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STATE OBSERVERS FOR TUBULAR REACTORS WITH UNKNOWN KINETICS

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Abstract: In this paper, the extension to tubular reactors of asymptotic observers originally developed for STR is first discussed and illustrated with real-life data on an non-isothermal fixed bed reactor. Then it will be shown how to design *exponential* observers, which are also independent from the process kinetics but for which the rate of convergence may be arbitrarily fixed (unlike the asymptotic observers for which the rate of convergence depends on the operating conditions). *Copyright © 1998 IFAC*

1 Introduction

A key question in process control is how to monitor reactant and product concentrations in a reliable and cost effective manner. However, it appears that, in many practical applications, only some of the concentrations of the components involved and critical for quality control are available for on-line measurement. For instance, dissolved oxygen concentration in bioreactors, temperature in non-isothermal reactors and gaseous flowrates are available for on-line measurement while the values of the concentration of biomass, reactants and/or products are often available via off-line analysis. An interesting alternative which circumvents and exploits the use of a model in conjuction with a limited set of measurements is the use of Luenberger or Kalman observers.

One of the reasons for the popularity of the EKF is that it is easy to implement since the algorithm can be derived directly from the state space model. However, since (as the extended Luenberger observer) it is based on a linearized model of the process, the stability and convergence properties are essentially local and valid around some equilibrium point, and it is rather difficult to guarantee its stability over wide ranges or operation. [9] shows that the EKF for state and parameter estimation of linear systems may give biased estimates or even diverge if it is not carefully initialized.

One reason for the problem of convergence of EKF is that, in order to guarantee the (arbitrarily chosen) exponential convergence of the observer, the process must be locally observable, i.e. the linearized tangent model must be observable and fulfil the classical observability rank condition. This condition, as it turns out, is restrictive in many practical situations and may account for the failure of EKF to find widespread application (e.g. [1]). Another problem is that the theory for the extended Luenberger and Kalman observers is developed using a perfect knowledge of the system parameters, in particular of the process kinetics : it is difficult to develop error bounds and there is often a large uncertainty on these parameters. It appears from the above remarks that there is a clear incentive to develop new methodologies for the on-line estimation of the unmeasured concentration variables in (bio)chemical reaction systems that do not only rely on the explicit use of kinetic models. This has resulted in the design and application of *asymptotic* observers based on the well-known nonlinear model of the process without the knowledge of the process kinetics being necessary ([1], [4]).

In this paper, the extension to tubular reactors of asymptotic observers originally developed for stirred tank reactors is first considered (see also [3]) and illustrated with real-life data on an non-isothermal fixed bed reactor. Then it will be shown how to design *exponential* observers, which are also independent from the process kinetics but for which the rate of convergence may be arbitrarily fixed (unlike the asymptotic observers for which the rate of convergence depends on the operating conditions). The exponential observers are applicable to multi-tank reactors, a class of reactors for which the tubular reactor models in their discretized form are a sub-class.

2 Dynamic Model of Tubular Reactors

Let us consider a tubular rector with N components and M reactions. From mass and energy balance, we can deduce the following *general dynamical model for tubular reactors with axial dispersion*:

$$\frac{\partial x}{\partial t} = -u \frac{\partial x}{\partial z} + D_a \frac{\partial^2 x}{\partial z^2} + \widetilde{Kr}(x) + U$$
(1)

with :

$$x = \begin{bmatrix} C \\ T \end{bmatrix} , \quad \widetilde{K} = \begin{bmatrix} K \\ -\frac{\Delta H^{T}}{\rho C_{p}} \end{bmatrix}$$
(2)

$$U = \begin{bmatrix} -\frac{R_h}{\rho C_p} \\ 0 \end{bmatrix} , \quad D_a = \begin{bmatrix} D_{ma} I_N & 0 \\ 0 & \frac{\lambda_{ca}}{\rho C_p} \end{bmatrix}$$
(3)

