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Stochastic axial dispersion model for tubular equipment

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HIGHLIGHTS

- A stochastic model is proposed for the fluid dynamics of tubular equipment.
- The SDE was built by inserting randomness in the dispersion coefficient.
- A convergence analysis was carried out for numerically solving of SDE.
- An estimator function was developed to calculate the stochastic term.
- The computational confidence intervals were calculated using the Monte Carlo method.

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ABSTRACT

A stochastic model based on the axial dispersion model was proposed for the mathematical representation of the fluid dynamics of tubular equipment with irregular behavior. The differential equation was built by inserting randomness in the dispersion coefficient, which added a stochastic term to the model. This term was capable of simulating fluctuations that may arise in the characterization of tubular equipment using the stimulus-response technique. The model was validated by comparing sample paths and computational confidence intervals with three experimental data sets of a tubular milli-reactor for polystyrene production with different configurations. A convergence analysis was carried out in order to determine the number of elements needed for time discretization. An estimator function was developed to calculate the parameter of the stochastic term, while the parameter of the deterministic term was estimated by the least squares method. The stochastic differential equation was discretized and solved by the Euler-Maruyama method. The computational confidence intervals were calculated using the Monte Carlo method. The results were considered satisfactory, once the model was capable of representing the irregular fluid dynamics of a tubular reactor.

1. Introduction

Continuous production is very important in the industry due to the possibility of achieving higher capacity when compared to batch or semi-batch regimes. Tubular equipment is commonly chosen for continuous operation, since it has a simple geometry, which reduces costs and facilitates maintenance. Reactors, for example, are a fundamental type of equipment in the chemical industry and are often designed as a tube. Stirred tank is also very common, but tubular reactors present some advantages, such as higher heat transfer capacity due to the higher surface to volume ratio (Vega et al., 1997).

Tubular reactors can be represented by a plug-flow reactor (PFR) model, which is an ideal one. It considers that every element of the effluent has the same age and there are no radial gradients along the reactor. Most reactors can be described by an ideal model (Levenspiel, 1998); however, a few of them may have significant nonidealities that require a more detailed representation. An easy and simple way of characterizing a nonideal reactor is using its residence time distribution (RTD) curve. RTD curves can help to diagnose channeling and dead zones and to indicate how to model a flow pattern, since it cannot evaluate the whole system performance alone (Vianna Jr. and Nichele, 2010).

Although there are more sophisticated tools for characterizing equipment, e.g. CFD, RTD curves are still commonly employed for that purpose due to the simplicity of the experimental procedure. Different chemical processes have been analyzed and characterized using the RTD curve, such as separators (Schuur et al.,

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Nomenclature

b	model's stochastic term parameter	t	time
C	tracer concentration	u	fluid velocity
$\mathcal{D}$	Fick's law diffusion coefficient	W	Wiener process
D	axial dispersion parameter	x	relative axial position
F	response curve for a step input using stimulus-response technique	z	actual axial position
L	length of tubular equipment		
Pe	Peclet number		

2012), mixers (Rakoczy et al., 2014), rotary calciners (Gao et al., 2013) and tubular reactors (Hweij and Azizi, 2015). RTD can be expressed mathematically for simulating or predicting equipment performance. Wörner (2010) developed a model for the RTD of laminar flow in a straight rectangular channel from a velocity profile expression for this type of flow. Fan et al. (1995), Harris et al. (2002), and Vianna Jr. and Nichele, (2010) used a stochastic approach for developing an expression for RTD. Fan et al. (1995) proposed a transient RTD expression derived from the stochastic population balance of the elements in a system. Harris et al. (2002) developed a stochastic model based on the Markov chain for simulating the RTD of particles in a riser. Vianna Jr. and Nichele (2010) proposed a stochastic axial dispersion model that could reproduce the irregularities in the experimental responses of a tubular polymerization reactor.

