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Implementation of Multi-Kalman Filter to detect Runaway Situations and Recover Control

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Abstract

This work should concentrate on developing a tool able to detect runaway conditions in a batch reactor and act on the reactor to recover a safer condition. Parallel Kalman filters are implemented, corresponding to some possible models that potentially can describe the system (i.e. parallel or consecutive reactions). Acting over each one of the filters, the Bayes' theorem allows determining the probability of success of each filter and, finally, estimating the divergence of the system. If the divergence were positive, a runaway situation is detected and prevention and protection procedures should be activated dangerous situations. Using the divergence criterion, a runaway situation is detected at very early stages, giving time enough to decide and apply the most convenient actions.

Keywords: Kalman filter, divergence, runaway, control, batch reactor

1. Introduction

Calculation of the divergence of the trajectory of a chemical reaction carried out in an industrial reactor has demonstrated [2] to be an excellent method to early detecting runaway situations. However, noise on the measures and a lack of knowledge of a suitable kinetic and transport model of the system make the task of calculating the divergence some more difficult. Kalman filters are able to be used both to reduce the level of noise of a signal and to adjust a model.

A Kalman filter is essentially a set of mathematical equations that implement a predictor-corrector type estimator that is *optimal* in the sense that it minimises the estimated *error* covariance when some presumed conditions are met (scheme show in Figure 1) [1]. This occurs in large part to advances in digital computing that makes the filter useful, but also to the relative simplicity and robust nature of the filter by itself. Rarely do the conditions necessary for the optimal application of the filter, however, the filter works well for many applications.

However, the model-based Kalman filter is only possible thanks to a great deal of a prior information about the process put together in a mathematical model. This is the

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most time consuming step in the application of the model single Kalman filter. Equations necessary to compute the filter are indicated in Figure 2.

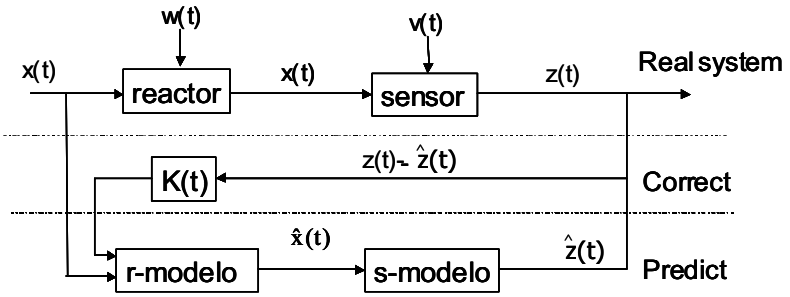

Figure 1. Structure of Kalman filter

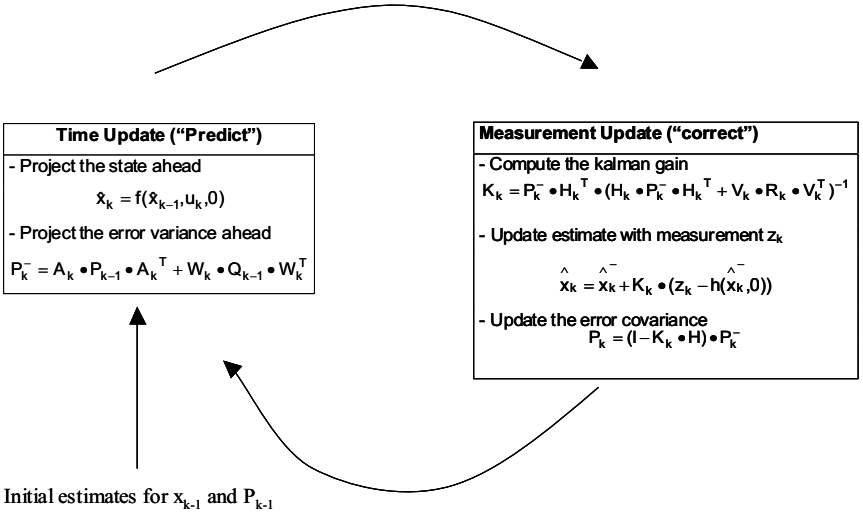

Figure 2. Computing Kalman filter.

