Kalman Filter Design for a Second-order Model of Anaerobic Digestion

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Abstract: The paper deals with the state estimation of a second-order model of anaerobic digestion. This estimation is necessary to implement the sophisticated control algorithms that have already been developed for this process. Hereby design and performance of a classical Kalman filter (compared with other two deterministic estimation approaches) for the main variables of this model have been discussed and analysed by simulations. The performance analysis has been conducted at realistic random perturbations, comparable with experimental data, on the one hand, and on the other – with and without parameter perturbations. Although at random perturbations alone the Kalman filter has a clear advantage over the two equivalent deterministic estimators, at the presence also of parameter perturbations, to which the Kalman filter is more sensitive, no such advantage is guaranteed.

Keywords: Anaerobic digestion, State and parameter estimation, Kalman filter, Robustness.

Introduction
Anaerobic digestion (AD) is a biotechnological process widely used in life sciences and a promising method for solving some energy and ecological problems in agriculture and agro-industry. In such kind of processes, usually carried out in continuously stirred tank bioreactors (CSTR), the organic matter is depolluted by microorganisms into biogas (mainly methane and carbon dioxide) and compost in the absence of oxygen [4].

Many mathematical models of this process in CSTR are known [3, 5, 9]. They are systems of nonlinear ordinary differential equations with a great number of unknown coefficients. The estimation of these coefficients is a very difficult task [5, 9]. Quite often one obtains only local solutions and it is impossible to validate the model in a large domain of experimental conditions.

In practice, only biogas flow rate can be easily measured on-line. However, to control this complex and strongly nonlinear process, sophisticated algorithms have been developed [3]. These algorithms include some unmeasurable variables that must be estimated.

For the unmeasurable state variable estimation, when only the biogas flow rate is measurable, various estimators have been proposed [2, 3].
The aim of the paper* is to design a classical Kalman filter for the main variables of a simple nonlinear AD model and to quantify the robustness of the filter to step-wise model parameter perturbations. The real stochastic environment of the process is taken into account.

**Model description**
Consider the continuous AD state-space model presented in [9]:

\[
\begin{align*}
\frac{dX}{dt} &= (\mu - D)X \\
\frac{dS}{dt} &= -k_1\mu X + D(s_i - S) \\
Q &= k_2\mu X
\end{align*}
\]  

(1)

where \([X S]^T\) is the state vector of the concentrations \([g \cdot dm^{-3}]\) of biomass \(X\) and substrate \(S\); \(D\) is the control input – dilution rate \([day^{-1}]\); \(Q\) is the output – biogas flow rate \([dm^3 \cdot day^{-1}]\); constant parameters: \(k_1\) and \(k_2\) are yield coefficients; \(s_i\) is the input substrate concentration \([g \cdot dm^{-3}]\); the variable parameter \(\mu\) is the specific growth rate of bacteria \([day^{-1}]\) assumed to be of Monod type:

\[
\mu = \frac{\mu_m S}{k_s + S}
\]  

(2)

where \(\mu_m\) and \(k_s\) are kinetic coefficients.

The operational domain of the process is the constraint:

\[
0 < D < D_{sup}
\]  

(3)

where \(D_{sup}\) is the value at which washout of microorganisms takes place.

**Estimator design via Kalman filter**
Before using the Kalman filter, a preliminary linearisation [1, 7] of the AD model (1)-(2) is performed in the neighbourhood of a triple of trajectories: a chosen operating control input trajectory \(D_0(t)\) and corresponding to \(D_0(t)\) solutions \(X_0(t)\) and \(S_0(t)\) of the state equations in (1).

