# A Scaling Procedure for the Structural and Interaction Analysis of Dynamic Models

Many techniques that are used for analyzing the structure of large-scale, interactive systems (including the structural dominance analysis and singular-value decomposition methods) require a careful scaling of input and output variables to yield useful results. A suitable scaling procedure motivated by physical arguments and aimed at expressing input and output variables in common terms is presented and illustrated through several examples, including nonlinear lumped-parameter and distributed-parameter models.

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## Introduction

Mathematical models are widely used to design, analyze, and control industrial processes. Steady state models are very useful at the design stage, but for the investigation of start-up and control strategies dynamic models are needed. This work considers dynamic phenomenological models that are developed for the purpose of analyzing a system, determining an appropriate control structure, and designing a robust controller. These phenomenological models are obtained through careful modeling of the process using physical laws and conservation equations.

A model is then a consistent system representation, indicating the output behavior as a function of inputs and initial conditions:

$$\dot{\underline{x}} = \underline{f}(\underline{x}, \underline{u}) \quad \underline{x}(0) = \underline{x}_0$$
$$\underline{y} = \underline{g}(\underline{x}, \underline{u})$$

Even though the functionalities $\underline{f}$ and $\underline{g}$ are highly dependent on the choice of units for the input, state, and output variables, the model responses usually can be computed or a controller can be designed without a scaling of the variables. Recently, however, several powerful numerical methods of analysis have been proposed for multivariable, interactive systems, e.g., the relative gain array method (Bristol, 1966; McAvoy, 1983), the component cost analysis method (Skelton, 1980; Skelton and Yousuff, 1983), the selective modal analysis method (Perez-Arriaga et al., 1980, 1981), the structural dominance analysis method (Litz, 1979; Bonvin and Mellichamp, 1982), and singular-value decomposition methods (Stewart, 1973; Lau et al., 1985; Lau and Jensen, 1985). Unfortunately, many of these methods are scaling- (or units-) dependent, and therefore can be applied only if the system model is scaled appropriately. Since the choice of variable units in developing a model is generally quite arbitrary, real system models are unsuited for analysis with such methods unless a scaling that is directly related to the objective of the analysis technique is applied. In order to overcome the scaling problem with singular-value decomposition methods, Morari and Doyle (1986) suggested using structured singular values. Other approaches consist of optimizing the scaling in such a way that the condition number is minimized (Prasad, 1984; Palazoglu et al., 1985).

Paige (1981) clearly separated the two steps of scaling (based on the physical properties of the system) and analysis (using numerical algorithms). The scaling has to be such that the mathematical problem accurately reflects the sensitivity of the physical problem. The choice of scaling is best handled by the engineer abstracting the mathematical model from the physical system.

This study demonstrates the need for appropriate input and output variable scaling in connection with both the structural dominance analysis and singular-value decomposition methods. Furthermore, a suitable scaling procedure that brings output, state, and input variables onto a common basis is proposed. The scaled variables are extensive variables that indicate directly the amount of a chosen reference quantity present in each system state variable, or measured by each output variable, or brought into the system by each input variable. Because of its physical basis, the technique cannot be used blindly as a tool suitable to scale every dynamic model. As an example, it is not suited to scale the state and input variables of a state-space model given exclusively by the $\underline{\underline{A}}$, $\underline{\underline{B}}$, and $\underline{\underline{C}}$ matrices, i.e., in the absence of full knowledge of the conservation equations. Rather, it should be used by the system designer as a way to weight the input and

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output variables of a physical system model before analyzing for design of the control system, e.g., to condition the system equations when the goal is to compare input and output variables as extensive quantities.

The scaling factors depend implicitly on steady state values and therefore are valid only in the vicinity of an operating point. Nevertheless, this kind of scaling can greatly increase the applicability of many general methods for analyzing the importance of input and output variables in physical models. When used in conjunction with structural dominance analysis and singular-value decomposition methods, this procedure can provide valuable help to:

1. Locate the best measured and manipulated variables
2. Specify a multiloop or multivariable control structure
3. Measure the amount of interaction between various control loops
4. Investigate the structural characteristics of a large-scale system
5. Choose the order of a reduced-order model
6. Select the retained states and modes for modal model reduction and singular perturbation methods, etc.

## A Need for Scaling

In the analysis of large-scale systems it often is necessary to measure the real strength of the input/output couplings through each mode, as is done with the structural dominance analysis method (SDA) (Bonvin and Mellichamp, 1982). Such an analysis provides useful information concerning possible controller structures (e.g., input/output pairings for multiloop control) as well as the size and structure of reduced-order models. The method, however, uses a direct numerical comparison of measures derived for each input and output variable, and thus it is only meaningful after an appropriate scaling of input and output variables has made apparent the intrinsic system properties (Lau and Jensen, 1985).

