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Global-nonlinear stochastic estimation of exothermic reactors with temperature measurement

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Abstract: In this work, the problem of estimating the concentration of exothermic rectors with temperature measurement is addressed. The problem is treated within a global nonlinear stochastic framework, according to the Fokker Plank-based Kushner filtering theory. The on-line solution of the associated two-dimensional partial differential equation driven by the temperature measurements yields the evolution of the conditioned concentration-temperature probability density function (PDF), with considerable more information than the one provided by standard EKF based on a local-nonlinear approach. A catalytic reactor with deterministic multistability, experimental data, and previously addressed with EKF is addressed as case example, yielding: (i) the on-line evolution of the (possibly bimodal) conditioned concentration probability density function, and (ii) mean uncertainty values which are better than the ones drawn with EKF.

Keywords: Nonlinear filtering, estimation, Kushner, catalytic reactor

1. INTRODUCTION

The problem of nonlinear estimation is of great importance for chemical process systems, where state variables like, e.g., concentrations, are not often continuously available on-line and needs to be inferred from secondary measurements. In the chemical process systems engineering field, the Extended Kalman Filter (EKF) has been by far the most tested and accepted state estimation technique. On the basis of a local-nonlinear approach, the EKF provides estimates of the state mean and of its error covariance. In the EKF implementations, the uncertainty characterization is used as a means to draw the state mean and not to on-line assess its error covariance. This is so because, in the linear-to-nonlinear passage, the stochastic meaningfulness of the linear Kalman filter is somehow lost. According to the global-nonlinear stochastic estimation theory (Jazwinski, 1970): (i) the general solution to the estimation problem is given by the Kushner Filter (KF) which on-line solves the multidimensional Fokker Plank-like PDE which describes the (possibly multimodal) measurement-conditioned state probability density function (PDF), (ii) the nonlinear EKF is the local case of the global-nonlinear KF, assuming that, in a neighborhood of the state motion, the error covariance propagation is given by the linear part of the state dynamics, and consequently, that the associated PDF is Gaussian (i.e., monomodal), and (iii) as a consequence, the infinite-dimensional linear PDE of the KF becomes the familiar finite-dimensional matrix Riccati nonlinear ODE of the EKF. The EKF applies to nonlinear systems, but it can be inadequate when: (i) the initialization is poor (Sharma et al., 2006), (ii) there are significant system nonlinearities and constraints (Kolas et al, 2009 and reference there in), and (iii) there is PDF multimodality due to deterministic model (Tronci et al., 2009; Oberlack, 2000). It must be pointed out that deterministic multiplicity due to kinetics non-monotonicity with respect to concentration concerns an important class of chemical (or bio) reactors with reaction inhibition described by Langmuir-Hinshelwood (or Haldane) kinetics (Aris, 1965). The interplay between deterministic (mono/multi) stability and stochastic (mono/multi) modality in the context of a global-nonlinear stochastic chemical reactor modeling problem (without measurements) can be seen in a recent study (Tronci et al., 2009).

The KF theory, based on the global-nonlinear probabilistic description of the Fokker Planck equation, was developed sometime ago. However, due to the complexity and difficulty of having to on-line numerically solve a PDE with independent variables equal to the number of states, the KF applications was not used until the advent of modern computing technology. Recently, motivated by the need of designing system probabilistic descriptions and the availability of more powerful and reliable computational tools, the development of numerical schemes and packages to handle Fokker-Plank equations has become a subject of intense research (Kushner and Budhiraja, 2000; Sharma et al., 2006; Germani et al., 2007; Budhiraja et al., 2007; Xu and Vedula, 2009; Sharma, 2009). As far as we know, the KF

theory has not been applied in chemical process systems engineering field, even if the characteristics of those systems (e.g. deterministic multistability) can take advantage of a global nonlinear estimation approach.

