POPULATION BALANCE EQUATION: A TOOL FOR DYNAMIC MODELING OF PARTICULATE PROCESSES

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Abstract

Particulate processes are often encountered in industry. The polydispersity of some key properties characterizes particulate processes and makes them ill-suited to be modeled within the framework of conventional conservation equations only. In the mid 60s a tool called Population Balance Equation was developed to quantify the dynamics of particulate processes. This paper aims to give an introduction to the Population Balance Equation and review its state of the art.

Introduction

Particulate processes are encountered in many applications and are widely used in the production of valuable industrial products. Crystallization, biochemical processes, polymerization, leaching, comminution, and aerosols are just some examples of particulate processes. Such processes differ considerably from one another but they all are characterized by the presence of a continuous phase and a dispersed phase comprised of entities with a distribution of properties, such as size, chemical composition, etc. The entities typically interact with one another as well as with the continuous phase. Such interactions may vary from entity to entity. Therefore, the polydispersity of particulate processes affects significantly the behavior of such systems, thus affecting the quality of the final products. Moreover, the polydispersity makes particulate processes ill-suited to be modeled within the framework of conventional conservation equations only.

This paper deals with the Population Balance Equation, a tool to quantify the dynamics of particulate processes, which was developed in the mid 60s and since then has experienced wide acceptance and use in the field of particulate processes. This paper describes the formulation of the Population Balance Equation, and reviews the strenghts, the weaknesses and the status of this approach.

Formulation

The Population Balance Equation was originally derived in 1964, when two groups of researchers studying crystal nucleation and growth recognized that many problems involving change in particulate systems could not be handled within the framework of the conventional conservation equations only, see Hulbert & Katz (1964) and Randolph (1964) . They proposed the use of an equation for the continuity of particulate numbers, termed population balance equation, as a basis for describing the behavior of such systems. This balance is developed from the general conservation equation

$$\text{Accumulation} = \text{Input} - \text{Output} + \text{Net Generation} \qquad (1)$$

applied to the number of entities having a specified set of n properties ζ_i i = 1,2...n. The properties ζ_i to be considered for the number balance will depend on the application. Typical examples are the entity's size diameter, entity's chemical composition, entity's age... In equation 1, all the terms represent number of entities with the specified property in a given interval, each term being related to certain transport, generation or destruction processes. Thus the accumulation term is the change of number of entities in a given property interval by accumulation in the system, the input and output terms are related to convective flow, the generation term includes both generation and destruction by continuous or discrete processes. Examples of continuous processes are chemical reaction or precipitation. Discrete generation processes are those giving birth or death of entities in a given property interval such as nucleation (birth), agglomeration (birth) or breakage (death).

The derivation of the Population Balance Equation is equivalent to the development of the conventional equations of change, i.e. the number balance shown in equation 1 is applied to a volume element of the system $\Delta x\ \Delta y\ \Delta z$ fixed in the space, the resulting equation is divided by the volume element and the limit as Δx Δy Δz go to zero is taken. By doing this, the microscopic Population Balance Equation is obtained

$$\frac{\partial \Psi}{\partial t} = -\frac{\partial (v_x \Psi)}{\partial x} - \frac{\partial (v_y \Psi)}{\partial y} - \frac{\partial (v_z \Psi)}{\partial x} - \sum_{i=1}^{n} \frac{\partial (v_{\zeta_i} \Psi)}{\partial \zeta_i} + B - D \qquad (2)$$

where $\Psi(t, x, y, z, \zeta_1, \zeta_2, ..., \zeta_n)$ is the number density distribution, v_j j = x, y, z is the velocity of propagation of entities along the spatial coordinate axes x, y, z , whereas $v_{\zeta j}$ is the velocity of property coordinate axes ζ_i, D is the rate of death of entities and B is the rate of birth of entities. Therefore, the partial derivative with respect to time represents the accumulation term, the partial derivatives with respect to the spatial coordinate axes represent the convective transport term, the partial derivatives with respect to the property coordinate axes represent the continuous generation term and D and B give the discrete generation term. For more details about the derivation of the Population Balance Equation, the reader is referred to the original work by Hulburt & Katz (1964) and Randolph (1964).