Stochastic models are generally used when the phenomenon to be represented is influenced by probabilistic factors, which can be external disturbances, an intrinsic randomlike characteristic or even a way of simplification. Many authors have worked with stochastic models in the field of chemical engineering. For instance, there are models developed for chemical reactions (Gillespie, 2007; Higham, 2008), simulation of transport in porous media (Fayazi and Ghazanfari, 2015; Stalgorova and Babadagli, 2012), and bioreactors with uncertainties in its environment (Chen and Zhang, 2012).

Here, a mathematical model capable of representing tubular equipment with irregular fluid dynamic behavior is proposed and applied to a tubular milli-reactor for polystyrene synthesis (Vianna Jr. and Nichele, 2010). This model is similar to the one proposed by Vianna Jr. and Nichele (2010), but in this case it is mathematically more consistent. It was developed from the classical axial dispersion equation and its final expression presents a stochastic term, resulting in a stochastic differential equation. This equation was numerically solved by a semi-implicit Euler-Maruyama method. The model has two parameters, Peclet number and a parameter b. The latter was estimated using a methodology proposed by Kelly et al. (2004). To be validated, the model was applied to irregular F curves obtained with three different configurations of a polymerization milli-reactor (Vianna Jr. and Nichele, 2010). The experimental data in question were better represented by this model than by a previously proposed one (Vianna Jr. and Nichele, 2010).

2. Model formulation

The idea of this work was to propose a model capable of simulating residence time distribution (RTD) of tubular equipment with random behavior. At first the (deterministic) axial dispersion model was used to represent the experimental F curve. *Pe* was estimated using the least square method to best fit the experimental data. However, the model could not reproduce the irregular behavior of the experimental F curves. Therefore, a stochastic model was needed for a better representation of those irregularities. This behavior has already been observed in multiphase flows, e.g., slug and stratified flows (Issa and Kempf, 2003).

Nonetheless, the concept of RTD became fundamental in the study of fluid dynamics after Danckwerts (1953) published a paper analyzing different RTD curves. In a nutshell, a RTD curve represents the age of small portions of material when they leave the equipment. It is a good and simple tool and, therefore, very practical for evaluating equipment performance (Levenspiel, 1998).

A RTD curve can be experimentally determined by the stimulus-response technique. In a steady state system, an inert tracer is injected into the entrance and its concentration is monitored at the exit. The most common stimuli are the pulse and step inputs. Using the latter, one obtains the F curve, which is the cumulative distribution function (CDF) of the tracer concentration. It is represented by

$$F(t) = \frac{C(t) - C_0}{C_\infty - C_0} \tag{1}$$

when normalized.

Nonidealities of tubular equipment follow the fluid dynamics of a tube, which is well known. If Reynolds number is high, turbulent flow will be observed, and a PFR model can be assumed. However, if Reynolds number is low, the flow will be laminar, and the velocity profile, a parabola. This profile can be seen like a non-ideality of the PFR model. Axial mixing and molecular diffusion can be sources of non-idealities as well.

For non-ideal tubular equipment, the F curve can be mathematically expressed by the axial dispersion model. It is mostly used for reactor analysis (Palma and Giudici, 2003; Wang, 1995), but it has also been employed to describe other types of equipment, such as heat exchangers (Roetzel and Balzereit, 2000) and rotary calciners (Sudah et al., 2002). An axial dispersion parameter *D*, which represents the degree of axial mixing, is defined and the model is expressed by

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial z^2} - u\frac{\partial C}{\partial z} \tag{2}$$

in an analogy with Fick's law,

$$\frac{\partial C}{\partial t} = \mathcal{D}\frac{\partial^2 C}{\partial z^2}. \tag{3}$$

It is important to emphasize that this parameter *D* and the parameter defined by Fick's law are different despite having the same unit of measurement. *D* is related to the fluid flow and includes nonidealities associated with radial mixing, molecular diffusion and velocity-profile deviations, while $\mathcal{D}$ only represents molecular diffusion (Vianna Jr. and Nichele, 2010).

Taking this into consideration, the initial step for developing the proposed model is assuming that *D* is not necessarily constant and can assume different random values at each instant of time. It is then possible to connect this variation of *D* with oscillations that