



# Symmetries of population balance equations for aggregation, breakage and growth processes



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## ABSTRACT

The integro-differential population balance equation describing aggregation processes was proposed almost 100 years ago. Aggregation is an important size enlargement process in many industries; the modeling and design of the process can be done using the population balance framework, however it is typically impossible to obtain analytical solutions: in almost every case a numerical solution of the equations must be obtained. In this paper, we present the developed group analysis method for the one-dimensional population balance equation for aggregation in a well-mixed batch system including a crystal growth term. The determining equations are solved, the optimal system, invariant solutions and all the reduced equations are obtained. Furthermore, finding the determining equation by use of the preliminary group classification is also considered.

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## 1. Introduction

We investigate analytical solutions of the population balance equation (PBE) describing an agglomerating system with a crystal growth term. The PBE was discussed in [1–5], however in general the application of initial conditions and auxiliary equations to the population balance results in a multidimensional set of integro-partial-differential equations, for which analytical solutions can rarely be found.

The PBE for a well-mixed batch system of constant volume is given by Randolph and Larson [5]. Hulburt and Katz [2] developed a population balance model for aggregation using volume as the internal coordinate. One-dimensional population balance models for both batch and continuous processes as special cases of the generalized population balance model are more frequently applied to industrial granulation processes than its generalized format.

For a well-mixed batch system with only one internal coordinate  $\bar{x}$  (particle size, volume), the general PBE [1,6] for a system having aggregation and breakage, and also crystal growth is reduced to the form

$$\begin{aligned} \frac{\partial \bar{f}(\bar{x}, \bar{t})}{\partial \bar{t}} = & -\frac{\partial}{\partial \bar{x}} [G\bar{f}(\bar{x}, \bar{t})] + \frac{1}{2} \int_0^{\bar{x}} K(\bar{x} - \bar{y}, \bar{y}) \bar{f}(\bar{x} - \bar{y}, \bar{t}) \bar{f}(\bar{y}, \bar{t}) d\bar{y} \\ & - \bar{f}(\bar{x}, \bar{t}) \int_0^{\infty} K(\bar{x}, \bar{y}) \bar{f}(\bar{y}, \bar{t}) d\bar{y}, \end{aligned} \quad (1.1)$$

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where  $\bar{t}$  denotes the time,  $\bar{f}$  is the one-dimensional number density function, representing the particle number distribution in property space, location space and time space.  $G$  is known as the growth rate function. The growth rate function is not related to aggregation, but to the growth of clusters by mass transfer of solute from solution to the cluster. The symmetric nonnegative kernel function  $K(\bar{x}, \bar{y})$  will be introduced below. The second term on the right hand side of Eq. (1.1) accounts for the formation of a cluster of volume  $\bar{x}$  resulting from the merger of two clusters with respective volumes  $\bar{y}$  and  $\bar{x} - \bar{y}$ ,  $\bar{y} \in (0, \infty)$ , i.e., the coagulation of smaller particles to produce one of volume  $\bar{x}$ . The third term on the right hand side of Eq. (1.1) describes the loss of the cluster of volume  $\bar{x}$  by coagulation with other clusters, i.e., removal of particles of volume  $\bar{x}$  as they in turn coagulate to produce larger particles.

The integro-differential PBE was first proposed by Müller [7] based on Smoluchowski's ground-breaking work for coagulation processes and this equation is in the form of Eq. (1.1) if  $G = 0$ .

The PBE for continuous systems involving aggregation and crystal growth with one internal coordinate  $\bar{x}$  and one external coordinate  $\bar{y}$  is given by

$$\begin{aligned} \frac{\partial \bar{f}(\bar{x}, \bar{y}, \bar{t})}{\partial \bar{t}} &= -\frac{\partial}{\partial \bar{x}}[G\bar{f}(\bar{x}, \bar{y}, \bar{t})] - \frac{\partial}{\partial \bar{y}}[Z\bar{f}(\bar{x}, \bar{y}, \bar{t})] \\ &+ \frac{1}{2} \int_0^{\bar{x}} K(\bar{x} - \bar{z}, \bar{z})\bar{f}(\bar{x} - \bar{z}, \bar{y}, \bar{t})\bar{f}(\bar{z}, \bar{y}, \bar{t}) d\bar{z} - \bar{f}(\bar{x}, \bar{y}, \bar{t}) \int_0^{\infty} K(\bar{x}, \bar{z})\bar{f}(\bar{z}, \bar{y}, \bar{t}) d\bar{z}, \end{aligned} \tag{1.2}$$