vector $(kg.m^{-3}, T)$ is the temperature (K), λ_{ea} is the cal equations are independent of the reaction rate r(x). axial energy dispersion coefficient $(kJ.m^{-1}.s^{-1}.K^{-1})$, The equations (6) (7) are the basis for the derivation of I_N is the identity matrix of dimension N, U (K.s⁻¹ is the asymptotic observer. The dynamical equations of an external transfer vector (which is only includes the ζ are used to calculate an estimate of ζ on-line, which external heat exchange rate R_h , ΔH is the reaction is used, via equation (6) and the on-line data of x_1 , to heat vector $(kJ.kg^{-1})$: $\Delta H^T = [\Delta H_1, \Delta H_2, ..., \Delta H_M]$ derive an estimate of the unmeasured component x_2 : ρ is the fluid density (kg/m^3) , C_p is the specific heat $(kJ.kg^{-1}.K^{-1})$, r(x) is the reaction rate vector $(kg.m^{-3}.s^{-1}): r^{T}(x) = [r_{1}(x), r_{2}(x), ..., r_{M}(x)]. R_{h}$ is the external heat exchange rate $(kJ.s^{-1}.m^3)$, and K is the stoichiometric coefficient matrix. In a tubular reactor, R_h is often given by the following expression :

$$R_h = \frac{4h}{d}(T - T_w) \tag{4}$$

where h, d and T_w are, respectively, the wall heat transfer coefficient $(kJ.m^{-2}.K^{-1}.s^{-1})$, the reactor diameter (m) and the coolant temperature (K).

3 Design of the Asymptotic Observer

The derivation of the asymptotic observer equations is based on the following assumptions:

1. M components (including the temperature) are measured on-line along the reactor.

2. The influent concentrations x_{in} , the coolant temperature T_w , and the fluid superficial velocity u are known either by measurement or by choice of the user.

3. The stiochiometric coefficient matrix K, and the parameters ΔH , ρ , C_p , h, d, D_{ma} and λ_{ea} are known. 4. The reaction rate vector r is unknown.

5. The M reactions are irreversible and independent, i.e. rank(K) = R = M

From assumption 1, we can define the following state partition :

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$
(5)

where x_1 and x_2 hold for the measured component concentrations and the unmeasured ones, respectively.

Let us consider the following state transformation ζ :

$$\zeta = x_2 - K_2 K_1^{-1} x_1 \tag{6}$$

where K_1 and K_1 are the submatrices associated to x_1 and x_2 . If the M measured components and the M reactions are independent, then K_1 will be invertible. In order to simplify the notations and without loss of generality, let us consider that the temperature T is the first entry of x_1 . Then if we consider c_a the first column of $C_a = K_2 K_1^{-1}$, the dynamics of ζ are given by the following set of PDE's :

$$\frac{\partial \zeta}{\partial t} = -u \frac{\partial \zeta}{\partial z} + D_{ma} \frac{\partial^2 \zeta}{\partial z^2} + c_a U_T - (\frac{\lambda_{ea}}{\rho C_p} c_a - D_{ma} \mathbf{1}_{N-M}) \frac{\partial^2 T}{\partial z^2}$$
(7)

and where C is the process component concentration with $1_{N-M}^T = [1, 1, ..., 1]$. Note that the above dynami-

$$\frac{\partial \hat{\zeta}}{\partial t} = -u \frac{\partial \hat{\zeta}}{\partial z} + D_{ma} \frac{\partial^2 \hat{\zeta}}{\partial z^2} + c_a U_T - (\frac{\lambda_{ea}}{\rho C_p} c_a - D_{ma} \mathbf{1}_{N-M}) \frac{\partial^2 T}{\partial z^2}$$
(8)

$$\hat{x}_2 = \hat{\zeta} + K_2 K_1^{-1} x_1 \tag{9}$$

Remark : note that, in presence of reversible reactions, the matrix K will not be full column rank because it will contain two identical columns. However a simple way to treat the asymptotic observation problem of reversible reactions is to consider each reversible reaction as one global reaction (whose rate may then be positive or negative) and therefore characterized by only one column in the matrix . This means that if the "forward" and "backward" reactions are characterized by a reaction rate r_f and r_b respectively, we consider, for the observation, one global reaction characterized by one global reaction $r_g = r_f - r_b$.