In this work the global-nonlinear Kushner filter (Jazwinski, 1970) approach is applied to solve the on-line estimation of the composition in continuous exothermic reactors with deterministic bistability due to kinetics non-monotonicity with respect to concentration. A catalytic reactor with deterministic bistability, experimental data, and previously addressed with EKF (Baratti et al., 1993) is considered as representative case example, yielding: (i) the on-line evolution of the (possibly bimodal) conditioned concentration probability density function, and (ii) mean uncertainty values which are better than the ones drawn with EKF. The numerical implementation issue and the tuning aspects (which are substantially different than the familiar ones of the EKF) are discussed.

2. REACTOR ESTIMATION PROBLEM

Consider exothermic continuous reactor with volume V, where a reactant is fed with volumetric flow F at concentration C_e and temperature T_e, and converted into product via a Lipschitz-continuous reaction rate R with Arrhenius dependency on temperature T and isotonic (growing) or nonmonotonic (growing-decreasing) dependency on concentration C. The actual reactor dynamics are given by:

$$\begin{aligned} \dot{C} &= \theta(C_e - C) - r(C,T) + w_c(t) = f_1(C,T) + w_C(t) \\ \dot{T} &= \theta(T_e - T) + \beta r(C,T) + \delta(T_a - T) + w_T(t) = f_2(C,T) + w_T(t) \\ y &= T + v(t),\ v(t) \sim N(0, q_w) \end{aligned} \quad (1)$$

$$\mathbf{w}(t) \sim N(0,\mathbf{Q}),\ \mathbf{w}(t) = \begin{pmatrix} w_C(t) \\ w_T(t) \end{pmatrix},\ \mathbf{Q} = \begin{pmatrix} q_{CC} & q_{CT} \\ q_{TC} & q_{TT} \end{pmatrix},\ q_{CT} = q_{TC}$$

where θ is the dilution rate (F/V), β is the heat of reaction ($-\Delta H$) divided by the volumetric specific heat capacity (ρc_p), δ is the mixture-jacket heat transfer coefficient divided by the heat capacity ($V\rho c_p$), and $\mathbf{w}(t)$ is a white noise vector with zero-mean and noise intensity matrix $\mathbf{Q}$.

Our *global-nonlinear estimation problem* consists in on-line computing the conditional probability density function $\pi(C,T)$ on the basis of the stochastic model (1) in conjunction with the temperature measurement (y). For illustration and comparison purposes, a catalytic reactor with deterministic bistability, experimental data, and previously considered with the local-nonlinear EKF approach (Baratti et al., 1993) is addressed as representative case example.

3. GLOBAL-NONLINEAR ESTIMATOR

In the Bayesian framework, where the statistical models are available for the state and the measurements, the filtering problem consists in obtaining the states PDF at time t, given all the measurements until t (Gelb, 1988). The conditional probability density function of C(t), $\pi(C(t)|\mathbf{Y}(t_k))$, with $\mathbf{Y}(t_k)$ being the vector of measurements collected until $t_k \leq t$, is the complete solution of the filtering problem because it contains all the statistical information according to the measurements and initial conditions. In case of linear filtering, the conditional distribution is Gaussian and it is simply characterized by the state mean and its covariance matrix. In the EKF for nonlinear system (Gelb, 1988; Jazwinski 1970), a Gaussian PDF approximation is used in terms of its two moments, on the basis of the linearization of the dynamic model around the current state estimate. EKF functioning improvements can be obtained by increasing the filter order (Gelb, 1988, Sharma, 2009). However, the main disadvantage of the EKF is the impossibility of handling the non-Gaussian (i.e., asymmetric and/or multimodal) state PDF features associated with strong nonlineariti y and deterministic multistability phenomena (Tronci et al., 2009; Oberlack et al., 2000).

