in the variables are used. We have

$$y \text{ intensive : } \sum_{u_e} \frac{\partial y/y}{\partial u_e/u_e} = 0 \quad (28)$$

$$y \text{ extensive : } \sum_{u_e} \frac{\partial y/y}{\partial u_e/u_e} = 1 \quad (29)$$

## 4.2 Derivation of the Scaling Relationship

For a given case the scaling consistency relationship is derived using the following procedure:

**Step 1.** Identify the independent *extensive* variables.

**Step 2.** Physical assumption: Scaling all the independent extensive variables by a factor  $k$  (with the independent *intensive* variables constant), scales all the dependent extensive variables by the same factor  $k$  and keeps *all* the dependent intensive variables constant.

**Step 3.** Formulate the physical insight from Step 1 and 2 mathematically and use Euler's Theorem to derive the consistency relationship (Eq.27).

The key idea in Step 2 is that the properties of the system may be maintained when the throughput is increased. The use of this method is best illustrated by examples as shown below.

Note from the derivation of Eq.27 that the independent extensive variables must be truly independent. Also note that *all* intensive variables (both independent and dependent) must be constant when the independent extensive variables are scaled by a factor  $k$ . If there is an

intensive variable which will vary, then we must introduce an additional extensive variable to keep it constant in order to apply Euler's Theorem.

One underlying assumption for Step 2 is that the "efficiency" of the system, which may be viewed as an intensive variable, is unchanged. For example, in the mixing tank example we must assume that the separator efficiency is unchanged when the load is increased. Similarly, for a distillation column we must assume that the tray efficiency remains constant. This assumption is generally satisfied if the data are obtained by simulations using a theoretical model. However, if data are obtained from a real system this may not apply exactly.

## 5 Applications of the Scaling Relationship

### 5.1 Flash Tank with chemical reaction.

*Example 1.* Consider again the flash tank in Fig.1. We now include the possibility that the approach to equilibrium ("efficiency") may vary. This will be the case, for example, if there is a chemical reaction in the liquid phase. We must then include an additional extensive variable which we may adjust to keep the efficiency constant. We make the physical assumption that the efficiency depends on the liquid residence time,  $\tau_L = V_L/F$ . We must then add the liquid volume,  $V_L$ , as an additional variable. We shall use the three-step procedure to obtain consistency relations.

1. Independent extensive variables are  $F, Q$  and  $V_L$  and the linear model becomes

$$dy = g_{yF}dF + g_{yQ}dQ + g_{yV_L}dV_L + \dots \quad (30)$$

where  $y$  is any dependent variable.<sup>1</sup>

2. Physical assumption: Increasing the extensive variables  $F, Q, V_L$  by the same factor keeps all intensive variables constant.
3. Using Eq.27 (or equivalently, integrate Eq.30 from zero to actual conditions) yields

$$h \cdot y = g_{yF}F + g_{yQ}Q + g_{yV_L}V_L \quad (31)$$

where  $h = 0$  if  $y$  is an intensive variable and  $h = 1$  if  $y$  is an extensive variable.

Consider two special cases:

*Case 1.*  $g_{yV_L} = 0$ . In this case the liquid residence time has no effect on the steady-state operation and the product streams are in equilibrium. This is the case considered in the introduction, where  $y$  was chosen to represent an intensive variable. Here, let  $y$  represent the vapor flow,  $F_V$ , which is an extensive variable. We derive the consistency relationship

$$g_{F_V F}F + g_{F_V Q}Q = F_V \quad (32)$$

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<sup>1</sup>The additional terms which are indicated as dots in Eq.(30) are related to changes in the independent intensive variables. For example, we will have a term  $g_{yz}dz$  for the effect of changes in feed composition.



or

$$\left(\frac{\partial F_V/F_V}{\partial F/F}\right)_{Q,z} + \left(\frac{\partial F_V/F_V}{\partial Q/Q}\right)_{F,z} = 1 \quad (33)$$

As a numerical example assume that the first term in Eq.33 is 0.8, that is, a 10% increase in  $F$  increases  $F_V$  by 8% (neglecting nonlinear effects). Eq.33 then tells us that the second term must be 0.2, that is a 10% increase in  $Q$  must increase  $F_V$  by 2%.