In formulating classical optimization problems, the use of objective function terms of the form $\underline{x}^T\underline{x} + \underline{u}^T\underline{u}$ presupposes that the various state and input variables can be compared directly, and therefore that they are expressed in similar quantities. The use of weighting matrices, generally incorporated in these problems, represents an indirect, often fairly subjective way of scaling the problem.

In applications involving parameter identification, inappropriate scaling of the variables may lead to a defective experimental design and, consequently, to highly correlated estimates. Similarly, in multivariate regression problems, the specific choice of combinations of the various responses can be crucial to the validity of the parameter estimates. Finally, the singular-value decomposition (SVD) method furnishes a powerful tool for analysis of multivariable control problems and for balanced model reduction. However, the computed condition number and total interaction measures (Lau et al., 1985) or the second-order modes (Moore, 1981) are highly dependent on the problem scaling (Prasad, 1984; Lau and Jensen, 1985; Bonvin, 1986).

## Scaling Methods

There are many ways of scaling the input and output variables in a process model; the choice of a scaling approach depends highly on the primary use for the scaled model. In this work, the goal of the scaling is:

1. To adjust the numerical values of input, state, and output variables so as to eliminate the arbitrariness associated with the choice of units
2. To keep the relative strength of input/output couplings
3. To put all of the variables on a common basis so as to facilitate comparison between variables of various types

In matrix representation, the original input, state, and output variables are multiplied by the diagonal matrices $\underline{\underline{W}}$, $\underline{\underline{P}}$ and $\underline{\underline{V}}$, respectively:

$$\tilde{\underline{u}} = \underline{\underline{W}}\,\underline{u}$$
$$\tilde{\underline{x}} = \underline{\underline{P}}\,\underline{x}$$
$$\tilde{\underline{y}} = \underline{\underline{V}}\,\underline{y}$$

A scaling with respect to the steady state values is clearly inadequate since it considers only the variables without their ranges. Scaling with respect to the range of each variable is certainly a step in the right direction and has been used extensively (Ostrach, 1982; McAvoy, 1983; Denn, 1985); its application yields variables that vary between 0 and 1. The approach, however, has a major drawback for the goals stated above: it is either very subjective without a good knowledge of the process, or the scalings introduce some gain characteristics in an effort to reduce subjectivity. (It is obvious that "less important" variables are made numerically equivalent to "more important" variables after both are scaled with respect to their individual ranges.) Similarly, scaling with respect to input/output gains completely eliminates the relative strengths of the various couplings. Even so, it has been used in some structural dominance studies (Litz, 1979; Litz and Roth, 1981; Gatica et al., 1984.)

Recently, Lau and Jensen (1985) studied the effects that a scaling of the steady state system matrix has on the results obtained with SVD; they concluded that a scaling based on physical considerations by limiting the variability of the system variables was preferable to more empirical methods such as row and column equilibration or geometric scaling.

In this study, we propose to put input and output variables on a common physical basis, thus enabling a direct comparison of their numerical values and providing information concerning their sensitivity (outputs) and effectiveness (inputs). The scaling procedure starts by scaling the state variables—choosing the common basis and determining its relationship to the various states through consideration of the accumulation terms. Although the approach requires a good knowledge of the process and of its environment, it is not unduly subjective as are some other procedures. It is worth emphasizing here the difference between this proposed scaling procedure and the nondimensionalizing scaling methods typically found in the literature on process modeling (see Denn, 1985, for an excellent treatment of scaling).

For the latter approaches, the idea of scaling is to obtain dimensionless variables of order unity. This approach leads to dimensionless differential equations in which all variables and their derivatives are of order unity, and to neglecting the terms with small coefficients. Such an approach permits simplification of the model, as well as estimation of useful characteristic quantities representing the process that otherwise would require solution of a differential equation system.

The scaling developed in this study is also aimed at making

the input and output variables more comparable, but their magnitudes are not necessarily all of order unity. The scaled variables are extensive quantities. If a variable is associated with a less important process, its magnitude will be small. The main goal of the scaling is to facilitate the analysis of the importance of input and output variables.

The two scaling approaches are in a sense complementary. The first one facilitates model simplification using physical arguments; the second—the proposed method—is best tailored to reduce the model using mathematical reduction methods.

## Proposed Scaling Procedure

Each state variable in a dynamic model is described by a differential equation representing the conservation (or balance) of some physical quantity such as energy, mass, or momentum. One of these quantities can be chosen as the reference quantity for the entire dynamic model: it is here denoted by the symbol $\pi$. (Depending on the objectives of the investigation, the designer alternatively could choose another reference quantity, most likely of the extensive type.) The idea behind this scaling approach is to express state, input, and output variables in terms of the quantity $\pi$ using physical arguments.