Introducing the denotation:

\[
Q_0 = k_2\mu(S_0)X_0,
\]  

(4)

the linearised model can be expressed as:

* Parts of the results presented herewith were published in the proceedings of the Int. Conf. “Automatics and Informatics’08” and “Automatics and Informatics’09” held in Sofia, Bulgaria.
\[
\frac{dY}{dt} = AY + B \begin{pmatrix} \Delta D \\ \Delta F \end{pmatrix}, \quad Y = \begin{pmatrix} \Delta X \\ \Delta S \end{pmatrix}
\]

\[Q - Q_0 = CY\]

where

\[\Delta D = D - D_0; \Delta X = X - X_0; \Delta S = S - S_0.\] (6)

\(\Delta F\) is a term provisioned to reflect disturbances as described below and the matrices \(A, B, C\) are:

\[
A = \begin{pmatrix}
\frac{\mu_s S_0}{k_s + S_0} & -\frac{k_m X_0}{(k_s + S_0)^2} \\
-\frac{k_m X_0}{(k_s + S_0)^2} & \frac{\mu_s S_0}{k_s + S_0} - D_0
\end{pmatrix}, \quad
B = \begin{pmatrix}
-X_0 \\
1 - S_0 
\end{pmatrix}, \quad
C = \begin{pmatrix}
\frac{k_m S_0}{k_s + S_0} & \frac{k_m X_0}{(k_s + S_0)^2}
\end{pmatrix}.\] (7)

It is assumed that the internal process perturbations are revealed in \(\Delta D\) and in the additional disturbance term \(\Delta F\). The latter is introduced as an extension to the linearised form of the model (1)-(2) where all internal perturbations were referred to \(\Delta D\). This extension makes sense, since the checked small sensitivity of \(Q\) to changes in \(\Delta D\) suggests that \(\Delta D\) alone is able to present only a part of the internal perturbations.

Both \(\Delta D\) and \(\Delta F\) are considered zero-mean Gaussian white noises with covariances respectively \(E[\Delta D(t)\Delta D(\tau)] = q_1\delta(t - \tau)\) and \(E[\Delta F(t)\Delta F(\tau)] = q_2\delta(t - \tau)\). Besides, another additive uncorrelated (with \(\Delta D\) and \(\Delta F\)) zero-mean Gaussian white noise with covariance \(r\delta(t - \tau)\) acts on the output \(Q\) in the course of measurement. It is supposed also that the initial state \(Y(0)\) of the linearised model (5) is a zero-mean Gaussian random vector.

The Kalman filter providing optimal mean-square estimate \(\hat{Y}\) of \(Y\) is [10]:

\[
\frac{d\hat{Y}}{dt} = (A - KC)\hat{Y} + K(Q - Q_0), \quad \hat{Y}(0) = 0
\]

(8)

where

\[K = \frac{1}{r}PC^T\]

(9)

is the filter gain matrix, and the error covariance matrix \(P\) is obtained from the Riccati matrix differential equation:

\[
\frac{dP}{dt} = AP - \frac{1}{r}PC^T CP + PA^T + BNB^T, \quad P(0) > 0, \quad N = \text{diag}(q_1, q_2).
\]

(10)
Estimators for comparison

**Differential algebraic estimator**

On the basis of the differential algebraic approach, an exponentially stable estimator first for specific growth rate $\mu$ and then for biomass and substrate concentrations (respectively $X$ and $S$) was obtained in [2] and is further compared with the Kalman filter.

**Classical adjustable estimator**

Introducing transformations and an auxiliary variable, an estimator first for $\mu$ and $Q$ and then, as above, for biomass and substrate concentrations, was obtained in [8] and is also used for comparison.

**Simulation studies**

*Performance analysis at random perturbations*

The model coefficients have the following values [9]: $k_1 = 6.7$; $k_2 = 16.8$; $s_i = 7.4$ g·dm$^{-3}$; $\mu_m = 0.35$ day$^{-1}$; $k_3 = 2.3$ g·dm$^{-3}$. The model initial conditions: $X(0) = 0.450$ g·dm$^{-3}$; $S(0) = 0.383$ g·dm$^{-3}$ are strongly non-equilibrium and supposed unknown to the three estimators having rather different initial estimates: 0.179 g·dm$^{-3}$ for $X(0)$ and 1.335 g·dm$^{-3}$ for $S(0)$.

