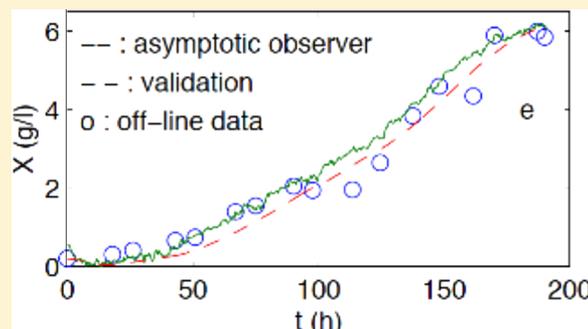


Some Structural Properties of Reaction Systems Useful For Estimation and Control

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ABSTRACT: The objective of this text is to give an overview of some structural properties of the dynamical models of reaction systems, in particular (but not uniquely) of chemical and biochemical systems as well as environmental and ecological systems, that can be interesting for the analysis and the design of process estimation and control tools. We shall in particular consider the notion of reaction invariants (that will allow us to rewrite part of the system dynamics in a way that is independent of the reaction kinetics) and of singular perturbations (slow/fast dynamics) (that will allow us to generalize the notion of quasi steady states). We also consider a transformation that allows us to diagonalize the stoichiometric coefficient matrix (useful in the implementation of some parameter estimators) and a simple condition based on the system reaction network that allows us to emphasize the possible presence of inverse response/nonminimum phase. Finally, the link between adaptive linearizing control and PI control will be discussed. Links with some important research of Dominique Bonvin will also be emphasized.



■ FOREWORD

This paper had been prepared with the objective of being included in a special issue prepared in the honor of Dominique Bonvin. It rapidly became obvious that the best contribution I could provide should emphasize a research activity in which we both have been very active over the years: the analysis of the properties of reaction systems and their use for identification, estimation, and control. If some of the properties presented here have no connection with the work of Dominique Bonvin, some exhibit a strong link even if their use, although similar, is not fully identical.

1. INTRODUCTION

The chemical, biochemical, environmental, and ecological systems are the key elements of the class of the reaction systems. To know and understand well the properties of this class of systems can be particularly useful when the purpose is to understand their specific features and develop and implement monitoring (software sensors) and control tools. The main objective of this paper is to illustrate this viewpoint by emphasizing some structural properties of models of reaction systems and their link with the design and implementation of monitoring and control tools for reaction systems.

In this paper, we concentrate on homogeneous reaction systems, i.e., those whose dynamics is characterized by ordinary differential equations (ODE's). Yet several properties emphasized here can be rather straightforwardly extended to the nonhomogeneous system (tubular reactors,¹ for instance) where partial differential equations are used to characterize the system dynamics. We begin by introducing the dynamical

model that we call the “general dynamical model for reaction systems in homogeneous medium” (Section 2). Section 3 is devoted to a state transformation that is related to the notion of reaction invariants and is useful for the design of state observers that are independent of the reaction kinetics. In Section 4, we consider model reduction and the notions of singular perturbations and slow/fast systems. Section 5 is dedicated to the introduction of another transformation that allows us to diagonalize the stoichiometric coefficient matrix. This transformation is useful in different situations including the calibration of the design parameters of a parameter estimator independently of the (nonlinear) system dynamics. The last two sections are dedicated to control. In Section 6, the link between adaptive linearizing control and PI control is discussed, whereas Section 7 will show under which conditions inverse response/nonminimum phase behavior can take place.

2. GENERAL DYNAMICAL MODEL OF REACTION SYSTEMS IN HOMOGENEOUS MEDIUM

Let us consider a reaction system in which n components interact via a number of reactions equal to m . Let us also consider that the reaction medium is homogeneous or confined (as is the case for a perfectly mixed reactor). The reactions are possibly nonisothermal. The dynamical equations of the system can then be obtained from mass balance

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equations for the components and energy balance for the temperature. (Note that the latter is obtained by considering some simplifying assumptions for the internal energy balance and that a thermodynamically more consistent expression can possibly be considered, see refs 3 and 4 for examples.) These can be put under the following generic matrix form:²

$$\frac{dx}{dt} = Kr(x) + F - Q - \frac{q}{V}x + U(T) \quad (1)$$

where x represents the vector of the concentrations of the components (reactants, products, biomass, species, resources, etc.) of the reaction system (g/L) and of the temperature (K) of the reaction medium (for nonisothermal systems). The matrix K is the stoichiometric coefficient matrix (these coefficients usually called yield coefficients in biological systems), $r(x)$ (g/(L h)) is the reaction rate vector, F (g/h) is the feed rate vector, Q (g/h) is the gaseous outflow rate vector, and $U(T)$ (K/h) is the heat exchange vector related to the cooling or heating system (this term is usually a function of the temperature of the reaction medium). q (L/h) is the volumetric inlet flow rate and V is the volume of the reaction medium. It is important to note (or more prosaically, to recall) that a fundamental aspect of this model is that the dynamics of a reaction system is generically the sum of a conversion term $Kr(x)$ and of a transport dynamics term $F - Q - qx/V + U(T)$. It is also worth noting that this model is valid whatever the operating mode, batch, fed-batch, or continuous.⁵ The only necessary modification is the addition of a volume balance

$$\frac{dV}{dt} = q \quad (2)$$

in the fed-batch operating mode.