### *Basis for state variable scaling*

For each state equation, the accumulation term is reexpressed in terms of an accumulation of the common variable $\pi$ by defining an appropriate equivalence factor. For example, a holdup (number of moles) can be related to an energy through use of a potential energy factor such as the heat of reaction or a heat of vaporization. This step requires a good insight into the physics of the process. Each state equation is then multiplied throughout by its appropriate equivalence factor. The state scaling factor $p_s$ for the $s$th state equation relates accumulation of a particular state quantity $x_s$ to an accumulation of $\pi$. The numerical values of $x_s$ and $p_s$ depend on the choice of units for $x_s$, whereas the numerical value of the scaled state variable, $\tilde{x}_s$, does not.

### *Basis for input scaling*

Once each dynamic equation has been expressed as an *ad hoc* balance of the reference quantity $\pi$, each term involving an input indicates a flow of the quantity $\pi$ into or out of the system. The scaling factor $w_{si}$ for the $i$th input in the $s$th equation is simply the multiplicative term relating $u_i$ to the corresponding flow of $\pi$. Again, the numerical values of $u_i$ and $w_{si}$ depend on the choice of units for $u_i$ (but not on the choice of units for $x_s$ since the state variables have already been scaled in terms of $\pi$). More importantly, the scaled input $\tilde{u}_i$ is independent of the choice of units for $u_i$. Since each equation may produce a separate scaling for any given input, we propose to define the scaling factor for that input as the maximum of the absolute values of the individual factors rather than as a value weighted over the various state equations.

### *Basis for output scaling*

With the state variables expressed in terms of $\pi$, each output equation indicates the amount of information, in terms of $\pi$, observed through the corresponding output. The scaling factor $1/v_{os}$ for the $o$th output is simply the multiplicative term relating $y_o$ to the amount of $\pi$-information contained in $\tilde{x}_s$. While the values of $y_o$ and $v_{os}$ depend on the choice of units for $y_o$, the scaled output $\tilde{y}_o$ is independent of that choice of units. Since each output equation may contain contributions from several state variables, the scaling factor for the output is chosen as the maximum of the absolute values of the individual factors.

### *Procedure*

For the $n$-dimensional dynamic system with an $r$-dimensional input vector and $m$-dimensional output vector

$$\dot{\underline{x}} = \underline{f}(\underline{x}, \underline{u}) \quad \underline{x}(0) = \underline{x}_0 \tag{1}$$

$$\underline{y} = \underline{g}(\underline{x}) \tag{2}$$

the scaling procedure consists of three steps:

1. Consider the $n$ conservation equations and choose the conserved quantity with the highest level of information as the reference quantity $\pi$ (usually the ordering would be energy before mass, component mass before overall mass, etc.). As mentioned above, other choices are also possible. Define equivalence factors relating each quantity to $\pi$ and multiply each equation throughout by the appropriate equivalence factor.

Express the accumulation of each state variable $x_s$ ($s = 1, \ldots n$) as an accumulation of $\pi$, defining the state scaling factors $p_s$.

Scale the state variables accordingly:

$$\underline{\pi} = \underline{\tilde{x}} = \underline{\underline{P}}\,\underline{x} \tag{3}$$

with

$$\underline{\underline{P}} = \text{diag}\,\{p_s\} \quad p_s > 0 \tag{4}$$

After state variable scaling, Eqs. 1 and 2 read:

$$\dot{\underline{\pi}} = \dot{\underline{\tilde{x}}} = \underline{\tilde{f}}(\underline{\tilde{x}}, \underline{u}) \tag{5}$$

$$\underline{y} = \underline{\tilde{g}}(\underline{\tilde{x}}) \tag{6}$$

or for the $s$th state variable and $i$th input:

$$\dot{\tilde{x}}_{si} = \tilde{f}_{si}(\underline{\tilde{x}}, u_i) \tag{7}$$

and for the $s$th state variable and $o$th output:

$$y_{os} = \tilde{g}_{os}(\tilde{x}_s) \tag{8}$$

2. Relate changes in $u_i$ to changes in the flow of $\pi$ into the subsystem associated with state $s$ by evaluating the input scaling factor

$$w_{si} = \left.\frac{\partial \tilde{f}_{si}}{\partial u_i}\right|_{ss} \tag{9}$$

where $ss$ indicates that the expression is evaluated at steady state. Define the input scaling factor $w_i (i = 1, \ldots, r)$

$$w_i = \max_s \{|w_{si}|\} \tag{10}$$

with

$$\underline{\underline{W}} = \text{diag}\,\{w_i\} \quad w_i > 0 \tag{11}$$

3. Relate changes in $y_o$ to changes in $\tilde{x}_s$ (i.e., in the observed flow of information, again in terms of $\pi$):

$$\frac{1}{v_{os}} = \left.\frac{\partial \tilde{g}_{os}}{\partial \tilde{x}_s}\right|_{ss} \tag{12}$$