A single Kalman Filter is useful if the model of the system is really known but cannot predict any change of the behaviour of the system, involving a change in the model. To solve this problem, this work demonstrates that parallel Kalman filters corresponding each one to a different possible model, which are supposed to describe the studied system. Over each one of the filters, the Bayes' theorem allows determining the probability of each filter.

2. Theory

Consecutive equilibrium and Parallel reactions (A⇄B→C)

$$\frac{du_A}{dt} = -f_1 \cdot u_A^{n_1} + \rho \cdot f_2 \cdot u_B^{n_2} \tag{1}$$

$$\frac{du_B}{dt} = f_1 \cdot u_A^{n_1} - \rho \cdot f_2 \cdot u_B^{n_2} - \varepsilon \cdot f_3 \cdot u_C^{n_3} \tag{2}$$

$$\frac{d\theta}{dt} = \alpha \cdot (f_1 \cdot u_A^{n_1} - \rho \cdot \varepsilon \cdot f_3 \cdot u_B^{n_3}) + \alpha \cdot \lambda \cdot \rho \cdot f_2 \cdot u_B^{n_2} - \beta \cdot (\theta - 1) \quad (3)$$

Two parallel reactions (A→B and A→C)

$$\frac{du_A}{dt} = -f_1 \cdot u_A^{n_1} + \rho \cdot f_2 \cdot u_B^{n_2} - \varepsilon \cdot f_3 \cdot u_B^{n_3} \quad (4)$$

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$$\frac{du_B}{dt} = f_1 \cdot u_A^{n_1} - \varepsilon \cdot f_3 \cdot u_B^{n_3} \quad (5)$$

$$\frac{d\theta}{dt} = \alpha \cdot (f_1 \cdot u_A^{n_1} - \varepsilon \cdot f_3 \cdot u_B^{n_3}) + \alpha \cdot \lambda \cdot \rho \cdot f_2 \cdot u_B^{n_2} - \beta \cdot (\theta - 1) \quad (6)$$

Where ρ is the reaction rate constant, λ is the head of reaction rate, α is the dimensionless heat of reaction, and β is the dimensionless heat transfer constant.

All the reactions are assumed to be n^{th} order respecting reactants, and agreeng the Arrhenius law:

$$f_i = e^{\gamma_i \cdot \frac{\theta - 1}{\theta}} \qquad \gamma_i = \frac{E_i}{R \cdot T_w} \quad (7)$$

Multi Kalman filter

When some independent filters are applied in parallel, the Bayes' theorem (Equation 8) can be used to decide which of them better describes the system.

$$P(E_i \mid A) = \frac{P(A \mid E_i) \cdot P(E_i)}{\sum_{j=1}^{n} \{P(A \mid E_i) \cdot P(E_j\}} \quad (8)$$

When a particular event E_i occurs on condition of the event A, the posterior probability $P(E_i|A)$ of the event E_i is actualised. In order to judge the state of the objective system by Bayes' theorem combined with Kalman filter, "the system in observation is considered to correspond to a model M_i" is associated with event E_i. Likewise "the hypothesis is assumed to be correct" is associated with the A. Also the posterior probability in a prior step is to be a priori probability of the new step.

Furthermore if the actual system corresponds to a certain model, with respect to the residual from Kalman filter, the output is to be followed with the normal distribution of the average 0 and variance $(\det(Vi(k))^{0.5}$.

$$N(\xi) = \frac{e^{0.5 \cdot \xi^T(k) \cdot Vi(k)^{-1} \cdot \xi(k)}}{2 \cdot \pi^{(m/2)} \cdot (\det V_i(k))^{0.5}} \quad (9)$$

Therefore, regarding ξ (the difference between measure and prediction, z(k)-h(x(k)), which represents the residual obtained from the Kalman filter of model M_i, its probability density function is provided as N (Equation 9). From equations 8 and 9 the probability $P_i(t)$ corresponding to a specific model M_i is obtained from the recursion Equation 10.

$$P_i(k) = \frac{N_i \cdot P_i(k-1)}{\sum_{j=1}^{n} N_j \cdot P_j(k-1)} \quad (10)$$

If the probability concerning the model M_i exceeds the probability of the other models, it can be concluded that model M_i is the better description of the system.