As a matter of illustration, let us consider the Van de Vusse reaction scheme:⁶



If we consider nonisothermal reactions, we can choose the following state vector and reaction rate vector:

$$x = \begin{bmatrix} T \\ C_{A1} \\ C_{A2} \\ C_{A3} \\ C_{A4} \end{bmatrix}, r = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix} \quad (4)$$

where C_{A_i} ($i = 1-4$) and r_j ($j = 1-3$) represent the concentrations of the components A_i ($i = 1-4$) and the rates of reactions 1, 2, 3, respectively. If there is no product in the gaseous phase, the matrix K and the vectors F , Q , and U are written as follows:

$$K = \begin{bmatrix} -\frac{\Delta H_1}{\rho C_p} & -\frac{\Delta H_2}{\rho C_p} & -\frac{\Delta H_3}{\rho C_p} \\ -1 & 0 & -2 \\ 1 & -1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, F = \begin{bmatrix} \frac{q}{V}T_{in} \\ \frac{q}{V}C_{in} \\ 0 \\ 0 \\ 0 \end{bmatrix}, Q = 0, U = \begin{bmatrix} \frac{hA}{\rho C_p V}(T_c - T) \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (5)$$

with ΔH_i ($i = 1-3$), ρ , C_p , T_{in} , C_{in} , h , A , and T_c being the enthalpies of each reaction, the density, the specific heat of the fluid, the inlet temperature, the inlet component concentration, the heat exchanger coefficient, its exchange area, and the temperature of the fluid in the exchanger, respectively.

3. STATE TRANSFORMATION, REACTION INVARIANTS, AND DESIGN OF ASYMPTOTIC OBSERVERS

Let us define by p the rank of the matrix K in model (1). Generally speaking, if the considered reactions are independent, p will be equal to the number of reactions ($p = m$). (A typical case of dependent reactions is the reversible reaction where two reactions with the same stoichiometric coefficients and reactions rates of opposite signs are considered. It is worth noting that in that case, a single reaction whose reaction rate is the difference of the rates of the forward reaction and of the backward reaction (i.e., which can be either positive or negative) can be considered.) Let us consider the following state partition:

$$x = \begin{bmatrix} x_a \\ x_b \end{bmatrix} \quad (6)$$

such that the submatrix K_a corresponding to x_a is full rank ($\text{rank}(K_a) = p$). We can then rewrite the model under the following form:

$$\frac{dx_a}{dt} = K_a r(x) + F_a - Q_a - \frac{q}{V}x_a + U_a(T) \quad (7)$$

$$\frac{dx_b}{dt} = K_b r(x) + F_b - Q_b - \frac{q}{V}x_b + U_b(T) \quad (8)$$

We can then state the following structural property: for the system (1), there exists a state transformation

$$z = A_0 x_a + x_b \quad (9)$$

with A_0 solution of the matrix equation:

$$A_0 K_a + K_b = 0 \quad (10)$$

such that the dynamical system (1) can be written under the following form:

