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Exact solutions of population balance equation

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ABSTRACT

Population balance equations have been used to model a wide range of processes including polymerization, crystallization, cloud formation, and cell dynamics, but the lack of analytical solutions necessitates the use of numerical techniques. The one-dimensional homogeneous population balance equation with time dependent but size independent growth rate and time dependent nucleation rate is investigated. The corresponding system of equations is solved analytically in this paper.

1. Introduction

The current work presents analytical solutions of the population balance equation for a batch crystallizer. Firstly, we present background for the meaning and uses of the population balance equation. The population balance is an equation of continuity for discrete entities (particles, crystals, emulsion droplets, bubbles, and people, among others) having a particular characteristic, which could be a measure of size (diameter or volume of a particle), age, chemical activity, or other characteristic. In our use of it, the population consists of particles or crystals within a crystallizer, or a particular subsection of a crystallizer, and the characteristic of most significance is the particle size based on a particular linear dimension [1,2]. In a well mixed system having only one particle characteristic of interest, the characteristic lengths of the population of particles in the system, the population balance has two independent variables, the particle size, and the time from the initiation of the crystallization. The dependent variable is the population density of crystals of a particular size L at the time t, which is a probability distribution defined for all non-negative values of size and time.

The population balance equation was discussed in [1–3], however it is typically impossible to obtain solutions to these equations for all but the most simple of the realistic industrial systems (for instance steady-state crystallizers with a fully mixed suspension, plug flow crystallizers in the absence of agglomeration or breakage, etc.). The major difficulty is not the ability to produce a fundamental, analytical model of the processes, but the ability to solve models, except numerically. Clearly it would be preferable to have analytical solutions that can describe a range of conditions with a single set of solutions. The problem with the equations describing the systems is that they typically involve both a partial differential equation (the population balance), an integral equation (the equation that represents the time-dependent mass of crystal

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as a function of the crystal population density), and an algebraic equation (the calculation of the growth rate from the concentration of the solute, which is dependent on the mass of crystal). Such systems of equations are typically impossible to find solutions for in most realistic cases.

Many chemical processes, including crystallization, aerosol formation, polymerization, and growth of cell populations, are best described by the population balance equation [4]. In the following we consider the one-dimensional homogeneous population balance equation as used for batch crystallization units

$$\bar{G}(\bar{c}) = k_g\left(\frac{\bar{c}-c_{sat}}{c_{sat}}\right)^g, \quad \bar{B}_0(\bar{c}) = k_b\left(\frac{\bar{c}-c_{sat}}{c_{sat}}\right)^b, \tag{1.1}$$

$$\frac{\partial \bar{f}}{\partial \bar{t}} + \bar{G}(\bar{c})\frac{\partial \bar{f}}{\partial \bar{L}} = 0, \tag{1.2}$$

$$\frac{\partial \bar{c}}{\partial \bar{t}} = -3\rho_{\bar{c}} k_v \bar{G}(\bar{c}) \int_0^\infty \bar{f}\bar{L}^2\, d\bar{L}, \tag{1.3}$$

where $\bar{t}$ denotes the time, $\bar{c}$ is the solution concentration, $\bar{L}$ is an internal coordinate, the characteristic length of the particle (it can also represent age, composition, or other characteristics of an entity in a distribution depending on the system being modeled, although this may alter the mass balance equation), $\bar{f}(\bar{L},\bar{t})$ is the probability distribution representing the number concentration of particles of a particular size, $\bar{L}$, at the time $\bar{t}$ (this is commonly known as the population density), $G(\bar{c})$ is the crystal growth rate, and $\bar{B}_0(\bar{c})$ is the rate of nucleation of particles of zero size. For a seeded batch crystallizer the dominant mechanism of crystal birth is secondary nucleation, and the nucleation kinetics are typically in power-law form [5,6]. Constants k_b, b, k_g and g are the kinetic parameters, $\rho_{\bar{c}}$ is the crystal density, and c_{sat} is the saturated solution concentration. The constant k_v depends on geometry of crystals, in particular, $k_v = 1$ for crystals with the shape of a cube. The integro-differential Eq. (1.3) is a mass balance which gives the solution concentration.

There are a small number of exact solutions to the population balance for a batch crystallizer already known. Largely these come from the work of Tavare et al. [7]. These solutions are for very limited cases – for instance maintaining a constant concentration driving force via evaporation, or a desupersaturation crystallization where the nuclei population density is held constant – that are generally not physically realistic. In addition some solutions may depend on arbitrary and unusual constraints such as the initial values of all moments being equal to zero. Thus, much work has been made in the use of numerical methods to find solutions to the population balance equation. These solutions are less powerful than exact solutions since the system of equations needs to be resolved for any new case considered, however appear necessary because of the lack of exact solutions.

An accurate numerical solution of the population balance equation can be challenging since $\bar{f}(\bar{L},\bar{t})$ can extend many orders of magnitude in size and time, and the rate of change in the distribution can be very sharp at some points. This has led to the development of many specialized algorithms for solving the population balance equation; these methods can be roughly divided into eight categories: variations of the method of moments [8–13], the method of characteristics [14–17], the method of weighted residuals or orthogonal collocation [18,19], Monte Carlo simulation [20–23], spectral methods [24,25], the finite element method [26–29], the finite volume method [30–33], and the method of classes [34,35]. The method of moments approximates the distribution by its moments [3] reducing the dimensionality of the population balance equation. Under certain conditions, the moment equations are closed, that is, the differential equations for the lower order moments do not depend on values for the higher-order moments. If there are only two independent variables, for instance particle size and time, this results in a small number of ordinary differential equations that can be solved very efficiently and accurately using ordinary differential equation solvers. The use of moments reduces the dimensionality of the system (1.1)–(1.3) by taking different averages of the population density along the length $\bar{L}$ axis, by the use of the integral of the population density $\bar{f}(\bar{L},\bar{t})$ with respect to $\bar{L}$. This can directly result in the partial differential Eq. (1.2) representing the population balance to be converted to a series of ordinary differential equations with respect to the moments M_i, $(i = 0, 1, \ldots)$, which simplifies the solution greatly. In particular assume that the zeroth moment is a constant, i.e. $\frac{dM_0}{dt} = 0$, this system was solved for some cases in [7]. However, the main weakness of the method of moments is the moment closure conditions are violated for more complex systems. If $\frac{dM_0}{dt} = C$ the solution is known for the case that $M_i(t=0) = 0$ for all $i \neq 0$. However, if $\frac{dM_0}{dt} \neq C$ then the solution is currently not known.

The principal aim of group analysis approaches [36] is to obtain exact solutions and admitted symmetries, which allow one to make sound decisions in more detailed applied investigations. Classical Lie group theory provides a universal tool for calculating symmetry groups for systems of differential equations. Consequently, group theoretical methods appear efficient in analyzing different phenomena using mathematical models that employ differential equations. However Lie's methods cannot be directly applied to integro-differential equations, e.g. Eq. (1.3). Hence, it is natural to extend the ideas of modern group analysis to these mathematical objects that up to recently were not in mainstream of classical group theoretical approaches. The main obstacle for the application of Lie's infinitesimal technique to integro-differential equation is their nonlocality. Some approaches to overcome these difficulties were proposed by Grigoriev and Meleshko [37]. There are several heuristic ways for overcoming this difficulty. Among these ways the following are known [38,39]:

(1) finding a representation of an admitted group or a solution (on the basis of a priory assumption);