Define the output scaling factors $v_o (o = 1, \ldots, m)$

$$v_o = \max_s \{|v_{os}|\} \tag{13}$$

with

$$\underline{\underline{V}} = \text{diag}\,\{v_o\} \quad v_o > 0 \tag{14}$$

The effects of scaling can be summarized as follows:

- A unit change in a scaled state variable corresponds to a unit change in the reference quantity.
- A unit change in a scaled input brings one additional unit of the reference quantity into the strongest state variable.
- A unit change in the scale output contains one unit of the reference quantity as information concerning the strongest state variable.
- There is no need with this procedure to rescale the independent variable time. This feature is certainly desirable because it leaves the eigenvalues of the system model unchanged.

Further, note that the procedure is limited to dynamic models since it requires the accumulation terms to determine the equivalence factors for the state variables.

## Application Examples

### *Example 1*

Two continuous stirred-tank reactors (CSTR's) in series, with a first-order exothermic reaction, jacket or coil cooling, and a by-pass around the second reactor are shown in Figure 1.

The conservation equations for the reaction system are:

Component balances, gmol/s

$$V_1 \frac{dc_1}{dt} = q(c_i - c_1) - V_1 k_0 e^{-E/RT_1} c_1 \tag{15}$$

$$V_2 \frac{dc_2}{dt} = \alpha q(c_1 - c_2) - V_2 k_0 e^{-E/RT_2} c_2 \tag{16}$$

Energy balances, $J/s$

$$V_1 \rho c_p \frac{dT_1}{dt} = q\rho c_p(T_i - T_1) + (-\Delta H)V_1 k_0 e^{-E/RT_1} c_1 + (UA)_1(T_{c1} - T_1) \tag{17}$$

$$V_2 \rho c_p \frac{dT_2}{dt} = \alpha q \rho c_p(T_1 - T_2) + (-\Delta H)V_2 k_0 e^{-E/RT_2} c_2 + (UA)_2(T_{c2} - T_2) \tag{18}$$

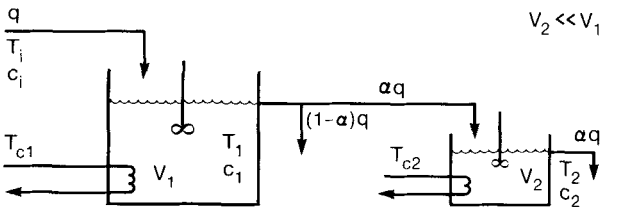


**Figure 1. Two CSTR's in series.**

The model involves the conservation of two physical quantities (number of moles of key component and energy), four state variables ($c_1$, $c_2$, $T_1$, $T_2$), and six input variables ($q$, $T_i$, $c_i$, $T_{c1}$, $T_{c2}$, $\alpha$). It is assumed that the four state variables are measurable but that the four sensors provide differing units:

$$c_{1m}(\text{gmol/L}) = c_1 \tag{19}$$

$$c_{2m}(\text{gmol/m}^3) = 1{,}000\, c_2 \tag{20}$$

$$T_{1m}(°\text{C}) = T_1 \tag{21}$$

$$T_{2m}(°\text{F}) = 1.8\, T_2 \tag{22}$$

Following the procedure given above, energy is chosen as the reference quantity $\pi$, and Eqs. 15 and 16 are multiplied throughout by the equivalence factor $(-\Delta H)$. The accumulation of each state variable is then expressed as an accumulation of $\pi$ as follows:

$$\dot{\pi}_1 = (-\Delta H)V_1 \dot{c}_1 \tag{23}$$

$$\dot{\pi}_2 = (-\Delta H)V_2 \dot{c}_2 \tag{24}$$

$$\dot{\pi}_3 = V_1 \rho c_p \dot{T}_1 \tag{25}$$

$$\dot{\pi}_4 = V_2 \rho c_p \dot{T}_2 \tag{26}$$

Concentration and temperature changes are then related to changes in energy through the following state variable scaling factors:

$$p_{c_1} = V_1(-\Delta H) \quad p_{c_2} = V_2(-\Delta H)$$
$$p_{T_1} = V_1 \rho c_p \quad p_{T_2} = V_2 \rho c_p$$

By considering the input variables in the scaled, dynamic equations, the following input scaling factors are obtained:

$$w_q = \max\{|(-\Delta H)(\bar{c}_i - \bar{c}_1)|, |(-\Delta H)\bar{\alpha}(\bar{c}_1 - \bar{c}_2)|, \cdot |\rho c_p(\bar{T}_i - \bar{T}_1)|, |\bar{\alpha}\rho c_p(\bar{T}_1 - \bar{T}_2)|\}$$
$$w_{T_i} = \bar{q}\rho c_p \quad w_{T_{c1}} = (UA)_1$$
$$w_{c_i} = |(-\Delta H)\bar{q}| \quad w_{T_{c2}} = (UA)_2$$
$$w_\alpha = \max\{|(-\Delta H)\bar{q}(\bar{c}_1 - \bar{c}_2)|, |\bar{q}\rho c_p(\bar{T}_1 - \bar{T}_2)|\}$$

where a bar over a variable indicates its steady state value.