It has been shown in ([3]) that the practical implementation of the asymptotic observer will be asymptotically stable if the eigenvalues of the matrix $D_{ma}\tilde{C}_2$ $u ilde{C}_1$ are stable, where $ilde{C}_1$ and $ilde{C}_2$ are the matrices associated to the approximation (e.g. finite differences or orthogonal collocation) of the first and second order space derivatives :

$$\frac{\partial^{k}}{\partial z^{k}} \begin{bmatrix} x(z=z_{1}) \\ x(z=z_{2}) \\ \vdots \\ x(z=z_{q}) \end{bmatrix} \cong \begin{bmatrix} \tilde{c}_{k} \mid \tilde{C}_{k} \end{bmatrix} \begin{bmatrix} x(z=z_{0}) \\ x(z=z_{1}) \\ \vdots \\ x(z=z_{q}) \end{bmatrix}$$
(10)

k = 1, 2, with dim $(\tilde{c}_k = q \ge 1 \text{ and } \dim(\tilde{C}_k = q \ge q)$.

Note that the stability of the asymptotic observer only depends on the axial mass transfer and not on the kinetics. In other words, the reactor may be unstable (due to the kinetics like in the classical exothermic reactor example with Arrhenius kinetics) while the asymptotic observer is asymptotically stable (because of stable hydrodynamics).

3.1 Example 1 : a simple nonisothermal reactor

Let us consider a tubular reactor with one nonisothermal reaction :

$$A + bB \longrightarrow dD$$
 (11)

Its dynamics are described by equations (1) with :

$$C = \begin{bmatrix} C_A \\ C_B \\ C_D \end{bmatrix}, \quad K = \begin{bmatrix} -1 \\ -b \\ d \end{bmatrix}$$
(12)



Figure 1: Estimation results of ethanol

= C, and the auxiliary variables ζ is equal to :

$$\zeta = \begin{bmatrix} C_A - \frac{\rho C_p}{\Delta H} T \\ C_B - b \frac{\rho C_p}{\Delta H} T \\ C_D + d \frac{\rho C_p}{\Delta H} T \end{bmatrix}$$
(13)

and the asymptotic observer then specializes as follows:

$$\frac{\partial \hat{\zeta}_1}{\partial t} = -u \frac{\partial \hat{\zeta}_1}{\partial z} + D_{ma} \frac{\partial^2 \hat{\zeta}_1}{\partial z^2} - \frac{\lambda_{ea} - D_{ma} \rho C_p}{\Delta H} \frac{\partial^2 T}{\partial z^2} - \frac{\rho C_p}{\partial z} U_T$$
(14)

$$\frac{\partial \hat{\zeta}_2}{\partial t} = -u \frac{\partial \hat{\zeta}_2}{\partial z} + D_{ma} \frac{\partial^2 \hat{\zeta}_2}{\partial z^2} - \frac{\lambda_{ea} - D_{ma} \rho C_p}{\Delta H} \frac{\partial^2 T}{\partial z^2} - \frac{\lambda_{ea} - D_{ma} \rho C_p}{\Delta H} \frac{\partial^2 T}{\partial z^2}$$
(15)

$$\frac{\partial \hat{\zeta}_3}{\partial t} = -u \frac{\partial \hat{\zeta}_3}{\partial z} + D_{ma} \frac{\partial^2 \hat{\zeta}_3}{\partial z^2} + \frac{\lambda_{ea} - D_{ma} \rho C_p}{\Delta H} \frac{\partial^2 T}{\partial z^2}$$

$$+d\frac{\rho c_p}{\Delta H}U_T \tag{16}$$
$$= \hat{c}_1 + \frac{\rho C_p}{2}T \tag{17}$$