Divergence.

Divergence establishes a universal criterion to detect unsafe situations in chemical reactors. The divergence in a reactor is defined as the trace of Jacobian that is the sum of he partial derivatives of the difference equations 1, 2 and 3 (consecutive reactions) or 4, 5 and 6 (parallel reactions). If the divergence is positive, a runaway situation is detected [2].

2. Results and discussion

Figure 3 exposes the decision structure used to maintain the reactor within safer limits.

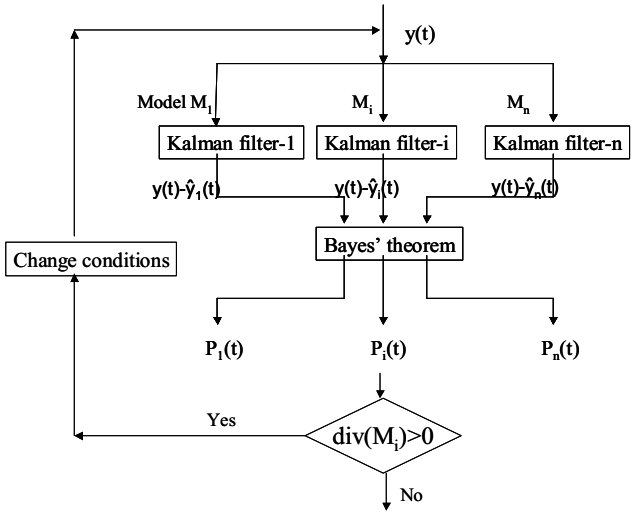

Figure 2. Structure of Multi-Kalman filters

It is assumed that the parameters of the systems are invariant during the reaction, so the transition matrix A of the Kalman filters is set as the identity matrix. The measurement matrix is the Jacobian of the set of equations 1 to 3 or 4 to 6. Those systems do not have analytical solution, so the matrix H is calculated numerically.

γ1	γ2	γ3	ρ	λ	ε	α	β	n1	n2	n3
30	40	25	0.5	0.3	0.7	0.53	30	1	1	1

Table 1. Condition of simulation Figure 4-1.

Table 1 shows the parameter set used to simulate the system of parallel reactions. A stochastic noise with variance of 0.01 was added to the simulated profiles. When the two parallel filters were applied to the simulated measured profiles, the filter with a parallel reaction model produces the best estimation of composition. On the other hand, the filter with equilibrium model produces wrong predictions. Temperature estimates by both filters are quite similar to the real (Figure 4). The probability of each filter using the Bayes' theorem is shown in Figure 5. When the adimensional time reaches a value

of 0.03, the probability of the parallel model is about 76% and at a time of 0.05, the probability is near to 100%. This filter is able to differentiate both mechanisms after short intervals of time. In addition, the multi-Kalman filter is very efficient reducing the measured variables.

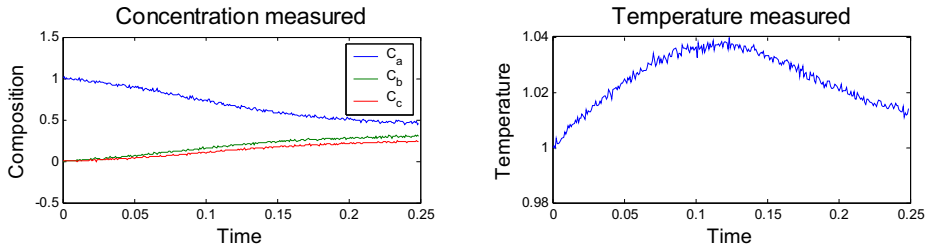

Figure 4. Temperature and composition measured.