Similarly, by considering the output variables in the scaled

output equations, the output scaling factors are:

$$v_{c_{1m}} = |V_1(-\Delta H)| \quad v_{c_{2m}} = \left| \frac{V_2(-\Delta H)}{1{,}000} \right|$$

$$v_{T_{1m}} = V_1 \rho c_p \quad v_{T_{2m}} = \frac{V_2 \rho c_p}{1.8}$$

The model given by Eqs. 15–18 was evaluated numerically using the reactor data given in the Appendix. The plant, input, and output matrices for the original and scaled, linearized systems, as well as the scaling matrices, are also given in the Appendix. Note that the columns of $\underline{\underline{\tilde{B}}}$ and rows of $\underline{\underline{\tilde{C}}}$ have been normalized such that the absolute value of the largest element equals one.

Structural dominance analysis (Bonvin and Mellichamp, 1982) was used to analyze the internal model structure. The dominance elements shown in Table 1 were computed without mode weighting and then were normalized with respect to the largest element in the table. Hence, the elements in the table can be interpreted as relative energetic changes in the output or state variables caused by unit energetic changes in the inputs. The mode most strongly associated with an input/output path is also given in parentheses. The eigenvalues for the system are

$$\lambda_1 = -1.21*10^{-3}$$

$$\lambda_2 = -2.28*10^{-3}$$

$$\lambda_{3,4} = -1.10*10^{-2} \pm 2.8*10^{-4}j$$

This analysis shows that, as expected, $T_{1m}$ and $c_{1m}$ represent the most energetic outputs; $T_i$, $c_i$, and $T_{c1}$ are the most energetic inputs; modes 1 and 2 are the most important: the input $q$ is strongest through mode 2, whereas $T_i$, $c_i$, and $T_{c1}$ affect both modes 1 and 2. The second reactor is most excited by the inputs $T_{c2}$ and $\alpha$ through the complex modes 3 and 4. In an attempt to control the four outputs, one would most likely choose the following pairings: $T_{1m}/T_i$ or $T_{1m}/T_{c1}$, $c_{1m}/q$, $T_{2m}/T_{c2}$, and $c_{2m}/\alpha$.

Clearly, the results would have been different without a meaningful scaling since, for example, the simple fact of expressing the volume in $m^3$ rather than in L would change some of the dominance elements by a factor of $10^{-3}$ or $10^3$ while leaving the others unchanged. Obviously, structural dominance analysis cannot be used effectively without appropriate input and output scaling.

The reaction system was then analyzed using the singular-value decomposition (SVD) method as proposed by Lau et al. (1985). The condition number of the original static gain matrix $\underline{\underline{G}} = -\underline{\underline{C}}\underline{\underline{A}}^{-1}\underline{\underline{B}}$ is 39,240. The nodal decomposition is totally uninformative with respect to the amount of physical interaction that is present between input and output variables. The following pairings are suggested: $c_{2m}/\alpha$, $T_{2m}/c_i$, $T_{1m}/q$, and $c_{1m}/T_{c2}$, which is physically meaningless. The largest singular value is associated with $c_{2m}/\alpha$—mainly because $c_{2m}$ (expressed in gmol/$m^3$) has the largest numerical value and not because the coupling $c_{2m}/\alpha$ is dominant in the system.

Since it is well known that the SVD is highly dependent on the choice of units, the scaled gain matrix $\underline{\underline{\tilde{G}}} = -\underline{\underline{\tilde{C}}}\underline{\underline{\tilde{A}}}^{-1}\underline{\underline{\tilde{B}}} = \underline{\underline{V}}\,\underline{\underline{G}}\,\underline{\underline{W}}^{-1}$ with a condition number of 22.6 was then analyzed. Nodal decomposition suggests the following output/input pairings: $T_{1m}/T_i$ or $T_{1m}/T_{c1}$, $c_{1m}/q$, $c_{2m}/\alpha$, and $T_{2m}/T_{c2}$. These results agree entirely with those obtained using structural dominance analysis.

A complete mathematical conditioning of the model, obtained through row and column equilibration of the steady state gain matrix, produced a condition number of 2.5. However, with the new system model it is impossible to distinguish important from unimportant variables because the normalization has put them all on a numerically (more or less) similar basis. Thus, the largest singular value, for example, would point equally to any of the 24 possible pairings.