$$\frac{dz}{dt} = K_a r(x) + F_a - Q_a - \frac{q}{V}z + U_a(T) \quad (11)$$

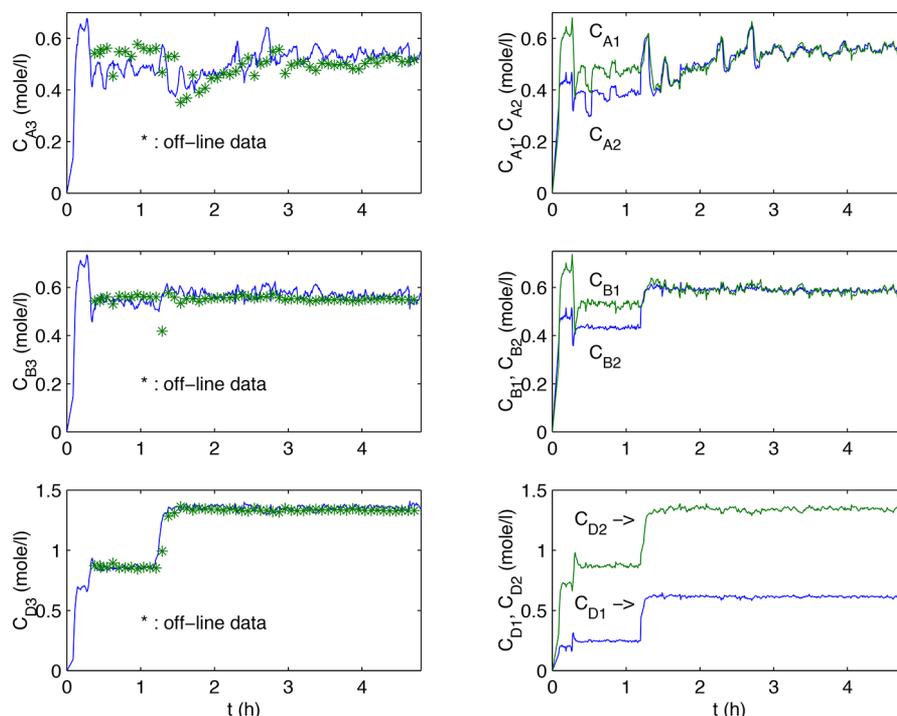


Figure 1. Asymptotic observer applied to a ETBE synthesis process.

$$\frac{dz}{dt} = -\frac{q}{V}z + A_0(F_a - Q_a + U_a(T)) + F_b - Q_b + U_b(T) \quad (12)$$

The interest of this property is that it provides a model description whose a part of the dynamics (eq 12) is independent of the kinetics $r(x)$. This notion corresponds to the notion of reaction invariants⁷ for closed systems ($F = Q = U = q = 0$). Observe that then eq 12 reduces to $\frac{dz}{dt} = 0$, which explains the notion of reaction invariants, which is then a mathematical invariant. The use of reaction invariants in automatic control dates back from works of Fjeld and co-workers.⁸ It is also at the core of a large part of the research activities of Dominique Bonvin starting from his 1990 seminal paper.⁹ This activity developed (and is still developing) methods for estimation and control around the notion of variants, invariants and extents, and results in a impressive number of scientific publications^{10–16} (to cite a few).

The reaction invariant property can be very useful in the design of software sensors that allow reconstruction of the unmeasured variables of a reaction system. It is well-known that the balance models are the basis for modeling the dynamics of reaction systems. (Originally, we were not aware of the fact that the above property was the invariant reaction property, and our source of inspiration was a paper by Aborhey and Williamson (1978),¹⁸ where the authors had been designing an observer for the biomass concentration by using the measurement of substrate concentration in the scalar version of the above transformation in a simple microbial growth system. We indeed originally used it to rewrite the dynamics of the system in the context of the online estimation of specific growth rates in biological systems.¹⁹) The modeling of the kinetics is often their weak point (because of the lack of appropriate models and/or experimental data sufficiently informative to provide sufficiently reliable models). It is therefore important to be able to be free from the knowledge

of the kinetics to provide reliable values of the unmeasured variables. This is the case of the “asymptotic” observer.^{2,5,17}

Let us consider that q variables (concentrations and possibly temperature in the nonisothermal case) are measured on line, with $q \geq p$. Let us call x_1 the vector of the measured variables and let us put in a vector x_2 the unmeasured variables. We can therefore rewrite the state vector x with the following new state partition:

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad (13)$$

We can rewrite z as a function of x_1 and x_2 :

$$z = A_1x_1 + A_2x_2 \quad (14)$$

The asymptotic observer computes the value of x_2 on the basis of eqs 12 and 14:

$$\frac{d\hat{z}}{dt} = -\frac{q}{V}\hat{z} + A_0(F_a - Q_a + U_a(T)) + F_b - Q_b + U_b(T) \quad (15)$$

$$\hat{x}_2 = A_2^+(\hat{z} - A_1x_1) \quad (16)$$

where A_2^+ is a left inverse of the matrix A_2 . In the frequent case when $q = p = m$, A_2^+ is the inverse of A_2 ($A_2^+ = A_2^{-1}$). Let us draw attention to the fact that the submatrix K_1 associated with the vector of the measured variables has to be full rank (it is the case if the reactions are independent and if the variables of the vector x_1 are independent). (One example of the loss of independence of the variables is the case of the respiratory quotient equal to one in an aerobic biological system.⁵)

Figure 1 presents implementation results of the asymptotic observer for a fixed bed reactor used in the synthesis of ethyl tertio-butyl ether (ETBE), used in particular as additive in unleaded gasoline.^{17,20} The reactants of the synthesis of ETBE are ethanol and isobutene:



and the reaction is exothermic ($\Delta H = -40$ kJ/kmol). The measured variable used for the asymptotic observer is the temperature. This one is measured at 4 locations in the reactor (including the inlet and the outlet) and in the heat exchanger. Figure 1 illustrates the reconstruction of the concentrations in ethanol C_A , isobutene C_B , and ETBE C_D at both internal locations of the reactor (indices 1 and 2) and at the outlet (index 3).