where  $\bar{t}$  denotes the time,  $\bar{f}$  is the one-dimensional population density function,  $G$  is the growth rate function. The spatial velocity is defined as the rate of change of position on the  $\bar{y}$ -axis with respect to time  $\bar{t}$ , that is

$$Z = \frac{d\bar{y}}{d\bar{t}}.$$

The merging of clusters of volume  $\bar{x}$  and volume  $\bar{y}$  to produce clusters of volume  $\bar{x} + \bar{y}$  occurs at a rate modulated by a symmetric nonnegative kernel function  $K(\bar{x}, \bar{y})$ , i.e.

$$K(\bar{x}, \bar{y}) = K(\bar{y}, \bar{x}) \geq 0. \tag{1.3}$$

It is affected by two major factors: (I) the collision probability of the specified pair of particles, and (II) successful coalescence or rebounding after collision. The first factor mainly depends on the particle sizes, granulator configuration, particle flow patterns and operating conditions. The second issue has been intensively studied by [8] with the identification of the following aspects as being most important in the success of coalescence: elastic-plastic properties, viscous fluid layer, energy of the collision, and the energy balance. The wider class of coagulation kernels [6,9,10] arising in applications are homogeneous. That is, there is  $\gamma$  such that

$$K(\alpha\bar{x}, \alpha\bar{y}) = \alpha^\gamma K(\bar{x}, \bar{y}), \tag{1.4}$$

for every  $\alpha, \bar{x}, \bar{y} > 0$ . By means of homogenous kernel (1.4), it is easy to show that

$$\bar{x}K_{\bar{x}}(\bar{x}, \bar{y}) + \bar{y}K_{\bar{y}}(\bar{x}, \bar{y}) = \gamma K(\bar{x}, \bar{y}), \tag{1.5}$$

then the general solution to Eq. (1.5) is given by

$$K(\bar{x}, \bar{y}) = \bar{y}^\gamma H\left(\frac{\bar{x}}{\bar{y}}\right), \tag{1.6}$$

here  $H$  is an arbitrary differentiable function of one variable. Particular cases of homogeneous kernel (1.4) are

$$K(\bar{x}, \bar{y}) = k_0, \quad k_1(\bar{x} + \bar{y}), \quad k_2\bar{x}\bar{y}, \tag{1.7}$$

where  $k_0, k_1$  and  $k_2$  are positive constants. These kernels are amenable to a complete mathematical analysis, and provide valuable heuristic hints for general kernels; they are also of physical interest and of particular interest to specialists.

Although the integro-differential PBE has been proposed for nearly 100 years [7], an exact analytical solution for it nearly cannot be achieved in realistic industrial systems. For instance, the PBEs (1.1) and (1.2) are a strong non-linear equation with the same mathematical structure as Boltzmann's transport equation; they are frequently applied to industrial granulation processes. However, the analytical solution of these equations still remains a challenging issue.

Group analysis was developed especially for differential equations [11]. The major obstacle for the application of Lie's infinitesimal techniques to integro-differential equations or infinite systems of differential equations is that the frames (see, e.g. [11]) of these equations are not locally defined in the space of differential functions. Consequently, the vital idea of splitting of the determining equations into over-determined systems, usually used in the classical Lie group analysis, fails. Some approaches to overcome these difficulties were proposed in [12]. There are several heuristic ways [13,14] for overcoming this difficulty.

There are some different known approaches to calculating symmetry group for integro-differential equations. Loosely speaking, these approaches can be divided into two large groups: indirect and direct methods.

The first indirect method is the method of moments: the system of basic integro-differential equations that usually contains nonlocal terms depending on moments is reduced to an infinite system of differential equations for these moments.

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