The entire control input range of practical interest is covered by choosing the nominal control input $D_0$ values between 0.03 and 0.09 day$^{-1}$ (the latter value equals to 90% of the value maximising the equilibrium $Q$ under the above coefficient values). The transition to an equilibrium takes from 0th to 80th day for the nominal (corresponding to $D_0$) model variables under $D_0 = 0.06$ day$^{-1}$. This period suffices to compare the convergence times of the initial estimator estimates to the corresponding model variables under constant control input. Afterwards consecutive transitions (smaller than that above) to other equilibrium states in the mentioned range at each 10 days (sufficient for the transitions) are performed under the following (on Fig. 1) time profile of $D_0$ [day$^{-1}$]: 0.075 – day 80 to 90; 0.09 – day 90 to 100; 0.075 – day 100 to 110; 0.06 – day 110 to 120; 0.045 – day 120 to 130; 0.03 – day 130 to 140; 0.045 – day 140 to 150; 0.06 – day 150 to 180.

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![Fig. 1 Control input](image)

The term $\Delta F$ is considered additive also to the first equation of (1). The process uncertainties and perturbation levels are modelled by choosing the values of the covariance parameters as...
follows. The small value of $q_1 = 1.27 \times 10^{-4}$ day$^{-2}$ guarantees the observance of the operational constraint (3) for the entire considered range of $D_0$, as depicted on Fig. 1. Yet it should be considered to contain a referred noise component, since $q_1 \approx (0.2D_0)^2$. The choice of $q_2 = 1.27 \text{[g·dm}^{-3}·\text{day}^{-1}]^2$ together with that of $q_1$ determines the level of the internal perturbations. The measurement noise level is determined by $r = 2.5 \times 10^{-3}$ (dm$^{-3}·$day$^{-1}$)$^2$. The average relative disturbances of the output $Q$ due to internal perturbations and to measurement noise up to the current simulation time are shown on Fig. 2. The curves on this figure are realistic, since they are comparable with experimental data.

Fig. 2 Influence of internal perturbations and measurement noise on output

The simulations require also adjusting estimator parameters as follows: for the Kalman filter, the initial condition of Eq. (10) is chosen large enough, viz. $P(0) = 50I_2$, with $I_2$ denoting the 2×2 identity matrix; and the tuning parameter $h \approx 2$ was checked to ensure the best performance of the classical adjustable estimator.

The properties of the three estimators are compared for the variable $\mu$ and states $X$ and $S$ by simulations shown on Fig. 3 to Fig. 8 under the above conditions. The estimation of $\mu$ is presented on Fig. 3 for the Kalman filter and for the classical adjustable estimator, and on Fig. 4 for the differential algebraic estimator. On about day 40, the average relative errors of the first and second estimator are checked to be equal. The convergence time of the initial estimate to the model $\mu$ is about 50 days for the first one, whereas for the second one on about day 15 the maximum possible convergence is reached, being rather unstable in the remaining simulation time and especially after day 80.
The behaviour of the differential algebraic estimator on Fig. 4 is very close to that of the classical adjustable estimator. Although producing more fluctuating estimates, its average relative error at any simulation time was checked to be nearly the same as that of the latter.

The estimation of $X$ is presented on Fig. 5 for the Kalman filter and for the classical adjustable estimator, and on Fig. 6 for the differential algebraic estimator. The first estimator mostly tracks the model $X$, except mainly for about 30 days – from about day 90 to 120, when it is inexact, with rare full failures and mostly equipollent with the second one. However, the second one is inexact from about day 30 on. The estimates of the differential algebraic estimator on Fig. 6 are nearly the same as those of the classical adjustable estimator.
Fig. 5 Estimation of $X$ by Kalman filter and classical adjustable estimator

Fig. 6 Estimation of $X$ by differential algebraic estimator

Fig. 7 Estimation of $S$ by Kalman filter and classical adjustable estimator
The estimation of $S$ is presented on Fig. 7 for the Kalman filter and for the classical adjustable estimator, and on Fig. 8 for the differential algebraic estimator. The above about the estimation of $\mu$ holds with respect to $S$ too.