3.1 Nonlinear stochastic filter

In the absence of measurements, the evolution of the normalized concentration PDF function π, associated with the stochastic model (1), is given by the solution of the Fokker-Planck PDE:

$$\frac{\partial \pi}{\partial t} = \frac{1}{2} q_{CC} \frac{\partial^2 \pi}{\partial C^2} + \frac{1}{2} q_{TT} \frac{\partial^2 \pi}{\partial T^2} + q_{CT} \frac{\partial^2 \pi}{\partial C \partial T} - \frac{\partial (f_1 \pi)}{\partial C} - \frac{\partial (f_2 \pi)}{\partial T} \quad (2)$$

$$\pi(C, T, 0) = \pi_o(C, T)$$

$$f_1(0,T)\pi(0,T) - \frac{1}{2} q_{CC} \left.\frac{\partial \pi}{\partial C}\right|_{C=0} - \frac{1}{2} q_{CT} \left.\frac{\partial \pi}{\partial T}\right|_{C=0} = 0,$$

$$\left.\frac{\partial \pi}{\partial C}\right|_{C=\infty} = 0,\ \forall T,\ t > 0$$

$$f_2(C,0)\pi(C,0) - q_{TT} \left.\frac{\partial \pi}{\partial T}\right|_{T=0} - \frac{1}{2} q_{CT} \left.\frac{\partial \pi}{\partial C}\right|_{C=0} = 0,$$

$$\left.\frac{\partial \pi}{\partial T}\right|_{T=\infty} = 0,\ \forall C,\ t > 0$$

Without restricting the approach, and for the sake of clarity, let us recall the nonlinear stochastic observer, called Kushner Filter, for the discrete measurements case (Jazwinsky, 1970):

Initialization at t = 0: $\pi(C, T, 0) = \pi_o(C, T)$ (3a)

Evolution over $[t_k, t_{k+1}]$:

$\pi_o(C, T) = \pi^+(C, T, t_k)$, $\pi^-(C, T, t_{k+1}) = \pi(C, T, t_{k+1})$ (3b)

Update at t_{k+1}:

$$\pi^+(C,T,t_{k+1}) = \frac{\pi^-(C,T,t_k)\mu(T)}{\int_0^\infty \mu(\tau) \int_0^\infty \pi^-(\xi,\tau,t_k) d\xi d\tau} \quad (3c)$$

where μ is the measurements error (possibly not gaussian) PDF, π^- is the *a priori* (before measurements) concentration PDF according to Fokker-Planck equation-based prediction along $[t_k, t_{k+1}]$ (3b), $\pi+$ is the a posteriori (after measurements) concentration PDF according to the conditioned (Bayesian) PDF formula at t_{k+1} (3c). It must be pointed out that: (i) the update step (3c) consists of a rather straightforward double integration, and (ii) consequently, the

complexity of the NLS filter resides in the evolution step (3b), or equivalently, in the integration of the Fokker-Planck parabolic linear PDE (2) with two "spatial" independent variables (C and T).

3.2 Numerical scheme

To tackle the numerical integration of the FPE, including the fulfillment of the PDF positivity and normalization conditions, efficient and accurate integration methods from the field of Computational Fluid Dynamics are recalled. Specifically, we apply the technique employed in the simulation of mass or heat transport in a conveying fluid, according to the fundamental mechanisms of advection (drift of elementary mass particles due to the mean fluid velocity) and diffusion (related to, e.g., Brownian motion, described by the Fickian flux model, heat conduction, with the Fourier law, or turbulent diffusion). It should be noted that the analogy is not merely formal: the advection-diffusion equation (ADE) is indeed a FPE, with the mass concentration divided by total mass representing the PDF of mass location in the physical space,

Even though the ADE (and the FPE) are formally parabolic for non vanishing diffusivities, all the major problems related to its numerical solution are related to its hyperbolic part, i.e. the transport equation for pure advection. Therefore, the positivity condition is more difficult to fulfill in advection dominated problems characterized by high Péclet numbers.

