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On the global nonlinear stochastic dynamical behavior of a class of exothermic CSTRs

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ABSTRACT

The problem of assessing the short and long time effects of stochastic fluctuations on the global-nonlinear dynamics of a class of closed-loop continuous exothermic reactors with temperature control and mono or bistable isothermal dynamics is addressed. The consideration of the problem within a Fokker–Planck (FP) stochastic framework yields: (i) the characterization of the global-nonlinear stochastic dynamics, and (ii) the connection between the deterministic and stochastic modeling approaches. The evolution of the state probability density function (PDF) is explained as the result of a complex interplay between deterministic dynamical features, initial PDF shape, and noise intensity. The correspondence between stationary PDF mono (or bi) modality and deterministic mono (or bi) stability is established, and the stochastic settling time is put in perspective with the deterministic, noise-diffusion, and escape times. The conditions for the occurrence of a retarded response, with respect to deterministic and noise-diffusion times, are identified. The proposed approach: (i) is illustrated with representative case class example, and (ii) constitutes an inductive step towards the development of a general-purpose stochastic modeling approach in chemical process systems engineering.

1. Introduction

Industrial chemical process systems operate subjected to persistent fluctuations, which are due to variations around mean values of actuators, measurements, and high-frequency parasitic dynamics. Since the fluctuation frequencies are faster than the deterministic dynamics, they can be modeled as an exogenous stochastic noise input for the deterministic system. Depending on the system and its operating condition, the stochastic and deterministic modeling approaches can yield similar or considerably different results. For instance, in chemical reactive systems the presence of noise fluctuations can induce or eliminate a steady-state or a limit cycle [1,2] or may explain atypical long term behavior observed in experimental catalytic systems [3,4].

The global dynamical behavior of a stochastic nonlinear system is described by the evolution of the (possibly multimodal) state probability density function (PDF). The related stochastic modeling problem has been addressed with the simulation-oriented Monte Carlo (MC) and the analysis-oriented Fokker–Planck (FP) approaches.

In the *MC approach* [5] a suitable sample of initial conditions and exogenous inputs (including time-invariant parameters) deviations are set, a bundle of discrete-time state motions is generated by running the nonlinear deterministic system over the data sample, and PDF identification-fitting techniques are applied to draw the evolution of the state PDF. The MC method is conceptually simple, can handle high-dimensional (up to ten-state) systems with a diversity of specialized numerical algorithms [5], but becomes cumbersome or intractable when the PDF is multimodal [6], and breaks down when the deterministic system evolves in close-to-bifurcation condition [1,7]. The state of the art on the application of the MC method for chemical processes in general [5] and exothermic reactors [8] can be seen elsewhere, and here it suffices to mention that the MC method is one of the most widely applied stochastic modeling techniques in chemical process.

In the FP approach the PDF dynamics are described by a multidimensional (with one dimension per state) linear partial differential equation (PDE), by a fundamental probability conservation principle with diffusive-convective transport mechanism [9,10]. The FP approach can *a priori* relate, in a qualitative way, important (mono/multimodality, settling time, and metastability) characteristics of the state (possibly multimodal) PDF dynamics with (mono/multistability, SS attractivity, dissipativity) features of the nonlinear deterministic dynamics. Due to the difficulty of solving the underlying FP PDE over an n-dimensional space (with one dimension per state), the quantitative evolution of the state PDF can be drawn for systems with up to four states [11–17]. The capabili-

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