This example clearly demonstrates that for the purpose of analyzing input and output variables, an appropriate scaling is indeed needed. Furthermore, a purely mathematical conditioning may subvert the intended purpose if it eliminates the intrinsic strength of inputs and outputs. The proposed physically based scaling procedure will now be briefly demonstrated with two other examples.

**Table 1. Structural Dominance Analysis for Example 1 (scaled)**

| | Inputs | | | | | |
|---|---|---|---|---|---|---|
| Outputs | $q(2)$ | $T_i(1)$ | $c_i$ | $T_{c1}(1)$ | $T_{c2}(3,4)$ | $\alpha(3,4)$ |
| $c_{1m}$ | 0.29 | −0.25 | 0.09(2) | −0.25 | 0.0 | 0.0 |
| $c_{2m}$ | 0.003 | −0.002 | 0.0004(2) | −0.002 | −0.005 | 0.07 |
| $T_{1m}$ | −0.13 | 1.0 | 0.66(1) | 1.0 | 0.0 | 0.0 |
| $T_{2m}$ | −0.008 | 0.009 | 0.007(1) | 0.009 | 0.08 | 0.003 |

### *Example 2*

A mixing tank with a hot and a cold stream and with variable volume is depicted in Figure 2.

The conservation equations for the mixing system are:

Mass balance, g/s

$$\rho \frac{dV}{dt} = q_h + q_c - q \tag{27}$$

Energy balance, J/s

$$V\rho c_p \frac{dT}{dt} = q_h c_p (T_h - T) + q_c c_p (T_c - T) \tag{28}$$

The model involves the conservation of two physical quantities (mass and energy), two state variables ($V$ and $T$), which are

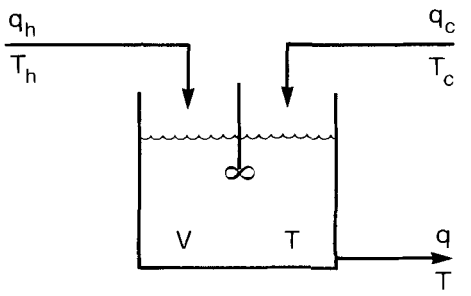


**Figure 2. Mixing tank with variable volume.**

both measured, and five inputs ($q_h$, $q_c$, $q$, $T_h$, $T_c$). After choosing energy as the reference quantity, we need to multiply Eq. 27 by an equivalence factor. However, since there is no reaction involved in this system, a potential energy factor of the form $(-\Delta H)$ is not appropriate. Rather, we define a weighted $(c_p\Delta T)$ term of dimension J/g:

$$c_p\Delta T \triangleq \frac{|\bar{q}_h c_p(\bar{T}_h - \bar{T})| + |\bar{q}_c c_p(\bar{T}_c - \bar{T})| + |\bar{q} c_p(\bar{T} - \bar{T})|}{|\bar{q}_h| + |\bar{q}_c| + |\bar{q}|} = \frac{\bar{q}_h}{\bar{q}} c_p(\bar{T}_h - \bar{T}) \quad (29)$$

Note that this definition is not valid in the trivial case $\bar{T}_h = \bar{T}_c = \bar{T}$. The individual scaling factors are easily deduced:

$$p_V = v_V = \rho(c_p\Delta T) = \rho \frac{\bar{q}_h}{\bar{q}} c_p(\bar{T} - \bar{T})$$

$$p_T = v_T = \bar{V}\rho c_p$$

$$w_{q_h} = \max\{|c_p\Delta T|, |c_p(\bar{T}_h - \bar{T})|\} = c_p(\bar{T}_h - \bar{T})$$

$$w_{q_c} = \max\{|c_p\Delta T|, |c_p(\bar{T}_c - \bar{T})|\} = \frac{\bar{q}_h}{\bar{q}_c} c_p(\bar{T}_h - \bar{T})$$

$$w_q = |-c_p\Delta T| = \frac{\bar{q}_h}{\bar{q}} c_p(\bar{T}_h - \bar{T})$$

$$w_{T_h} = \bar{q}_h c_p$$

$$w_{T_c} = \bar{q}_c c_p$$

### *Example 3*

An adiabatic packed-bed tubular reactor is shown in Figure 3.

