Measure of Closed-Loop Nonlinearity and Interaction for Nonlinear Chemical Processes

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A new approach for assessing nonlinear interaction effects and closed-loop nonlinearity in multivariable processes is presented. It is based on a differential geometric interpretation of the relative gain array that leads naturally to systematic procedures for describing interaction effects of higher order and for assessing closed-loop nonlinearity effects in nonlinear processes. Two types of nonlinear effects associated with the behavior of a process are introduced. Between-channel nonlinearity is associated with the nonlinear dependence of an output channel on other input–output pairings. Within-channel nonlinearity is used to identify the nonlinear effects that result from the inherent nonlinearity of an individual output channel. A root-mean-squared measure of nonlinearity is introduced and is used to evaluate the significance of local nonlinear effects. Nonlinear interaction measures are derived that provide tools for assessing input–output pairings in a nonlinear process. This new approach extends the standard techniques and provides an estimate of the effect of nonlinearity on closed-loop interactions.

Introduction

The performance of closed-loop multivariable processes can be highly influenced by interactions between individual control loops. For many applications involving linear dynamics, the relative gain array (RGA) (Bristol, 1966) provides an effective tool for the evaluation of potential control-loop pairings for multiloop controller design. Quantitative measures of interaction such as the RGA have been used successfully in linear controller design for chemical processes and continue to be of considerable importance, especially with respect to the study of robust stability (Grosdidier and Morari, 1987; Skogestad and Morari, 1987) and performance of ill-conditioned plants (Nett and Manousiouthakis, 1987; Skogestad and Morari, 1987; Skogestad et al., 1988).

Since the RGA is basically a first-order measure of interaction, its interpretation for nonlinear processes relies heavily on the direction of the input (or output) perturbations used to estimate gains (Koung and MacGregor, 1992). Problems can be encountered in the study of gain–asymmetric processes where interpretation of the RGA may often yield misleading results. Interaction measures that take the gain nonlinearity of the process into account can prove beneficial in overcoming these problems in a number of cases.

Very few measures of interactions for nonlinear processes have been proposed. Daoutidis and Kravaris (1992) used a differential geometric approach to develop a methodology for the evaluation of control configurations in nonlinear control–affine processes. With this approach various control configurations are evaluated in terms of their corresponding relative order. Input–output pairings are selected by virtue of the most immediately related (or less sluggish) pairs. Assuming the availability of a detailed state-space description of the process, this control pairing selection methodology constitutes a very useful strategy for providing insight into the structure of nonlinear systems. While information is provided about the dynamic lags in the process, no information is provided regarding the magnitudes of output changes in response to input changes.

Manousiouthakis and Nikolaou (1989) developed a nonlinear block relative gain array measure using an operator-based

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approach that elegantly demonstrated the need to consider nonlinear effects in the assessment of interaction in nonlinear plants. This approach, although very general and appealing, can constitute a considerable challenge when applied to complex plants. Other approaches to this problem include that of Mijares et al. (1985), who developed a methodology for assessing nonlinear interaction from evaluation of first-order gains.

Piette et al. (1995) have presented a graphical interpretation of the relative gain array in terms of intersections of constant output contours and the degree of rotation of constant output norm contours. A graphical assessment for nonlinear problems is also proposed that consists of relative gain surfaces and constant output norm contours. Nonlinear effects are identified by deformations in the contours, and by changes in the relative gains over the operating region. This latter approach is consistent with the approaches identified earlier, in which changes in linear approximations are used to identify nonlinearity and nonlinear interactions. The main drawback of graphical methods is their inherent subjectivity and the dependence on the particular graphical representation employed.

The purpose of this article is to present an alternative geometric interpretation of the RGA that extends directly to the treatment of higher- (in particular, second) order interactions in nonlinear processes. Furthermore, the problem of interaction is identified fundamentally as the result of input and output coordinate choices. Standard linear techniques such as the relative gain array identify interactions in coordinate choices arising at the first-order level. The approach presented is based on the framework proposed in Guay et al. (1995) for the assessment of open-loop nonlinearity of steady-state nonlinear processes. In the development presented in the current article, methods are proposed for assessing nonlinearity within and between input–output channels. This leads to the definition of a measure of higher-order interaction, and also leads to the concept of closed-loop nonlinearity.

As is the case for linear control problems, control-loop interaction can be assessed using both steady-state and dynamic information. This article proposes interaction measures, based on steady-state information, that describe nonlinear interaction behavior appearing in the "gain" relationships of the process. While measures based on steady-state information cannot provide definitive answers regarding dynamic interaction, they can be used to identify potential interaction problems.

For a nonlinear closed-loop process operating at steady state without offset, it follows that the extent of open-loop nonlinearity, that is, nonlinearity associated with input variation, is exactly counterbalanced by the control-law nonlinearity. From a differential geometric perspective, this is because either the inputs or the outputs can be used to parametrize the same space at steady state. By viewing the inputs and outputs as two coordinate systems on an abstract surface, we can establish, through differential geometry, a number of interesting identities that provide local measures of interaction. A direct consequence of this construction is the recognition of a certain arbitrariness in the choice of coordinates. We do not distinguish, *a priori*, between input and output variables. Interchangeability of input and output coordinates has been widely discussed by system theorists, particularly with respect to the development of behavioral approaches in the study of dynamical systems (Willems, 1991) and closely related differential algebraic methods (Fliess et al., 1995). In this approach, it becomes more natural to let the underlying structure of the system dictate appropriate choices for the inputs and outputs.

The advantages of interchangeability of coordinate systems is demonstrated here in the development of interaction measures for nonlinear steady-state processes. It is shown that this approach provides a natural, rigorous framework for studying interaction effects for both linear and nonlinear systems, which provides a fundamental basis for the development of measures of closed-loop nonlinearity and new measures of nonlinear interaction. The result is a set of nonlinear interaction tables that provide easy interpretation of the contribution of nonlinear effects to interaction effects. A continuous stirred-tank reactor (CSTR) model is used to demonstrate the application of the method.

The main concepts of this article are illustrated using a conventional approach to control system structure. Then, differentiable manifolds and pseudo-Riemannian geometry are discussed, as well as the differential geometric basis for this analytical procedure and a number of identities derived. The application of these identities to the assessment of closed-loop nonlinearity for nonlinear processes is presented using a simple chemical-reactor example. Nonlinear interaction measures are also discussed using two chemical process examples.

Motivation

Figure 1 shows the Internal Model Control (IMC) form of the block diagram of a closed-loop process subjected to setpoint changes. For a general nonlinear process and controller, the closed-loop expressions are given by the following implicit algebraic equations:

$$u = C\{r - [P(u) - P_m(u)]\}$$
$$y = P(u), \tag{1}$$

where $u \in U \subset \mathbb{R}^P$, $y \in Y \subset \mathbb{R}^P$, and $r \in S \subset \mathbb{R}^P$ are the process inputs, outputs, and setpoints, respectively, of the closed-loop process, and the subscript m denotes model. In the general nonlinear case, P, P_m, and C are the process, process model, and controller operators (see, for example, Economou et al., 1986). These operators are assumed to be

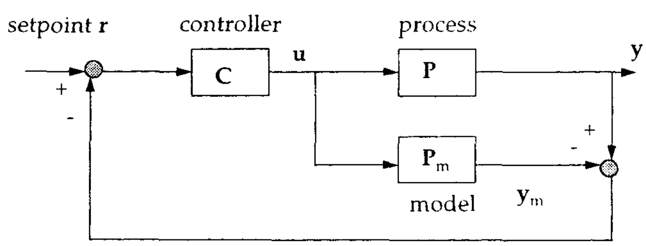

Figure 1. Internal model control (IMC) block diagram of a closed-loop process under set-point changes.

twice differentiable and unbiased [i.e., $P(0)=0$, $C(0)=0$]. Note that dynamic results can be derived by considering the maps as Fréchet differentiable operators and examining the first- and second-order Fréchet derivatives. Such an approach is used by Guay (1996) to provide a measure of open-loop dynamic nonlinearity. A measure of dynamic interaction will be the subject of a future article.

The corresponding steady-state maps can be viewed as vectors of functions. In the linear case, these quantities are P by P transfer function matrices corresponding to the process, process model, and the controller, respectively. At steady state, the transfer-function matrices yield gain matrices. Note that for the linear case, Eq. 1 can be solved explicitly for u and y in terms of r, yielding the standard expressions for linear IMC control.

Since the focus of this article is the development of interaction measures using steady-state process and controller information, consider Eq. 1 in its steady-state form. If the process model is perfect (at least at steady state), Eq. 1 simplifies to

$$u = C(r)$$
$$y = P[C(r)].$$

The controller is typically chosen to the approximate inverse of the process model, and at steady state the controller must be the inverse of the process map for perfect setpoint tracking (no offset). The perfect setpoint tracking requirement implies that the composition of the process and controller maps is the identity map, or $y=r$. This observation leads to the following identities, which can be obtained by differentiation and application of the chain rule:

$$\left.\frac{\partial y}{\partial r}\right|_{u_0,r_0} = \left.\frac{\partial y}{\partial u}\right|_{u_0,r_0} \left.\frac{\partial u}{\partial r}\right|_{u_0,r_0} = I \tag{2}$$

and

$$\left.\frac{\partial^2 y}{\partial r \partial r'}\right|_{u_0,r_0} = \left.\frac{\partial y}{\partial u}\right|_{u_0,r_0} \left.\frac{\partial^2 u}{\partial r \partial r'}\right|_{u_0,r_0} + \left.\frac{\partial u'}{\partial r}\right|_{u_0,r_0} \left.\frac{\partial^2 y}{\partial u \partial u'}\right|_{u_0,r_0} \left.\frac{\partial u}{\partial r}\right|_{u_0,r_0} = \mathbf{0}. \tag{3}$$

Finally, under perfect tracking the setpoints can be identified directly as the outputs and the derivative identities in Eqs. 2 and 3 can be rewritten as

$$\left.\frac{\partial y}{\partial y}\right|_{y_0} = \left.\frac{\partial y}{\partial u}\right|_{u_0} \left.\frac{\partial u}{\partial y}\right|_{y_0} = I \tag{4}$$

$$\left.\frac{\partial^2 y}{\partial y \partial y'}\right|_{y_0} = \left.\frac{\partial y}{\partial u}\right|_{u_0} \left.\frac{\partial^2 u}{\partial y \partial y'}\right|_{y_0} + \left.\frac{\partial u'}{\partial y}\right|_{y_0} \left.\frac{\partial^2 y}{\partial u \partial u'}\right|_{u_0} \left.\frac{\partial u}{\partial y}\right|_{y_0} = 0.$$

When examining these identities, it is important to remember that the partial derivative with respect to a given control input implies that the other inputs are fixed at the nominal point ("other loops open"), while the partial derivative taken with respect to a specific output implies that the other outputs are constant ("other loops closed").

The significance of the relative gain to closed-loop performance, and specifically the relationship between the outputs and the setpoints, was presented for the linear RGA case by Manousiouthakis et al. (1986). The identities just given extend this result to the nonlinear case by examining second-order effects.

Perfect setpoint tracking implies that the relationship between the setpoints and the outputs is decoupled, that is, one setpoint affects one output. In practice, this decoupling may be difficult to achieve when individual inputs affect more than one output. The difficulty in decoupling channels of a multi-input, multioutput (MIMO) process is commonly assessed using the RGA, which measures the relative contributions of each input channel to the unit diagonal elements of the identity matrix in Eq. 2. The magnitudes of the elements of the RGA provide some indication of the invertibility of the gain matrix. Large elements indicate potential singularity in the process and poor robustness (Kuong and MacGregor, 1992).

For a nonlinear process, it is possible to obtain an appreciation of the extent of interaction by perturbing the process over a range of input values and evaluating the RGA as a function of the inputs. The RGA still provides an indication of the extent of interaction locally. However, such an approach measures the change of *linear* interaction over a specific range and considers only the interaction in the process subject to linear control. It does not provide a measure of nonlinear interaction that is applicable for nonlinear controllers.

A natural way to extend the RGA is to consider higher-order identities of the form of Eq. 3. This equation indicates how the second-order derivative of the process map must relate to the second-order derivative of its inverse under perfect tracking. It is conceptually similar to Eq. 2, except that it also takes into account the local *nonlinear* inversion of the process. The purpose of this article is to introduce the application of such identities to the study of nonlinear processes.

