HYBRID EXTENDED LUENBERGER-ASYMPTOTIC OBSERVER FOR BIOPROCESS STATE ESTIMATION

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Abstract: State observers provide estimates of non-measured variables based on a mathematical model of the process and some available hardware sensor signals. On the one hand, exponential observers, such as Luenberger observers or Kalman filters, have an adjustable rate of convergence, but strongly rely on the accuracy of the process model. On the other hand, asymptotic observers use a state transformation in order to avoid using the (usually uncertain) kinetic model, but have a rate of convergence imposed by the process dilution rate. In an attempt to combine the advantage of both techniques, a hybrid observer is developed, which estimates a level of confidence in the process model and, accordingly, evolves between the two above-mentioned limit cases (model perfectly known or kinetic model unknown). In particular, attention is focused on a hybrid "Luenberger-asymptotic" observer, for which a rigorous stability/convergence analysis is possible. The efficiency and usefulness of the proposed observer is illustrated with an application example.

Keywords: State observers, nonlinear systems, biotechnology, fermentation processes.

INTRODUCTION

Bioprocess modelling, monitoring and control are important developments in order to ensure optimal operation and product quality. As the bioprocess becomes more complex (in terms of reactor design, biocatalysts, products...) more information about the dynamics of the main constituents is required. Whereas sensors for process variables such as dissolved oxygen, pH and temperature are widespread, key biological state variables such as biomass and products of interest, usually require more sophisticated measurement devices, which can have several drawbacks, e.g. sterilisation, discrete-time (and often rare) samples, relatively long processing (analysis) time, hardware and maintenance costs, degradation of reactor hydrodynamics. A solution to these latter problems can be found through the design of software sensors, which combine some available hardware sensors signals and a mathematical model, in order to provide time-continuous estimates of non-measured variables on-line. The estimation algorithm is called a state observer.

Several estimation techniques considering the non-linear models involved in bioprocesses have been proposed in the literature. Usually, state observers are classified as exponential or asymptotic observers (Bastin and Dochain 1990). The former class of algorithms have an adjustable rate of convergence towards the true state, which is defined by one or several tuning parameters. The main drawback of exponential observers is that their efficiency strongly rely on the model quality. The extended Kalman filter, the extended Luenberger observer, and the high gain observer belong to this class. On the other hand, asymptotic observers (Bastin and Dochain 1990) do not require any knowledge about the kinetic model, which is most of the time difficult to identify with good accuracy. However, the price to pay is that the rate of convergence is completely determined by the experimental conditions (namely the dilution rate). This may lead to very slow convergence in the case of low dilution rate or no converge at all in the case of batch cultures.

In order to combine the advantages of exponential observers (i.e. fast convergence with an accurate model) and asymptotic observers (i.e. convergence without any knowledge about the kinetic model), hybrid observers have recently been developed. The principle of these observers is to evolve between two limit cases (corresponding rigorously to an exponential and an asymptotic observer) according to the quality of the kinetic model. This evolution is ensured by the introduction of a confidence parameter in the kinetic model within the observer structure. Besides the stability and convergence analysis of the observer, the tuning of the confidence parameter is a key element in the development of hybrid observers. In the extended Kalman-asyptotic hybrid observer (Bogaerts 1999) and the full horizon-asymptotic observer (Hulhoven and Bogaerts 2002) the evolution of the observer structure is driven by a confidence parameter which is evaluated on-line. The main drawback of the extended Kalman-asymptotic observer is the absence of proof of stability. This was the motivation for subsequently developing a full horizon-asymptotic observer, whose stability could in principle be analysed (this work has however not been completed so far). In the hybrid high gain-asymptotic observer (Lemesle and Gouzé 2001), the stability properties are well described. However, the structure evolution is driven by an, *a priori*, fixed confidence parameter. In this contribution, a new hybrid observer is proposed, which allows both aspects to be addressed at the same time, i.e. the automatic tuning of a confidence parameter and the development of a complete, rigorous, stability/convergence analysis. This latter observer is based on the extended Luenberger observer.

This paper is organized as follows. The next section briefly introduces macroscopic reaction schemes and the associated mass balance equations, which are used for bioprocess modelling. Based on this modelling framework, Section 2 and 3 present the basic principles of the extended Luenberger and the asymptotic observers. Section 4 is devoted to the development of a new hybrid extended Luenberger-asymptotic observer. The performance of this observer is illustrated with a simulation example in section 5. Finally, Section 6 is devoted to some conclusions.