For the purpose at hand, let us re-write equation (2) in compact vector notation:

$$\frac{\partial \pi}{\partial t} + \nabla \cdot \left(\mathbf{f}\pi - \frac{1}{2}\mathbf{Q}\nabla\pi \right) = 0 \tag{4}$$

where $\nabla \equiv (\partial/\partial C, \partial/\partial T)$ is the Nabla operator, $\mathbf{f} \equiv (f_1, f_2)$ is the corresponding drift "velocity" vector. Recall the divergence of a vector field represents the net outgoing flow across the walls of an infinitesimal parallelepiped control volume, per unit volume, Eq. (4), express the rate of local change of the PDF in terms of advective ($\mathbf{f}\pi$) and diffusive ($\mathbf{D}\nabla\pi$) flows, integrate Eq. (4) over an arbitrary and fixed surface of finite extent on the phase space Ω, (denominated control volume with boundary Γ), and applying the divergence theorem to obtain (Hirsch, 1991)

$$\frac{\partial}{\partial t}\int_{\Omega} \pi \, d\Omega + \int_{\Gamma} \left(\mathbf{f}\pi - \frac{1}{2}\mathbf{Q}\nabla\pi \right) \cdot \mathbf{n} \, d\Gamma = 0 \tag{5}$$

where $\mathbf{n}$ is the unit outgoing normal. This states that the local variation of probability associated with a finite portion Ω of the phase space equals the ingoing probability from outside the control volume, so that the total probability over the whole phase space must be conserved. A numerical method based on such concept, called a *finite volume method* (FVM), by definition conserves the total (unit) probability *regardless of its overall accuracy*. This is why equation (4) (written in *divergence form*) is also (more often) referred to as equation in *conservation form*.

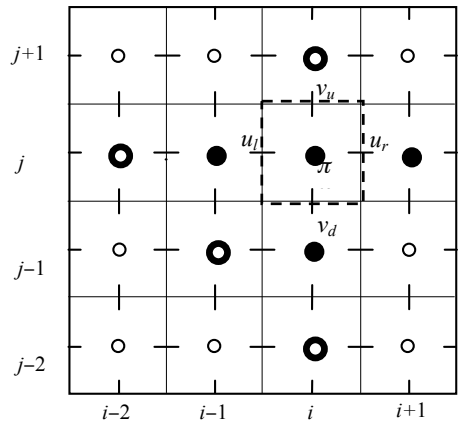

Figure 1. Arakawa-C grid with control volume and computational stencil for $u > 0$ and $v > 0$ (full points involved in definition of flux $F_{i+1/2,\,j}$; empty, bold points involved in scheme for control volume).

The FVM-based numerical scheme requires a partition of the computational domain, with non overlapping elements of arbitrary form. Since our FPE has a regular domain a structured mesh can be used, implying high degree of algorithmic simplicity. Thus, the numerical scheme is based on the staggered Arakawa-C Cartesian grid shown in Figure 1, with rectangular elements (cells) of sides ΔC and ΔT, PDF values defined in cell centers as $\pi_{i,j} = \pi(C_i, T_j)$ and drift velocity defined on cell sides as normal components. Accordingly, the discretized form of equation (5) reads:

$$\pi^{n+1}_{i,j} = \pi^{n}_{i,j} - \tau_C (F_{i+1/2,j} - F_{i-1/2,j}) - \tau_T (G_{i,j+1/2} - G_{i,j-1/2}) \tag{6}$$

where $\tau_C = \Delta t/\Delta C$ and $\tau_T = \Delta t/\Delta T$, Δt is the step of time advancement of the scheme with related index n, such that $t^n = n\Delta t$, and F and G are numerical approximations of time averages over the interval $[t^n, t^{n+1}]$ of the flux $\mathbf{f}\pi - \mathbf{D}\nabla\pi$ across the cell sides ΔT and ΔC, respectively. Note that Eq. (6) is an approximation of the FPE (4) according to a finite-difference (FD) scheme. The actual FVM/FD method depends on the expression of the average numerical fluxes F and G, with schemes based on explicit time advancement being very efficient and particularly well-suited for transient problems.