One interpretation of the first- and second-order conditions identified in Eqs. 2 and 3 can be provided by considering the steady-state behavior of the second-order approximation of the process (considered as the "true process") under an IMC control law in which the process model is a first-order approximation of the process, and a linear controller is used. The process, model and controller expressions are

$$P \approx P_1 u + \frac{1}{2} u' P_2 u = \left.\frac{\partial P}{\partial u}\right|_0 u + \frac{1}{2} u' \left.\frac{\partial^2 P}{\partial u \partial u'}\right|_0 u$$
$$P_m = P_1 u \tag{5}$$
$$C \approx C_1[r-(y-y_m)] = \left.\frac{\partial C}{\partial r}\right|_0 [r-(y-y_m)],$$

where the variables are assumed to be in deviation form for simplicity. The approximation is calculated about the nominal operating point. The model mismatch consists exclusively of the second-order term in the process, and the relationship between the control input and the setpoint is given by

$$u = C_1 r - \frac{1}{2} C_1 u' P_2 u. \tag{6}$$

Note that although the controller is linear, the closed-loop relationship between $\boldsymbol{u}$ and $\boldsymbol{r}$ is second order because of the feedback through the second-order process. This expression can be used to determine the first- and second-order derivatives of the process output with respect to setpoints by using Eq. 1 and the chain rule from calculus:

$$\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{r}} = [\boldsymbol{I} + \boldsymbol{C}_1 \boldsymbol{P}_2 \boldsymbol{u}]^{-1} \boldsymbol{C}_1$$

$$\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{r}} = (\boldsymbol{P}_1 + \boldsymbol{P}_2 \boldsymbol{u})[\boldsymbol{I} + \boldsymbol{C}_1 \boldsymbol{P}_2 \boldsymbol{u}]^{-1} \boldsymbol{C}_1 \tag{7}$$

$$\frac{\partial^2 \boldsymbol{y}}{\partial \boldsymbol{r} \partial \boldsymbol{r}'} = (\boldsymbol{P}_1 + \boldsymbol{P}_2 \boldsymbol{u}) \frac{\partial^2 \boldsymbol{u}}{\partial \boldsymbol{r} \partial \boldsymbol{r}'} + \frac{\partial \boldsymbol{u}'}{\partial \boldsymbol{r}} \boldsymbol{P}_2 \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{r}}.$$

When the derivative expressions are evaluated at the nominal operating point and the linear controller is chosen to be the inverse of the process first-order gain matrix at the nominal point, the identities in Eqs. 2 and 3 are obtained. Thus, the linear IMC controller consisting of the inverse process gain matrix provides perfect tracking at the nominal operating point as expected, since first-order behavior is being matched. Furthermore, the setpoints can be identified as the outputs given the perfect setpoint tracking. The second derivative identity describes how the second-order process nonlinearity (the second term in the expression) must be compensated by the controller.

It should be emphasized that for perfect tracking using a nonlinear controller, the first and second derivative identities in Eqs. 2 and 3 must be satisfied over the entire operating region. In contrast, the linear IMC controller satisfies these identities strictly at the nominal operating point.

When designing controller configurations for processes, control applications engineers are presented with a set of variables describing the process. Poor choices in control-loop pairings can lead to nonminimum phase behavior, serious control-loop interactions, and potentially instability. This behavior arises from the complex physical relationships in the process. Mathematically, this behavior is associated with the choice of "coordinates" for the process. Selecting input and output variables amounts to choosing coordinate systems for the process, and the interaction behavior can be seen mathematically in the interaction or exchange of these coordinates.

The development of the derivative identities will be presented based on a classic differential geometric setting that provides a natural interpretation of interaction effects in linear and nonlinear processes. First, some basic notions of differential geometry are presented.

Differential Geometric Tools

The identities in Eqs. 2 and 3 were obtained by recognizing the implications of perfect tracking and differentiating the resulting relationship between outputs and setpoints. They are in fact a manifestation of an underlying "coordinate" representation for the process. The concept of coordinate charts can be illustrated by considering the operation of a distillation column. The steady-state profile for a distillation column consists of temperatures, pressures, holdups, and compositions. The column operation evolves in a high dimension operating "space" (consisting of, for example, 150 variables). However, there are relatively few degrees of freedom (e.g., five degrees of freedom that are typically "free" variables such as reflux flow rate and vapor boilup). Specifying values for the free variables fixes the column profile in the high dimension operating space because of the constraints posed by energy and material balances, and equilibrium relationships. In many cases, the free variables are identified as manipulated variables; determining the column profile for given values of the inputs corresponds to the "rating" problem in steady-state process design simulation. Alternatively, output variables such as distillate composition can be specified and the simulation can determine the necessary input variables. This corresponds to the "design" calculation in process design.

The column operation can be seen to evolve on a surface in the high dimension operating space. The degrees of freedom represent the number of variables required to specify an operating point on this surface. Thus, although the column operation might evolve in a space of 150 variables, the operating point can be identified by specifying the values of five variables. The operating surface is in fact a "five-dimensional surface" embedded in a higher dimensional space. Choosing values of variables to satisfy the degrees of freedom amounts to specifying coordinates on this operating surface. In this article, we argue that interaction between input and output channels is associated with the exchange of such coordinate systems for the process. Interaction between a multiloop controller configuration without decoupling arises because we try to impose a coordinate system that ignores the linkages in the process. Determining the manipulated variable coordinates for a desired operating point using this approximate coordinate system produces coordinates for a different operating point in the actual process. Although this will be seen mathematically, it should be remembered that the structure of the interaction arises from the underlying physical phenomena, as represented by the balance and constitutive equations in the process model.

The fundamental coordinate relationships in this article are properly developed using classic differential geometric tools (see Boothby, 1986), which were developed in part to study the behavior of surfaces under different coordinate representations. Some details pertaining to differential geometrical approaches for process control are provided in Kravaris and Kantor (1990a,b). The notion of a differentiable manifold is first defined.

Definition 3.1. An n-dimensional differentiable manifold M is an abstract set of points with the following properties:

1. We can partition M into open sets (i.e., M is Hausdorff with countable base, and we can define the concept of a continuous function on M).
2. M is the union of a collection of open sets U_i, $M \subset \bigcup_i U_i$, $i \in A$, where A is an indexing set.
3. For each $i \in A$, there exists a continuous equivalence between U_i and $\mathbb{R}^n$. More precisely, there exists a diffeomorphism $\phi_i : U_i \to \mathbb{R}^n$ called a coordinate chart of M. A mapping is a diffeomorphism if it is a one-to-one correspondence and is infinitely continuously differentiable.
4. For any two intersecting coordinate charts $U_i \cap U_j$, the change of coordinate map expressed as the composition $\phi_i \circ \phi_j^{-1}$ is a smoothly differentiable map (see Figure 2).

The collection $\{(U_i, \phi_i) \mid i \in A\}$ is called an atlas of charts on the manifold M.

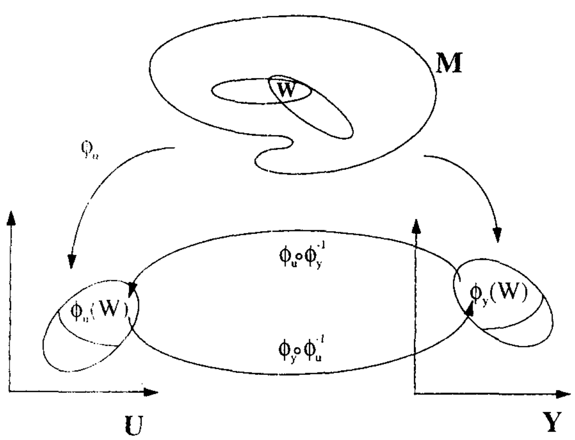

Figure 2. Coordinate systems on a differentiable manifold.

Conceptually, a differentiable manifold is an abstract space that locally looks like a Euclidean space. The purpose of the atlas is to cover this space completely using local coordinate maps. The maps allow the application of familiar operations from differential calculus to abstract manifolds. For example, the ideal gas law describes a pressure–volume–temperature (PVT) surface for a gas (given one mole of gas). We can identify a point on this surface by specifying values for any two of the three variables (P,V,T). We might want to specify different coordinate charts for this surface by deciding to use volume and temperature to characterize one part of the surface, while using pressure and temperature for another region. Another example of coordinate charts is the use of cylindrical coordinates to describe tubular reactors. The tube section is mapped to a subset of the "rectangular" Euclidean space $\mathbb{R}^3$.

Property 4 in Definition 3.1 endows the manifold M with a differentiable structure. Since the map $\phi_i \circ \phi_j^{-1}: A \subset \mathbb{R}^n \to B \subset \mathbb{R}^n$ is diffeomorphic, it follows that the notion of differentiability of functions is preserved at every point on M. This notion allows the definition of a tangent space on a manifold that is related to the familiar concept of a tangent space in $\mathbb{R}^n$. Consider a point $x \in \mathbb{R}^n$. The tangent space $T_x\mathbb{R}^n$ at x is the set of tangent vectors to $\mathbb{R}^n$ at x. $T_x\mathbb{R}^n$ is in fact a copy of $\mathbb{R}^n$. In the coordinate system $\{x_1, x_2, \ldots, x_n\}$, the natural basis of $T_x\mathbb{R}^n$ is denoted by

$$\left\{ \frac{\partial}{\partial x_1}\bigg|_x, \ldots, \frac{\partial}{\partial x_n}\bigg|_x \right\}.$$

In this notation, the tangent space is associated with the differentiation of the family of smooth functions of $\mathbb{R}^n$. At each point x, the tangent space is generated by the derivation of smooth functions of x with respect to the coordinate basis. A corresponding basis for the tangent space to a manifold M at a point p, denoted T_pM, can be identified as follows.

Consider a manifold of dimension n and let $p \in M$. Let (U, ϕ) be a coordinate chart in a neighborhood of p. For $v \in T_{\phi(p)}\mathbb{R}^n$, define

$$\phi_*(p)v = \frac{\partial \phi^{-1}}{\partial x}[\phi(p)]v.$$

The expression $\phi_*(p)v$ is the image of v in T_pM via the local coordinate representation. The tangent space T_pM at p is defined as

$$T_pM = \text{span}_{C^\infty(M)}\left\{ \phi_*(p) \frac{\partial}{\partial x_k}\bigg|_{\phi(p)}, k = 1, \ldots, n \right\}.$$

The elements of T_pM are called tangent vectors at p. Since ϕ is a diffeomorphism, the mapping $\phi_*(p): T_{\phi(p)}\mathbb{R}^n \to T_pM$ is a linear isomorphism. Hence the vectors

$$\frac{\partial}{\partial \phi_k}\bigg|_p = \phi_*(p) \frac{\partial}{\partial x_k}\bigg|_{\phi(p)}, \qquad k = 1, \ldots, n$$

form a basis of T_pM. By defining a tangent space to each point of M, a tangent space is defined for the manifold M.

Definition 3.2. The set $TM = \{(p,v) \mid p \in M,\ v \in T_pM\}$ is called the tangent bundle of M.

Note that the definition of T_pM coincides with the intuitive notion of the tangent space to a surface in $\mathbb{R}^n$. It is important to note that its definition is also independent of the choice of local coordinates.

Associated with the tangent bundle is a mapping that identifies a vector at each point $p \in M$. This can be formalized in the form of a mapping called a vector field.

Definition 3.3. A vector field v on M is a mapping that assigns a tangent vector $v(p) \in T_pM$ to each point $p \in M$. A vector field is smooth if for each $p \in M$ there exists a coordinate chart (U, ϕ) around p and smooth functions $v_1, \ldots, v_n$ on M, such that for any point $\bar{p} \in U$, $v(\bar{p}) = \sum_{i=1}^n v_i(\bar{p}) \partial / \partial\phi_i|_{\bar{p}}$, that is, v can be expressed in terms of the basis vector fields with smooth coefficient functions.

The concept of vector field is very important in the study of dynamical systems. Such systems are often described as evolving on differentiable manifolds. The movement of a particle is described by a time-dependent path $\alpha(t)$ with velocity $d\alpha(t)/dt$. There exists a vector that gives the velocity at any point of the manifold. In a neighborhood U of a point $\alpha(t_0)$, the vector field may be described by a set of differential equations $dx(t)/dt = f(x(t))$ where $x \in \mathbb{R}^N$ is a coordinate representation of the manifold in U. Nonlinear control systems are often described using vector fields. In a system of the form, $dx(t)/dt = f[x(t)] + \sum_{i=1}^P g_i[x(t)]u_i(t)$, the vector $f[x(t)]$ is often called the drift vector field and $\{g_i[x(t)]\}$, the steering vector fields.

In order to describe the geometry of this abstract set, the extent of variation of the tangent space T_pM to the manifold must be evaluated in a neighborhood of each point $p \in M$. This is provided by the introduction of an inner product on a manifold. The process of assigning an inner product to each point p of M is summarized by a tensor called the metric tensor.