1. MACROSCOPIC REACTION SCHEMES AND MASS BALANCES FOR BIOPROCESS MODELLING

A bioprocess can be described by a reaction scheme defined by a set of M reactions (Bastin and Dochain 1990). Such a reaction scheme can be expressed by:

$$\sum_{i\in R_k}(-\nu_{i,k})\xi_i \xrightarrow{\varphi_k} \sum_{j\in P_k}\nu_{j,k}\xi_j \qquad k\in[1,M] \quad (1)$$

where
- $\nu_{i,k}$ and $\nu_{j,k}$ are the pseudo-stoichiometric coefficients or yield coefficients;
- φ_k is the reaction rate;
- ξ_i is the i^{th} component;
- $R_k(P_k)$ is the set of ξ_i which are reactants (products) in the reaction k;
- M is the number of reactions.

Assuming that the bioprocess takes place in a perfectly stirred bioreactor, the system dynamics can be described by a model resulting from mass balances for the macroscopic species involved in the reaction scheme:

$$\frac{d\xi(t)}{dt} = K\varphi(\xi(t)) - D(t)\xi(t) + F(t) - Q(t) \quad (2)$$

where
- $\xi \in \Re^N$ is the vector of concentrations;
- $K \in \Re^{N\times M}$ is the pseudo-stoichiometric coefficients matrix ($M \leq N$);
- $\varphi \in \Re^M$ is the vector of reaction rates;
- $D \in \Re$ is the dilution rate;
- $F \in \Re^N$ is the vector of external feed rates;
- $Q \in \Re^N$ is the vector of gaseous outflow rates.

In the sequel, the external feed rates and gaseous outflow rates are put together in a vector

$$u(t) = F(t) - Q(t) \quad (3)$$

In the context of state observation the state vector can be subdivided into two vectors:

$$\xi(t)^T = [\xi_1^T \quad \xi_2^T] \quad (4)$$

where $\xi_1 \in \Re^L (L \leqslant N)$ contains the elements of ξ which are measured :

$$\xi_1 = C\xi = [I_L \quad O_{L,N-L}]\xi \quad (5)$$

These measurements are in the form of discrete samples $y(t_k)$:

$$y(t_k) = C\xi(t_k) + \epsilon(t_k) \quad (6)$$

ϵ being a white noise sequence normally distributed with $E[\epsilon(t_k)] = 0$ and $E[\epsilon(t_k)\epsilon^T(t_k)] = \delta_{k,l}Q(t_k)$. C is the measurement matrix.

The other elements $\xi_2 \in \Re^{(N-L)}$ of ξ are the variables which are not measured.

2. THE EXTENDED LUENBERGER OBSERVER

In the field of bioprocesses, the extended Luenberger observer can be described by (in the sequel, the time dependence of the variables will no longer be specified for simplicity of notations):

$$\frac{d\hat{\xi}_1}{dt} = K_1\varphi(\hat{\xi}) - D\hat{\xi}_1 + u_1 + \gamma_1(\hat{\xi})[y - C\hat{\xi}] \quad (7)$$

$$\frac{d\hat{\xi}_2}{dt} = K_2\varphi(\hat{\xi}) - D\hat{\xi}_2 + u_2 + \gamma_2(\hat{\xi})[y - C\hat{\xi}] \quad (8)$$

where γ_1 and γ_2 are the tuning parameters of the observer.

The objective of a state observer is to generate an accurate estimation of the non-measured state variables. In practice, there is an estimation error $(\tilde{\xi})$ which is defined by the difference between the true state (ξ) and the estimated state $(\hat{\xi})$.

$$\tilde{\xi} = \hat{\xi} - \xi$$

The convergence of an observer is related to the dynamics of the estimation error, i.e. the rate at which the estimation error tends towards zero. The convergence properties of the extended Luenberger observer can be analysed on the basis of state estimation error equations which are obtained by linearization along the estimated trajectory :

$$\frac{d}{dt}\begin{bmatrix}\tilde{\xi}_1\\ \tilde{\xi}_2\end{bmatrix} \approx A(\tilde{\xi})\begin{bmatrix}\tilde{\xi}_1\\ \tilde{\xi}_2\end{bmatrix} \quad (9)$$

where

$$A(\tilde{\xi}) = \begin{bmatrix} K_1G_{\xi_1} - D - \gamma_1(\hat{\xi}) & K_1G_{\xi_2} \\ K_2G_{\xi_1} - \gamma_2(\hat{\xi}) & K_2G_{\xi_2} - D \end{bmatrix}$$

where $G_{\xi_1} = \left.\frac{\partial\varphi(\xi)}{\partial\xi}\right|_{\xi=\hat{\xi}}$ and $G_{\xi_2} = \left.\frac{\partial\varphi(\xi)}{\partial\xi_2}\right|_{\xi=\hat{\xi}}$