*Case 2.*  $Q = 0$ . This is the case with no heat input. Let  $y$  denote an intensive variable, for example, the fractional conversion. Eq.31 yields

$$\left(\frac{\partial y/y}{\partial F/F}\right)_{V_L,z} + \left(\frac{\partial y/y}{\partial V_L/V_L}\right)_{F,z} = 0 \quad (34)$$

In words, this equation tells us that the effect of an increase in the feed rate  $F$  by, say, 1% is equivalent to a decrease in the volume  $V_L$  by 1%. This is of course no surprise since both these changes correspond to a decrease in the residence time  $\tau = V_L/F$  by 1%.

## 5.2 Blending system.

*Example 2.* Stephanopolous (1984, p. 502-503) considers the blending system shown in Fig.3. Two streams with flow rates  $F_1 = 133.4$  mol/h and  $F_2 = 66.6$  mol/h are mixed to form a product stream with flow rate  $F$ . Let  $x_1, x_2$ , and  $x$  represent some property of these streams, eg. density, mole fraction, temperature or pH. The linear steady-state model becomes

$$dF = g_{FF_1}dF_1 + g_{FF_2}dF_2 + \dots \quad (35)$$

$$dx = g_{xF_1}dF_1 + g_{xF_2}dF_2 + \dots \quad (36)$$

Assume that the total material balance  $F = F_1 + F_2$  applies. We then have  $dF = dF_1 + dF_2$ , and the gains in (35) become

$$g_{FF_1} = 1; \quad g_{FF_2} = 1 \quad (37)$$

Now, assume we want to use  $F_1$  and  $F_2$  (inputs) to control  $F$  and  $x$  (outputs) using single loops. To decide on an appropriate pairing we shall compute the Relative Gain Array (RGA) (Bristol, 1966). The relative gain between  $F$  and  $F_1$  is defined as

$$\lambda_{11} = \frac{(\partial F/\partial F_1)_{F_2}}{(\partial F/\partial F_1)_x} = \frac{g_{FF_1}}{\hat{g}_{FF_1}} \quad (38)$$

which is equivalent to (recall Eq.16):

$$\lambda_{11} = \left(1 - \frac{g_{FF_2}g_{xF_1}}{g_{FF_1}g_{xF_2}}\right)^{-1} = \left(1 - \frac{g_{xF_1}}{g_{xF_2}}\right)^{-1} \quad (39)$$

*Stephanopolous approach.* To compute the remaining two gains, one might expect that a model of the blending process is needed. For example, Stephanopolous (1984) assumed  $x_1, x_2, x$  to represent mole fractions and used the steady-state component balance

$$Fx = F_1x_1 + F_2x_2 \quad (40)$$

to evaluate the relative gain numerically and obtained  $\lambda_{11} = 0.60$ .

*General approach.* We shall now use the scaling consistency relationship to show that the correct value is 0.67. The reason for the error in Stephanopolous is numerical round-off errors. However, more importantly, we shall show that the value of the relative gain is independent of what property  $x$  represents (that is, Eq.40 is not needed). We have

1. Independent extensive variables:  $F_1$  and  $F_2$ .
2. Physical assumption: Increasing  $F_1$  and  $F_2$  by the same factor keeps all intensive variables constant.
3. The scaling relationship (Eq.27) yields for the intensive variable  $x$

$$0 = g_{xF_1}F_1 + g_{xF_2}F_2 \quad (41)$$

Note that this relationship is derived *without* using any model of the blending process. Our only assumption is that the blending property,  $x$ , is unaffected if both blending streams,  $F_1$  and  $F_2$ , are scaled equally. Inserting Eq.41 into Eq.39 yields

$$\lambda_{11} = (1 + F_2/F_1)^{-1} = F_1/F = 0.67 \quad (42)$$

Thus, the value of the relative gain between  $F_1$  and  $F$  is equal to  $F_1/F$  *irrespective* of what property  $x$  represents. Consequently, if we use the rule that one should pair variables with relative gains close to 1 (Bristol, 1966), one should use the larger stream to control the flow rate of the blend and the smaller stream to control the property of the blend. This is indeed consistent with most engineers intuition.

