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Open and closed-loop stochastic dynamics of a class of nonlinear chemical processes with multiplicative noise

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ABSTRACT

The open and closed-loop global state probability density function behavior of a class of single-state nonlinear chemical processes subjected to additive and multiplicative white noises is characterized with analytic formulae through Fokker Planck (FP) theory, in terms of: (i) stationary state probability density function (PDF), (ii) PDF evolution along deterministic, diffusion, and escape time scales, (iii) conditions for PDF metastability along escape time scale, and (iv) dependency of PDF motion on deterministic dynamics. Comparing with noise additivity, multiplicativeness can yield similar or substantially different open-loop PDF evolution behavior. The application of control to an open-loop (possibly fragile and metastable) multimodal PDF yields a closed-loop robust monomodal PDF with mode regulation capability. The developments and findings are illustrated with numerical simulations of FP's PDE equation.

1. Introduction

Industrial chemical processes operate subjected to exogenous (flow, composition, heat exchange rates, etc.) and endogenous (imperfect mixing-transport, quasi-stationary dynamics, etc.) fluctuations. These processes are modeled by adding additive or multiplicative exogenous noise to first-principle deterministic nonlinear models. Additive and multiplicative noises enter the system through constant and state-dependent gains, respectively, additive noise with respect to deterministic dynamics introduces a state probability density (PDF) distribution with extrema (maxima, minima and inflections) at the deterministic steady-states, and noise multiplicativeness against additivity can create or destroy PDF extrema [1–3]. The need of modeling processes with noise is motivated by a diversity of problems in kinetics and transport modeling [4,5], as well as in safe process [6], monitoring [7] and control [8–10] designs.

The global dynamical behavior of a nonlinear system with noise is formally described by the state PDF evolution, along deterministic, diffusion and escape (related to metastibility) time scales, that satisfies Fokker-Planck's (FPs) partial differential equation (PDE) [1,3,11]. Since the computational load of FP's PDE grows rapidly with dimension, it is solved with: (i) standard (finite difference, element, volume) PDE solvers for the few-state systems [12,13], or (ii) specialized Monte Carlo (MC)-based PDE solvers for many-state systems [14,15]. The FP approach, which has the capability of connecting stochastic and deterministic dynamics, has been applied to a diversity of physics, chemistry, biology, electronic engineering problems [16,17].

While the design of stochastic controllers for linear systems with additive noise is a mature field [18,19], the design of nonlinear systems with multiplicative noise lags far behind. Nonlinear optimal controllers that ensure mean PDF convergence in probability along deterministic time scale for nonlinear systems with multiplicative disturbances have been designed on the basis of a stochastic variation of Hamilton-Jacobi-Isaacs (HJI) nonlinear PDE equation [2]. This approach provides existence-like solvability results and insight, but the control construction is a complicated task, and a complete multiscale PDF description is not provided. Recently, a combined HJI-FP PDE approach has been proposed to perform control design with complete PDF description [20]. This motivates an aim of the present study: the FP-based PDF motion characterization for a single-state nonlinear chemical process system with multiplicative disturbances and PDF mode regulation through linear proportional control.

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Most of the studies on stochastic chemical process systems have been performed with local (about a deterministic SS) MC for open-loop stationary regime with unstructured additive noise, by determining PDF mean and variance through the numerical integration of an ODE [that approximates Langevin's stochastic differential equation (SDE)] forced by random steps [4,5,21]. When the PDF is nearly Gaussian, this MC method yields an adequate PDF mean-variance result, but yields atypical results or breakdown when the stationary PDF is multimodal, especially in close to extrema bifurcation condition. Stationary PDFs have been tractably described with orthogonal polynomial basis representation [22–24]. Dabke et al. [25] reported that, in the additive-to-multiplicative noise passage, a reactor with Brusselator kinetics with flowrate noise underwent induction of limit cycling behavior. Vesterinen and Ritala [26] employed a global version of the SDE-based MC method to describe the bimodal PDF evolution of a two-state bioreactor along deterministic time scale. Ratto [8] and Ratto and Paladino [9] reported that for a two state-chemical reactor with stabilizing linear PI control and temperature noise, the local MC method functioned well in away from deterministic bifurcation, but broke down in close to bifurcation. It was concluded that the assessment of the close-to-bifurcation case requires a complete global-nonlinear PDF modeling approach. The local and global ODE-based MC methods employed in previous chemical process studies cannot: (i) describe the evolution along diffusion time scale and metastability along escape time scale, and (ii) connect stochastic and deterministic dynamics. The global-nonlinear FP PDE-based approach has been applied to formally (with analytic formulae) characterize single-state nonlinear systems with white noise: the stationary PDF of an adiabatic combustion reactor [27], and the PDF evolution along deterministic, diffusion and escape time scales of an isothermal reactor with Langmuir Hinshelwood kinetics [28]. The more complex case with multiplicative noise has been addressed for linear heat exchange systems [29]. These open-loop studies are methodological points of departure for the present study on open and closed-loop single-state nonlinear systems with multiplicative noise.