In this work, the two-dimensional FPE was efficiently solved by using MOSQUITO (Balzano et al., 1999) explicit numerical scheme for the advective part of FPE, and second-order accurate in space and first order in time explicit scheme to handle diffusion term. Letting $f_1 = u$ and $f_2 = v$ to simplify the notation, the numerical difference scheme can be written as follows (for positive u and v):

$$F^{n}_{i+1/2,j} = u_{i+1/2,j}\,\bar{\pi}_{i+1/2,j} - \frac{q_{CC}}{2}\frac{\pi^{n}_{i+1,j} - \pi^{n}_{i,j}}{\Delta C} - \frac{q_{CT}/2}{2\Delta T}\frac{\left(\pi^{n}_{i+1,j+1} + \pi^{n}_{i,j+1}\right) - \left(\pi^{n}_{i,j-1} + \pi^{n}_{i,j-1}\right)}{2} \tag{7}$$

with $\bar{\pi}_{i+1/2} = a_d \pi^{n}_{i+1,j} + a_u \pi^{n}_{i,j} + a_{uu} \pi^{n}_{i-1,j} + a_{uT} a_{uu} \pi^{n}_{i,j-1}$,

involving the full points shown in Figure (1), and

$$a_d = \tfrac{1}{6}(2 - 3c_{Cr} + c_{Cr}^2) \qquad a_{uu} = \tfrac{1}{6}(c_{Cr}^2 - 1)$$
$$a_u = \tfrac{1}{6}(5 + 3c_{Cr} - 2c_{Cr}^2 - 3\bar{c}_{Tr}) \qquad a_{uT} = \tfrac{1}{2}\bar{c}_{Tr} \qquad (8)$$

where:

$$c_{Cr} = u^n_{i+1/2,j}\Delta t / \Delta C, \quad \bar{c}_{Tr} = \bar{v}^n_{i+1/2,j}\Delta t / \Delta T$$

are the Courant numbers, and the average T velocity component is given by:

$$\bar{v}^n_{i+1/2,j} = \tfrac{1}{4}\left(v^n_{i+1,j+1/2} + v^n_{i,j+1/2} + v^n_{i+1,j-1/2} + v^n_{i,j-1/2}\right).$$

The location of the mesh points used in the scheme (stencil) is *upwind biased*, with more information being provided from upstream, reflecting the physical mechanism of pure advective transport in a mean velocity field. Analogous expressions are derived for the T flux and for different signs of the velocity components, according to the upwind concept.

The boundary of the rectangular domain is assumed to be closed, i.e. it does not allow for probability to leave nor enter the domain. Zero fluxes are then prescribed. In a transient problem this is appropriate if the support of the asymptotic PDF is always located entirely away from the boundary.

The truncation error is $0(\Delta t^2, \Delta t\Delta C, \Delta t\Delta T)$ for unsteady advection. Nonetheless, based on computational tests, MOSQUITO was proved to be as accurate as, but more efficient than, third-order-in-space and second-order-in-time implicit models (for further details see Balzano, 1999).

Because a stability condition for the advection-diffusion scheme cannot be expressed in closed form, guidance for selecting the time step can be given by the sufficient stability conditions of the schemes for pure advection (MOSQUITO) and pure diffusion, deduced from Fourier analysis. This is $\max\{c_x, c_y\} \le 1$ for MOSQUITO, whereas for the scheme for pure diffusion both $\delta_{CC} + \delta_{TT} \le 1$ and $\delta_{CC} + \delta_{TT} + \delta_{CT} \le 1$ must be fulfilled, where $\delta_{CC} = 1/2 q_{CC}\Delta t/\Delta C^2$, $\delta_{TT} = 1/2 q_{TT}\Delta t/\Delta T^2$ and $\delta_{CT} = 1/2 q_{CT}\Delta t/\Delta C\Delta T$ are diffusion numbers.

It must be pointed out that an adaptation of the ULTIMATE flux limiter (Leonard, 1991) has been employed, even though the limiter was originally designed for 1D advection schemes. This scheme has effectively avoided PDF approximations with appreciable negative values, meaning that a basic drawback of most, if not all, previous FPE numerical methods has been adequately resolved.