It is therefore not surprising that equation 2 shows an obvious resemblance with the conventional equations of transport. For example, the equation of continuity is given by (Bird, Stewart & Lightfoot, 2002)

$$\frac{\partial \rho}{\partial t} + \frac{\partial (v_x \rho)}{\partial x} + \frac{\partial (v_y \rho)}{\partial y} + \frac{\partial (v_z \rho)}{\partial x} = 0 \qquad (3)$$

Nevertheless, note some important differences between the conventional equations of transport and the Population Balance Equation. First, the discrete generation term does not have a counterpart in the conventional equations of transport. But, more importantly, the Population Balance Equation is a functional equation not a scalar equation. The latter explains why the Population Balance is typically more difficult to solve mathematically than the conventional equations of transport.

There are many examples in physical modeling where the spatial variation might be neglected, and where the interest lies in studying the global behavior of the system. This led to the development of the macroscopic balances in transpor phenomena theory. Similarly, there are many instances in the field of particulate processes in which the macroscopic behavior is of main interest. Therefore, a macroscopic version of the Population Balance Equation was developed

$$\frac{1}{V}\frac{d(V\overline{\psi})}{dt} = \frac{1}{V}\left(Q_{in}\overline{\psi}_{in} - Q_{out}\overline{\psi}_{out}\right) - \sum_{i=1}^{n} \frac{\partial (v_{\zeta_i} \overline{\psi})}{\partial \zeta_i} + \overline{B} - \overline{D} \qquad (4)$$

where $\overline{\psi}$ $(t, \zeta_1, \zeta_2, ..., \zeta_n)$ is the geometrically averaged number distribution, i.e. it represents the number of entities in the given property interval per unit volume. In equation 4, the derivative with respect to time represents the accumulation term, the first two terms on the r.h.s represent the convective transport term, the derivative terms with respect to the property coordinate represent the net continuous generation term and the averaged birth rate $\overline{B}$ minus the averaged death rate $\overline{D}$ represent the net discrete generation term.

The macroscopic Population Balance Equation is the version that has been most widely used in practical applications, and the version that has attracted most attention.

Pros and cons of the Population Balance Equation

The secret of the success of the Population Balance Equation for dynamic modeling of particulate processes lies in its ability to describe systematically the polydispersity of such processes. Moreover, the Population Balance Equation is able to describe mathematically a wide range of complex events affecting such processes. Some good examples of complex events that can be accounted for in the Population Balance Equations are the nucleation phenomena taking place in crystallization, the disintegration of particles in comminution, the aggregation event in polymerization, etc. Finally, another advantage of this tool comes from its general character and wide application. Any advance that might be obtained for one certain application can easily be extended to other applications. For a good review of applications, the reader is referred to Ramkrishna (2000).

However, the application of the Population Balance Equation presents also certain drawbacks. The main problem is that the resulting formulations may be mathematically challenging. The macroscopic balance equation, when all terms are used, typically yields to an integrodifferential equation. Analytical solution of integrodifferential equations is in most cases impossible. Fortunately, extensive research has been devoted to the solution of Population Balance Equations. The method of moments, as developed by Hulburt & Katz (1964), is the most widely used method to reduce integro-differential equations into a set of Ordinary Differential Equations (ODEs), but it is not always applicable because this method may lead to an open set of equations. Examples of numerical solution methods proposed in the literature (Ramkrishna, 1985; Ramkrishna, 2000) are: the method of weighted residuals, the method of self-preserving distributions, Monte Carlo simulation techniques, the size interval-by-size marching method and discretization via fixed/moving pivot techniques. Discretization techniques are widely used and might lead to a system of Differential and Algebraic Equations (DAEs). An example about the use and solution of a Population Balance Equation yielding a DAE system can be found in Dueñas Díez, Ausland, Fjeld & Lie (2002).