### 5.3 Distillation Column Control.

Consider the distillation column in Fig.2.

1. Assumption: Independent extensive variables are  $L, V$  and  $F$ . Here  $L$  is the reflux rate,  $V$  may represent boilup rate, heat input or steam rate (note that  $V$  here is a flow or heat rate and not a volume), and  $F$  is the feed rate. This choice of independent variables is usually called the  $LV$ -configuration or  $LV$ -structure. The column model is then given by

$$y = y(L, V, F, \dots) \quad (43)$$

where the dots denote the independent intensive variables, e.g.,  $z_F, p, q_F$  and  $N$ . The linearized model becomes

$$dy = g_{yL}^{LV}dL + g_{yV}^{LV}dV + g_{yF}^{LV}dF + \dots \quad (44)$$

where  $y$  may represent, for example, the product flow rates  $D, B$  or the product compositions  $y_D, x_B$ .

2. Physical assumption: Increasing  $L$ ,  $V$  and  $F$  by the same factor  $k$  keeps all intensive variables constant.
3. The scaling consistency relationship Eq.27 yields

$$h \cdot y = g_{yL}^{LV} L + g_{yV}^{LV} V + g_{yF}^{LV} F \quad (45)$$

If  $y$  is an intensive variable, for example, top compositions  $y_D$  then Eq.45 yields

$$g_{y_DF}^{LV} = -g_{y_DL}^{LV} \frac{L}{F} - g_{y_DV}^{LV} \frac{V}{F} \quad (46)$$

or on matrix form for both top and bottom composition

$$\underline{g}_F^{LV} = -G^{LV} \begin{pmatrix} L/F \\ V/F \end{pmatrix} \quad (47)$$

where

$$\underline{g}_F^{LV} = \begin{pmatrix} g_{y_DF}^{LV} \\ g_{x_B F}^{LV} \end{pmatrix}; \quad G^{LV} = \begin{pmatrix} g_{y_DL}^{LV} & g_{y_DV}^{LV} \\ g_{x_B L}^{LV} & g_{x_B V}^{LV} \end{pmatrix} \quad (48)$$

This result tells us that we may compute the effect of a change in feed rate, if we know the effects of changes in reflux and boilup. The result may seem trivial, but in fact seems to be unknown in the literature. The following example shows that published data for the much quoted Wood and Berry column does not satisfy these consistency relationships.

### 5.3.1 Numerical examples

Wood and Berry column example (Example 3). From pulse testing of an experimental column separating methanol and water the following gain data were obtained (Wood and Berry, 1973)

$$G^{LV} = \begin{pmatrix} 12.8 & -18.9 \\ 6.6 & -19.4 \end{pmatrix} \quad (49)$$

Here  $y_D$  and  $x_B$  represent wt.% methanol in the products,  $L$  is the reflux rate, and  $V$  is the steam rate to the reboiler. Data for compositions and flows at the nominal operation point are given in Table I. Note that all the flows are in mass units. This means that although the assumption of constant molar flows applies quite well to the methanol-water system, the mass flows will vary through the column due to variations in mole weight. The reflux is not saturated, but is heated to a constant temperature, which may be viewed as an additional independent variable. However, since this is an *intensive* variable, Eq.47 still applies, and we obtain the estimate of the feed gains

$$\underline{g}_F^{LV} = - \begin{pmatrix} 12.8 & -18.9 \\ 6.6 & -19.4 \end{pmatrix} \begin{pmatrix} 1.95/2.45 \\ 1.71/2.45 \end{pmatrix} = \begin{pmatrix} 3.0 \\ 8.3 \end{pmatrix} \quad (50)$$

These values should be compared with the experimental gains (Berry, 1973)

$$\underline{g}_F^{LV} \text{ exp} = \begin{pmatrix} 3.8 \\ 4.9 \end{pmatrix} \quad (51)$$

We see that the feed gain for  $y_D$  is reasonably consistent, but the one for  $x_B$  is not. Note that the material balance consistency relationships, eg.,  $Dg_{y_D L} + Bg_{x_B L} = -(y_D - x_B)g_{DL}$  (similar to Eq.22) cannot be used to check consistency in this case since experimental data for  $g_{DL} = (\partial D/\partial L)_V$  is not given.