The design of asymptotic observers has been extended to distributed parameter tubular reactor models.¹⁷ In that paper it is also shown how to introduce design parameters in the observer in the case of multitank systems to arbitrarily assign the observer dynamics. Another interesting extension of the asymptotic observers are the interval observers^{21,22} that take advantage of the cooperativity properties of the system.²³

Note also that the notion of reaction invariants and the related transformation appears to be very useful when identifying the parameters of a reaction system. Indeed, because it allows us to provide a dynamical description that is independent of the reaction kinetics, the use of the dynamical equations of the variable z allows us to proceed with the identification of the yield/stoichiometric coefficients and of the transfer coefficients independently of the choice of kinetic models (and therefore of the calibration of the parameters of the selected kinetic models). This calibration can be performed subsequently once the calibration of the other parameters has been validated by coming back to the original mass and energy balance model. This approach is discussed in particular in^{5,24}

4. DIAGONALIZATION OF THE STOICHIOMETRIC COEFFICIENTS AND CALIBRATION OF PARAMETER ESTIMATORS

Let us go back to the general dynamical model (1) for which we consider m variables of the state vector x that we shall call y such that the submatrix of the stoichiometric coefficients K_y is full rank. Then the dynamical equations of y are written:

$$\frac{dy}{dt} = K_y r - \frac{q}{V} y + F_y - Q_y + U_y \quad (18)$$

Let us consider the following transformation ζ :

$$\zeta = K_y^{-1} y \quad (19)$$

The dynamical equations of ζ are then written as follows:

$$\frac{d\zeta}{dt} = -\frac{q}{V} \zeta + r + K_y^{-1}(F_y - Q_y + U_y) \quad (20)$$

We observe that the dynamics of ζ has the property that one reaction rate is associated with each entry of ζ , i.e., for all $i = 1$ to m :

$$\frac{d\zeta_i}{dt} = -\frac{q}{V} \zeta_i + r_i + f_i \quad (21)$$

where f_i is the i th row of $K_y^{-1}(F_y - Q_y + U_y)$.

This property is useful for, for instance, the calibration of parameter estimators, in particular for the online estimation of reaction rates (observer-based estimators).²⁵ In this case, we are often not interested in the online estimation of the complete reaction rate but rather to one parameter of the kinetic expression. For instance, the objective will be to reconstruct the online evolution of the specific growth rate μ of a growth reaction ($r = \mu X$), where X is the biomass

concentration; or the kinetic constant k_0 for a reaction of order α ($r = k_0 C^\alpha$). The vector of the reaction rates r can then be rewritten as the product of a diagonal matrix $G(x)$ (which is, generally speaking, a function of the system variables) and of a vector of parameters to be estimated on line θ : $r = G(x)\theta$. Then eq 18 becomes

$$\frac{dy}{dt} = K_y G(x) \theta - \frac{q}{V} y + F_y - Q_y + U_y \quad (22)$$

We can then use the following software sensor⁵²⁵ to estimate θ on the basis of the measurements of y :

$$\frac{d\hat{y}}{dt} = K_y G(x) \hat{\theta} - \frac{q}{V} y + F_y - Q_y + U_y - \Omega(y - \hat{y}) \quad (23)$$

$$\frac{d\hat{\theta}}{dt} = [K_y G(x)]^T \Gamma (y - \hat{y}) \quad (24)$$

The matrices Ω and Γ are the gains of the estimator. The calibration of the estimator may be performed via the choice of appropriate values of the entries of Ω et Γ . The basic rule is that the matrix $\Omega^T \Gamma + \Gamma \Omega$ has to be negative definite. This being said, it is important to know that the convergence speed of the estimator depends on the value of the variables x via $G(x)$. Indeed, the state matrix of the estimation error system

$$e = \begin{bmatrix} y - \hat{y} \\ \theta - \hat{\theta} \end{bmatrix} \quad (25)$$

is equal to

$$A = \begin{bmatrix} \Omega & K_y G(x) \\ -(K_y G(x))^T \Gamma & 0 \end{bmatrix} \quad (26)$$

This difficulty can be circumvented by using the above transformation. Indeed, in that case, the parameter estimator takes the following form:

$$\frac{d\hat{\zeta}}{dt} = G(x) \hat{\theta} - \frac{q}{V} \zeta + K_y^{-1}(F_y - Q_y + U_y) - \Omega(\zeta - \hat{\zeta}) \quad (27)$$

$$\frac{d\hat{\theta}}{dt} = \Gamma(\zeta - \hat{\zeta}) \quad (28)$$

Because $G(x)$ is diagonal and by choosing diagonal matrices for Ω and Γ

$$\Omega = \text{diag}\{-\omega_i\}, \Gamma = \text{diag}\{\gamma_i\}, \omega_i > 0, \gamma_i > 0, i = 1 \dots p \quad (29)$$

we see that we obtain a system of second-order differential equations that allows us to estimate each unknown parameter independently of the other parameters. Let us now see how to make the dynamics of the estimator independent of the operating conditions of the system. To do so, let us redefine the estimation error

$$e = \begin{bmatrix} \zeta - \hat{\zeta} \\ \theta - \hat{\theta} \end{bmatrix} \quad (30)$$

whose dynamics can be derived from eqs 20, 27, and 28):