Definition 3.4. A metric tensor g smoothly assigns to each point p of a manifold M an inner product, $g_p = \langle\ ,\ \rangle$, on the tangent space T_pM. Let $\{x_1, \ldots, x_n\}$ be a coordinate system on $U \subset M$. The components of g on U are

$$g_{ij} = \left\langle \frac{\partial}{\partial x_i}, \frac{\partial}{\partial x_j} \right\rangle$$

for $1 \leq i,j \leq n$. If $v = \Sigma_i v_i \partial/\partial x_i$ and $w = \Sigma_j w_j \partial/\partial x_j$ are vector fields on M, their inner product at a point p is

$$g(v,w) = \sum_{i=1}^{n} \sum_{j=1}^{n} g_{ij} v_i w_j.$$

The metric tensor defines a notion of length and orientation of vectors on the tangent space. One also needs to consider the rate of change of one vector w in the direction of a second vector v. This leads to the definition of a new vector field, $\nabla_v w$. In $\mathbb{R}^n$ this vector field is defined as

$$\nabla_v w = \sum_{k=1}^{n} v(w_k) \frac{\partial}{\partial x_k}.$$

This vector field is generally called the natural covariant derivative of w in the direction of v.

To define such an object on a manifold, care must be taken to account for the changing nature of the tangent space as we move around the manifold. We must first formalize the definition of the operator ∇, which is called a connection.

Definition 3.5. A connection ∇ on a smooth manifold M is a mapping $\nabla: TM \times TM \rightarrow TM$ such that

(i) for smooth functions f and g on M, $\nabla_{v(f+g)} w = \nabla_{v(f)} w + \nabla_{v(g)} w$

(ii) for real numbers a and b, $\nabla_v (a+b) w = \nabla_v (a) w + \nabla_v (b) w$

(iii) for a smooth function f on M, $\nabla_v f w = v(f) w + f \nabla_v w$.

$\nabla_v w$ is called the covariant derivative of w with respect to v for the connection ∇.

This definition demonstrates that the connection behaves differently under changes of coordinates. This property is exploited in the following sections to develop a nonlinear interaction measure. The concept of a coordinate system is used extensively in the article.

Definition 3.6. Let $\{x_1, \ldots, x_n\}$ be a coordinate system on a neighborhood U of a point p belonging to a manifold M endowed with a metric g. The connection coefficients for this coordinate system are real-valued functions Γ_{ij}^k in U such that

$$\nabla_{\partial/\partial x_i} \frac{\partial}{\partial x_j} = \sum_{k=1}^{n} \Gamma_{ij}^k \frac{\partial}{\partial x_k}.$$

The connection coefficients are symmetric in i and j, that is, $\Gamma_{ij}^k = \Gamma_{ji}^k$. Γ_{ij}^k is the kth component of the vector representing the rate of change of the jth basis vector in the direction of the ith basis vector. The connection coefficients can also be written in the form

$$\Gamma_{ijk} = \sum_{i=1}^{m} \Gamma_{ij}^m g_{mk} = \left\langle \nabla_{\partial/\partial x_i} \frac{\partial}{\partial x_j}, \frac{\partial}{\partial x_k} \right\rangle.$$

From Definition 3.6, it follows that, for a vector field $w = \Sigma_j w_j \partial/\partial x_j$, we can write

$$\nabla_{\partial/\partial x_i} \left(\sum_{j=1}^{n} w_j \frac{\partial}{\partial x_j} \right) = \sum_{k=1}^{n} \left\{ \frac{\partial w_k}{\partial x_i} + \sum_{j=1}^{n} \Gamma_{ij}^k w_j \right\} \frac{\partial}{\partial x_k}.$$

These basic notions from differential geometry are used in the following section to develop nonlinear identities that are closely linked with interaction effects in nonlinear processes.

Nonlinear Interaction Identities

Formally, the dynamic input–output relationship for a nonlinear process can be described by an implicit relationship of the form

$$G(x_0, y, y^{(1)}, y^{(2)}, \ldots, y^{(N)}, u, u^{(1)}, u^{(2)}, \ldots, u^{(N)}) = 0, \quad (8)$$

which, at steady state, gives a relationship of the form

$$G(x_0, y, u) = 0. \quad (9)$$

The state variables, x, evolve on an N-dimensional manifold. The outputs, y, and the inputs, u, belong to a P-dimensional Euclidean space. The subscript 0 denotes initial conditions that specify an initial position in the state space.

Assuming that the state-space behavior of a nonlinear system described by

$$\dot{x} = f(x, u) \quad (10)$$

is such that the Jacobian matrix $[\partial f(x,u)/\partial x]$ evaluated at (x_0, u_0) is stable and invertible and the sensitivity matrix $[\partial f(x,u)/\partial u]$ has rank P in a neighborhood of x_0, then Eq. 9 describes a P-dimensional submanifold of $\mathbb{R}^P \times \mathbb{R}^P$, called the steady-state process graph of the input–output relationship in the following way. For a given x_0 it is assumed that the steady-state input–output relationship can be described by an expression of the form

$$G(y, u) = G[P(u), u] = 0, \quad (11)$$

where $y \in Y \subset \mathbb{R}^P$ and $u \in U \subset \mathbb{R}^P$ and P is the process steady-state map in the output coordinates.

Equation 11 defines a P-dimensional manifold, M, modeled on $\mathbb{R}^P$. It follows from Eqs. 9 and 11 that M can be locally expressed in either u or y coordinates. By definition, this implies the existence, for every point p of M, of an open neighborhood diffeomorphic to some open set of $\mathbb{R}^P$ such that M is completely covered by the union of such open neighborhoods. Let $u_1, \ldots, u_P$ and $y_1, \ldots, y_p$ represent local coordinate representations in open neighborhoods U and Y, respectively, of a point p of M. Let $W = U \cap Y \neq \emptyset$ be an open set in M. By the definition of coordinate neighborhoods for differentiable manifolds, it follows that there exists a diffeomorphism between the input and output coordinates for every point p of W. This diffeomorphism represents the usual process steady-state map in the u and y coordinates. This is shown in Figure 3. Note that it is not necessary to represent u and y as coordinate systems for all of M.

For every point $p \in W$ let $\partial/\partial u_i$, $1 \leq i \leq P$, and $\partial/\partial y_j$, $1 \leq j \leq P$, represent local bases of T_pM, the tangent space to M at p expressed in the u_i and y_j coordinates, respectively. The exchange of bases on TM at p, expressed in Einstein summation notation, is given by

$$\frac{\partial}{\partial u_j} = \frac{\partial y^i}{\partial u_j} \frac{\partial}{\partial y_i} \quad (12)$$

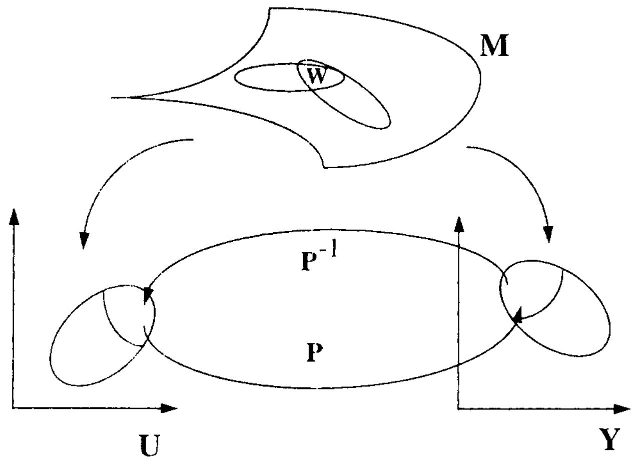

Figure 3. Inputs and outputs as coordinate systems on a differentiable manifold.

in the y coordinates, and by

$$\frac{\partial}{\partial y_i} = \frac{\partial u^k}{\partial y_i}\frac{\partial}{\partial u_k} \tag{13}$$

in the $\boldsymbol{u}$ coordinates. Note that the Einstein summation notation is used to express summations in the following way

$$\frac{\partial u^k}{\partial y_i}\frac{\partial}{\partial u_k} = \sum_{k=1}^{P}\frac{\partial u_k}{\partial y_i}\frac{\partial}{\partial u_k},$$

where the superscript indicates the index of summation. By this construction, variations in one coordinate system are immediately expressed in the other through the action of a diffeomorphism on $\boldsymbol{W}$. Thus, if one considers a tangent vector in one coordinate system, it is possible to express it in terms of the other coordinate system. Clearly, for consistency, the tangent vector must be recoverable by the inverse mapping to the original coordinate system. To illustrate this, substitute Eq. 13 into Eq. 12. This gives

$$\frac{\partial}{\partial u_j} = \frac{\partial y^i}{\partial u_j}\frac{\partial u^k}{\partial y_i}\frac{\partial}{\partial u_k}$$

which yields the identities

$$\frac{\partial y^i}{\partial u_j}\frac{\partial u_k}{\partial y_i} = \begin{cases} 0, & j \neq k \\ 1, & j = k. \end{cases} \tag{14}$$

The usual RGA formula appears within this expression

$$\Lambda_{ij} = \frac{\partial y_i}{\partial u_j}\frac{\partial u_j}{\partial y_i}. \tag{15}$$

The RGA identities of Eq. 14 simply reflect the fact that the sum of the RGA elements from the same column is equal to 1. In this setting, the relative gain array adopts a very nice and natural interpretation. The RGA reflects the ability to exchange bases on $\boldsymbol{TM}$. It gives a measure of how individual components are mapped through the process map and its inverse.

Note that Eq. 15 can be written in the standard form

$$\Lambda = \boldsymbol{K} \otimes \boldsymbol{K}^{-T}$$

where $\boldsymbol{K}$ is the steady-state gain of the process, and $\otimes$ denotes the Hadamard product of two matrices (see Horn and Johnson, 1991, p. 300). Recall that the Hadamard product of two matrices corresponds to elementwise multiplication. Letting $\boldsymbol{K}^{-1} = \partial \boldsymbol{u}/\partial \boldsymbol{y}$ and $\boldsymbol{K} = \partial \boldsymbol{y}/\partial \boldsymbol{u}$ in this expression automatically yields the standard definition of the RGA.

Summarizing, the RGA condition has been obtained by changing coordinates and then mapping back to the original coordinate system. Consistency of coordinates imposes the RGA condition. This approach forms a basis for deriving additional conditions.

In order to handle nonlinear situations, higher-order effects must be considered. First define a metric in either the y coordinates

$$g_{ij} = \left\langle \frac{\partial}{\partial y_i}, \frac{\partial}{\partial y_j} \right\rangle, \qquad 1 \leq i, j \leq P,$$

or the $\boldsymbol{u}$ coordinates

$$g_{ab} = \left\langle \frac{\partial}{\partial u_a}, \frac{\partial}{\partial u_b} \right\rangle, \qquad 1 \leq a, b \leq P,$$

The metric is a quantity that allows one to define and measure the distance between two points on an abstract manifold. It follows that the metric associated with one system of coordinates can be related to the other coordinate metric by considering

$$g_{ab} = \frac{\partial y^i}{\partial u_a}\frac{\partial y^j}{\partial u_b} g_{ij}$$

and

$$g_{ij} = \frac{\partial u^a}{\partial y_i}\frac{\partial u^b}{\partial y_j} g_{ab}$$

from the exchange of bases. Note that the Einstein summation is over two indices in each case, and corresponds to double summation. The consistency requirement is imposed by substituting again, yielding

$$g_{ab} = \frac{\partial y^i}{\partial u_a}\frac{\partial y^j}{\partial u_b}\frac{\partial u^c}{\partial y_i}\frac{\partial u^d}{\partial y_j} g_{cd}.$$

This gives a second type of RGA identity of the form

$$\frac{\partial y^i}{\partial u_a}\frac{\partial y^j}{\partial u_b}\frac{\partial u_c}{\partial y_i}\frac{\partial u_d}{\partial y_j} = \begin{cases} 1, & c = a, \quad d = b \\ 0, & c \neq a, \quad d \neq b \end{cases}$$

for $b \geq a$. The identities

$$\frac{\partial y^i}{\partial u_a}\frac{\partial y^j}{\partial u_b}\frac{\partial u_a}{\partial y_i}\frac{\partial u_b}{\partial y_j}=1$$

can be written in terms of the elements of the RGA matrix, Λ, as

$$\sum_{i=1}^{P}\sum_{j=1}^{P}\Lambda_{ia}\Lambda_{jb}=1.$$

This development demonstrates how a tensor, such as the metric tensor g, behaves under changes of coordinates. Because of the linearity of the tensor, nothing is gained by considering the effects of changes of coordinates on such objects.