$$\hat{C}_{A} = \hat{\zeta}_{1} + \frac{1}{\Delta H} \hat{T}$$

$$\hat{C}_{B} = \hat{\zeta}_{1} + b \frac{\rho C_{p}}{T} T$$
(18)

$$\hat{C}_B = \hat{\zeta}_1 + b \frac{\Delta H}{\Delta H}$$

$$\hat{C}_D = \hat{\zeta}_1 - d \frac{\rho C_p}{\Delta H} T$$
(18)
(19)

$$C_D = \zeta_1 - d \frac{\gamma}{\Delta H} T \tag{19}$$
(20)

3.2 Experimental Result

The above asymptotic observer has been implemented with data from a chemical reactor used for the synthesis of ethyl tertio-butyl ether (ETBE), a powerful octane enhancer which can be added to unleaded gasoline, see [6]. The reaction is characterized by the following reaction scheme :

$$Ethanol + Isobutene \rightleftharpoons ETBE \tag{21}$$

in presence of an acidic catalyst (a solid sulfonic resin). The reaction is exothermic. In order to shift the equilibrium to the right and have a high conversion, the reaction has to be carried out at low temperature (323 - 363 K). Under usual operating conditions, the selectivity of the reaction is close to 100 %: this means that the effect of the side reactions may be neglected. The reaction takes place in a fixed bed reactor (a 8.5 mm diameter and 0.6 m long tube with a cooling jacket). Online temperature measurements are collected at four positions ($z_0 = 0$, $z_1 = 0.05$ m, $z_2 = 0.13$ m, $z_3 = 0.6$ m) and in the cooling fluid (water). On-line measurement of the reaction components at the reactor output is performed via a HPLC (high performance liquid chromatograph). The dynamics of the process are characterized by the model (1) with :

The asymptotic observer has been implemented by considering a backward difference approximation for both first and second order space derivatives. The sampling rate is equal to 30 s. The auxiliary variables $\hat{\zeta}$ have been initialised as follows :

$$\tilde{\zeta}_i(z_1, 0) = 11.8 \ mol/l, \ \tilde{\zeta}_i(z_2, 0) = 11.81 \ mol/l$$

 $\tilde{\zeta}_i(z_3, 0) = 11.83 \ mol/l, \ i = 1, 2$

This corresponds to set the initial values of the estimates of C_a and C_b to zero. The results of the asymptotic observer for the ethanol (C_A) and isobutene (C_B) concentrations at the two internal points and at the reactor output (where it is compared with the on-line data) are shown in Figures 1 and 2, while the operation variables $(u, C_{A,in} \text{ and } C_{B,in})$ and the data of the different temperatures are shown in Figures 3 and 4.

4 Design of the Exponential Observer

One of the main advantage of the asymptotic observers consists of incorporating the process dynamics without requiring the usually uncertain process kinetics. One of the disadvantages is that its dynamics are completely dependent on the process operating conditions or characteristics. This does not appear a major problem in the experimental result presented in the preceding section (where the convergence rate appears to be quite fast), but it seems interesting to look if it is possible to design an observer which presents the same advantages as the asymptotic observer while allowing the user to fix arbitrary observer dynamics. The design of such observers (that we shall call *exponential* observers, in order to make the connection with the *asymptotic* observers, but by also suggesting that there is a "plus" with respect to these) is possible for multi-tank (possibly interconnected) cascade reactors. This class of systems covers in particular the approximation of tubular reactor models (either by finite differences or with orthogonal collocation).

The design of the *exponential* observer is based on the same ideas as for the asymptotic observer, and also on works on state observers with unknown inputs [8], [5], [7], [10] (with respect to the process dynamics, the kinetics term can be viewed as a system input).