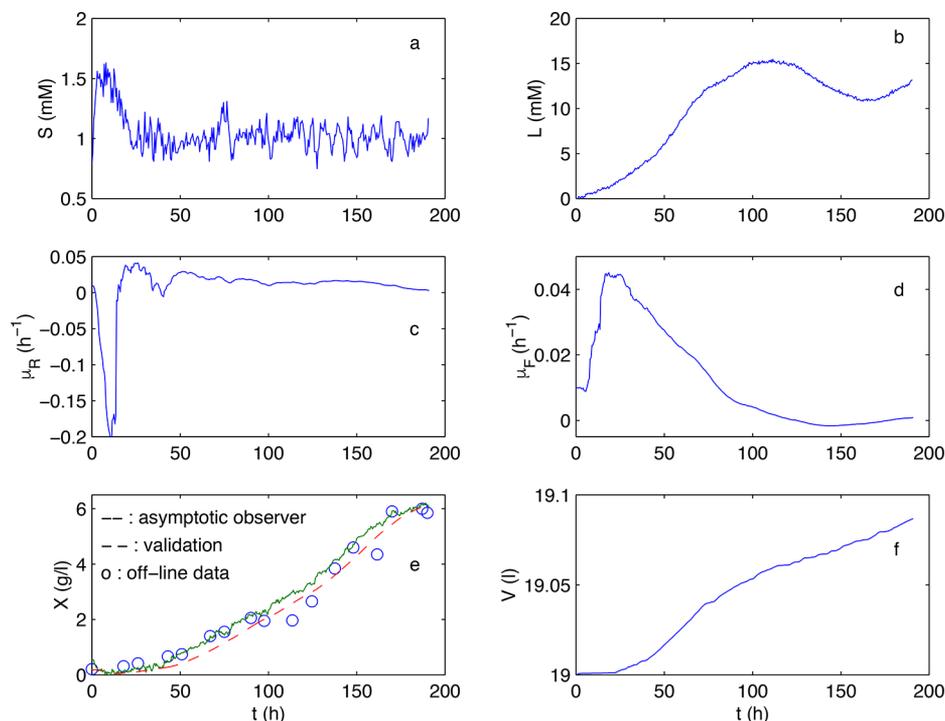


Figure 2. Estimation of specific growth rates for an animal cell culture.

$$\frac{de}{dt} = Ae + b \quad (31)$$

where A is a block-diagonal matrix with blocks of dimension 2:

$$A = \text{diag}\{A_i\}, A_i = \begin{bmatrix} -\omega_i & g_i(x) \\ -\gamma_i & 0 \end{bmatrix}, i = 1a'p \quad (32)$$

and where b is equal to

$$b = \begin{bmatrix} 0 \frac{d\theta_1}{dt} 0 \frac{d\theta_2}{dt} \dots 0 \frac{d\theta_p}{dt} \end{bmatrix}^T \quad (33)$$

The characteristic polynomial associated with the matrix A , $\det(\lambda I - A)$, is here written as follows:

$$\det(\lambda I - A) = \prod_{i=1}^p (\lambda^2 + \omega_i \lambda + \gamma_i g_i(x)) \quad (34)$$

The central idea of the choice of the calibration parameters consists of choosing each γ_i inversely proportional the corresponding term $g_i(x)$ (that has to be different from zero):

$$\gamma_i = \frac{\bar{\gamma}_i}{g_i(x)}, \bar{\gamma}_i > 0, i = 1a'p \quad (35)$$

We can then rewrite the characteristic eq 34 as follows:

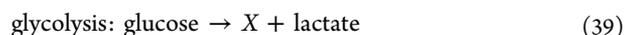
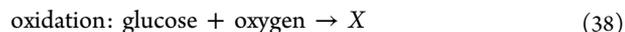
$$\det(\lambda I - A) = \prod_{i=1}^p (\lambda^2 + \omega_i \lambda + \bar{\gamma}_i) \quad (36)$$

In other words, the dynamics of the estimator is now independent of the operating conditions. Such a choice of the calibration parameters de calibration corresponds to a Lyapunov transformation.²⁶ An interesting choice consists of considering double poles, i.e.:

$$\bar{\gamma}_i = \frac{\omega_i^2}{4} \quad (37)$$

In such a case, the calibration of each estimator reduces to the choice of only one ω_i . This allows to have a calibration procedure that has the double advantage to be simple (a single calibration parameter per unknown parameter) and flexible (each calibration parameter may have a value which is different depending on the rate of variation of each unknown parameter).