Having endowed M with a metric, it is natural to consider similar identities based on the coefficients of the metric connection. Recall that the connection coefficients give rise to the covariant derivative given by $\nabla_A B$ of a vector field B in the direction of the vector field A. By definition, the connection coefficients are uniquely determined by the covariant derivatives expressed in the basis vector fields. In the current situation, they are given by

$$\Gamma_{abc}=\langle \nabla_{\partial/\partial u_a}\partial/\partial u_b,\ \partial/\partial u_c\rangle$$

in the input coordinates and by

$$\Gamma_{ijk}=\langle \nabla_{\partial/\partial y_i}\partial/\partial y_j,\partial/\partial y_k\rangle$$

in the output coordinates. The connection coefficients adopted for a coordinate system reflect the fact that the coordinate system is a nonlinear coordinate system. Intuitively, the coefficients Γ_{abc} express the effect of the nonlinear dependence of the bth input component on the ath input component when one moves an infinitesimal distance in the direction of the cth input component of the coordinate basis.

Connection coefficients in the output coordinates can be obtained from the coefficients in the input coordinates from the identity

$$\Gamma_{ijk}=\Gamma_{abc}\frac{\partial u^a}{\partial y_i}\frac{\partial u^b}{\partial y_j}\frac{\partial u^c}{\partial y_k}+\frac{\partial u^a}{\partial y_k}\frac{\partial^2 u^b}{\partial y_i\partial y_j}g_{ab} \tag{16}$$

and, similarly,

$$\Gamma_{abc}=\Gamma_{ijk}\frac{\partial y^i}{\partial u_a}\frac{\partial y^j}{\partial u_b}\frac{\partial y^k}{\partial u_c}+\frac{\partial y^i}{\partial u_c}\frac{\partial^2 y^j}{\partial u_a\partial u_b}g_{ij}. \tag{17}$$

The consistency condition is imposed by substituting the expression for Γ_{ijk} from Eq. 16 into Eq. 17

$$\Gamma_{abc}=\left\{\Gamma_{a'b'c'}\frac{\partial u^{a'}}{\partial y_i}\frac{\partial u^{b'}}{\partial y_j}\frac{\partial u^{c'}}{\partial y_k}+\frac{\partial u^{a'}}{\partial y_k}\frac{\partial^2 u^{b'}}{\partial y_i\partial y_j}g_{a'b'}\right\}\times\frac{\partial y^i}{\partial u_a}\frac{\partial y^j}{\partial u_b}\frac{\partial y^k}{\partial u_c}+\frac{\partial y^i}{\partial u_c}\frac{\partial^2 y^j}{\partial u_a\partial u_b}g_{ij},$$

where a', b' and c' are additional indices. This yields

$$\Gamma_{abc}=\Gamma_{abc}+\frac{\partial u^{a'}}{\partial y_k}\frac{\partial^2 u^{b'}}{\partial y_i\partial y_j}g_{a'b'}\frac{\partial y^i}{\partial u_a}\frac{\partial y^j}{\partial u_b}\frac{\partial y^k}{\partial u_c}+\frac{\partial y^i}{\partial u_c}\frac{\partial^2 y^j}{\partial u_a\partial u_b}g_{ij}.$$

Substituting for g_{ij},

$$\Gamma_{abc}=\Gamma_{abc}+\frac{\partial u^{a'}}{\partial y_k}\frac{\partial^2 u^{b'}}{\partial y_i\partial y_j}g_{a'b'}\frac{\partial y^i}{\partial u_a}\frac{\partial y^j}{\partial u_b}\frac{\partial y^k}{\partial u_c}+\frac{\partial y^i}{\partial u_c}\frac{\partial^2 y^j}{\partial u_a\partial u_b}\left\{\frac{\partial u^{a'}}{\partial y_i}\frac{\partial u^{b'}}{\partial y_j}g_{a'b'}\right\},$$

or, upon simplification, using identities, Eq. 14,

$$\Gamma_{abc}=\Gamma_{abc}+\frac{\partial y^i}{\partial u_a}\frac{\partial^2 u_{b'}}{\partial y_i\partial y_j}\frac{\partial y^j}{\partial u_b}g_{cb'}+\frac{\partial u^{b'}}{\partial y_j}\frac{\partial^2 y^j}{\partial u_a\partial u_b}g'_{cb}.$$

The following identity is then obtained:

$$\frac{\partial u_c}{\partial y_j}\frac{\partial^2 y^j}{\partial u_a\partial u_b}+\frac{\partial y^i}{\partial u_a}\frac{\partial^2 u_c}{\partial y_i\partial y_j}\frac{\partial y^j}{\partial u_b}=0, \tag{18}$$

which holds for all $1 \leq a,b,c \leq P$. This is a *second-order* "relative-gain-type" identity for a nonlinear process.

Under the assumption of perfect control (i.e., integral action), the composition of the process map and its inverse is required to yield the identity map on W. Clearly, this implies that Eq. 18 must also hold on W. Figure 4 illustrates the implication of the cancellation implied by Eq. 18. The controller is decomposed into a linear gain part (L_c) and a nonlinear gain part (N_c), which can be represented locally by

$$L_C=\frac{\partial \boldsymbol{u}}{\partial y}\qquad\text{and}\qquad N_C=\frac{\partial^2 \boldsymbol{u}}{\partial y\partial y'}$$

respectively. Similarly, the output response can be decomposed into a linear gain part (L_p) and a nonlinear gain part (N_p) represented by

$$L_p=\frac{\partial y}{\partial \boldsymbol{u}}\qquad\text{and}\qquad N_p=\frac{\partial^2 y}{\partial \boldsymbol{u}\partial \boldsymbol{u}'},$$

respectively.

From Figure 4, it is seen that, in the absence of a nonlinear gain controller ($N_C=0$), Eq. 18 cannot hold unless the process is linear ($N_p=0$). When the process is nonlinear, the extent of mismatch experienced by the closed-loop system as a result of the nonlinearity of a process is measured by the first term of Eq. 18

$$\frac{\partial u_c}{\partial y_i}\frac{\partial^2 y^i}{\partial u_a\partial u_b}.$$

This term is called a mismatch term, and is a measure of the

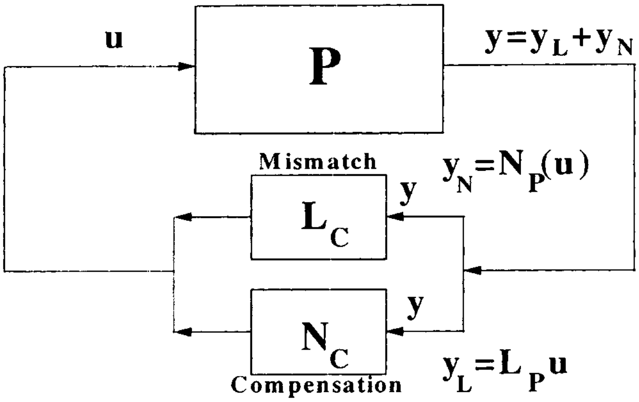

Figure 4. Second-order identities for a closed-loop nonlinear process.

input mismatch experienced by a nonlinear process controlled by a linear gain controller.

Consequently, the second term of Eq. 18

$$\frac{\partial y^i}{\partial u_a}\frac{\partial^2 u_c}{\partial y_i \partial y_j}\frac{\partial y^j}{\partial u_b}$$

can be interpreted as a measure of the extent of controller gain nonlinearity required to compensate for that mismatch. It is called the mismatch compensation term.

Note that Eq. 18 summarizes the closed-loop nonlinearity of a nonlinear process expressed in terms of the input coordinates. A similar identity can be obtained in the output coordinates:

$$\frac{\partial u^a}{\partial y_i}\frac{\partial^2 y_k}{\partial u_a \partial u_b}\frac{\partial u^b}{\partial y_j} + \frac{\partial y_k}{\partial u_a}\frac{\partial^2 u^a}{\partial y_i \partial y_j} = 0. \qquad (19)$$

The first term of this expression is a measure of the output mismatch experienced by a nonlinear process controlled by a linear gain controller. The second term gives the extent of nonlinearity of a controller that removes the output error.

Following a differential geometric argument, a more precise interpretation can be developed for each of these identities. When considering the geometry of a manifold, the curvature associated with a particular choice of connection indicates the extent of local nonlinearity of the manifold. A connection is said to possess zero curvature if there exists a local coordinate representation for which the corresponding connection coefficients vanish.

To understand the implication of the exchange of bases, suppose that the manifold M admits a connection with zero curvature and that the output coordinates provide a representation in which the connection coefficients vanish ($\Gamma_{ijk} = 0$), that is a flat coordinate system of M. From Eq. 18, the connection coefficients expressed in the input coordinates are given by

$$\Gamma_{abc} = \frac{\partial y^i}{\partial u_c}\frac{\partial^2 y^j}{\partial u_a \partial u_b} g_{ij}.$$

Substitution into Eq. 17 gives

$$\frac{\partial y^{i'}}{\partial u_c} g_{i'j'} \frac{\partial^2 y^{j'}}{\partial u_a \partial u_b}\frac{\partial u^a}{\partial y_i}\frac{\partial u^b}{\partial y_j}\frac{\partial u^c}{\partial y_k} + \frac{\partial u^a}{\partial y_k}\frac{\partial^2 u^b}{\partial y_i \partial y_j} g_{ab} = 0,$$

which yields, upon substitution of the expression of g_{ab} in the output coordinates, the identity

$$\frac{\partial y^{i'}}{\partial u_c} g_{i'j'} \frac{\partial^2 y^{j'}}{\partial u_a \partial u_b}\frac{\partial u^a}{\partial y_i}\frac{\partial u^b}{\partial y_j}\frac{\partial u^c}{\partial y_k} + \frac{\partial u^a}{\partial y_k}\frac{\partial^2 u^b}{\partial y_i \partial y_j}\frac{\partial y^{i'}}{\partial u_a}\frac{\partial y^{j'}}{\partial u_b} g_{i'j'}$$

$$= \frac{\partial^2 y^{j'}}{\partial u_a \partial u_b}\frac{\partial u^a}{\partial y_i}\frac{\partial u_b}{\partial y_j} g_{kj'} + \frac{\partial^2 u^b}{\partial y_i \partial y_j}\frac{\partial y^{j'}}{\partial u_b} g_{kj'} = 0,$$

similar to Equation 19. Satisfying this identity is therefore equivalent to requiring that the manifold M admit a connection with zero curvature whose coefficients vanish in the output coordinates. Furthermore, satisfying this identity is independent of the metric employed.

Under the assumption that rank $\{\partial y/\partial u\} = P$ at every point p of M, it can be seen that the geometry of M is essentially the geometry of a flat metric space with metric g_{ij}. By letting $g_{ij} = \delta_{ij}$ (where δ_{ij} is the Kronecker delta), M can be identified with a subset of $\mathbb{R}^P$ along with coordinates $y_1, \ldots, y_P$.

These simple identities establish the relationship between the nonlinearity of the input–output map and the nonlinearity of its inverse, that is, between open-loop nonlinearity and control-law nonlinearity. More importantly, they hightlight the interaction between linear and nonlinear components of a closed-loop process. As a result, they are very useful in the assessment of nonlinearity of closed-loop nonlinear processes. In the following sections, these identities are used to study nonlinear interaction effects and closed-loop nonlinearity in nonlinear processes.

Nonlinearity of Closed-loop Processes

In this section, the identities in Eqs. 18 and 19 are used to develop a method to assess the nonlinearity of closed-loop processes. This measure of nonlinearity is based on the decompositions of the mismatch term and the compensation term of Eq. 18 into their individual components. This gives an assessment of the contribution of each individual term to the overall mismatch and compensation effects and provides information about the nature of the nonlinear relationship existing between given input–output pairs.

As earlier, the mismatch from Eq. 18 is denoted by

$$\gamma_{abc} = \frac{\partial u_a}{\partial y_i}\frac{\partial^2 y^i}{\partial u_b \partial u_c},$$

where the individual components of the sum are given by

$$\gamma^i_{abc} = \frac{\partial u_a}{\partial y_i}\frac{\partial^2 y_i}{\partial u_b \partial u_c}.$$

The individual component describes how the nonlinearity in y_i associated with changes in u_b and u_c passes through the linear controller determining u_a. Alternatively, this quantity can be interpreted as the ratio of the second-order gain of inputs b and c acting on output i with the other loops open, to the first-order gain for the $y_i - u_a$ pair with the other loops closed. The latter interpretation is similar in spirit to the empirical definition of the relative gain as the ratio of the open-loop (first-order) gain to the loop (first-order) gain with all other control loops closed; thus, judgments are made in reference to the closed-loop gains.