Simulation of Wood and Berry column (Example 4). Tray-by-tray simulations using the data in Table I gave an almost exact match to the published steady-state data of Wood and Berry. Tray temperatures were consistently about 1.5°C higher than reported, but otherwise matched the experimental profile. The results were obtained using 8 theoretical stages, the UNIQUAC equation to describe the non-ideal vapor-liquid equilibrium, and assuming the enthalpy contents of the steam to be 2150 kJ/kg.

Steady-state gains were obtained numerically using a commercially available process simulator. In Tables II and III we summarize the results obtained by making increases in the independent variables  $L$ ,  $V$  and  $F$  of magnitudes 0.1% and 1.0%, respectively. The individual gain elements are quite similar for the two cases. However, the effect of nonlinearity is more evident when checking consistency of the gains. We note that whereas the feed gains obtained from small changes in the flows (Table II) are reasonably consistent, the ones based on large changes are not. For example, for a 1% increase in feed rate the numerical value of  $g_{x_B F}$  was found to be 4.13, whereas the value obtained from the scaling consistency relationship is only 0.64. Note that the gains are obtained from a simulation model where the physical assumptions for the scaling consistency relationship hold exactly.

Another striking difference is that the relative gain for the two cases is 9.1 and -2.0, respectively. The last value is obviously in error since it may be shown that the relative gain for the LV-configuration should always be larger than 1 (Skogestad et al., 1990). For comparison, the relative gain of the experimental gain matrix (Eq.49) is 2.0.

The results above clearly illustrate the difficulties in obtaining consistent steady-state gains for distillation columns even when using an accurate simulation program. The results may be improved, for example, by using two-sided difference approximations or by evaluating the gains with  $D$  constant (to get a good estimate of the effect of changes in internal flows, Skogestad, 1988). Of course, the difficulties in obtaining consistent gains from experiments are even larger. Actually, the inconsistencies in the experimental gains found between Eqs.50 and 51, and the differences between experimental and simulated gains, are surprisingly small.

Waller et al. example (Example 5). This example is chosen because the authors specifically state that the model has been reconciled to satisfy the material balance consistency relationships. From experiments on a 15 stage pilot plant column separating ethanol and water Waller et al. (1988) obtained the following gains

$$\begin{pmatrix} dT_4 \\ dT_{14} \end{pmatrix} = \begin{pmatrix} -0.045 & 0.048 \\ -0.23 & 0.55 \end{pmatrix} \begin{pmatrix} dL \\ dV \end{pmatrix} + \begin{pmatrix} -0.001 \\ -0.16 \end{pmatrix} dF \quad (52)$$

where  $T_4$  and  $T_{14}$  are temperatures at selected trays in the column and  $V$  is the steam flow to the reboiler. The nominal flow rates in kg/h are  $F = 200$ ,  $L=60$  and  $V = 72$ . Reflux temperature is assumed constant. The gains were reconciled to satisfy the material balance consistency relationships (similar to Eq.22) but they do not satisfy the scaling consistency relationships: Using Eq.47 we derive

$$\underline{g}_F = \begin{pmatrix} 0.045 \cdot 60/200 - 0.048 \cdot 72/200 \\ 0.23 \cdot 60/200 - 0.55 \cdot 72/200 \end{pmatrix} = \begin{pmatrix} -0.004 \\ -0.13 \end{pmatrix} \quad (53)$$

which in relative terms is significantly different from the reported values of  $\begin{pmatrix} -0.001 \\ -0.16 \end{pmatrix}$ .

### 5.3.2 Some distillation extensions

Unsaturated reflux. If the reflux temperature may vary due to subcooling then the overall cooling duty  $Q_D$  is no longer a dependent variable. It must then be added as a independent variable and the independent extensive variables become  $F, L, V$  and  $Q_D$ . In this case an additional term  $g_{yQ_D} Q_D$  must be added to Eq.45 and the other gains must be evaluated with  $Q_D$  constant. However, if the reflux temperature is kept constant (even though it may be subcooled) then  $Q_D$  is not an independent variable, and Eq.45 holds as dicussed in the Wood and Berry example above.