Figure 2 illustrates the application of this result to the estimation of 2 specific growth rates μ_R (oxidation reaction) and μ_F (glycolysis reaction) in a fed-batch process of production of animal cells in a pilot reactor of 22 L.²⁷ The associated reaction scheme can be put under the following form:



Glucose (Figure 2a) and lactate (Figure 2b) are measured via a biosensor of the FIA (Flow Injection Analysis) type. In the absence of reliable models for the specific growth rates, the validation of the estimation has been performed on the basis of biomass concentration data: Figure 2e compares the off-line biomass data (o) with the estimation X_v (dotted line) of the biomass computed from the balance equation and the estimated values of the specific growth rates $\hat{\mu}_R$ and $\hat{\mu}_F$:

$$\frac{dX_v}{dt} = \hat{\mu}_R X_v + \hat{\mu}_F X_v - \frac{q}{V} X_v \quad (40)$$

This diagonalization transformation appears to be also of interest in other situations, for instance, in the design of observers where the structure of the kinetic model is known while the parameters of the kinetic model are known (or at least poorly known).^{28,29}

Note that this transformation allows us to make another strong link with the work of Dominique Bonvin because the same transformation has been considered to emphasize the dynamics of reaction variants with a number of methodological developments, in particular, in the context of identification and parameter estimation, yet in a different context.^{13–1530}

5. SLOW–FAST DYNAMICS AND MODEL REDUCTION

The models of reaction systems can rapidly become high-order ones once the number of components and reactions that are taken into account is increasing. In practice, it can be of interest to use models of reduced complexity that appear to be more reliable from parameter identification, monitoring, or control design viewpoints.

The notion of slow/fast dynamics and the singular perturbations techniques are tools that allow order reduction of dynamical models³¹ and in particular of reaction system models.³² In very simple terms, the central idea is to separate the model dynamics into fast and slow dynamics and to keep only the slow dynamics while reducing the fast dynamics into algebraic equations. Singular perturbations are applicable in particular to slow and fast reactions and low solubility gaseous products. Let us concentrate here on a typical example of slow and fast reactions. Let us consider the following sequential reaction scheme:



where the first reaction is slow and the second is fast. The dynamical balance of the components gives the following equations:

$$\frac{dC_{A1}}{dt} = \frac{q}{V} C_{in} - \frac{q}{V} C_{A1} - r_1 \quad (42)$$

$$\frac{dC_{A2}}{dt} = -\frac{q}{V} C_{A2} + a_2 r_1 - r_2 \quad (43)$$

$$\frac{dC_{A3}}{dt} = -\frac{q}{V} C_{A3} + a_3 r_2 \quad (44)$$

where the reaction rates r_1 and r_2 , in agreement with the chemical kinetics laws, can take the following form

$$r_1 = k_{01} C_{A1} \phi_1(C_{A1}, C_{A2}), r_2 = k_{02} C_{A2} \phi_2(C_{A2}, C_{A3}) \quad (45)$$

with ϕ_1 and ϕ_2 positive (and possibly nonlinear) functions ($\phi_1 > 0$, $\phi_2 > 0$) of the components intervening in the reaction (for instance in the case of first-order reactions, $\phi_1 = 1$ et $\phi_2 = 1$). The fact that the reaction is slow can be formalized via the kinetic constants as follows: $k_{01} \ll k_{02}$. At the limit, k_{02} is very large or, in other words, its inverse $\varepsilon = \frac{1}{k_{02}}$ tends to zero.

Let us consider the following auxiliary variable: $\tilde{C} = a_3 C_{A_2} + C_{A_3}$. Its dynamics is directly obtained from eqs 43 and 44:

$$\frac{d\tilde{C}}{dt} = -\frac{q}{V} \tilde{C} + a_2 a_3 r_1 \quad (46)$$

Moreover by introducing the kinetic expressions and by dividing by k_{02} , we can rewrite the dynamical balance of A_2 (eq 43) as follows:

$$\varepsilon \frac{dC_{A2}}{dt} = -\varepsilon \frac{q}{V} C_{A2} + \varepsilon a_2 k_{01} C_{A1} \phi_1(C_{A1} - C_{A2} \phi_2(C_{A2}, C_{A3})) \quad (47)$$

If k_{02} is very large, ε tends to zero, and the above equation becomes

$$0 = -C_{A2} \phi_2(C_{A2}, C_{A3}) \quad (48)$$

Because $\phi_2 > 0$, this implies that $C_{A2} = 0$. Coming back to eq 46, we obtain

$$\frac{dC_{A3}}{dt} = -\frac{q}{V} C_{A3} + a_2 a_3 r_1 \quad (49)$$

In other words, since the intermediate product C_{A2} does not accumulate, this results in considering only one reaction



This result is similar to the one that would be obtained by considering the hypothesis of quasi steady-state (QSS) well-known in chemical engineering. The singular perturbations and the notion of slow–fast allow us to provide a formal mathematical framework for this type of model order reduction methods.³²

Another typical case of application of the singular perturbation techniques is the case of gaseous products P that have a low solubility. The mass balance equation can then be written as follows:

$$\frac{dP}{dt} = -\frac{q}{V} P - Q + r \quad (51)$$

We can show⁵ that in this case we can rewrite the balance equation under the following algebraic form:

$$Q = r \quad (52)$$

A typical case is the production of CH_4 in anaerobic digestion processes.