The term γ^i_{a**} is used to denote the P-by-P matrix associated with the ath input channel and the ith output channel. These terms can be summarized in a table of the following form

$$
\begin{array}{ccccc}
 & y_1 & y_2 & \cdots & y_P \\
u_1 & \begin{pmatrix} \gamma^1_{111} & \gamma^1_{112} & \cdots & \gamma^1_{11P} \\ \gamma^1_{121} & \gamma^1_{122} & \cdots & \gamma^1_{12P} \\ \vdots & \vdots & & \vdots \\ \gamma^1_{1P1} & \gamma^1_{1P2} & \cdots & \gamma^1_{1PP} \end{pmatrix} & \begin{pmatrix} \gamma^2_{111} & \gamma^2_{112} & \cdots & \gamma^2_{11P} \\ \gamma^2_{121} & \gamma^2_{122} & \cdots & \gamma^2_{12P} \\ \vdots & \vdots & & \vdots \\ \gamma^2_{1P1} & \gamma^2_{1P2} & \cdots & \gamma^2_{1PP} \end{pmatrix} & \cdots & \begin{pmatrix} \gamma^P_{111} & \gamma^P_{112} & \cdots & \gamma^1_{11P} \\ \gamma^P_{121} & \gamma^P_{122} & \cdots & \gamma^P_{12P} \\ \vdots & \vdots & & \vdots \\ \gamma^P_{1P1} & \gamma^P_{1P2} & \cdots & \gamma^P_{1PP} \end{pmatrix} \\
u_2 & \begin{pmatrix} \gamma^1_{211} & \gamma^1_{212} & \cdots & \gamma^1_{21P} \\ \gamma^1_{221} & \gamma^1_{222} & \cdots & \gamma^1_{22P} \\ \vdots & \vdots & & \vdots \\ \gamma^1_{2P1} & \gamma^1_{2P2} & \cdots & \gamma^1_{2PP} \end{pmatrix} & \begin{pmatrix} \gamma^2_{211} & \gamma^2_{212} & \cdots & \gamma^2_{21P} \\ \gamma^2_{221} & \gamma^2_{222} & \cdots & \gamma^2_{22P} \\ \vdots & \vdots & & \vdots \\ \gamma^2_{2P1} & \gamma^2_{2P2} & \cdots & \gamma^2_{2PP} \end{pmatrix} & \cdots & \begin{pmatrix} \gamma^P_{211} & \gamma^P_{212} & \cdots & \gamma^1_{21P} \\ \gamma^P_{221} & \gamma^P_{222} & \cdots & \gamma^P_{22P} \\ \vdots & \vdots & & \vdots \\ \gamma^P_{2P1} & \gamma^P_{2P2} & \cdots & \gamma^P_{2PP} \end{pmatrix} \\
\vdots & \vdots & \vdots & \cdots & \vdots \\
u_P & \begin{pmatrix} \gamma^1_{P11} & \gamma^1_{P12} & \cdots & \gamma^1_{P1P} \\ \gamma^1_{P21} & \gamma^1_{P22} & \cdots & \gamma^1_{P2P} \\ \vdots & \vdots & & \vdots \\ \gamma^1_{PP1} & \gamma^1_{PP2} & \cdots & \gamma^1_{PPP} \end{pmatrix} & \begin{pmatrix} \gamma^2_{P11} & \gamma^2_{P12} & \cdots & \gamma^2_{P1P} \\ \gamma^2_{P21} & \gamma^2_{P22} & \cdots & \gamma^2_{P2P} \\ \vdots & \vdots & & \vdots \\ \gamma^2_{PP1} & \gamma^2_{PP2} & \cdots & \gamma^2_{PPP} \end{pmatrix} & \cdots & \begin{pmatrix} \gamma^P_{P11} & \gamma^P_{P12} & \cdots & \gamma^1_{P1P} \\ \gamma^P_{P21} & \gamma^P_{P22} & \cdots & \gamma^P_{P2P} \\ \vdots & \vdots & & \vdots \\ \gamma^P_{PP1} & \gamma^P_{PP2} & \cdots & \gamma^P_{PPP} \end{pmatrix},
\end{array}
$$

which is called a "mismatch nonlinearity" table.

For each input channel, u_a, the table gives the contribution of each output channel, y_j, $1 \le j \le P$, to the second-order effects displayed by the process subject to variations of u_a. For each input–output pair, the $P \times P$ submatrix γ^i_{a**} measures the impact of second-order effects due to the inputs. For the input–output pair, $u_a - y_i$, the corresponding (a, i)th submatrix of the mismatch table is a measure of the nonlinearity due to fluctuations of the inputs on this pairing. By construction, it is related to the nonlinearity experienced by a nonlinear process subject to a linear controller with fixed gain. Thus for a given input–output pair, $u_a - y_i$, each $P \times P$ submatrix gives the extent of mismatch of the ath input channel due to the nonlinear effects of the inputs on the ith output channel. This is called *within-channel nonlinearity*, since it gives the extent of nonlinearity of the inputs on the input mismatch. This type of nonlinearity can be removed without affecting the output channels by introducing nonlinear transformations of the inputs.

If a particular input–output pairing is selected, one must also consider the effect of the other output channels on that pairing. This can be detected by the presence of nonzero submatrices in the entries of the mismatch table corresponding to that input and the remaining output channels. Accordingly, it is called *between-channel nonlinearity*. This type of effect is related to the existence of a nonlinear relationship between two output channels. It can only be removed by pairings of the input channels with nonlinear combinations of the output channels.

These nonlinearity effects are scale dependent and so their interpretation is subject to the scaling of the system variables. The problem of scaling can be handled as described in Guay et al. (1995). Since the identities expressed in the input coordinates in Eq. 18 (or alternatively in the output coordinates in Eq. 19) are invariant under output (or alternatively input) scaling, we need only define a region of interest in the input (or alternatively output) space and rewrite the identities in Eq. 18 (or alternatively in Eq. 19) in terms of the scaled coordinates. That is, scaled inputs can be defined as

$$v = S(u - u_0),$$

where S is a $P \times P$ matrix whose elements define the scaling region in the input space. From Eq. 18, it is seen that the scaling of v leads to the scaling of each submatrix by post-multiplying by S^{-1}. In what follows, each scaled submatrix is written as $\hat{\gamma}^i_{abc} = \gamma^i_{abc} S^{-1}$. To avoid bias in the measures, each channel is scaled independently by using a diagonal scaling matrix.

A mean squared measure, c^2_{ai}, can be associated with each submatrix $\hat{\gamma}^i_{a**}$, where

$$c_{ai}^2 = \int_A \left(\sum_{b=1}^{P} \sum_{c=1}^{P} \hat{\gamma}_{abc}^i v_b v_c \right)^2 dA$$

and A is the area of the unit sphere $\| v \|^2 = 1$ in the scaled input space. The resulting value is

$$c_{ia}^2 = \frac{1}{P(P+2)} \left[2 \sum_{b=1}^{P} \sum_{c=1}^{P} (\hat{\gamma}_{abc}^i)^2 + \left(\sum_{d=1}^{P} \hat{\gamma}_{add}^i \right)^2 \right].$$

The root-mean-squared (rms) measure, c_{ia}, is then used as a measure of significance of the nonlinear effects. An rms measure of 0.3 is usually considered to be significant, as it leads to a 15% deviation from linearity for every unit step in the scaled input.

When a nonlinear process is controlled using a linear controller, the nonlinearity measures and the table obtained using the procedures described earlier provide a precise description of the nature of the nonlinear effects in the closed-loop process. If a nonlinear controller is used, it should be designed so that the identities in Eqs. 18 and 19 are satisfied and nonlinear effects are removed. Information about the overall extent of closed-loop nonlinearity can be obtained from the table given earlier; however, it does not yield information about the local nature of the nonlinear transformation required to remove the between-channel nonlinear effects. To provide this information, the table given earlier can be complemented by a second table obtained from mismatch and compensation terms in the identities in Eqs. 18 and 19.

Consider the compensation terms of Eq. 18, denoted by

$$\delta_{abc} = \frac{\partial y^i}{\partial u_b} \frac{\partial^2 u^a}{\partial y_i \partial y_j} \frac{\partial y^j}{\partial u_c}.$$

The measure of the nonlinearity arising from the control action u_a required to compensate for output changes in y_i and y_j can be locally represented by the individual components of δ_{abc}, given by

$$\delta_{abc}^{ij} = \frac{\partial y_i}{\partial u_b} \frac{\partial^2 u_a}{\partial y_i \partial y_j} \frac{\partial y_j}{\partial u_c}.$$

This component can be interpreted as the nonlinear control compensation required in u_a in response to changes in the ith and jth outputs that have been produced by the actions of inputs u_b and u_c on these outputs, respectively. Alternatively, this component can be interpreted as the ratio of the second-order controller action in u_c from changes in the ith and jth outputs with the other control loops closed, to the product of the linear control actions in $u_a - y_i$ and $u_b - y_i$ with the other control loops open.

In analogy with the table given earlier, these components are arranged in a table of the following form, which is called a compensation table:

$$
\begin{array}{ccccccccc}
 & y_1 y_1 & & y_1 y_2 & \cdots & y_1 y_P & \cdots & y_P y_P \\
u_1 & \begin{pmatrix} \delta_{111}^{11} & \delta_{112}^{11} & \cdots & \delta_{11P}^{11} \\ \delta_{121}^{11} & \delta_{122}^{11} & \cdots & \delta_{12P}^{11} \\ \vdots & \vdots & & \vdots \\ \delta_{1P1}^{11} & \delta_{1P2}^{11} & \cdots & \delta_{1PP}^{11} \end{pmatrix} & & \begin{pmatrix} \delta_{111}^{12} & \delta_{112}^{12} & \cdots & \delta_{11P}^{12} \\ \delta_{121}^{12} & \delta_{122}^{12} & \cdots & \delta_{12P}^{12} \\ \vdots & \vdots & & \vdots \\ \delta_{1P1}^{12} & \delta_{1P2}^{12} & \cdots & \delta_{1PP}^{12} \end{pmatrix} & \cdots & \begin{pmatrix} \delta_{111}^{1P} & \delta_{112}^{1P} & \cdots & \delta_{11P}^{1P} \\ \delta_{121}^{1P} & \delta_{122}^{1P} & \cdots & \delta_{12P}^{1P} \\ \vdots & \vdots & & \vdots \\ \delta_{1P1}^{1P} & \delta_{1P2}^{1P} & \cdots & \delta_{1PP}^{1P} \end{pmatrix} & \cdots & \begin{pmatrix} \delta_{111}^{PP} & \delta_{112}^{PP} & \cdots & \delta_{11P}^{PP} \\ \delta_{121}^{PP} & \delta_{122}^{PP} & \cdots & \delta_{12P}^{PP} \\ \vdots & \vdots & & \vdots \\ \delta_{1P1}^{PP} & \delta_{1P2}^{PP} & \cdots & \delta_{1PP}^{PP} \end{pmatrix} \\
u_2 & \begin{pmatrix} \delta_{211}^{11} & \delta_{212}^{11} & \cdots & \delta_{21P}^{11} \\ \delta_{221}^{11} & \delta_{222}^{11} & \cdots & \delta_{22P}^{11} \\ \vdots & \vdots & & \vdots \\ \delta_{2P1}^{11} & \delta_{2P2}^{11} & \cdots & \delta_{2PP}^{11} \end{pmatrix} & & \begin{pmatrix} \delta_{211}^{12} & \delta_{212}^{12} & \cdots & \delta_{21P}^{12} \\ \delta_{221}^{12} & \delta_{222}^{12} & \cdots & \delta_{22P}^{12} \\ \vdots & \vdots & & \vdots \\ \delta_{2P1}^{12} & \delta_{2P2}^{12} & \cdots & \delta_{2PP}^{12} \end{pmatrix} & \cdots & \begin{pmatrix} \delta_{211}^{1P} & \delta_{212}^{1P} & \cdots & \delta_{21P}^{1P} \\ \delta_{221}^{1P} & \delta_{222}^{1P} & \cdots & \delta_{22P}^{1P} \\ \vdots & \vdots & & \vdots \\ \delta_{2P1}^{1P} & \delta_{2P2}^{1P} & \cdots & \delta_{2PP}^{1P} \end{pmatrix} & \cdots & \begin{pmatrix} \delta_{211}^{PP} & \delta_{212}^{PP} & \cdots & \delta_{21P}^{PP} \\ \delta_{221}^{PP} & \delta_{222}^{PP} & \cdots & \delta_{22P}^{PP} \\ \vdots & \vdots & & \vdots \\ \delta_{2P1}^{PP} & \delta_{2P2}^{PP} & \cdots & \delta_{2PP}^{PP} \end{pmatrix} \\
\vdots & \vdots & & \vdots & \cdots & \vdots & \cdots & \vdots \\
u_P & \begin{pmatrix} \delta_{P11}^{11} & \delta_{P12}^{11} & \cdots & \delta_{P1P}^{11} \\ \delta_{P21}^{11} & \delta_{P22}^{11} & \cdots & \delta_{P2P}^{12} \\ \vdots & \vdots & & \vdots \\ \delta_{PP1}^{11} & \delta_{PP2}^{11} & \cdots & \delta_{PPP}^{11} \end{pmatrix} & & \begin{pmatrix} \delta_{P11}^{12} & \delta_{P12}^{12} & \cdots & \delta_{P1P}^{12} \\ \delta_{P21}^{12} & \delta_{P22}^{12} & \cdots & \delta_{P2P}^{12} \\ \vdots & \vdots & & \vdots \\ \delta_{PP1}^{12} & \delta_{PP2}^{12} & \cdots & \delta_{PPP}^{12} \end{pmatrix} & \cdots & \begin{pmatrix} \delta_{P11}^{1P} & \delta_{P12}^{1P} & \cdots & \delta_{P1P}^{1P} \\ \delta_{P21}^{1P} & \delta_{P22}^{1P} & \cdots & \delta_{P2P}^{1P} \\ \vdots & \vdots & & \vdots \\ \delta_{PP1}^{1P} & \delta_{PP2}^{1P} & \cdots & \delta_{PPP}^{1P} \end{pmatrix} & \cdots & \begin{pmatrix} \delta_{P11}^{PP} & \delta_{P12}^{PP} & \cdots & \delta_{P1P}^{PP} \\ \delta_{P21}^{PP} & \delta_{P22}^{PP} & \cdots & \delta_{P2P}^{PP} \\ \vdots & \vdots & & \vdots \\ \delta_{PP1}^{PP} & \delta_{PP2}^{PP} & \cdots & \delta_{PPP}^{PP} \end{pmatrix}
\end{array}.
$$