The design is based on the discretized model of the tubular reactor obtained after lumping the partial differential equations of the model. Then the dynamics of the approximated model are then given by the following set of differential equations :

$$\frac{dx_r}{dt} = (-uC_1 + D_aC_2)x_r + \bar{K}\bar{r} + U_r + (-uc_1 + D_ac_2)x_f(z=0,t) \quad (22)$$

Let consider the following state partition :

$$x_r = \left[\begin{array}{c} x_1\\ x_2 \end{array}\right] \tag{23}$$

where x_1 is the vector of the measured variables $(\dim(x_1) = p)$, and x_2 the vector of the unmeasured ones $(\dim(x_2) = N.q - p)$, where N is the number of process components, i.e. reactants, products, and temperature in non-isothermal reactors). Assume also that K_1 is full rank $(\operatorname{rank}(K_1) = \operatorname{rank}(\bar{K}) = R.q)$. As it will be seen below, the number of measured variables need to be larger than the rank of the yield coefficient matrix \bar{K} (p > R.q).

According to the state estimation problem, the dynamical equations (22) can be formally rewritten as follows:

$$\frac{d}{dt} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = A \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} K_1 \\ K_2 \end{bmatrix} \bar{r} + \begin{bmatrix} U_1 \\ U_2 \end{bmatrix}$$
(24)

with :

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = -uC_1 + D_aC_2 (25)$$
$$\begin{bmatrix} U_1 \\ U_2 \end{bmatrix} = U_r + (-uc_1 + D_ac_2)x_f(0,t)$$
(26)

By considering the auxiliary variable ζ , the following observer equations can be introduced :

$$\frac{d\zeta}{dt} = F\zeta + Gx_1 - LU_1 + U_2 \qquad (27)$$
$$\hat{x}_2 = \zeta + Lx_1 \qquad (28)$$

$$F = A_{22} - LA_{12}$$

$$G = FL + A_{21} - LA_{11} \tag{30}$$

$$0 = K_2 - LK_1$$
 (31)

Assuming that p > R.q, the general solution of (31) can be written as follows :

$$L = K_2 K_1^+ + S(I_p - K_1 K_1^+)$$
(32)

where K_1^+ is a left inverse of K_1 . The poles of the observer (27) (28) are determined by the matrix F, in which the degrees of freedom for acting the observer dynamics are given by the matrix L, which is the observer gain. The observer may be *exponential* (in the sense that its dynamics may be arbitrarily fixed) if we are able to arbitrarily determine the poles of F via the matrix L is the observer for K_1 .

gain matrix L, i.e. if the pair (A_{22}, A_{21}) is observable. Note that if the number of measured variables was equal to the rank of K_1 (p = R.q), the matrix L would reduce to $K_2K_1^{-1}$: then there is no more degree of freedom for fixing the observer dynamics. Therefore this confirms that a minimal requirement is that : p > R.q. Before expliciting some rules, let us first try to clarify the question via a simple example.

4.1 A Simple Example

Let us consider a non-isothermal plug flow reactor with one reaction. Assume that the reactor model is approximated by three cascade reactors (finite difference approximation), that the temperature is measured online at the reactor input and output, and at the two internal positions of the approximation z_1 and z_2 , that the concentration of the reactant A, C_A is measured on-line at the reactor output, and that the objective to reconstruct the concentration of the reactant A in the reactor.

This means that here N = 3, p = 4, R = 1 and q = 3. Then x_1 and x_2 are equal to :

$$\boldsymbol{x}_{1} = \begin{bmatrix} T_{1} \\ T_{2} \\ T_{3} \\ C_{A3} \end{bmatrix}, \ \boldsymbol{x}_{2} = \begin{bmatrix} C_{A1} \\ C_{A2} \end{bmatrix}$$
(33)

This means that the matrices A_{ij} and K_j are equal to:

$$A = -\frac{u}{\Delta z} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{bmatrix}$$

$$K_{1} = \begin{bmatrix} -\frac{\Delta H}{\rho C_{p}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\Delta H}{\rho C_{p}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\Delta H}{\rho C_{p}} & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & -\frac{\Delta H}{\rho C_{p}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ \hline 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline r & r & r & r(z_{1}) & r(z_{2}) & r(z_{3}) & r(z_{3})$$