In this study the problem of formally characterizing (with analytic formula as much as possible) with FP theory the PDF evolution of a class of open and closed-loop single-state multi-noise input nonlinear chemical process systems with additive (unstructured) and multiplicative (structured) noises is addressed, in understanding that, in spite of its simplicity, the class of systems addressed captures the most relevant phenomena that occur in many-state stochastic chemical processes with complex dynamics. The aims are to identify the dependency of the stochastics on deterministic dynamics, and to characterize the PDF evolution in terms of: (i) open- closed-loop stationary state and control PDF, (ii) deterministic, diffusion, and escape time scales along which PDF evolution occurs, and (iii) conditions for PDF metastability along escape time. The development and findings are illustrated with a representative case example, studied before with FP theory for the case of only unstructured additive noise [28]: a nearly isothermal reactor with Langmuir-Hinshelwood kinetics and structured multiplicative noise.

2. Stochastic modeling problem

Consider the nonlinear open-loop process made by the interconnection of the first-principle model (1a) with state x and characteristic time t_x, and unmodeled parasitic dynamics (1b) [30] with state $\boldsymbol{\xi}$ and comparatively smaller characteristic time t_{ξ}:

$$\dot{x} = f(x, \boldsymbol{p} + \tilde{\boldsymbol{p}}) + \tilde{f}\left[x; \boldsymbol{\xi}, \tilde{\boldsymbol{p}}, \boldsymbol{w}_e(t)\right], \quad x(0) = x_o; \quad x \in X \tag{1a}$$

$$\dot{\boldsymbol{\xi}} = \tilde{f}_{\boldsymbol{\xi}}\left[x; \boldsymbol{\xi}(t), \boldsymbol{w}_e(t)\right], \quad \boldsymbol{\xi}(0) = \boldsymbol{\xi}_o; \quad \boldsymbol{\xi} \in X_{\boldsymbol{\xi}}, \quad \boldsymbol{p} \in P \tag{1b}$$

where

$$\tilde{f}(x; \mathbf{0}, \mathbf{0}) = 0, \quad \tilde{f}_{\boldsymbol{\xi}}(x; \mathbf{0}, \mathbf{0}) = \mathbf{0}, \quad dim\boldsymbol{\xi} = n_{\boldsymbol{\xi}}, \quad \boldsymbol{\xi} \in X_{\boldsymbol{\xi}},$$

$\boldsymbol{p}$ is the model parameter and $\tilde{\boldsymbol{p}}$ its error, and $\boldsymbol{w}_e$ is an exogenous input that fluctuates abouts its nominal value $\overline{\boldsymbol{w}}_e = 0$, the nominal value of $\boldsymbol{\xi}$ is $\bar{\boldsymbol{\xi}} = 0$, S is the set of n_s roots $(\bar{x}_i)$ of the nonlinear algebraic equation $f(x, \boldsymbol{p}) = 0$, X, $X_{\boldsymbol{\xi}}$ and P are bounded sets. The term $\tilde{f}$ in Eq. (1a) manifests the effect of the unmodeled parasitic dynamics (1b) on the modeled dynamics [4,5,8,28]. The unmodeled parasitic dynamics (1b) arise from quasi-steady state assumptions like perfect mixing, fast species in a reaction network, and so on. The input fluctuations $(\boldsymbol{w}_e)$ are due to feed flow, composition and temperature variations around mean value. The parasitic error dynamics (1b) are robustly input(x, $\boldsymbol{w}_e$)-to-state($\boldsymbol{\xi}$) stable (in a sense to be precised later) [2], with characteristic time t_{ξ} comparatively shorter (faster) than the one (t_x) of subsystem (1a), i.e.,