This table describes in detail the nature of the nonlinear dependencies between the inputs and the various output channels. Interpretation of this table is closely related to that of the corresponding table for the mismatch terms, γ_{abc}^i. It is clear that, by construction, addition of each submatrix δ_{abc}^{ij} of the compensation table with the corresponding entry in the table for the mismatch terms γ^i_{abc} for the ath input channel yields a null matrix. Note, however, that only nonredundant terms have been included. As a result, submatrices corresponding to the off-diagonal terms of the form y_i, y_j $(i \neq j)$ must be counted twice for the identity in Eq. 18 to hold.

In considering a given pairing, $u_a - y_i$, the presence of within-channel nonlinear effects can removed by using a nonlinear input transformation, $v_a = \phi(u)$, which locally eliminates within-channel nonlinearity. The corresponding terms of the matrix γ^i_{a**} given by

$$\gamma^i_{abc} = \left(\frac{\partial \Phi_a}{\partial u_a}\frac{\partial u_a}{\partial y_i}\right)\left(\frac{\partial u_b}{\partial \Phi_b}\frac{\partial^2 y_i}{\partial u_b \partial u_c}\frac{\partial u_c}{\partial \Phi_c}\right)$$

vanish locally where

$$\Phi_i = \begin{cases} v_i = u_i, & i \neq a \\ v_i = \phi(u_1, \ldots, u_P), & i = a. \end{cases}$$

The corresponding compensation terms are given by

$$\delta^{ij}_{abc} = \left(\frac{\partial \Phi_a}{\partial u_a}\right)\left(\frac{\partial u_b}{\partial \Phi_b}\frac{\partial y_i}{\partial u_b}\frac{\partial^2 u_a}{\partial y_i \partial y_j}\frac{\partial y_j}{\partial u_c}\frac{\partial u_c}{\partial \Phi_c}\right).$$

This construction implies that the pairing of the new inputs, v_a with y_i yields a locally linear response

$$\frac{\partial^2 v_a}{\partial y_i \partial y_i} = \frac{\partial y_i}{\partial u_b}\frac{\partial^2 v_a}{\partial y_i \partial y_i}\frac{\partial y_i}{\partial u_c} = 0$$

for all b and c. This suggests that the resulting table, reexpressed in terms of v_a, contains a null submatrix in the (y_i, y_i) entry. The remaining nonzero submatrices corresponding to the u_a input channel indicate the nature of the between-channel nonlinearity effects. The extent of between-channel effects implied by any given pairing , $u_a - y_i$, is explicitly indicated by the presence of a nonzero submatrix among the (y_k, y_l) entries in the compensation table where $1 \leq k,l \leq P$ with $l \neq i$. This second table can be seen to complement the mismatch table by indicating, through the existence of nonzero submatrices, the relationship between a particular input and higher-order output terms such as y_k^2 and $y_k y_l$.

In the next section, a simple CSTR model is used to illustrate the application of the second-order identities in the evaluation of local nonlinear effects in a nonlinear process.

Example 1

Consider the following model of a CSTR due to Nikolaou (1993),

$$\frac{dx_1}{dt} = -x_1 - Da_1 x_1^2 + 1 + u_1,$$

$$\frac{dx_2}{dt} = Da_1 x_1^2 - x_2 - Da_2 x_2^{1/2} + u_2$$

with output functions, $y_1 = x_1$ and $y_2 = x_2$. At steady state

$$u_1 = y_1 + Da_1 y_1^2 - 1$$

$$u_2 = -Da_1 y_1^2 + y_2 + Da_2 y_2^{1/2}.$$

The values of the first- and second-order inverse gain matrices can be isolated by differentiating each expression with respect to y_1 and y_2:

$$\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{y}} = \begin{pmatrix} 1 + 2Da_1 y_1 & 0 \\ -2Da_1 y_1 & \dfrac{1}{2}\dfrac{2\sqrt{y_2} + Da_2}{\sqrt{y_2}} \end{pmatrix},$$

$$\frac{\partial^2 \boldsymbol{u}}{\partial \boldsymbol{y} \partial \boldsymbol{y}^T} = \left\{ \begin{matrix} \begin{pmatrix} 2Da_1 & 0 \\ 0 & 0 \end{pmatrix} \\ \begin{pmatrix} -2Da_1 & 0 \\ 0 & -\dfrac{1}{4}\dfrac{Da_2}{y_2^{3/2}} \end{pmatrix} \end{matrix} \right\}.$$

Differentiating with respect to u_1 and u_2 and solving for the required derivatives gives

$$\left.\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{u}}\right|_{u=\Phi^{-1}(y)} = \begin{pmatrix} \dfrac{1}{1 + 2Da_1 y_1} & 0 \\ \dfrac{4\sqrt{y_2}\, Da_1 y_1}{\left(2\sqrt{y_2} + Da_2\right)(1 + 2Da_1 y_1)} & \dfrac{2\sqrt{y_2}}{2\sqrt{y_2} + Da_2} \end{pmatrix}$$

$$\left.\frac{\partial^2 \boldsymbol{y}}{\partial \boldsymbol{u} \partial \boldsymbol{u}^T}\right|_{u=\Phi^{-1}(y)} = \left\{ \begin{matrix} \begin{pmatrix} \dfrac{-2Da_1}{(1 + 2Da_1 y_1)^3} & 0 \\ 0 & 0 \end{pmatrix} \\ \begin{pmatrix} \dfrac{4Da_1\left(2Da_1 y_1^2 Da_2 + 4Da_1^2 y_1^3 Da_2 + 4y_2^{3/2} + 4y_2 Da_2 + \sqrt{y_2}\, Da_2^2\right)}{\left(2\sqrt{y_2} + Da_2\right)^3 (1 + 2Da_1 y_1)^3} & \dfrac{4Da_1 y_1 Da_2}{\left(2\sqrt{y_2} + Da_2\right)^3 (1 + 2Da_1 y_1)} \\ \dfrac{4Da_1 y_1 Da_2}{\left(2\sqrt{y^2} + Da_2\right)^3 (1 + 2Da_1 y_1)} & \dfrac{2Da_2}{\left(2\sqrt{y_2} + Da_2\right)^3} \end{pmatrix} \end{matrix} \right\}.$$

For the steady-state conditions, $y=\{0.61803399, 0.03085002\}^T$, $u=\{0,0\}^T$, with $Da_1=1$ and $Da_2=2$,

$$\frac{\partial \boldsymbol{u}}{\partial y}=\begin{pmatrix} 2.236 & 0 \\ -1.236 & 6.696 \end{pmatrix}, \quad \frac{\partial^2 \boldsymbol{u}}{\partial y \partial y^T}=\left\{\begin{matrix} \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix} \\ \begin{pmatrix} -2 & 0 \\ 0 & -92.388 \end{pmatrix} \end{matrix}\right\},$$

and

$$\frac{\partial y}{\partial \boldsymbol{u}}=\begin{pmatrix} 0.447 & 0 \\ 0.0826 & 0.149 \end{pmatrix}, \quad \frac{\partial^2 y}{\partial \boldsymbol{u} \partial \boldsymbol{u}^T}=\left\{\begin{matrix} \begin{pmatrix} -0.179 & 0 \\ 0 & 0 \end{pmatrix} \\ \begin{pmatrix} 0.121 & 0.170 \\ 0.170 & 0.308 \end{pmatrix} \end{matrix}\right\}.$$

This gives

$$\frac{\partial \boldsymbol{u}}{\partial y_i}\frac{\partial^2 y^i}{\partial \boldsymbol{u}\partial \boldsymbol{u}^T}=\left\{\begin{pmatrix} -0.40 & 0 \\ 0. & 0 \end{pmatrix}\begin{pmatrix} 1.0297 & 1.1391 \\ 1.1391 & 2.0607 \end{pmatrix}\right\}^T, \tag{20}$$

and

$$\frac{\partial y^i}{\partial \boldsymbol{u}}\frac{\partial^2 \boldsymbol{u}}{\partial y_i y_j}\frac{\partial y^j}{\partial \boldsymbol{u}}=\left\{\begin{pmatrix} 0.4 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} -1.0297 & -1.1391 \\ -1.1391 & -2.0607 \end{pmatrix}\right\}^T. \tag{21}$$

Each term in Eq. 20 is obtained by adding overall output channels. The contribution of each output channel can be obtained by isolating the corresponding term of the sum that gives, for example,

$$\frac{\partial u_1}{\partial y_1}\frac{\partial^2 y_1}{\partial u_1^2}=-0.4, \qquad \frac{\partial u_2}{\partial y_1}\frac{\partial^2 y_1}{\partial u_1^2}=0.2211,$$

and so forth. Tabulating these values as described above,

$$\begin{matrix} & y_1 & y_2 \\ u_1 & \begin{pmatrix} -0.4 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \\ u_2 & \begin{pmatrix} 0.2211 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0.8086 & 1.1391 \\ 1.1391 & 2.0607 \end{pmatrix} \end{matrix}.$$

The latter table demonstrates that the nonlinear behavior of the process causes both between- and within-channel nonlinear effects. The between-channel effect arises from the nonlinear effect of y_1 on the u_2-y_2 pairing. The related submatrix contains a nonzero off-diagonal term, 0.2211. The nature of this submatrix with one nonzero entry in the (1,1) position indicates only dependence on y_1 as confirmed from the steady-state relationships. This type of interaction can only be removed by pairing u_2 with a nonlinear function of y_1 and y_2. The null upper right submatrix indicates that there is no nonlinear effect of y_2 on the u_1-y_2 pairing. This is clearly supported by the steady-state expressions for u_1 and u_2 given earlier. Furthermore, the null submatrix also suggests that the linear RGA resulting from input variations in a neighborhood of the steady-state point will remain an identity matrix. The u_2 steady-state response depends nonlinearly on y_1 and y_2, while u_1 depends only on y_1.

Using the following input scaling,

$$\begin{pmatrix} v_1 \\ v_2 \end{pmatrix}=\begin{pmatrix} 1/0.5 & 0 \\ 0 & 1/0.5 \end{pmatrix}\begin{pmatrix} u_1 \\ u_2 \end{pmatrix},$$

the resulting second-order scaled interaction table is given by

$$\begin{matrix} & y_1 & y_2 \\ v_1 & \begin{pmatrix} -0.2 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \\ v_2 & \begin{pmatrix} 0.1106 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0.4043 & 0.5696 \\ 0.5696 & 1.0304 \end{pmatrix} \end{matrix}.$$

This table can be expressed in terms of rms measures as

	y_1	y_2
u_1	0.12247	0
u_2	0.067728	0.85195.