4. CASE EXAMPLE

The proposed reactor global-nonlinear stochastic KF was tested with experimental runs which correspond to a continuous reactor where carbon monoxide underwent catalytic oxidation to carbon dioxide, in the understanding that these experimental data have been treated with the EKF technique (Baratti et al., 1993). This reactor has a Langmuir-Hinshelwood nonmonotonic kinetics with quadratic inhibition, and open-loop multiplicity with two stable steady-states and an unstable one. Given the reactor deterministic bistability feature and its associated potential bimodality in the open-loop stochastic model system, this example can be seen as an extreme case of a class of industrial exothermic reactors with nonmonothonic kinetics.

4.1 Experimental apparatus

The oxidation of carbon monoxide took place over Pt catalyst pellets, in a continuous micro reactor (see details in Baratti et al., 1993). The reactor and wall temperatures were measured with thermocouples, and the wall temperature acted as a pre-programmed exogenous time-varying input. For stochastic model calibration and estimator behavior assessment purposes, the reactor concentration was on-line measured with a continuous non-dispersive infrared carbon dioxide analyzer.

4.2 Reactor model

In virtue that the reaction occurs in gas phase, the reactant concentration depends on temperature, and, consequently, the reactor model (1) acquires the following form

$$\frac{dx_1}{dt} = \theta(d_1 d_2 - x_1 x_2) - R(x,p) = f_1(x_1, x_2)$$
$$\frac{dx_2}{dt} = \kappa\theta(d_2 - x_2) + \beta R(x,p) + \delta(d_3 - x_2) = f_2(x_1, x_2) \qquad (9)$$
$$R(x,p) = k_0 x_1 \mathrm{Exp}\left[\gamma\left(1 - \frac{1}{x_2}\right)\right](1 + \sigma x_1)^{-2} \qquad y = x_2$$

where

$[x_1, x_2]^T = [C/C_r, T/T_r]^T$,

$[d_1, d_2, d_3]^T = [C_e T_e/(C_r T_r), T_e/T_r, T_w/T_r]^T$

$\gamma = E/(RT_r)$, $\beta = (-\Delta H)c_C/(\rho C_p T_r)$, $\kappa = (\rho c_p)_g/(\rho c_p)$,

$\delta = US/(\rho c_p)$

$\theta = 0.041\ s^{-1}$, $k_0 = 0.066\ s^{-1}$, $\gamma = 16.716$ (dimensionless)

$\sigma = 2.993$ (dimensionless), $\kappa = 0.0006\ s^{-1}$, $\delta = 0.0075\ s^{-1}$.

In dimensionless units (referred to $C_r = 1.052\ mol/m^3$, and $T_r = 463$ K), x_1 (or x_2) is the reactor concentration (or temperature), d_1 is the feed concentration, d_2 (or d_3) is the feed (or wall) temperature, and y is the temperature measurement signal. The product $(\rho c_p)_g$ is the gas-phase heat capacity at the reference temperature, and ρc_p is the overall heat capacity of the basket-pellet system. The parameter triplet (θ, κ, δ) was determined with mass and heat step response tests in the absence of reaction, and the kinetic parameter triplet (β, γ, σ) was determined with a set of isothermal steady-state experiments at various temperatures. The resulting parameter values are listed in (Baratti et al., 1993):

θ=0.041 s^{-1}, k_0=0.066 s^{-1}, γ=16.716 (dimensionless), σ =2.993 (dimensionless), κ =0.0006 s^{-1}, δ =0.0075 s^{-1}.

4.3 Estimator implementation

The implementation of the proposed global-nonlinear stochastic Kushner estimator was executed in a calibration step where the modeling error covariance matrix was tuned,

followed by a testing step where the performance of the KF was evaluated in two different cases.