More complex columns. If the column has a side stream (flow rate  $S$ ) or an intermediate cooler (duty  $Q_S$ ) then  $S$  and  $Q_S$  must be added as an independent extensive variable, and Eq.45 must be changed accordingly by adding the terms  $g_{yS} S + g_{yQ_S} Q_S$ .

Other control configurations. Depending on the control configuration a lot of other options for independent variables exist. For example, if  $L$  is used for reboiler level control then independent variables are  $D, V$  and  $F$  ( $DV$ -configuration), and a relationship similar to Eq.45 is derived:

$$h \cdot y = g_{yD}^{DV} D + g_{yV}^{DV} V + g_{yF}^{DV} F \quad (54)$$

Another configuration that is proposed as a good choice for many columns is the  $RS$ -configuration with  $F, R = L/D$  and  $S = V/B$  as independent variables. Since  $R$  and  $S$  are intensive variables the consistency relationship becomes

$$h \cdot y = g_{yF}^{RS} F \quad (55)$$

For example, if  $y$  represents top composition, then Eq.55 says that  $\left(\frac{\partial y_D}{\partial F}\right)_{R,S} = 0$ . This results simply says that product compositions are not affected by changes in feed rate provided all flow ratios are kept constant.

Compositions as independent variables. This may be the case, for example, if a feedback controller is used to manipulate  $L$  such that  $y_D$  is kept at a desired value. We may then view  $y_D$  as an independent variable instead of  $L$ . The scaling relationship yields

$$h \cdot y = \left(\frac{\partial y}{\partial V}\right)_{y_D, F} V + \left(\frac{\partial y}{\partial F}\right)_{y_D, V} F \quad (56)$$

A more extensive treatment of consistency relationships for distillation columns may be found in Skogestad (1988).

## 6 Steady-state models and thermodynamics

It should be clear by now that there are a number of similarities between the results presented in this paper and those of classical thermodynamics. Surprisingly, no one seem to have explicitly pointed out these similarities before. In both steady-state modelling and thermodynamics we assume steady state conditions or equilibrium and postulate a set of independent variables. For example, a basic postulate of equilibrium thermodynamics is that specifying temperature ( $T$ ), pressure ( $p$ ) and the number of moles ( $n_i$ ) of each species (independent variables) uniquely determines the state of the system (dependent variables). For example, consider the Gibbs energy ( $G$ ). We have

$$G = y(\{n_i\}, T, P) \quad (57)$$

where  $\{n_i\}$  represents the set of mole numbers  $n_1, n_2, \dots, n_c$ , and  $c$  is the number of components. This is the equivalence to Eq.4 and the equivalence to Eq.5 is the total differential of  $G$

$$dG = \sum_i \left( \frac{\partial G}{\partial n_i} \right)_{T, p, \{n_j, j \neq i\}} dn_i + \left( \frac{\partial G}{\partial T} \right)_{p, \{n_i\}} dT + \left( \frac{\partial G}{\partial p} \right)_{T, \{n_i\}} dp \quad (58)$$

Variable transformations are very common in thermodynamics. Volume ( $V$ ) is a dependent variable when  $p$ ,  $T$  and  $n_i$  are specified. However, we may want to use  $T$  and  $V$  as independent variables instead of  $T$  and  $p$ . The partial derivatives in this case, for example  $\left( \frac{\partial G}{\partial T} \right)_{V, \{n_i\}}$ , are of course related to those in Eq.58 through relations identical to the ones derived previously in Eq.16. A systematic method for this are the Jacobian transformations (eg., Callen, 1960, p.128).

However, we should note that there are also important differences between thermodynamics and steady state process control models. One is the laws of thermodynamics. These imply that the partial derivatives in thermodynamics are usually important variables in themselves. For example, Eq. 58 becomes

$$dG = \sum_i \mu_i dn_i - SdT + Vdp \quad (59)$$

where  $S$  is entropy and  $\mu_i$  is chemical potential. On the other hand, in process control usually only the numerical value of the partial derivatives (gains) are of interest. The powerful method of Legendre transformations used in thermodynamics (eg., Modell and Reid, 1983, p. 104) which forms the basis of the famous Bridgman tables, will therefore not generally have its equivalence for process control models.