For this example, there is no significant between-channel nonlinearity effect. The small off-diagonal term 0.067728 indicates a weak nonlinear dependency of the u_2-y_2 pairing on y_1. The larger value 0.85195 shows that there is evidence of strong within-channel interaction for the u_2-y_2 pairing. This could be removed by considering pairing the y_2 channel with a nonlinear combination of the inputs.

As discussed before, information about the nature of the nonlinearity is obtained by analysis of the mismatch compensation terms listed in the following table. Consider first the unscaled compensation table given by

$$\begin{matrix} & y_1,y_1 & y_1,y_2 & y_2,y_2 \\ u_1 & \begin{pmatrix} 0.40 & 0.0 \\ 0.0 & 0.0 \end{pmatrix} & \begin{pmatrix} 0.0 & 0.0 \\ 0.0 & 0.0 \end{pmatrix} & \begin{pmatrix} 0.0 & 0.0 \\ 0.0 & 0.0 \end{pmatrix} \\ u_2 & \begin{pmatrix} -0.40 & 0.0 \\ 0.0 & 0.0 \end{pmatrix} & \begin{pmatrix} 0.0 & 0.0 \\ 0.0 & 0.0 \end{pmatrix} & \begin{pmatrix} -0.6297 & -1.1391 \\ -1.1391 & -2.0607 \end{pmatrix} \end{matrix}.$$

This table provides considerable information about the structure of a nonlinear controller required to decouple this system. It can be seen from the u_1 channel that a simple quadratic transformation involving only y_1 would provide an appropriate controller. The quadratic nature of the relationship is deduced from the presence of the nonzero term 0.4 in the submatrix relating the u_1 channel to the term (y_1,y_1). Since this term is in the upper left corner of this submatrix, it involves only a second-order effect related to u_1. This indicates that the second-order term of the steady-state relationship expressing the dependence of u_1 on (y_1,y_1) can be written in terms of a second-order term involving u_1 only. This can only happen when u_1 becomes a quadratic function of y_1 at steady state.

For the interpretation of the u_2 channel, the previous table describing the mismatch can be used. Recall that only the terms in the upper left corner of each submatrix are associated with the between-channel interaction. As a result, all other nonzero entries are related to the within-channel interactions of the u_2-y_2 pairing, and can be removed by a nonlinear input transformation $v_2=\phi(u_1, u_2)$. From the compensation table, it can be seen that steady-state decoupling can be achieved locally by considering a nonlinear expression in y_1 and y_2. There are no terms of the form y_1y_2, indicating that the expression form required is

$$z_2=\beta_1(y_1)+\beta_2(y_2),$$

where $\beta_1(y_1)$ is a quadratic function of y_1 and $\beta_2(y_2)$ is a nonlinear function of y_2. This is supported by the model equations given earlier.

From this example, we see that inspection of the interaction table provides a good description of the nonlinear effects existing in closed-loop nonlinear processes. By using both the mismatch and compensation interaction tables, a good description of the required pairings is obtained. Furthermore, by using the tables along with the rms curvature measures, we can also provide an accurate description of the steady-state nonlinearity of a process.

In order to assess the importance of these nonlinear effects in the region using the prescribed scaling matrix, we can obtain the following table of rms measures:

	y_1,y_1	y_1,y_2	y_2,y_2
u_1	0.12247	0	0
u_2	0.12247	0	0.85195.

This table indicates that there are no significant nonlinear effects due to u_1. The u_1-y_1 pairing provides an approximately linear steady-state beahvior. Only the y_2,y_2 term has a significantly nonlinear effect on the u_2 channel. A nonlinear transformation of the form

$$z_2=\beta_2(y_2)$$

would provide an approximately linear steady-state behavior between u_2 and z_2.

This example illustrates the application of the method presented and the usefulness of the second-order identities derived in the fourth setion. As has been seen, considerable information about the extent and the nature of the nonlinear steady-state behavior of a closed-loop process can be obtained.

This analysis provides an effective tool for the assessment of nonlinearity in control problems and the extent of nonlinearity that must be addressed by a controller. The necessary second-order information about the process can be obtained from a mechanistic process model, numerical simulation experiments in the case of a complex process model (e.g., using a design simulator), or from plant data. A number of possible strategies exist for the assessment of second-order properties in steady-state processes. For this purpose, we can consider simple empirical model-building approaches, such as response surface methodology, or approximation methods, such as the secant approximation method (Goldberg et al., 1983).

The next two sections discuss the application of Eq. 18 for assessment of second-order interaction effects.

Nonlinearity and Interaction

As demonstrated in the fourth section, Eqs. 18 and 19 are closely related to second-order interaction effects. Equation 18 defines explicitly the inherent restrictions of input rotation experienced in a closed-loop nonlinear process. It describes the trade-off that must exist between process nonlinearity and controller nonlinearity, or between the mismatch and the compensation terms in Eq. 18. The mismatch term measures the extent of input rotation due to process nonlinearity, and the compensation term gives the corresponding rotation that must be supplied by the controller in order to achieve perfect control. Similarly, Eq. 19 defines restrictions in output rotation.

Consider the application of Eqs. 18 and 19 to the measurement of interaction effects in a nonlinear process. From Eq. 18, for a given input channel u_a, the following identity is obtained

$$\frac{\partial u_a}{\partial y_i}\frac{\partial^2 y^i}{\partial u_a \partial u_c}+\frac{\partial y^j}{\partial u_c}\frac{\partial^2 u_a}{\partial y_j \partial y_i}\frac{\partial y^i}{\partial u_a}=0.$$

Note that this identity can also be derived by differentiation of the equation

$$\frac{\partial u_a}{\partial y_i}\frac{\partial y^i}{\partial u_a}=1$$

with respect to u_c. However, the derivation using the exchange of basis requirements for connection coefficients identifies the coordinate representation issue that is the fundamental basis for interaction.

The second-order expression can also be decomposed into i individual terms

$$\gamma^i_{ac}=\frac{\partial u_a}{\partial y_i}\frac{\partial^2 y_i}{\partial u_a \partial u_c}+\frac{\partial y^j}{\partial u_c}\frac{\partial^2 u_a}{\partial y_j \partial y_i}\frac{\partial y_i}{\partial u_a}.$$

The term, γ^i_{ac}, measures the effect of u_c on the u_a-y_i pairing and its magnitude gives an estimate of the contribution of second-order effects to closed-loop interaction effects. These terms can be summarized in a table of the following form

	y_1	y_2	$\cdots$	y_P
u_1	γ_1^1	γ_1^2	$\cdots$	γ_1^P
u_2	γ_2^1	γ_2^2	$\cdots$	γ_2^P
$\cdot$	$\cdot$	$\cdot$	$\cdots$	$\cdot$
$\cdot$	$\cdot$	$\cdot$	$\cdots$	$\cdot$
$\cdot$	$\cdot$	$\cdot$	$\cdots$	$\cdot$
u_P	γ_P^1	γ_P^2	$\cdots$	γ_P^P,

where the terms γ_a^i are P-dimensional vectors whose elements are γ_{ac}^i. By construction, this table is symmetric. Furthermore, to satisfy Eqs. 18 and 19, the sum of all elements in each row must be zero. The sum of the elements of each column must also be zero. For a given direction in the input space, this table identifies the contribution of the nonlinearity to the interaction effects.

Using Eq. 19, the effect of variation of the outputs can also be estimated. As previously, for a particular output channel y_i,

$$\frac{\partial u^a}{\partial y_i}\frac{\partial^2 y_i}{\partial u_a \partial u_b}\frac{\partial u^b}{\partial y_j}+\frac{\partial y_i}{\partial u_a}\frac{\partial^2 u^a}{\partial y_i \partial y_j}=0,$$

which can be easily derived by differentiation of the equation

$$\frac{\partial y_i}{\partial u_a}\frac{\partial u^a}{\partial y_i}=1$$

with respect to y_j. Individual elements of Eq. 19 are given by

$$\delta_{ij}^a=\frac{\partial u_a}{\partial y_i}\frac{\partial^2 y_i}{\partial u_a \partial u_b}\frac{\partial u^b}{\partial y_j}+\frac{\partial y_i}{\partial u_a}\frac{\partial^2 u_a}{\partial y_i \partial y_j}.$$

This term measures the effect of y_j on the u_a-y_i pairing. As before, these terms can be arranged in a table of the form

	u_1	u_2	$\cdots$	u_P
y_1	δ_1^1	δ_1^2	$\cdots$	δ_1^P
y_2	δ_2^1	δ_2^2	$\cdots$	δ_2^P
$\cdot$	$\cdot$	$\cdot$	$\cdots$	$\cdot$
$\cdot$	$\cdot$	$\cdot$	$\cdots$	$\cdot$
$\cdot$	$\cdot$	$\cdot$	$\cdots$	$\cdot$
y_P	δ_P^1	δ_P^2	$\cdots$	δ_P^P.

This table displays the same properties as the table corresponding to Eq. 19.

Interpretation of these measures of interaction supplements the interpretation of the RGA calculated from the first-order gain of the nonlinear process. Of particular importance are the magnitudes of the terms γ_a^i and δ_i^a contained in the tables just given. Since these terms are not scale independent, we must consider appropriate scaling of the original variables. This can be performed as discussed in the fifth section. The result is a dimensionless measure of the contribution of the second-order terms to the interaction effects in a nonlinear closed-loop process. Naturally, large second-order effects within a prescribed region of operation indicate highly nonlinear behavior and the need for a nonlinear decoupling control strategy.

The choice of input–output pairings may also be affected by the second-order measures. For a given input–output pair, the corresponding P-dimensional vector entry from the second-order interaction tables measures the expected variation in interaction due to the second-order effects. They therefore provide a method to quantify the interaction effects in nonlinear processes where nonlinearity is the dominant source of interactions. The presence of large negative values in the second-order interaction terms associated with an input–output pair indicates large reverse effects due to the nonlinearity, indicating a poor choice of input–output pairing.

As mentioned earlier, the terms associated with Eqs. 18 and 19 are related to the extent of input rotation and output rotation, respectively. As a result, significantly large values of γ_a^i (or alternatively, δ_i^a) can be interpreted as an indication of significant variation in input (or alternatively, output) rotation in a prescribed region of operation. This is closely related to the effect of process nonlinearity on the input and output rotation components of the singular-value decomposition of the first-order gain (Morari and Zafiriou, 1989), as discussed in Koung and MacGregor (1991).

In the next section, two chemical-process examples are used to demonstrate the application of the tables discussed earlier in the assessment of nonlinear interaction effects. The first example is a continuation of the simple CSTR discussion in the previous section. The second example is an evaporator model described by Newell and Lee (1989).

Although both examples are based on process models, it should be noted that the analysis only requires the availability of first- and second-order gain information in a prescribed region of operation. The models presented in the next section are therefore only used to evaluate the gain information. Other empirical model descriptions such as second-order Volterra series (Maner et al., 1994), NARX or NARMAX models (Leontaritis and Billings, 1985), or simple steady-state models may often provide the necessary information.

Chemical Process Examples

Example 2

Let us consider again the simple CSTR discussed in the sixth section. As noted previously, this process was shown to display significant nonlinearity in the region of operation described by the scaling matrix

$$S=\begin{pmatrix}2 & 0\\ 0 & 2\end{pmatrix}.$$

The relative gain array of this process at the conditions considered is given by

$$\Lambda=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}.$$

The process displays no first-order closed-loop interaction; however, examination of the model equations indicates the presence of one-way interaction from u_1 to y_2. Recall that transmission interaction occurs when the action of one controller on an output is influenced by a path that includes other controllers. This is the type identified by the linear RGA.