In order to ensure stability (and therefore the exponential convergence) of this observer, the tuning of $\gamma_1$and γ_2 must be done in order to fulfill the following sufficient conditions.

$$\begin{aligned} &C1.\Re\{\lambda_i\left\{A(\hat{\xi})\right\}\} < 0 \quad \forall\hat{\xi},\ \forall i \\ &C2.\left\|A(\hat{\xi})\right\| \leq C_1 \quad \forall\hat{\xi} \\ &C3.\left\|\frac{d}{dt}(A(\hat{\xi})\right\| \leq C_1 \quad \forall\hat{\xi} \end{aligned} \quad (10)$$

Where C_1 and C_2 are positive constants

$\Re\{\lambda_i(.)\}$ represents the real part of the matrix eigenvalues.

Note that, rigorously, {C1, C2, C3} constitute a sufficient condition of stability of the time-varying linearized system (9), but in practice it is arduous to ensure that conditions C2 and C3 will be fulfilled for every value of the state estimate.

The main advantage of this observer is that it can be tuned by an appropriate choice of γ_1 and γ_2. However, its efficiency is strongly dependent on the model quality including the kinetic model.

3. THE ASYMPTOTIC OBSERVER

The derivation of the asymptotic observer (Bastin and Dochain 1990) is based on the following conditions : $\varphi(\xi)$ is unknown, K is known, $L = dim(\xi_1) \geqslant p = rank(K)$;

Hence, there always exists a partition

$$\xi^T = [\xi_a^T\ \xi_b^T] \quad (11)$$

so that the corresponding partition

$$K^T = [K_a^T\ K_b^T] \quad (12)$$

involves a matrix $K_a \in \Re^{p\times M}$ of full row rank. Given such a partition of K, the following matrix equation

$$A_0K_a + K_b = 0_{N-p,M} \quad (13)$$

has always a unique solution $A_0 \in \Re^{(N-p)\times M}$. It is therefore possible to define an auxiliary vector $Z \in \Re^{(N-p)}$.

$$Z = A_0\xi_a + \xi_b \quad (14)$$

whose dynamics is independent of the kinetics $\varphi(\xi)$:

$$\frac{dZ(t)}{dt} = -D(t)Z(t) + A_0u_a(t) + u_b(t) \quad (15)$$

where $u^T = [u_a^T\ \ u_b^T]$ is the partition of u corresponding to the partition of ξ. It is possible to write the vector Z as a linear combination of the vectors ξ_1 and ξ_2 of measured and non-measured states :

$$Z(t) = A_1\xi_1(t) + A_2\xi_2(t) \quad (16)$$

where $A_1 \in \Re^{(N-p)\times L}$ and $A_2 \in \Re^{(N-p)\times(N-L)}$.

The asymptotic observer is finally defined by :

$$\begin{cases} \dfrac{d\hat{Z}(t)}{dt} = -D(t)\hat{Z}(t) + A_1u_1(t) + A_2u_2(t) \\ \hat{\xi}_2(t) = A_2^+(\hat{Z}(t) - A_1\xi_1(t)) \end{cases}$$

where A_2^+ is a left pseudo inverse of the matrix A_2.

The dynamics of the state estimation error $\tilde{\xi}_2 = \hat{\xi}_2 - \xi_2$ is given by:

$$\frac{d\tilde{\xi}_2(t)}{dt} = -D(t)\tilde{\xi}_2(t) \quad (17)$$

It is therefore obvious that the convergence of the asymptotic observer is function of the experimental conditions (D). This observer may therefore not converge (batch process) or converge very slowly (low dilution rate).