The counterpart to the scaling consistency relationship is the integrated form of the Gibbs-Duhem equation. To show this consider Eq.(59). We know that  $G$  and  $n_i$  are extensive variables, while  $T$  and  $p$  are intensive variables. We also know from physical considerations

that an increase in all  $n_i$ 's by a factor  $k$  with  $T$  and  $p$  constant increases  $G$  by a factor  $k$ . The scaling consistency relationship (27) yields

$$G = \sum_i \mu_i n_i \quad (60)$$

Differentiation this equation and subtracting Eq.59 yields

$$SdT - Vdp + \sum_i n_i d\mu_i = 0 \quad (61)$$

which in fact is the Gibbs-Duhem equation of thermodynamics.

## 7 Discussion

If we use a model based on fundamental principles, such as material and energy balances, to evaluate the exact steady-state gains, then these gains will automatically be consistent and satisfy the scaling consistency relationship. Thus, the scaling consistency relationship does not contain any new information in addition to the fundamental principles. Rather, the advantage is that it gives an *overall* relationship, which the model equations, when *combined*, have to satisfy. This overall relationship may be derived based on physical insight about the extensive variables, and without detailed knowledge of the system. This is very similar to the use of the Gibbs-Duhem consistency relationships of thermodynamics.

The results in this paper are limited to steady-state. The consistency relationships based on steady-state material balances and the new scaling relationships cannot be extended to the dynamic case. On the other hand, the consistency results for variable transformations, e.g. Eq.16, can be extended if transfer functions are used instead of gains. However, this requires the assumption of perfect control (or at least some information about the controller). The reason is that a change in independent variables in a dynamic sense, physically must be caused some change in the control structure.

One might expect that the simple consistency relations derived in this paper were in common use. However, this is not the case as illustrated by examples based on i) the most widely used textbook in process control (Stephanopolous, Example 2), ii) the most commonly used model in process control (the Wood & Berry column, Example 3), and iii) a paper (Waller et al., Example 5) where it is specifically stated that the data are consistent. Using the scaling consistency relationship it was shown that all these models are inconsistent.

In general the scaling consistency relationship, (Eq.27), may be used for two purposes:

1. Check if the model is consistent.
2. If the model is known to be consistent, obtain “for free” gains for other independent variables (eg., a change in feed flow).

In Case 1 above, if a given set of data does *not* satisfy the scaling consistency relationships there are three possibilities:

1. There is something wrong in the physical assumption (Step 2) such that the relation does not apply.
2. The data are inconsistent due to nonlinearity in the process (the change made was too large or the operating point has changed).
3. The data are inconsistent due to, for example, measurement error or numerical errors.

It may be necessary to obtain additional data to find out which is the cause of inconsistency.

Obtaining consistent data from experiments is always very difficult. However, also steady-state simulations may yield inconsistent data as shown in Example 4. The scaling relationships may be used to decide on a reasonable magnitude of the perturbations for the simulations, and to check if the simulation model is correct.

It should be noted that even rather small errors in the individual gains may yield steady-state models which are almost useless for control purposes. This was shown in the numerical simulation of the Wood and Berry column (Example 4, Table III) where, because of nonlinearity, the gains obtained with “large” (1%) changes in the input variables, gave a gain matrix with wrong signs in the RGA-matrix. Note that the scaling consistency relationship indeed shows that the gains are inconsistent. Ignoring this relationship would in this case lead to the use of an incorrect model which was almost useless for control purposes. For example, if the incorrect gain matrix was used to select controller pairings the conclusion would be the opposite of the correct.

Another application of consistency relationships is in robust control. Here we may want to study the effect of variations in the gains. However, based on consistency relationships we may know that the gains cannot vary independently. For example, Skogestad et al. (1988) argue for distillation columns that the variations in the four elements of the gain matrix,  $G^{LV}$ , are strongly coupled, and may be captured using a single perturbation. This information may strongly reduce the conservativeness of the robustness analysis.

