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Approximate ODE models for population balance systems

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ABSTRACT

We propose an approximate polynomial method of moments for a class of first-order linear PDEs (partial differential equations) of hyperbolic type, involving a filtering term with applications to population balance systems with fines removal terms. The resulting closed system of ODEs (ordinary differential equations) represents an extension to a recently published method of moments which utilizes least-square approximations of factors of the PDE over orthogonal polynomial bases. An extensive numerical analysis has been carried out for proof-of-concept purposes. The proposed modeling scheme is generally of interest for control and optimization of processes with distributed parameters.

1. Introduction

A variety of methods and numerical integration schemes for first-order hyperbolic partial differential equations (PDEs) of the form:

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x}(G(x,t)f(x,t)) + h(x)f(x,t) = B(t)\delta(x), \tag{1}$$

and extensions thereof beyond advection and birth/death phenomena are spread across the engineering and applied mathematics literature. Such schemes include the method of characteristics (Kumar and Ramkrishna, 1997; Févotte and Févotte, 2010), quadrature method of moments (McGraw, 1997; Qamar et al., 2006; Grosch et al., 2007; Aamir et al., 2009; Marchisio and Fox, 2005), method of weighted residuals or orthogonal collocation (Singh and Ramkrishna, 1977; Rawlings et al., 1992; Chiu and Christofides, 1999), the Monte Carlo simulation (Smith and Matsoukas, 1998), the finite difference schemes/discrete population balances (Kumar and Ramkrishna, 1996), the high-resolution finite volume methods (Koren, 1993; Gunawan et al., 2004), schemes based on the method of characteristics (see, e.g., Kumar and Ramkrishna, 1997; Aamir et al., 2009), etc. A main impetus of the majority of these contributions has been enhancement of efficiency, accuracy and robustness of integration schemes for specific problem classes. New schemes or modifications thereof continue to develop as new applications and resulting numerical challenges arise in population balance systems. In a series of our papers we focused on the structural properties of the approximating models based on systems of ordinary differential equations (ODEs) which amount to various methods of moments. Our proposed scheme shall though not address the general structure of a population balance system, including aggregation and breakage kernels. Various numerical schemes, mainly based on the idea of the Gaussian quadrature have been developed for this purpose, but most of them necessarily need to dispense with a pure ODE structure. Our main concern is somehow opposite to this, as we focus on designing ODE models for process systems described by the PDE Eq. (1). Our approach is useful in the context of trajectory planning and optimal control in batch crystallization (see, e.g., Bajcinca, 2013), real-time model predictive control of population balances (Shi et al., 2005, 2006), robust control of uncertain population balance systems based on a reduced-order modeling approach (Chiu and Christofides, 2000), particle shape manipulation in multivariate crystallization (Patience and Rawlings, 2001; Lovette et al., 2008), etc.

In a previous work, we developed a variety of polynomial approximation methods for designing ODE models for the subclass of systems Eq. (1) with $h(x) \equiv 0$ (Bajcinca et al., 2011, 2014). A utilization thereof in the context of optimal control of batch crystallization for uni- and multivariate PDEs has been done in (Bajcinca, 2013) and in some related references therein. In the present paper, we focus on the extension of the general method of moments that

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Table 1
Nomenclature

Coordinates	
Time	t
Spatial (i.e. internal) coordinate	x
Transformed space coordinates	λ
Displacement in λ	τ
Process variables	
Density function	$f, \tilde{f}$
Initial density	$f_0, \tilde{f}_0$
Birth rate	B
Growth rate	G
Size-independent growth rate factor	G_0
Size-dependent growth rate factor	$\gamma(x)$
Filtering or removal factor	$h(x)$
Net volume referring to f	V_C
Monomial moments	μ_i
Polynomial moments	ν_i

was recently proposed in (Bajcinca et al., 2014) to the class of PDEs of the form Eq. (1) with a filtering term $h(x)f(x,t)$ introduced therein. Such models are useful, for instance, in batch crystallization involving dissolution of small crystal particles (referred to as fines removal or dissolution) or for design of efficient downstream processes by means of filtration. It turns out that in contrast to the case with the term $\gamma(x)$, more precisely, $\gamma(\lambda)$, in a transformed λ-domain introduced in Section 2, application of the least-square approximation techniques – as proposed in (Bajcinca et al., 2014) – directly into the factor $h(x)$, i.e., its corresponding $h(\lambda)$, leads necessarily to an open finite order ODE structure. To circuimvent this difficulty, in this work, we suggest the approximation of the products $h(\lambda)\phi_i(\lambda)$, $i \in \{0, \ldots, p\}$, instead, where $\{\phi_k\}_{k=0}^{p}$ corresponds to an underlying expansion basis of the orthogonal polynomials. We show that such an approach leads to a closed ODE structure. It turns out that thereby a trade-off between the structurally diminishing errors with increasing order p and the resulting numerical round-off errors in the least-square fitting, as well as ODE integration, has to be made. This typically leads to ODE schemes of a larger order than those in cases with $h(x) \equiv 0$ (see Bajcinca et al., 2014). This matter has been confirmed here by extensive numerical simulations in diverse case studies, indicating that generally the proposed method with the h-term introduced, may produce more fragile computational ODE schemes (primarily) with respect to the numerical round-off errors.