$$\boldsymbol{\xi}_o \neq 0, \quad (x, \boldsymbol{w}_e)(t) = 0 \Rightarrow \quad \boldsymbol{\xi}(t) \overset{4t_{\xi}}{\to} 0, \quad t_{\xi} \ll t_x \tag{1c}$$

2.1. Open-loop deterministic dynamics

The errorless modeled dynamics [Eq. (1a) with $(\tilde{\boldsymbol{p}}, \tilde{f}) = (0, 0)$] is given by the *deterministic ordinary differential equation* (ODE):

$$\dot{x} = f(x, \boldsymbol{p}), x(0) = x_o, x \in X = \left[x^-, x^+\right],$$

$$\boldsymbol{p} = \left(p_1, \ldots, p_{n_p}\right)^T \in P \tag{2a}$$

with n_s steady-state (SS) set

$$S = \left\{\bar{x}_1, \ldots, \bar{x}_{n_s}\right\}, \quad f(\bar{x}_i, \boldsymbol{p}) = 0, \quad \bar{x}_i \in X \tag{2b}$$

where X (or P) is the bounded state (or parameter) set. In general, in its parameter space P, this nonlinear system has multiplicity behavior regions delimited by saddle-node, transcritical and pitchfork bifurcation [31]. The solution of this ODE is a state versus time curve, called *motion* [32,33],

$$x(t) = \tau_{\boldsymbol{x}}(t, x_o) \overset{t_{sx}}{\to} \bar{x} \in S, \quad x(t) \in X \tag{3}$$

that reaches asymptotically, with settling time $t_{sx} \approx 4t_x$ where t_x is the characteristic time, one $(\bar{x})$ of the SS's, without nothing important happening thereafter [34,35].

In terms of the Taylor series expansion [2,36,37]

$$f(x, \boldsymbol{p} + \tilde{\boldsymbol{p}}) = f(x, \boldsymbol{p}) + l(x, \boldsymbol{p}; \tilde{\boldsymbol{p}}) + \sigma(x, \boldsymbol{p}; \tilde{\boldsymbol{p}})$$

about $\boldsymbol{p}$, with linear (l) and high-order (σ) terms, the process-error dynamics (1) are written as

$$\dot{x} = f(x, \boldsymbol{p}) + l(x, \boldsymbol{p}; \tilde{\boldsymbol{p}}) + \varpi(x, \boldsymbol{p}; \boldsymbol{w}_e), \quad x(0) = x_o \tag{4a}$$

$$\dot{\boldsymbol{\xi}} = \tilde{f}_{\boldsymbol{\xi}}\left[x; \boldsymbol{\xi}, \tilde{\boldsymbol{\zeta}}(t)\right], \quad \boldsymbol{\xi}(0) = \boldsymbol{\xi}_o \tag{4b}$$

where

$$l(x, \boldsymbol{p}; \tilde{\boldsymbol{p}}) = \sum_{i=1}^{n_p} \gamma_i(x, \boldsymbol{p}) \tilde{p}_i, \quad \gamma_i(x, \boldsymbol{p}) = \partial_{p_i} f(x, \boldsymbol{p}),$$

$$\partial_{p_i} f = \partial f / \partial p_i, \quad \varpi(x, \boldsymbol{p}; \boldsymbol{w}_e) = \tilde{f}[x; \boldsymbol{\xi}, \tilde{\boldsymbol{p}}, \boldsymbol{w}_e(t)] + \sigma(x, \boldsymbol{p}; \tilde{\boldsymbol{p}})$$

where l and σ are structured and unstructured modeling errors, respectively. For typical parameter error sizes $\tilde{\boldsymbol{p}}$, σ is appreciably smaller than l [4].

2.2. Open-loop stochastic dynamics

Following stochastic chemical process studies [4,5,28], let us assume that in Eq. (4): (i) the initial state x_o is a random variable