(29)

Let us consider the left pseudo-inverse of K_1 :

$$K_{1}^{+} = (K_{1}^{T}K_{1})^{-1}K_{1}^{T}$$

$$= \begin{bmatrix} -\frac{\rho C_{p}}{\Delta H} & 0 & 0 & 0\\ 0 & -\frac{\rho C_{p}}{\Delta H} & 0 & 0\\ 0 & 0 & \rho C_{p} \alpha & \frac{\alpha \rho^{2} C_{p}^{2}}{\Delta H} \end{bmatrix} (35)$$

$$\alpha = -\frac{\Delta H}{\Delta H^2 + \rho^2 C_p^2} \tag{36}$$

After some calculations by using expression (29) and denoting s_{ij} the entries of the matrix S, one obtains the following expression for the observer matrix F:

$$F = -\frac{u}{\Delta z} \begin{bmatrix} 1 & \alpha(\rho C_p s_{13} - \Delta H s_{14}) \\ -1 & 1 + \alpha(\rho C_p s_{23} - \Delta H s_{24}) \end{bmatrix}$$
(37)

with : Note that only the last two columns explicitly appears in the formulation of the matrix F. Moreover the entries of the last columns play a similar role in the matrix F (i.e. s_{13} and s_{14} on one hand, and s_{23} and s_{24} appear in an additive way in the entries (1,2)and (2,2) of F, respectively). Therefore only one of the last columns needs to be different from zero in order to assign the poles of F (i.e. to assign the dynamics of the observer). For instance if S is equal to :

$$S = \begin{bmatrix} 0 & 0 & s_{13} & 0 \\ 0 & 0 & s_{23} & 0 \end{bmatrix}$$
(38)

then the characteristic polynomial of F, $|\lambda I - F|$, is equal to :

$$\lambda^2 + \frac{u}{\Delta z} \left(2 + \alpha \rho C_p s_{23}\right) \lambda + \frac{u^2}{\Delta z^2} \left(1 + \alpha \rho C_p (s_{13} + s_{23})\right)$$

It is therefore possible to assign arbitrarily the poles of F via the choice of the parameters s_{13} and s_{23} .

The exercise can be repeated by considering the other combinations of the temperature T_1 , T_2 and T_3 , and one of the other concentrations C_{A1} or C_{A2} as the measured variables. It is routine to check that it is then not possible to assign the poles of the observer matrix F. The only good measurement in addition to the temperature measurements, is the reactant concentration at the reactor output.

This is consistent with the basic notion of observability, i.e. the possibility to "connect" the unmeasured variables to the measured ones. Here the observability properties are based on the transport dynamics (at the exclusion of the kinetics) : it is easy to check by simple inspection of the transport dynamics part of the finite difference approximation model :

$$\frac{dC_{A1}}{dt} = \frac{u}{\Delta z} C_{Ain} - \frac{u}{\Delta z} C_{A1}$$
(39)

$$\frac{dC_{A2}}{dt} = \frac{u}{\Delta z} C_{A1} - \frac{u}{\Delta z} C_{A2} \tag{40}$$

$$\frac{dC_{A3}}{dt} = \frac{u}{\Delta z}C_{A2} - \frac{u}{\Delta z}C_{A3} \tag{41}$$

that, for instance, the equation of C_{A1} does not contain will remain stable, i.e. the algorithm will still be able any information about the other two, C_{A2} or C_{A3} , and of reconstructing the state of the process and track the

that only the condition is fulfilled with C_{A3} (which can be connected to C_{A2} , which in turn can be connected to C_{A1}).

4.2 Generalization for Plug Flow Reactors

Let us consider a cascade reactor (e.g. a plug flow reactor approximated with finite differences). Thise generalisation can be formalized into the following theorem:

Theorem 1 The poles of the observer (27)(28) can be arbitrarily assigned if :

1.
$$rank(K_1) = rank(K) = R.q;$$

2. $p = R.q + N - R > R.q;$

3. among the p measured variables, R process components are measured at the q positions along the reactor and the N - R remaining process components are measured at the reactor output.