Therefore, we can then see that generically the singular perturbation techniques allow to reduce to algebraic equations the differential equations of low solubility gaseous products and of components intervening (only) as reactants in fast reactions. By noting x_i the concentration of each of those, we simply have to put both the derivative and the dilution term to zero: $\frac{dx_i}{dt} = 0$, $\frac{q}{V} x_i = 0$.

6. DESIGN OF LINEARIZING CONTROL LAWS AND PI CONTROL

The inflow rate q is often considered in (bio)process control as a potential control input. Many other options are possible but we shall concentrate on this option with the essential objective of simplicity. Let us also consider that at least one part of the feed rates are in the liquid phase and can therefore be written as $F_i = q x_{i, \text{in}} / V$, where $x_{i, \text{in}}$ is the inlet concentration of reactant x_i . In the case of a monovariable control problem (one control input, one controlled output), after having processed, if necessary, to an order reduction of the dynamical model, the dynamical equation of the controlled output can be written as follows:⁵

$$\frac{dy}{dt} = \frac{q}{V} (\alpha x_{\text{in}} - y) - \beta Q + \gamma r \quad (53)$$

where x_{in} is the inlet reactant concentration vector and α , β , and γ are vectors coming from the order reduction and are, generally speaking, nonlinear functions of the stoichiometric coefficients of matrix K . One rather natural way to design a control law is to use adaptive linearizing control, which simply

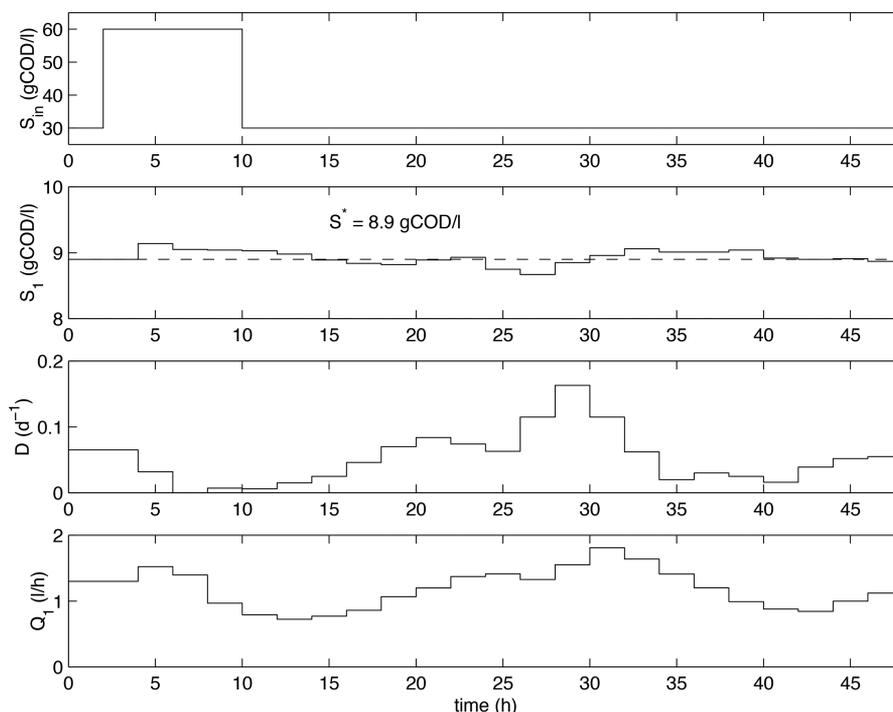


Figure 3. Control of the COD in an anaerobic digestion pilot process

consists to invert the output dynamical eq 53 by imposing a stable dynamics of the following type:

$$\frac{dy}{dt} = \lambda(y^* - y), \lambda > 0 \quad (54)$$

for a given set point value y^* while integrating a parameter adaptation law to estimate on line the badly known parameters of the model. In other words, by combining eqs 53 and 54 and if we consider only the parameter uncertainty in the yield coefficients and in the kinetics, the following control law is obtained:

$$q = \frac{V}{\hat{\alpha}x_{in} - y}(\lambda(y^* - y) + \hat{\beta}Q - \hat{\gamma}r) \quad (55)$$

where $\hat{\alpha}$, $\hat{\beta}$, are $\hat{\gamma}r$ are estimates of the “parameters” α , β , and γr . The parameter estimators will be for instance those presented above (Section 5). A Lyapunov-based design approach will also be considered (example here below). We shall also see later that these play the role of an integral action in the closed loop dynamics.