The conservation equations for this distributed-parameter reaction system are:

Component balance, gmol/s

$$V\epsilon \frac{\partial c}{\partial t} = -V\epsilon v \frac{\partial c}{\partial z} - V\epsilon R(c, T) \quad (30)$$

Energy balance for the gas phase, J/s

$$V\epsilon\rho c_p \frac{\partial T}{\partial t} = -V\epsilon v\rho c_p \frac{\partial T}{\partial z} + ha(T_s - T) + V\epsilon(-\Delta H)R(c, T) \quad (31)$$

Energy balance for the solid phase, J/s

$$V(1 - \epsilon)\rho_s c_{ps} \frac{\partial T_s}{\partial T} = ha(T - T_s) \quad (32)$$

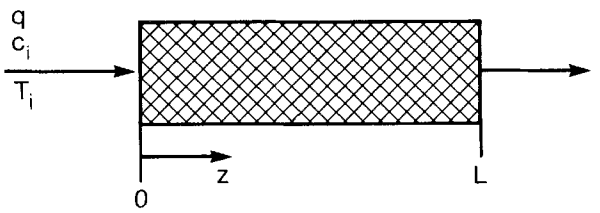


**Figure 3. Adiabatic packed-bed tubular reactor.**

The system has boundary conditions

$$\text{at} \quad z = 0: \quad c = c_i(t) \quad T = T_i(t) \quad (33)$$

The model involves the conservation of two physical quantities (number of moles of key component and energy), three states or measured outputs ($c$, $T$, $T_s$), and three inputs ($q$, $c_i$, $T_i$). Note that the mass flow rate $q$ is related to $v$ as

$$q = \rho A\epsilon v \text{ (kg/s)} \quad (34)$$

where $A$ is the cross-sectional area of the reactor. Again, energy can be chosen as reference quantity and Eq. 30 multiplied throughout by $(-\Delta H)$.

The state and output scaling factors are straightforward:

$$p_c = v_c = V\epsilon(-\Delta H)$$

$$p_T = v_T = V\epsilon\rho c_p$$

$$p_{T_s} = v_{T_s} = V(1 - \epsilon)\rho_s c_{ps}$$

Input scaling requires that a distinction be made between the local or global action of each input:

- The input $q$ acts globally on the reactor. From Eqs. 30 and 34 one can write:

$$w_q = \frac{1}{\rho A\epsilon} w_v \quad (35)$$

$$w_v(z) = \max\left\{\left| -(-\Delta H)V\epsilon\left(\frac{\partial c}{\partial z}\right)_{ss}\right|, \left| -V\epsilon\rho c_p\left(\frac{\partial T}{\partial z}\right)_{ss}\right|\right\} \quad (36a)$$

One way to eliminate the spatial dependency of $w_v$ is through the approximations:

$$\left(\frac{\partial c}{\partial z}\right)_{ss} \simeq \frac{\bar{c}_{\min} - \bar{c}_i}{L} \quad \text{for a reactant}$$

$$\left(\frac{\partial T}{\partial z}\right)_{ss} \simeq \frac{\bar{T}_{\max} - \bar{T}_i}{L} \quad \text{for an exothermic reaction}$$

and Eq. 36 becomes

$$w_v = \max\left\{\left| -(-\Delta H)V\epsilon\frac{\bar{c}_{\min} - \bar{c}_i}{L}\right|, \left| -V\epsilon\rho c_p\frac{\bar{T}_{\max} - \bar{T}_i}{L}\right|\right\} \quad (36b)$$

- The input $c_i$ acts through the first term on the righthand side of Eq. 30. Its scaling factor is:

$$w_{c_i} = \left| -(-\Delta H)\frac{V\epsilon\bar{v}}{L}\right| = \left| -(-\Delta H)\frac{1}{\rho}\bar{q}\right| \quad (37)$$

and similarly for $T_i$

$$w_{T_i} = \left| -\frac{V\bar{v}\rho c_p}{L}\right| = |-\bar{q}c_p| \quad (38)$$

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Constructive comments made by J. Keller at ETH, Zürich, as well as financial support from the National Science Foundation during part of this work are gratefully acknowledged.

## Notation

$A$ = cross-sectional area
$\underline{\underline{A}}$ = plant matrix
$\underline{\underline{B}}$ = input matrix
$\bar{c}$ = concentration
$c_p$ = heat capacity
$\underline{\underline{C}}$ = output matrix
$\bar{E}$ = activation energy
$f$ = function, Eq. 1
$g$ = function, Eq. 2
$G$ = static gain matrix
$-\Delta\bar{H}$ = reaction enthalpy
$ha$ = heat transfer coefficient times area
$k_o$ = preexponential factor
$L$ = reactor length
$m$ = number of outputs
$n$ = number of states
$P$ = diagonal state scaling matrix
$\bar{q}$ = flow rate
$r$ = number of inputs
$R$ = reaction rate, universal gas constant
$t$ = time
$T$ = temperature
$\underline{u}$ = input vector
$UA$ = heat transfer coefficient times effective area
$v$ = gas velocity
$V$ = reactor volume
$\underline{\underline{V}}$ = diagonal output scaling matrix
$\underline{\underline{W}}$ = diagonal input scaling matrix
$\underline{x}$ = state vector
$\underline{y}$ = output vector
$z$ = reactor axial coordinate