Proof : see [2]

The above result can be applied to tubular reactor with axial dispersion approximated by a finite difference when the second order space derivative is approximated by a backward difference (then the candidate invariant zero is $s = -\frac{u}{\Delta z} + \frac{D_{max}}{\Delta z^2}$). But extensions to other approximations (central difference for the second order space derivative, functional approximation) is not straightforward, even if it might be conjectured that in absence of any information about the kinetics, the measurement of each component at one position along the reactor, although not necessarily at the reactor output, should be a sufficient condition.

5 Conclusions

Here we have shown how to design state observers which are independent of the knowledge of the process kinetics in tubular reactors. A minimal requirement is that a number of process components at least equal to the number of independent reactions must be measured on-line to reconstruct the state. Then *asymptotic* observers can be implemented to observe the time evolution of the other unmeasured components. However the observer dynamics are then completely dependent on the process operating conditions. If in addition the value of each process component is known at the reactor output, then the state of the tubular reactor can be reconstructed via an *exponential* observer, the dynamics of which can be a priori arbitrarily determined.

It is worth noting that one of the key property of the proposed observers is their inherent stability properties which only depend on the hydrodynamics of the model. In other words, even if the process is unstable (typically because of unstable kinetics), the observer dynamics will remain stable, i.e. the algorithm will still be able of reconstructing the state of the process and track the time evolution of the process component concentrations and/or of the temperature.

An important practical example is the nonisothermal reactor with only one reaction : the concentration along the reactor of all the components can be estimated without the knowledge of the kinetics being required from temperature and thermal balance; in addition, the observer dynamics can be arbitrarily assigned if the concentration of the components at the reactor output are available for on-line measurement.

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References

- G. Bastin and D. Dochain. "On-line Estimation and Adaptive Control of Bioreactors". Elsevier, Amsterdam, 1990.
- [2] D. Dochain. Contribution to the Analysis and Control of Distributed Parameter Systems with Application to (Bio)chemical Processes and Robotics. Thèse d'Aggrégation de l'Enseignement Supérieur, UCL, Belgium, 1994.
- [3] D. Dochain and M. Perrier. Asymptotic observers for fixed bed reactors. Proc. ACC'93, pages 1179-1183, 1993.
- [4] D. Dochain, M. Perrier, and B.E. Ydstie. Asymptotic observers for stirred tank reactors. Chem. Eng. Sci., 47:4167-4178, 1992.
- [5] F.W. Fairman, S.S. Mahil, and L.Luk. Disturbance decoupled observer design via singular value decomposition. *IEEE Trans. Aut. Cont.*, AC-29 (1):84-86, 1984.
- [6] O. Francoisse. "Modélisation et Commande Adaptative de Réacteurs Tubulaires. Application a la Synthèse de l'Ethyl Tertio-butyl Ether". PhD thesis, UCL, Belgium, 1993.
- [7] M. Hou and P.C. Muller. Design of observers for linear systems with unknown inputs. *IEEE Trans. Aut. Control*, AC-37:871-875, 1992.
- [8] P. Kudva, N. Viswanadham, and A. Ramakrishna. Observers for linear systems with unknown inputs. *IEEE Aut. Cont.*, AC-25 (1):113-115, 1980.
- [9] L. Ljung. Asymptotic behavior of the extended kalman filter as a parameter estimator for linear systems. *IEEE Trans. Aut. Cont.*, 24:36-50, 1979.
- [10] H. Rafaralahy, M. Zasadzinski, C. Mechmeche, and M. Darouach. Unkonwn input observers for bilinear systems with gain optimization. *Proc. 13th IFAC World Cong.*, I:441-446, 1996.



Figure 2: Estimation results of isobutene



Figure 3: Experimental data of the influent



Figure 4: Experimental data of temperature