4. THE HYBRID EXTENDED LUENBERGER-ASYMPTOTIC OBSERVER

The principle of the hybrid extended Luenberger-asymptotic observer is to use the advantages of the extended Luenberger observer when the process model is in good agreement with the real system and to evolve towards the asymptotic observer when the confidence in the kinetic model decresases.

Let consider the auxiliary state variable $Z(t)$ defined in (16).

The process model (2) can be rewritten:

$$\begin{cases} \dfrac{d\xi_1}{dt} = K_1\varphi(\xi) - D\xi_1 + u_1 \\ \dfrac{dZ}{dt} = -DZ + A_1u_1 + A_2u_2 \\ \xi_2 = A_2^+(Z - A_1\xi_1) \end{cases} \tag{18}$$

The extended Luenberger observer for this model is:

$$\begin{cases} \dfrac{d\hat{\xi}_1}{dt} = K_1\varphi(\hat{\xi}) - D\hat{\xi}_1 + u_1 + \gamma_1(\hat{\xi})(y - \hat{\xi}_1) \\ \dfrac{d\hat{Z}}{dt} = -D\hat{Z} + A_1u_1 + A_2u_2 + \gamma_Z(\hat{\xi})(y - \hat{\xi}_1) \\ \hat{\xi}_2 = A_2^+(\hat{Z} - A_1\hat{\xi}_1) \end{cases} \tag{19}$$

In order to take account of the confidence in the kinetic model and to allow the evolution of this observer towards the asymptotic one according to this degree of confidence the following output injection is proposed:

$$\xi_1 \to \delta\xi_1 + (1-\delta)y \tag{20}$$

Introducing this in the second and the third equation of (19) yield

$$\begin{cases} \dfrac{d\hat{\xi}_1}{dt} = K_1\varphi(\hat{\xi}) - D\hat{\xi}_1 + u_1 + \gamma_1(\hat{\xi})(y - \hat{\xi}_1) \\ \dfrac{d\hat{Z}}{dt} = -D\hat{Z} + A_1u_1 + A_2u_2 + \gamma_Z(\hat{\xi})\delta(y - \hat{\xi}_1) \\ \hat{\xi}_2 = A_2^+(\hat{Z} - A_1(\delta\hat{\xi}_1 + (1-\delta)y)) \end{cases} \tag{21}$$

Within this system the hybrid behavior of the observer (i.e. its evolution between two limit cases) is insured by the definition of δ:

$$\delta = (e^{-\frac{(y-\hat{\xi}_1)^2}{\sigma^2}} - 1)(1 - e^{-\frac{t}{\tau}}) + 1 \tag{22}$$

where σ^2 corresponds to an *a priori* confidence in the kinetic model.

Using this function to define δ, the observer will evolve between the extended Luenberger and the asymptotic observer according to the estimation error on ξ_1. The two limit cases are $\delta = 1$ (corresponding rigorously to the extended Luenberger observer) and $\delta = 0$ (corresponding rigorously to the asymptotic observer). Note that the introduction of a time constant τ prevents the observer from evolving directly to the asymptotic observer in the first times, when the observation error on ξ_1 is due to a bad estimation of the initial condition rather than a bad kinetic model.

The linearized state estimation error of the hybrid observer is described by:

$$\frac{d}{dt}\begin{bmatrix} \tilde{\xi}_1 \\ \tilde{Z} \end{bmatrix} \approx A(\tilde{\xi}_1, \tilde{Z}) \begin{bmatrix} \tilde{\xi}_1 \\ \tilde{Z} \end{bmatrix} \tag{23}$$

where

$$A(\tilde{\xi}_1, \tilde{Z}) = \begin{bmatrix} K_1G_{\xi_1} - D - \gamma_1 & K_1G_Z \\ -\gamma_Z\delta & -D \end{bmatrix} \begin{bmatrix} \tilde{\xi}_1 \\ \tilde{Z} \end{bmatrix}$$

$$G_Z = \left.\frac{\partial\varphi(\xi)}{\partial Z}\right|_{\hat{\xi}=\xi}$$

The sufficient conditions to guarantee the stability of this hybrid observer ($O \le \delta \le 1$) are still given by (10) but applied to the matrix A given in (23).

A practical way to tune this hybrid observer is to tune the parameters γ_1 and γ_Z in the particular case $\delta = 1$ (i.e, extended Luenberger observer) and then to verify that the conditions (10) still hold for $O \le \delta \le 1$.