**Performance analysis at parameter perturbations**

Parameter perturbations are due to imprecise parameter values or to their unpredictable deterministic changes. Therefore, robustness analysis is an indispensable step of the estimator design.

The robustness of the estimators designed above have been investigated regarding parameters $k_1$, $\mu_m$ and $s_i$ at $D = 0.06 \text{ day}^{-1}$ for the variables $\mu$ and $X$. Some results are presented on Fig. 9 to Fig. 14. The perturbations of all the three parameters are applied at days 80 (+20%), 100 (−20%), 120 (−20%) and 140 (+20%). For the variable $\mu$, in all figures numbered “a” the respective model variable (with and without noise), the Kalman filter and classical estimator estimates are presented. On those figures numbered “b”, the respective model variable (with and without noise) together with the differential estimator estimates are shown. The same is for the variable $X$, except that the classical estimator estimates are shown on the “b” figures.

The Kalman filter tracks well the parameter perturbations at days 80 and 100 on Fig. 9a; all the four perturbations on Fig. 11a; all the perturbations but the one at day 100 on Fig. 12a and in these cases performs better than the two deterministic estimators. However, in the other perturbation cases it performs much worse, which cannot be avoided or provisioned. As in the case of random perturbations, the two deterministic estimators produce nearly the same average relative error when estimating $\mu$, or their estimates practically coincide when estimating $X$. The sensitivity of these estimators to parameter perturbations is low in all the considered cases.
Fig. 9a Estimation of $\mu$ at parameter perturbation of $k_1$ by Kalman filter and classical adjustable estimator

Fig. 9b Estimation of $\mu$ at parameter perturbation of $k_1$ by differential algebraic estimator
Fig. 10a Estimation of $X$ at parameter perturbation of $k_1$ by Kalman filter

Fig. 10b Estimation of $X$ at parameter perturbation of $k_1$ by classical adjustable and differential algebraic estimators
Fig. 11a Estimation of $\mu$ at parameter perturbation of $\mu_m$ by Kalman filter and classical adjustable estimator.

Fig. 11b Estimation of $\mu$ at parameter perturbation of $\mu_m$ by differential algebraic estimator.
Fig. 12a Estimation of $X$ at parameter perturbation of $\mu_m$ by Kalman filter

Fig. 12b Estimation of $X$ at parameter perturbation of $\mu_m$ by classical adjustable and differential algebraic estimators
Fig. 13a Estimation of $\mu$ at parameter perturbation of $s_i$ by Kalman filter and classical adjustable estimator

Fig. 13b Estimation of $\mu$ at parameter perturbation of $s_i$ by differential algebraic estimator
Fig. 14a Estimation of $X$ at parameter perturbation of $s_i$ by Kalman filter

Fig. 14b Estimation of $X$ at parameter perturbation of $s_i$ by classical adjustable and differential algebraic estimators

**Conclusion**

In this paper, three estimators, based only on the online measurement of $Q$, are compared by simulations taking into consideration random perturbations that may occur in a real process. The first one is a Kalman filter, and the other two are deterministic – a classical adjustable estimator and a differential algebraic estimator. The random perturbations deteriorate the performance of the deterministic estimators.

The convergence of the assumed initial estimates to the model variables is mostly commensurate for the three estimators. Presumably, considerable changes in the state of the nominal (unperturbed) model are harder to be tracked by any of the estimators. However, smaller changes (as those after simulation day 80) evidence the advantage of the Kalman filter over the two equipollent deterministic estimators despite the considerable change in $D_0$. 
The robustness analysis through simulations evidences that the two deterministic estimators again are of equal worth but substantially distinct from the Kalman filter. The latter is more sensitive to a series of parameter perturbations, especially to those of $k_1$ and $s_i$, for both variables $\mu$ and $X$, thus losing its advantage mentioned above. However, at lower values of the parameter perturbations or at rarer ones than those simulated, the Kalman filter’s robustness might rate higher and then it should be preferred.

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References
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