Calibration. The fact that EKF behavior can be improved with the employment of a non-diagonal 2x2 model error covariance (symmetric) matrix (Leu and Baratti, 2000), in conjunction with the global-nonlinear nature of the Kushner estimation approach, suggests the employment of a similar noise injection mechanism for the Kushner estimator design. Thus, one of the three experimental runs was dedicated to draw the three independent entries of the model error covariance matrix, according to the following procedure: the three parameters were obtained by performing a standard regression plus correlation assessment of model mismatch along the course of the reaction. The resulting error covariance entries are listed in Eq. (10a). The measurement uncertainty was set by looking at the instrument specifications and the standard deviation of the measurement signal, and setting the results in the form of a Gaussian PDF (10b).

$$q_{CC} = 0.38395 \text{ e-}4,\ q_{TT} = 0.2195 \text{ e-}5,\ q_{CT} = -0.8945 \text{ e-}4 \quad (10a)$$

$$\mu(T) = \exp[-(y-T)^2/(2q_w)],\ q_w = 0.187 \text{ e-}6 \quad (10b)$$

Implementation. For the Kushner estimator implementation stage, the error covariance terms q_{CC}, q_{TT} (10a) and q_w (10b) were kept fixed, and the cross error covariance term q_{CT} underwent some refinement. Thus, the model dynamics cross term is the only "tuning" parameter.

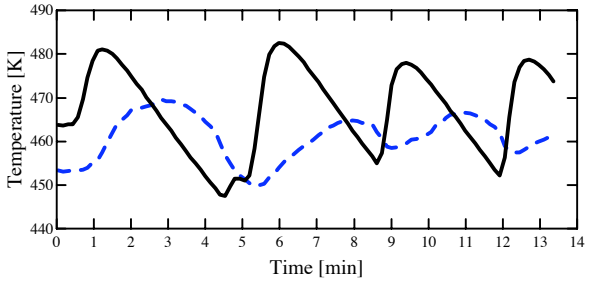

Figure 2. Enforced wall temperature (solid line) and reactor temperature (dotted line).

4.4 Estimator functioning

First, the reactor was subjected to the sequence of wall temperature ramps depicted in Figure 2, with constant inlet CO concentration (0.03). The Kushner implementation did not require any refinement of the model error covariance cross term. As expected, the PDF bimodality of the stochastic model without measurements (Tronci et al., 2009) was switched to monomodality due to the information injected by the measurements. The resulting marginal PDF evolution in contour plot form is presented in Figure 3. Observe how the PDF evolves, with larger uncertainty at high temperature with more model mismatch and stronger asymmetry (non gaussianity). The associated mean concentration estimate and its uncertainty expressed in the form of a standard covariance band are presented in Figure 4. Comparing with the results with standard EKF (Figure 6 in Baratti et al., 1993), the Kushner estimator provides the entire (possibly multimodal or non Gaussian monomodal) PDF, and a considerably better estimate uncertainty assessment (Figure 5). The wideness of the interval is due to the lack of information regarding the cross term in the covariance matrix, that determine the impossibility of reconstructing the second order statistics.

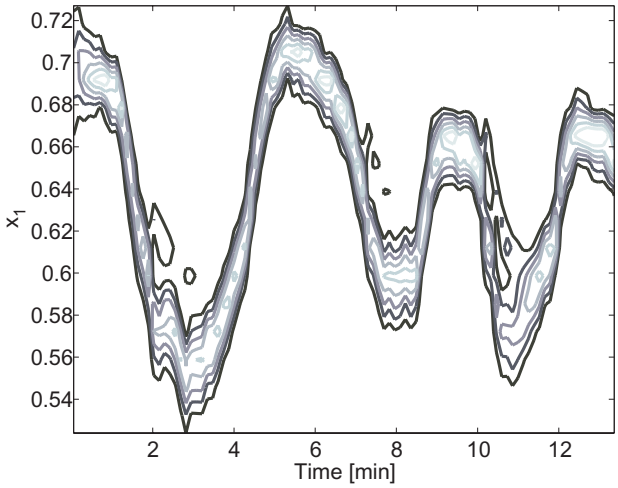

Figure 3. Kushner estimator functioning: PDF evolution in contour level form.