5. EXAMPLE: A SIMULATED FED-BATCH BACTERIAL CULTURE

Consider a fed-batch bacterial fermentation taking place in a perfectly stirred bioreactor. Consider the following reaction scheme :

$$\nu_S S \xrightarrow{\varphi} \overset{\frown}{X} \tag{24}$$

where S denotes the substrate, X the biomass, and ν_S the yield coefficient. $\overset{\frown}{X}$ denotes an autocatalytic reaction. The mass balance corresponding to this reaction scheme is :

$$\frac{dS}{dt} = \nu_S\varphi(C_S, X) - DC_S + DS^{in}$$
$$\frac{dX}{dt} = \varphi(C_S, X) - DX$$

where S and X are the substrate and biomass concentrations, D is the dilution rate, φ is the reaction rate and S^{in} is the substrate concentration in the feed medium. The reaction rate φ will be described using the Monod law:

$$\varphi = X\frac{\mu_m S}{K_m + S} \tag{25}$$

The numerical values used for the simulation are : $\nu_S = 0.5[g(10^{11}cell)^{-1}]$; $K_m = 12[gl^{-1}]$; $\mu_m = 1.4[h^{-1}]$; $S(0) = 12[gl^{-1}]$; $X(0) = 0.1410^{11}[cell\ l^{-1}]$; $S^{in} = 20[gl^{-1}]$; $D = \frac{0.3}{t_f}t[h^{-1}]$.

A simulation of this process is presented in figure 1.

In order to illustrate the performance of the extended Luenberger-asymptotic observer these simulation results are considered as the real process, the substrate is asumed to be measured on line and the biomass concentration is estimated thanks to the following state observer (26)

$$\begin{cases} \frac{d\hat{S}}{dt} = -\nu\varphi - D\hat{S} + DS^{in} + \gamma_1(y - \hat{S}) \\ \frac{d\hat{Z}}{dt} = -D\hat{Z} + A_1 DS^{in} + \gamma_Z(\delta y - \hat{S}) \\ \hat{X} = A_2^{+}(\hat{Z} - A_1(\delta\hat{S} + (1-\delta)y)) \end{cases} \tag{26}$$

5.1 *Tuning γ_1 and γ_Z*

As suggested in the last section, the hybrid observer is first tuned for $\delta = 1$ (in the case of the extended Luenberger observer). In order to fix both eigenvalues of the matrix A describing the linearized state estimation error at a value $-\frac{1}{\tau}$, the tuning parameter are given by:

$$\begin{aligned} \gamma_1 &= \frac{2}{\tau} - 2D + \nu G_S + G_X \\ \gamma_Z &= A_1\gamma_1 + A_2\gamma_2 \end{aligned} \tag{27}$$

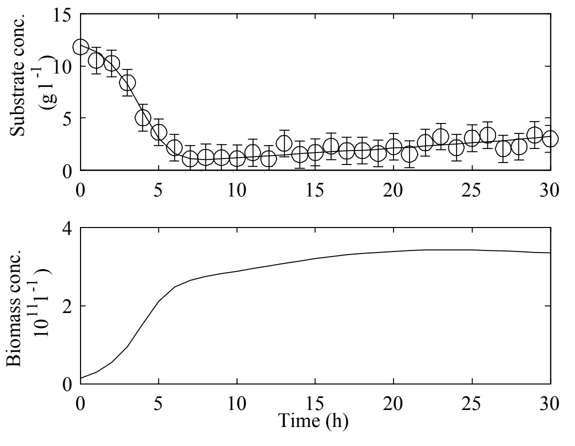

Fig. 1. Simulation of a fed-batch bacterial culture o :discrete noisy samples (with the 99 % confidence intervals),−continuous non measured signal.

where $G_S = \left.\frac{\partial\varphi(X,S)}{\partial S}\right|_{X=\hat{X},\ S=\hat{S}} = \frac{\mu_m}{(K_m+S)^2}X$ and $G_X = \left.\frac{\partial\varphi(\xi)}{\partial X}\right|_{X=\hat{X},\ S=\hat{S}} = \frac{\mu_m S}{(K_m+S)}$

and

$$\gamma_2 = \left(\frac{1}{\tau^2} - D\left(-\nu G_S - G_X + D + \gamma_1\right) + \gamma_1 G_X\right) * \frac{1}{\nu G_X}$$

Moreover, it is possible to proof that, in this case, the condition (10) (with the matrix A defined by (23)) are fulfilled for $O \leq \delta \leq 1\ \ (\forall\hat{\xi})$.