It is reasonable to ask whether the nonlinear effects contribute to transmission interaction effects in the closed-loop process. Using the first- and second-order gain information given in the sixth section, the entries in the interaction tables discussed previously can be evaluated as follows:

$$\gamma_{11}^1 = \frac{\partial u_1}{\partial y_1}\frac{\partial^2 y_1}{\partial u_1 \partial u_1} + \frac{\partial y_1}{\partial u_1}\frac{\partial^2 u_1}{\partial y_1 \partial y_1}\frac{\partial y_1}{\partial u_1} + \frac{\partial y_2}{\partial u_1}\frac{\partial^2 u_1}{\partial y_2 \partial y_1}\frac{\partial y_1}{\partial u_1}$$
$$= -0.4 + 0.4 + 0.0 = 0$$

$$\gamma_{12}^1 = \frac{\partial u_1}{\partial y_1}\frac{\partial^2 y_1}{\partial u_1 \partial u_2} + \frac{\partial y_1}{\partial u_2}\frac{\partial^2 u_1}{\partial y_1 \partial y_1}\frac{\partial y_1}{\partial u_1} + \frac{\partial y_2}{\partial u_2}\frac{\partial^2 u_1}{\partial y_2 \partial y_1}\frac{\partial y_1}{\partial u_1}$$
$$= 0.0 + 0.0 + 0.0 = 0$$

$$\gamma_{11}^2 = \frac{\partial u_1}{\partial y_2}\frac{\partial^2 y_2}{\partial u_1 \partial u_1} + \frac{\partial y_1}{\partial u_1}\frac{\partial^2 u_1}{\partial y_1 \partial y_2}\frac{\partial y_2}{\partial u_1} + \frac{\partial y_2}{\partial u_1}\frac{\partial^2 u_1}{\partial y_1 \partial y_2}\frac{\partial y_2}{\partial u_1}$$
$$= 0.0 + 0.0 + 0.0 = 0$$

$$\gamma_{12}^2 = \frac{\partial u_1}{\partial y_2}\frac{\partial^2 y_2}{\partial u_1 \partial u_2} + \frac{\partial y_1}{\partial u_2}\frac{\partial^2 u_1}{\partial y_1 \partial y_2}\frac{\partial y_2}{\partial u_1} + \frac{\partial y_2}{\partial u_2}\frac{\partial^2 u_1}{\partial y_1 \partial y_2}\frac{\partial y_2}{\partial u_1}$$
$$= 0.0 + 0.0 + 0.0 = 0$$

and, similarly, $\gamma_{21}^1 = \gamma_{22}^1 = \gamma_{21}^2 = \gamma_{22}^2 = 0$. The terms corresponding to Eq. 19 are

$$\delta_{11}^1 = \frac{\partial y_1}{\partial u_1}\frac{\partial^2 u_1}{\partial y_1 \partial y_1} + \frac{\partial u_1}{\partial y_1}\frac{\partial^2 y_1}{\partial u_1 \partial u_1}\frac{\partial u_1}{\partial y_1} + \frac{\partial u_2}{\partial y_1}\frac{\partial^2 y_1}{\partial u_2 \partial u_1}\frac{\partial u_1}{\partial y_1}$$
$$= 0.4 + -0.4 + 0.0 = 0$$

$$\delta_{12}^1 = \frac{\partial y_1}{\partial u_1}\frac{\partial^2 u_1}{\partial y_1 \partial y_2} + \frac{\partial u_1}{\partial y_2}\frac{\partial^2 y_1}{\partial u_1 \partial u_1}\frac{\partial u_1}{\partial y_1} + \frac{\partial u_2}{\partial y_2}\frac{\partial^2 y_1}{\partial u_2 \partial u_1}\frac{\partial u_1}{\partial y_1}$$
$$= 0.0 + 0.0 + 0.0 = 0$$

$$\delta_{11}^2 = \frac{\partial y_1}{\partial u_2}\frac{\partial^2 u_2}{\partial y_1 \partial y_1} + \frac{\partial u_1}{\partial y_1}\frac{\partial^2 y_1}{\partial u_1 \partial u_2}\frac{\partial u_2}{\partial y_1} + \frac{\partial u_2}{\partial y_1}\frac{\partial^2 y_1}{\partial u_1 \partial u_2}\frac{\partial u_2}{\partial y_1}$$
$$= 0.0 + 0.0 + 0.0 = 0$$

$$\delta_{12}^2 = \frac{\partial y_1}{\partial u_2}\frac{\partial^2 u_2}{\partial y_1 \partial y_2} + \frac{\partial u_1}{\partial y_2}\frac{\partial^2 y_1}{\partial u_1 \partial u_2}\frac{\partial u_2}{\partial y_1} + \frac{\partial u_2}{\partial y_2}\frac{\partial^2 y_1}{\partial u_1 \partial u_2}\frac{\partial u_2}{\partial y_1}$$
$$= 0.0 + 0.0 + 0.0 = 0.$$

It can be easily verified that $\delta_{21}^1 = \delta_{21}^2 = \delta_{22}^1 = \delta_{22}^2 = 0$.

These results indicate that the process nonlinearity does not introduce transmission interaction effects in the closed-loop system. From the steady-state point of view, the $u_1 - y_1$ and $u_2 - y_2$ control loops can be treated independently. However, one-way decoupling may be required to compensate for the action of u_1 on y_2.

Example 3

The approach discussed in the previous section is used to evaluate the extent of interaction in the 2×2 evaporator model of Newell and Lee (1989). In this process, the outlet product mass, y_1 (%), and operating pressure, y_2 (kPa), are controlled using the inlet steam pressure fed to the evaporator, u_1 (kPa), and the cooling-water flow rate to an overhead condenser, u_2 (kg/min). Guay et al. (1995) found that this process displays significant nonlinearity at the operating conditions $[y_1, y_2]^T = [25, 50.5]^T$ and $[u_1, u_2]^T = [194.7, 208.0]^T$. The first- and second-order gains are given by

$$\frac{\partial y}{\partial u} = \begin{pmatrix} 0.11677 & 0.045585 \\ 0.12807 & -0.049972 \end{pmatrix}$$

and

$$\frac{\partial y}{\partial u \partial u^T} = \begin{pmatrix} \begin{bmatrix} 8.1309\times 10^{-4} & 3.7307\times 10^{-4} \\ \cdot & -2.7355\times 10^{-4} \end{bmatrix} \\ \begin{bmatrix} -3.0467\times 10^{-4} & -1.7804\times 10^{-4} \\ & 3.8670\times 10^{-4} \end{bmatrix} \end{pmatrix}.$$

First- and second-order inverse gains are given by

$$\frac{\partial u}{\partial y} = \begin{pmatrix} 4.2268 & 3.9179 \\ 10.935 & -9.9704 \end{pmatrix}$$

and

$$\frac{\partial^2 u}{\partial y \partial y^T} = \begin{pmatrix} \begin{bmatrix} -1.6089\times 10^{-1} & -1.6163\times 10^{-6} \\ & -2.6744\times 10^{-6} \end{bmatrix} \\ \begin{bmatrix} 5.6258\times 10^{-2} & -9.4865\times 10^{-1} \\ & 9.5584\times 10^{-1} \end{bmatrix} \end{pmatrix}.$$

The relative gain array is given by

$$\Lambda = \begin{pmatrix} 0.498 & 0.502 \\ 0.502 & 0.498 \end{pmatrix},$$

indicating strong interaction effects. As suggested in Newell and Lee (1989), these results indicate that there is no clearly advantageous choice of input–output pairings in this case.

In order to analyze the second-order interaction effects, the first- and second-order gain information must be appropriately scaled. For the construction of the interaction table corresponding to Eq. 18, the inputs can be scaled by the scaling matrix

$$S = \begin{pmatrix} 0.016667 & 0 \\ 0 & 0.014286 \end{pmatrix}.$$

This matrix scales the inputs with respect to the expected range of variation of both channels during normal operation. The second-order interaction table is given by

$$\begin{array}{ccc} & y_1 & y_2 \\ u_1 & \begin{pmatrix} 7.1622\times 10^{-2} \\ 4.8834\times 10^{-2} \end{pmatrix} & \begin{pmatrix} -7.1622\times 10^{-2} \\ -4.8834\times 10^{-2} \end{pmatrix} \\ u_2 & \begin{pmatrix} -7.1622\times 10^{-2} \\ -4.8834\times 10^{-2} \end{pmatrix} & \begin{pmatrix} 7.1622\times 10^{-2} \\ 4.8834\times 10^{-2} \end{pmatrix}. \end{array}$$

This indicates that, for the region of operation described by the scaling matrix, the nonlinearity makes a mild contribution to closed-loop interactions. Furthermore, the positive diagonal elements in this table demonstrate a positive interaction effect due to nonlinearity in the u_1-y_1 and u_2-y_2 loop pairings. These loop pairings should therefore be adopted in this region of operation in order to prevent reverse effects due to nonlinearity. Thus this analysis of second-order effects complements linear techniques and improves the ability to assign appropriate input–output pairings in a nonlinear process.

Construction of the table from Eq. 19 for the output coordinates is now considered. This requires specification of scaling in the output region. Consider the region described by the scaling matrix

$$T=\begin{pmatrix}0.2 & 0\\ 0 & 0.14286\end{pmatrix}.$$

The corresponding interaction table is given by

$$\begin{array}{ccc} & y_1 & y_2 \\ u_1 & \begin{pmatrix}6.3612\times10^{-2}\\ -1.5953\times10^{-2}\end{pmatrix} & \begin{pmatrix}-6.3612\times10^{-2}\\ 1.5953\times10^{-2}\end{pmatrix} \\ u_2 & \begin{pmatrix}-6.3612\times10^{-2}\\ 1.5953\times10^{-2}\end{pmatrix} & \begin{pmatrix}6.3612\times10^{-2}\\ -1.5953\times10^{-2}\end{pmatrix}\end{array}.$$

Again, it can be seen that the nonlinearity of the process contributes significantly to the interaction effect. In this case, however, the components of each 2-dimensional vector in the interaction table are of opposite signs, indicating conflicting interaction effects for the closed-loop process due to the nonlinearity.

This situation complicates considerably the task of choosing appropriate input–output pairings. Many strategies can be envisaged. One simple solution is to allocate pairings based on the sign of the larger element in each vector. This is based on the assumption that, on average, the dominant components summarize the interaction effects observed. To facilitate the comparisons, one can normalize each P-dimensional element of the interaction table.

Applying this simple rule in this example, it is seen that the dominant effect of the nonlinearity is given by the term 6.3612×10^{-2}. Since this term appears as a positive term on the diagonal of the interaction table, the u_1-y_1 and u_2-y_2 pairings are selected for this process.

This example highlights the importance of choosing an appropriate scaling region. In this case, two scaling approaches were considered, and it was shown that the interpretation of the results generally depend on the choice of the scaling region. In the first case, a region defined by a diagonal matrix was used to evaluate interaction effects in the input coordinates. A direct effect of nonlinearity on closed-loop interactions was observed, which led to a clear choice of input–output pairings. The second analysis, based on the choice of a scaling region in the output coordinates, led to a different appreciation of the extent of nonlinear contributions to the interaction effects, requiring a more cautious interpretation of the results. The relationship between scaling and the orientation of a steady-state process has been in discussed in Guay et al. (1995) where an alternative scaling procedure was proposed.

Conclusions

A new approach for assessing closed-loop nonlinearity and interaction in nonlinear processes has been presented. It is based on a differential geometric interpretation of the relative gain array that leads to the derivation of second-order identities. These identities can be used to measure the extent and the nature of the nonlinearity of a closed-loop process under linear or nonlinear control. These identities can also be used in the analysis of higher-order interaction effects.

Two types of nonlinear closed-loop process behavior have been introduced. Between-channel nonlinearity is associated with the nonlinear dependence of output channels on other input–output pairings. Within-channel nonlinearity is used to identify the interaction effects that result from the inherent nonlinearity of each output channel. An rms measure of interaction has been introduced to evaluate the significance of local nonlinearity effects. Application of the approach has been illustrated using a two-input, two-output CSTR model, and the method has been shown to yield considerable information about the nature of the nonlinear behavior of that process.

An extension of the second-order identities to the measurement of nonlinear interaction effects has also been presented. The method yields a second-order interaction table that can be expressed in either the input or output coordinates to complement and extend the applicability of the relative gain array to nonlinear processes. Models describing a simple CSTR and an evaporator process have been used to demonstrate the application of the method. The CSTR model was shown to display no first- or second-order transmission interaction effects. Although this process is shown to display significant nonlinearity, the analysis demonstrates that the RGA captures very accurately the extent of interaction in the closed-loop process. The evaporator model displays both first- and second-order interaction effects. It has been shown that the choice of input–output pairings may be affected by consideration of the second-order effects under different scaling possibilities.

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Notation

A, B = vector fields
Da_1, Da_2 = kinetic constants
f = vector field describing the dynamics of a process on the state space
G = implicit vector-valued function of the inputs and the outputs
i,j,k = integer indices of output coordinates
N = dimension of the space of state variables
P = number of inputs and outputs
$\mathbb{R}$ = set of real numbers
$\mathbb{R}^P$ = P-dimensional real space
T = output scaling matrix
T = transpose of a matrix or vector
$u^{(k)}$ = kth time derivative of the input vector

v = scaled input vector

W = intersection of two open neighborhoods of a point p of a manifold M

$y^{(k)}$ = kth time derivative of the outputs

Y = open neighborhood of a point in $\mathbb{R}^P$

z = reparametrization of the outputs

$\hat{\gamma}_{abc}$ = scaled mismatch terms summed over all outputs

δ_a^i = P-dimensional vector element of the second-order interaction table expressed in the output coordinates

ϕ = nonlinear vector-valued function of the inputs

Φ = nonlinear vector-valued function of the inputs

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