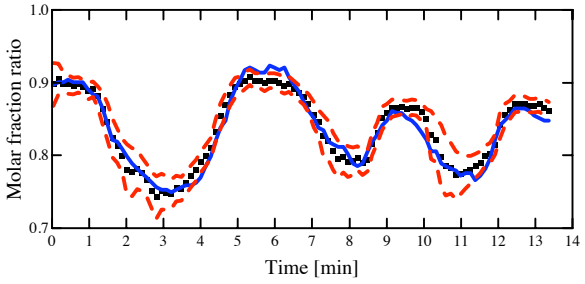

Figure 4. Kushner estimator functioning: CO estimated (or experimental) mole fraction ratio concentration - in red continuous (or black dotted) plot – and estimate uncertainty (blue dotted) band in ± standard deviation (σ) wideness.

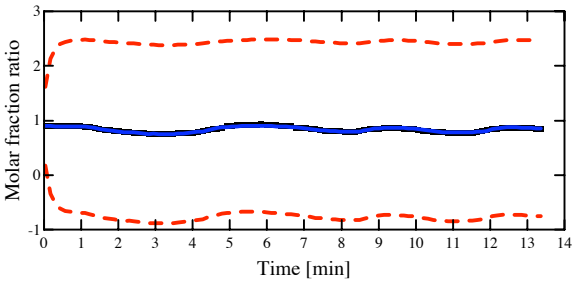

Figure 5. EKF estimate uncertainty (blue dotted) band in ± standard deviation (σ) wideness.

Then the reactor was run with another sequence of temperature ramps (Figure 6a), at a different inlet concentration (0.053), with the results depicted in Figure 6b, showing that: without any further retuning of the cross correlation term the results are similar than the ones of the previous experiment with Kushner estimation. Comparing with the previous experiment, in this case the advantage of

the Kushner over the EKF (see Figure 7 in Baratti et al., 1993) estimator is more pronounced.

It is worth noting that the computational time required by the Kusher estimator is higher with respect to the EKF, but it is still adequate for real time applications. In fact, the time required to simulate one characteristic time of the reactor (circa 30s) is 1.7s.

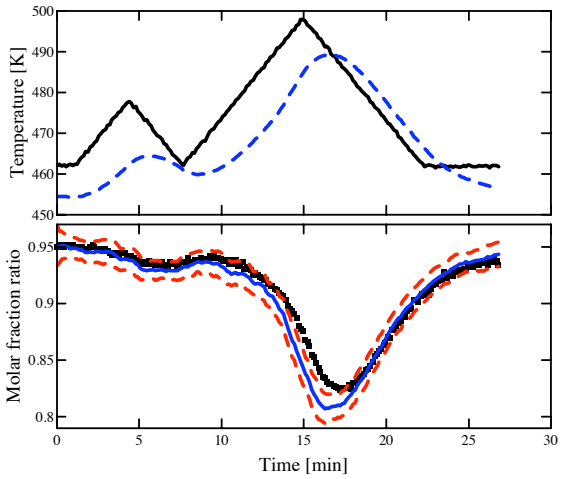

Figure 6. Analysis of the filter performance: (a) enforced wall temperature (solid line) and reactor temperature (dotted line); (b) CO estimated (or experimental) mole fraction ratio concentration - in red continuous (or black dotted) plot – and estimate uncertainty (blue dotted) band in ± standard deviation (σ) wideness.

5. CONCLUSIONS

The concentration estimation problem of exothermic rectors with temperature measurement has been addressed with a Kushner Filtering global-nonlinear stochastic approach, with results that: (i) are validated with experimental data, and (ii) outperform the ones obtained with EKF, in the sense that the entire concentration estimate (possibly multimodal) PDF evolution is obtained. The numerical integration of the FP partial differential equation was effectively and efficiently handled with an approach recalled from computational mechanics. These results evidence the tractability of the Fokker-Planck based Kushner estimation approach, and open the avenue for further studies on the subject, including: the consideration of batch reactor case, the exploitation of system characteristic and Bayesian estimation representation to draw PDF approximation in terms of interlaced low-dimensional Kushner estimators, as a generalization of the adjustable-structure geometric estimation studies for multicomponent distillation column (Frau et al., 2009).

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