State of the Art

In the last decade, the focus has been displaced from finding solution methods to using explicitely the Population Balance Equation models for control purporses. The first notable attempt was the controllability analysis suggested in Semino and Ray (1995) and applied to emulsion polymerization Semino and Ray (1995b). Chiu & Christofides (1999, 2000) successfully applied nonlinear output feedback controllers to a crystallization process. Model predictive control, which is a control framework that has spread in the process industry during the last decades, has also received a great deal of attention in the field of particulate processes in the last decade. Eaton & Rawlings (1990) used nonlinear programming to solve the nonlinear model predictive control formulation of a batch crystallizer. Nonlinear model predictive control was also used in Crowley, Meadows, Kostoulas & Doyle (2000) to optimize the performance of a semibatch emulsion polymerization reactor. Linear model predictive control has been proposed for the stabilization of oscillating microbial cultures in bioreactors Zhu, Zamamiri, Henson & Hjortsø (2000).

Conclusion

This paper gives an introduction to the Population Balance Equation, a tool for dynamic modeling of particulate processes which has received a great deal of acceptance due to its ability to describe the polydispersity and the complex events often encountered in particulate processes. The derivation of the Population Balance Equation is similar to the derivation of the equations of transport, but leads to functional equations which are difficult to solve. Indeed, the search for ways of overcoming the mathematical complexity of the resulting formulations focused during several decades all the attention and research effort. Nowadays several solution aproaches, both analytical and numerical, are available, and the main focus is to integrate the Population Balace Equation models with process control.

References

Bird, R.B., Stewart W.E. & Lightfoot, E.N. (2002), *Transport Phenomena*, John Wiley & Sons, Inc. 2nd Edition.

Chiu, T. & Christofides, P. (1999), 'Nonlinear control of particulate processes', *AIChE Journal* **45**(6), 1279–1297.

Chiu, T. & Christofides, P. (2000), 'Robust control of particulate processes using uncertain population balances',*AIChE Journal* **46**(2), 266–280.

Crowley, T. J., Meadows, E. S., Kostoulas, E. & Doyle, F. J. (2000), 'Control of particle size distribution described by a population balance model of semibatch emulsion polymerization', *Journal of Process Control* **10**, 419–432.

Dueñas-Díez, M., Ausland, G., Fjeld, M. & Lie, B. (2002), 'Simulation of a hydrometallurgical leaching reactor modeled as a DAE system', *Modeling, Identification and Control*, In press.

Eaton, J. W. & Rawlings, J. B. (1990), 'Feedback control of chemical processes using on-line optimization techniques', *Computers and Chemical Engineering* **14**(4), 469–479.

Hulburt, H. M. & Katz, S. (1964), 'Some problems in particle technology — A statistical mechanical formulation', *Chemical Engineering Science* **19**, 555–574.

Kalani, A. & Christofides, P. D. (2000), 'Modeling and control of a titania aerosol reactor', *Aerosol Science and Technology* **3**2, 369–391.

Ramkrishna, D. (1985), 'The status of population balances', *Reviews in Chemical Engineering* 3, 49–95.

Ramkrishna, D. (2000), *Population Balances. Theory and applications to particulate systems in engineering*, Academic Press.

Randolph, A. (1964), 'A population balance for countable entities', *The Canadian Journal of Chemical engineering* **4**2, 280–281.

Semino, D. & Ray, W. (1995a), 'Control of systems described by population balance equations — i. controllability analysis', *Chemical Engineering Science* **5**0(11), 1805–1824.

Semino, D. & Ray, W. (1995b), 'Control of systems described by population balance equations — II. emulsion polymerization with constrained control action', *Journal of Chemical Engineering* **5**0(11), 1825–1839.

Zhu, G.-Y., Zamamiri, A., Henson, M. A. & Hjortsø, M. A. (2000), 'Model predictive control of continuous yeast bioreactors using cell population balance models', *Chemical Engineering Science* **5**5, 6155–6167.