## 8 Conclusion

It has been shown that in many cases there exists a linearity in the direction of the extensive variables, and the gains related to changes in extensive variables are not independent. Their interdependence is given by the scaling consistency relationship

$$h \cdot y = \sum_{u_e} g_{yu_e} u_e \quad (27)$$

Its derivation and use is similar to that of the Gibbs-Duhem equation of thermodynamics.

In general, when obtaining gains from simulations or numerical differentiation there is a balance between numerical accuracy and avoiding nonlinear effects. Use of consistency relationships may help in obtaining a reasonable balance between these conflicting objectives, or may point out the need to use higher numerical accuracy in the calculations, or to use



a different technique for performing the linearization. To obtain consistent models from inaccurate numerical or experimental data one should reconcile the gains subject to the consistency constraints derived in this paper.

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## 9 Nomenclature

See also Eq.4-9.

$g_{y_i u_j} = g_{y_i u_j}^{u_k} = g_{ij} = \left( \frac{\partial y_i}{\partial u_j} \right)_{u_k \neq j}$  - steady state gain (effect of small change in  $u_j$  on  $y_i$ )

$h$  - integer variable which is 0 if  $y$  is intensive and 1 if  $y$  is extensive

$u$  - independent variable

$u_e$  - independent extensive variable

$y$  - dependent variable

$\lambda_{ij} = \frac{(\partial y_i / \partial u_j)_{u_k \neq j}}{(\partial y_i / \partial u_j)_{u_k \neq i}}$  - relative gain between variables  $y_i$  and  $u_j$ .

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**Table I.** Example 4. Data for simulation of Wood and Berry distillation column.

System	Methanol-Water
UNIQUAC parameters	-301.6449, 498.5938
Pressure (atm)	1.0
No. of theoretical stages, $N$	8
Feed stage, $N_F$ (1 is reboiler)	4
Feed composition, $z_F$ (wt.%)	46.5
Top composition, $y_D$ (wt.%)	96.0
Bottom composition, $x_B$ (wt.%)	0.5
Feed rate, $F$ (mass/time)	2.45
Distillate, $D$ (mass/time)	1.18
Bottom product, $B$ (mass/time)	1.27
Reflux, $L$ (mass/time)	1.95
Steam @ 2150 kJ/kg, $V$ (mass/time)	1.71
Feed liquid fraction, $q_F$	1.0
Saturated liquid reflux, total condenser	

**Table II.** Example 4. Simulations with small perturbations.

Gains obtained numerically by 0.1% increase in  $L$ ,  $V$  and  $F$ :

$$G^{LV} = \begin{pmatrix} 20.20 & -37.51 \\ 4.92 & -10.26 \end{pmatrix}; \quad g_F^{LV} = \begin{pmatrix} 10.10 \\ 3.25 \end{pmatrix}$$

Relative gain:

$$\lambda_{11}(G^{LV}) = 9.1$$

Feed gain from scaling consistency relationship, Eq.47:

$$g_F^{LV} = -G^{LV} \begin{pmatrix} L/F \\ V/F \end{pmatrix} = \begin{pmatrix} 9.79 \\ 3.42 \end{pmatrix}$$

**Table III.** Example 4. Simulations with large perturbations.

Gains obtained numerically by 1.0% increase in  $L$ ,  $V$  and  $F$ :

$$G^{LV} = \begin{pmatrix} 19.77 & -38.32 \\ 5.99 & -7.75 \end{pmatrix}; \quad g_F^{LV} = \begin{pmatrix} 9.72 \\ 4.13 \end{pmatrix}$$

Relative gain:

$$\lambda_{11}(G^{LV}) = -2.0$$

Feed gain from scaling consistency relationship, Eq.47:

$$g_F^{LV} = -G^{LV} \begin{pmatrix} L/F \\ V/F \end{pmatrix} = \begin{pmatrix} 11.02 \\ 0.64 \end{pmatrix}$$

### **Figure Captions**

1. **Figure 1.** Flash tank with heater.
2. **Figure 2.** Two product distillation column.
3. **Figure 3.** Blending system.