As a matter of illustration, let us consider the case of the control of the COD (chemical oxygen demand) in an anaerobic digestion process. The process can be characterized by the following (simple) reaction scheme:



where S_1 , S_2 , X_1 , X_2 , P_1 , P_2 represent the organic matter, the volatile fatty acids, the acidogenic and methanogenic bacteria, the CO_2 , and the CH_4 , respectively. If we consider that the variable to be controlled is the sum of the substrate concentrations $S = S_1 + S_2$, that the second reaction is fast, and that the methane is a low solubility product, we can rewrite the mass balance equation of S as follows:

$$\frac{dS}{dt} = \frac{q}{V}(S_{in} - S) - \beta Q \quad (58)$$

where S_{in} is the inlet COD concentration and Q is the methane gaseous outflow rate. Because the reaction scheme is already a simplification of the reality and we have performed a further model simplification, it is reasonable to think that the parameter β is most likely poorly known and might be time-varying. The control law will then take the following form:

$$q = \frac{V}{S_{in} - S}(\lambda(S^* - S) + \hat{\beta}Q) \quad (59)$$

where S^* is the set point for the COD. One way to compute on line the value of $\hat{\beta}$ is to consider the design of the control law by imposing Lyapunov stability criteria and by considering the Lyapunov function $\frac{1}{2}(S^* - S)^2$,⁵ which imply, in our example, to include the following adaptation law:

$$\frac{d\hat{\beta}}{dt} = \delta(S^* - S), \delta > 0 \quad (60)$$

If we integrate this equation by assuming for simplicity reasons that the initial value of $\hat{\beta}$ is equal to zero and that the flow rate of CH_4 is almost constant, the adaptive control law can be rewritten as follows:

$$q = \frac{V}{S_{in} - S} \left[\lambda(S^* - S) + \delta Q \int_0^t (S^* - S(\tau)) d\tau \right] \quad (61)$$

Therefore, we can note that our control law has the basic form of a PI controller²⁶ with a proportional action $\lambda(S^* - S)$ and an integral action $\delta Q \int_0^t (S^* - S(\tau)) d\tau$ (via the parameter adaptation) weighted by the term $\frac{V}{S_{in} - S}$, which is nothing but a feedforward action because it allows us via S_{in} to anticipate the effect of what is in our case a disturbance (S is nothing but the wastewater load that has to reduced below an acceptable

threshold). The behavior of such a controller is illustrated in Figure 3 in the case of a 60 L pilot reactor.³³

7. INVERSE RESPONSE AND LINEARIZING CONTROL

In the preceding section, we mentioned that the linearizing control law consisted in inverting the dynamical model of the reaction system. In control engineering words, this means that in the linear case, the open loop zeroes are poles of the controller. In other words if the system is nonminimum phase (i.e., exhibits an inverse response) (“unstable” zeroes), the control law will be unstable, which will destabilize the closed loop system. It is therefore important not to consider nonminimum phase models to design a linearizing control law.

The questions that we can then have is to know if the inverse response phenomenon can be present in a reaction system and, if yes, in which conditions it may appear. The response can be formulated in a few words: the inverse response phenomenon may appear once there are two sequential reactions in the case of the dynamical relation between the inlet flow rate q and the concentration of the product of the first reaction (which is also a reactant of the second reaction).³⁴ Let us go back to the simple case of the sequential reaction that we have considered above (41) in the case of first order kinetics: $r_1 = k_{01}C_{A1}$, $r_2 = k_{02}C_{A2}$. The transfer function between C_{A2} and q around the equilibrium point (noted by a bar above the value of the variable) is equal to

$$H(s) = \frac{-ak_{01}\bar{C}_{in}}{V\left(\frac{\bar{q}}{V} + k_{01}\right)\left(\frac{\bar{q}}{V} + k_{02}\right)} \frac{s + \left(\left(\frac{\bar{q}}{V}\right)^2 - k_{01}k_{02}\right)}{\left(s + \frac{\bar{q}}{V} + k_{01}\right)\left(s + \frac{\bar{q}}{V} + k_{02}\right)} \quad (62)$$

We therefore see that the system is minimum phase for any operating condition such that the square of the ratio of the inlet \bar{q} over the reactor volume V is smaller than the product of the kinetic constants $k_{01}k_{02}$.

Several solutions to circumvent the difficulty in the linearizing control framework are suggested in,³⁴ including the order reduction considered above or a dynamical version of the control law.

8. CONCLUSIONS

This paper was intended to emphasize some properties of reactions systems that may appear to be useful in the context of identification, estimation and control. The objective was double: to gather a number of analysis results about reaction systems that has been gathered within my research group and to connect some of them with those developed by Dominique Bonvin and his group. The potential of all the results (including many of those from Dominique Bonvin that have not been presented here) have proved to be very useful in many applications of identification, estimation and control of reaction systems.

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Notes

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