### *Greek letters*

$\alpha$ = fraction of flow out of reactor 1 going into reactor 2
$\epsilon$ = packed bed void fraction
$\lambda$ = eigenvalue
$\rho$ = density
$\pi$ = chosen reference quantity

### *Superscripts*

$T$ = transposed vector or matrix
$-$ = steady state value
$\sim$ = scaled quantity

### *Subscripts*

$c$ = cold
$h$ = hot
$i$ = input, inlet
$m$ = measured quantity
$o$ = output
$s$ = state, solid phase
$ss$ = steady state value
1 = reactor 1
2 = reactor 2

## Appendix

### *Numerical data used in example 1*

$$V_1 = 1{,}000\ \text{L} \quad V_2 = 10\ \text{L}$$

$$\bar{q} = 1\ \text{L/s} \quad \bar{\alpha} = 0.1$$

$$\rho c_p = 4{,}000\ \text{J/L°C} \quad (-\Delta H) = 10^5\ \text{J/gmol}$$

$$\bar{c}_i = 1\ \text{gmol/L} \quad \bar{c}_1 = 0.314\ \text{gmol/L}$$

$$\bar{c}_2 = 0.257\ \text{gmol/L} \quad \bar{T}_i = 20°\text{C}$$

$$\bar{T}_1 = 34.1°\text{C} \quad \bar{T}_2 = 34.3°\text{C}$$

$$\bar{T}_{c1} = \bar{T}_{c2} = 10°\text{C}$$

$$k_o = 5{,}000\ \text{s}^{-1} \quad E/R = 4{,}500\ \text{K}$$

$$(UA)_1 = 500\ \text{W/°C} \quad (UA)_2 = 20\ \text{W/°C}$$

### *Original A-, B-, and C-matrices*

$$\underline{\underline{A}} = \begin{bmatrix} -3.18 \times 10^{-3} & 0 & -3.26 \times 10^{-5} & 0 \\ 1.0 \times 10^{-2} & -1.22 \times 10^{-2} & 0 & -2.69 \times 10^{-5} \\ 5.45 \times 10^{-2} & 0 & -3.10 \times 10^{-4} & 0 \\ 0 & 5.5 \times 10^{-2} & 1.0 \times 10^{-2} & -9.83 \times 10^{-3} \end{bmatrix}$$

$$\underline{\underline{B}} = \begin{bmatrix} 6.86 \times 10^{-4} & 0 & 1.0 \times 10^{-3} & 0 & 0 & 0 \\ 5.7 \times 10^{-4} & 0 & 0 & 0 & 0 & 5.7 \times 10^{-3} \\ -1.41 \times 10^{-2} & 1.0 \times 10^{-3} & 0 & 1.25 \times 10^{-4} & 0 & 0 \\ -2 \times 10^{-3} & 0 & 0 & 0 & 5 \times 10^{-4} & -2 \times 10^{-2} \end{bmatrix}$$

$$\underline{\underline{C}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1{,}000 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1.8 \end{bmatrix}$$

### *Scaled A-, B-, and C-matrices*

$$\underline{\underline{\tilde{A}}} = \begin{bmatrix} -3.18 \times 10^{-3} & 0 & -8.15 \times 10^{-4} & 0 \\ 1.0 \times 10^{-4} & -1.22 \times 10^{-2} & 0 & -6.73 \times 10^{-4} \\ 2.18 \times 10^{-3} & 0 & -3.10 \times 10^{-4} & 0 \\ 0 & 2.2 \times 10^{-3} & 1.0 \times 10^{-4} & -9.83 \times 10^{-3} \end{bmatrix}$$

$$\underline{\underline{\tilde{B}}} = \begin{bmatrix} 1.0 & 0 & 1.0 & 0 & 0 & 0 \\ 8.31 \times 10^{-3} & 0 & 0 & 0 & 0 & 1.0 \\ -0.822 & 1.0 & 0 & 1.0 & 0 & 0 \\ -1.17 \times 10^{-3} & 0 & 0 & 0 & 1.0 & -0.140 \end{bmatrix}$$

$$\underline{\underline{\tilde{C}}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\underline{\underline{P}} = \text{diag}\,\{10^8, 10^6, 4 \times 10^6, 4 \times 10^4\}$$

$$\underline{\underline{W}} = \text{diag}\,\{6.86 \times 10^4, 4{,}000, 10^5, 500, 20, 5.7 \times 10^3\}$$

$$\underline{\underline{V}} = \text{diag}\,\{10^8, 10^3, 4 \times 10^6, 2.22 \times 10^4\}$$

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