The remainder of the article is organized as follows. In Section 2, we provide a preliminary analytical discussion and coordinate transformation leading to a form of the PDE Eq. (1) which is more suitable for the derivation of the method of moments in Section 3. Least square approximation and related numerical techniques are discussed in Section 4. The usability of our computational technique is illustrated in various scenarios on batch crystallization processes with kinetics involving size-dependent growth rate and fines dissolution in Section 6. Additionally, we invoke a numerical scheme based on the method of characteristics and a moving grid in Section 5, which shall serve as the reference computational scheme. The basic nomenclature and notation is given in Table 1.

2. Coordinate transformations and PDE models

In this work, we propose a generalized method of moments for the population balance equation (PBE) of the form:

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x}(G(x,t)f(x,t)) + h(x)f(x,t) = B(t)\delta(x), \tag{2a}$$

with given initial condition:

$$f(x,0) = f_0(x), \quad x \in [0, x_{\max}], \quad \text{otherwise} f(x,0) = 0. \tag{2b}$$

Here, $f(x,t)$, $G(x,t)$, $B(t)$, $h(x)$ and $\delta(x)$ represent the particle density function, the size-dependent growth rate, the birthrate, a fixed filtering function in x, and the Dirac function, respectively. Furthermore, we require the separability condition

$$G(x,t) = \gamma(x)G_0(t), \tag{2c}$$

where $\gamma(x)$ and $G_0(t)$ are both strictly positive functions. In most applications, including our case-study analysis in Section 6, the function $\gamma(x)$ is assumed to be continuous, while the functions $G_0 = G_0(t)$ and $B = B(t)$ are implicitly defined by

$$G_0 = G_0(u(t), \mu(t)), \quad B = B(u(t), \mu(t)), \tag{2d}$$

where $u(t)$ is an external manipulating variable and $\mu(t)$ refers to appropriate moments of the density function $f(x,t)$:

$$\mu_i(t) = \int_{-\infty}^{\infty} x^i f(x,t)\mathrm{d}x, \quad i = 0, 1, \text{etc.} \tag{3}$$

Remark 1. It has been a common practice in the literature to accept 0 rather than $-\infty$ as the lower bound in the latter integration. This is indeed non-critical as we have $f(x,\cdot) \equiv 0$ for $x < 0$. Yet, in light of the presence of the Dirac-term in Eq. (2a), the above moment definition will prove technically easier when deriving our approximate method of moments.

As already mentioned, in addition to the methodological inquisitiveness, there exists a physical motivation for considering the effects of the term $h(x)f(x,t)$ in Eq. (2a). In such applications, typically, the function $h(x)$ reflects a filtering effect, typically, in some interval $x \in [0, x_h]$, $x_h < x_{\max}$, see Section 6.

Remark 2 *(Size-dependent growth factor $\gamma(x)$).* The problem class Eq. (2) refers to a generalization of the problems investigated in our previous work (e.g., Bajcinca et al., 2011), where we studied the effects of the size-dependent term factor $\gamma(x)$ in

$$\frac{\partial f}{\partial t} + G_0(t)\frac{\partial}{\partial x}(\gamma(x)f(x,t)) = B(t)\delta(x). \tag{4}$$

Therein, a coordinate transformation $\lambda = \lambda(x)$ and the scaled density function $\tilde{f} = \tilde{f}(\lambda, t)$ have been introduced as

$$\frac{\mathrm{d}\lambda}{\mathrm{d}x} := \frac{1}{\gamma(x)}, \quad \text{i.e.,} \quad \lambda(x) = \int_0^x \frac{\mathrm{d}\zeta}{\gamma(\zeta)}, \quad \text{and} \tag{5a}$$

$$\tilde{f}(\lambda, t) := f(x(\lambda), t)\gamma(x(\lambda)). \tag{5b}$$

The function $\lambda(x)$ is monotonous, thus, its inverse $x(\lambda)$ is well-defined. With $x(0) = 0$ and $\mathrm{d}x/\mathrm{d}\lambda = \gamma(x)$, we have:

$$\delta(x(\lambda)) = \frac{\delta(\lambda)}{\gamma(0)}, \quad \gamma(0) \neq 0. \tag{5c}$$

Then, substitution of the conditions Eq. (5), transforms (2) (with $h(x) \equiv 0$) into an equation with size-independent growth rate:

$$\frac{\partial \tilde{f}}{\partial t} + G_0(t)\frac{\partial \tilde{f}}{\partial \lambda} = B(t)\,\delta(\lambda). \tag{6a}$$

The scaled density function $\tilde{f}$ is the new unknown function with the initial density $\tilde{f}_0(\lambda)$ defined by

$$\tilde{f}(\lambda, 0) = \gamma(x(\lambda))f_0(x(\lambda)) =: \tilde{f}_0(\lambda). \tag{6b}$$

Observe that in the latter derivation, we tacitly used the identity $\gamma(x)\delta(x) \equiv \gamma(0)\delta(x)$.

Following the same idea, Eq. (2) can be transformed to

$$\frac{\partial \tilde{f}}{\partial t} + G_0(t)\frac{\partial \tilde{f}}{\partial \lambda} + h(\lambda)\tilde{f}(\lambda, t) = B(t)\,\delta(\lambda), \tag{7}$$

where, here (and elsewhere), for convenience, we abuse the formal notation by adopting $h(\lambda) := h(x(\lambda))$.