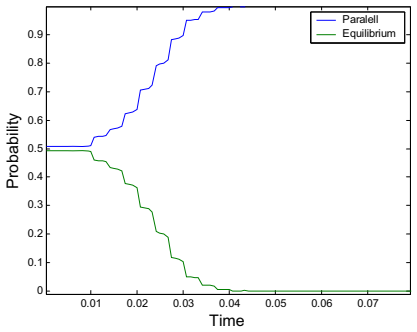

Figure 5. Probability of each reaction using Multi-Kalman filter

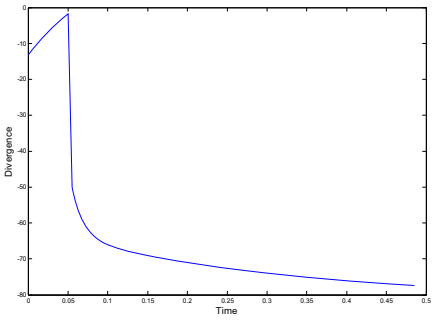

Figure 6. Divergence along the time.

At an adimensional time of 0.05 the divergence of the system (Figure 6) takes a positive value so the control system acts over the jacked temperature to recover the control. The reduced temperature changes only from 300K to 298K (Figure 7), but the divergence of the system becomes negative, indicating a very high sensitivity of the system.

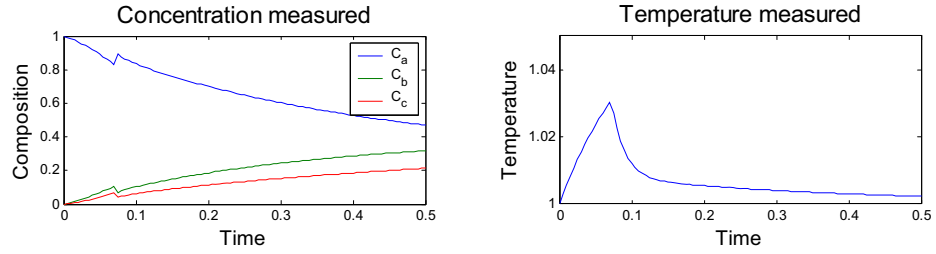

Figure 7. Composition and temperature profiles.

4. Conclusions.

The Kalman filter using temperature measures, composition measures or both of them reduces meaningfully the noise and avoids all false positive values of the divergence criterion for early warning runaway.

Kalman filters have demonstrated to be a robust and powerful tool for fitting kinetic parameters of a reaction, and to calculate the divergence of the system. In addition, Multi-Kalman filters help to select the most convenient model to describe a system.

The Multi-Kalman filter combined with the adjusted parameters solves the problem of the great amount of initial information needed to implement traditional Kalman filters, making efficient predictions in a wide range of possible cases. The combination of different Kalman filters using the Bayes' theorem and the divergence runaway criterion provide a tool to detect unsafe reaction conditions at a very early stages, providing time enough to decide actions to prevent the final runaway.

5. Symbols

C_p	Heat capacity.
E	activation energy.
n	reaction order
T_w	Jacket temperature, K
U	overall heat transfer coefficient, W/m^2K
ΔH_i	heat of the i-th reaction, J/mol
β	Damköhler number, $\beta = -(\nu_A) \cdot C_{B_0} \cdot k \cdot e^{-\frac{1}{\gamma}} \cdot t_{ref}$
α	dimensionless adiabatic temperature parameter, $\alpha = \frac{(-\Delta H_1) \cdot u_{Ao}}{\rho_f \cdot c_p \cdot T_w}$
γ_I	dimensionless activation energy, $\gamma_i = \frac{E_i}{R \cdot T_w}$
θ	dimensionless temperature $\theta = T/T_w$
τ	dimensionless time, $\tau = \frac{t}{t_{ref}}$
ρ, ε	reaction rate
x	state estimate
z	measured state
$\hat{x}_k$	a posteriori state estimate
$\hat{x}_k^-$	a priori state estimate
K	Kalman gain
P_k^-	*a priori* estimate error covariance
P_k	*a posteriori* estimate error covariance

6. References

[1] Gelb, A., *Applied Optimal Estimation*. Cambridge, MA:MIT Press., 1974

[2] J.M. Zaldívar, J. Cano, M.A: Alós, J. Sempere, R. Nomen, *Journal of Loss Prevention*, **2003**, 187-200.