Two cases are presented. First the use of the exact model (figure 2), second, the use of a very bad model (figure 3).

In this latter case, the comparison of the different observers can be made on the basis of the root of the mean square error of the biomass estimation. These values are 0.3211 [10^{11}cell l^{-1}] for the extended Luenberger observer, 0.4676 [10^{11}cell l^{-1}] for the asymptotic observer and 0.1749 [10^{11}cell l^{-1}] for the hybrid extended Luenberger-asymptotic observer.

6. CONCLUSION

The extended Luenberger observer is a well-known exponential observer, which has the typical advantages and drawbacks of this class of observers, i.e. an adjustable rate of convergence determined by an appropriate choice of the tuning parameters, and actual performances completely dependent on

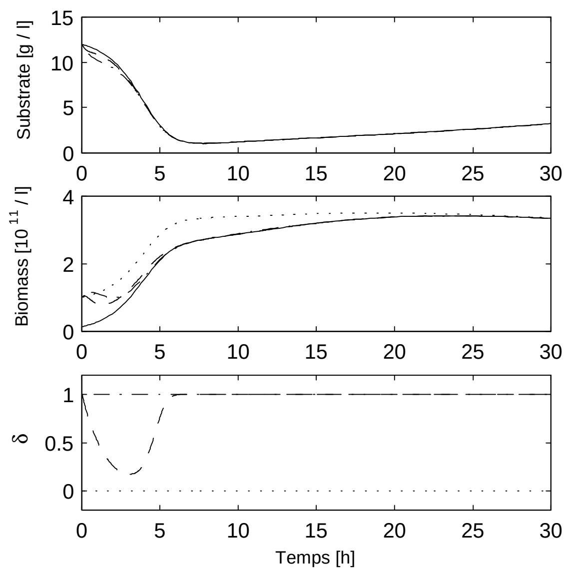

Fig. 2. Estimation of the substrate and the biomass concentrations (exact model).—: real signal, -.-. extended Luenberger observer, ...: asymptotic observer and – –: hybrid observer.

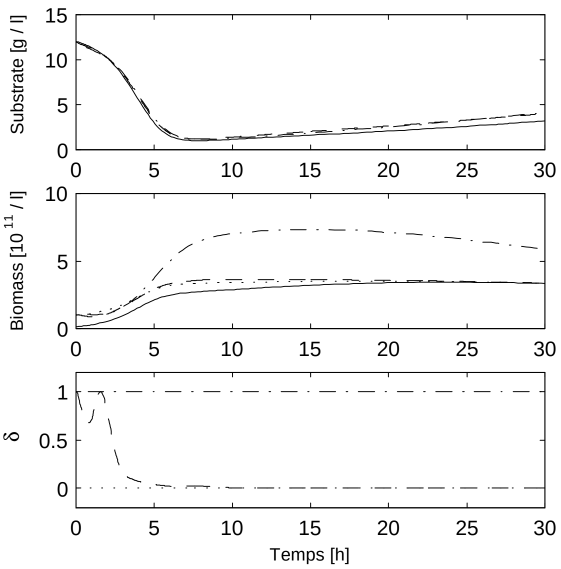

Fig. 3. Estimation of the substrate and the biomass concentrations (bad model). (modelling error : $\mu_{max} = 0.7h^{-1}$ and $K_m = 18gl^{-1}$ in place of $\mu_{max} = 1.4h^{-1}$ and $K_m = 12gl^{-1}$).—: real signal, -.-. extended Luenberger observer, ...: asymptotic observer and $--$: hybrid observer.

the model quality. On the other hand, the asymptotic observer is able to provide state estimates without any knowledge about the kinetic model. However, its convergence rate is completely defined by the process operating conditions (i.e. dilution rate).

In this contribution, a hybrid observer is proposed, which builds upon these two state estimation algorithms. This hybrid observer evolves between the extended Luenberger and the asymptotic observer according to the kinetic model quality. The evolution is driven by a parameter which is function of the estimation error on the measured variables. This parameter may vary between two limit values, 1 and 0, corresponding rigorously to the extended Luenberger observer (100% confidence in the kinetic model) and the asymptotic observer (0% confidence in the kinetic model). Moreover, sufficient stability conditions are discussed.

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