Stochastic Monte Carlo simulation for the solution of the dynamic population balance equation in batch particulate systems

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In the present wok, an efficient stochastic Monte Carlo (MC) algorithm is presented for the numerical solution of the dynamic population balance equation (PBE) in batch particulate processes undergoing simultaneous particle aggregation, growth and nucleation.

The general uni-variate population balance equation for a batch particulate system can be written as follows:

$$\frac{\partial n(V,t)}{\partial t} + \frac{\partial [G(V)n(V,t)]}{\partial V} = \int_{0}^{V/2} \beta (V-U,U) n (V-U,t) n (U,t) dU - (1)$$

$$n (V,t) \int_{0}^{\infty} \beta (V,U) n (U,t) dU + S(V,t)$$

where n(V,t)dV denotes the number of particles per unit volume in the size range [V, V+dV]. G(V) and S(V,t) are the particle volume growth rate and the particle nucleation rate, respectively and $\beta(V,U)$ is an aggregation rate kernel for particles of volumes V and U. In general, Eq. (1) will satisfy the following initial condition: $n(V,0) = n_0(V)$, where $n_0(V)$ is the initial number density function. If the value of the number density function at the minimum particle volume, $n(V_{min}, t)$, is known, the corresponding boundary condition for Eq. (1) takes the following form: $n(V_{min}, t) = n_1(t)$.

The general bi-variate PBE for a batch particulate system is given by:

$$\frac{\partial n(V, x, t)}{\partial t} + \frac{\partial [G_v(V, x)n(V, x, t)]}{\partial V} + \frac{\partial [G_x(V, x)n(V, x, t)]}{\partial x} =$$

$$+S(V, x, t) + \int_{V_{\min}}^{V/2} \int_{x_{\min}}^{x/2} \beta(V - U, x - z, U, z)n(V - U, x - z, t)n(U, z, t)dUdz$$

$$-\int_{V_{\min}}^{V_{\max}} \int_{x_{\min}}^{x_{\max}} \beta(V, U, x, z)n(V, x, t)n(U, z, t)dUdz$$
(2)

In accordance to the uni-variate PBE, n(V, x, t)dVdx denotes the number of particles per unit volume in the size range [V, V+dV] having the property x in the range [x, x+dx]. Furthermore, Licensed under the Creative Commons Attribution Noncommercial No Derivatives $\beta(V, U, x, z)$ denotes the aggregation rate kernel between particles with volumes V and U and internal properties x and z, respectively. The initial condition of Eq.(2) is $n(V, x, 0) = n_0(V, x)$ and the boundary conditions that may be used are $n(0, x, t) = n_x(x, t)$ and $n(V, 0, t) = n_V(V, t)$.

The stochastic Monte Carlo (MC) method is based on the principle that the dynamic evolution of an extremely large population of particles (e.g., 10^{12}) can be followed by tracking down the corresponding changes or events (i.e., growth, aggregation, nucleation) occurring in a smaller number of sample particles, (e.g., 10^5). Initially, the particle volume and/or the second internal property domains are divided into a number of discrete volume intervals using a logarithmic discretization rule. Subsequently, each particle in the sample population is assigned to an appropriately selected volume, V_i, and an appropriately selected value of the internal property, x_i, so that the particle array at time zero, N_s(0), closely represents the initial distribution, according to the "inverse transform method" (Rubinstein, 1981). Once all the particles in the sample population have been assigned to randomly selected volumes, the MC algorithm is initiated and the effects of particle aggregation, growth and nucleation mechanisms on the dynamic evolution of the particle population are stochastically simulated in a consecutive series of variable-duration time steps.

In problems involving particle aggregation, the time step can be determined in terms of the number of aggregation events, N_{agg} , that take place (Gooch et al., 1996). According to the above procedure, the time required for the occurrence of the duration of N_{agg} events, Δt , will be given by the following equation:

$$\Delta t = \int_{m_0}^{m_0 - \Delta m_0} \left[\int_0^{\infty} \left[B(V) - D(V) \right] dV \right]^{-1} dm_0$$
(3)

where $m_0(t)$ and $\Delta m_0(t)$ denote the total number of particles and the change in the total number of particles due to aggregation. In the absence of particle aggregation, the time step does not need to be explicitly calculated via Eq. (3) and, therefore, it can be arbitrarily set in the MC algorithm.

Numerical solution of the uni-variate PBE.

Detailed numerical simulations were carried out for several batch particulate processes undergoing particle aggregation, growth and nucleation and the calculated distributions were compared with available analytical solutions (Scott, 1968; Ramabhadran et al. 1976). Several particle aggregation rate functions (i.e., constant and sum aggregation kernels) and particle growth rate functions (i.e., size independent and size dependent) were considered. The particle nucleation rate function was size-dependent assumed to follow an exponential, functional form (i.e., $S(V,t) = (N_{0s}/V_{0s}) exp(-V/V_{0s})$, where N_{0s} and V_{0s} are some characteristic values of the distribution). Finally, the initial number density function, n(V, 0), was assumed to follow an exponential dependence with respect to the particle volume, $n(V,0) = (N_0 / V_0) exp(-V / V_0)$. For the presentation of the results, the following dimensionless aggregation, τ_a , and growth, τ_g , time constants were defined (Alexopoulos et al. 2004):

 $\tau_{_{a}}=\beta_{_{0}}V_{_{0}}^{^{\gamma}}N_{_{0}}t\qquad \qquad ;\qquad \qquad \tau_{_{g}}=t\,G_{_{v}}(V_{_{0}})/\,V_{_{0}}$

where β_0 , N₀ and V₀, are some characteristic values of the aggregation rate constant, particle number and particle volume, respectively.

In Fig. 1, the MC calculated distribution is compared with the analytical solution for the case of pure aggregation with a constant aggregation rate ($\beta(V,U) = \beta_0$), for two different values of the dimensionless aggregation time (i.e., $\tau_a = 10^3$ and $\tau_a = 10^6$). Fig. 2 depicts the comparison of the MC calculated PSD with the analytically calculated distribution for the case of sum particle aggregation ($\beta(V,U) = \beta_0(U+V)$). Fig. 3 depicts the comparison of the distributions calculated by the MC method with the analytical ones for the case of combined constant particle aggregation ($\beta(V,U) = \beta_0$) and constant particle growth ($G(V) = G_0$), for two different sets of aggregation and growth times (i.e., $\tau_a=10^2$, $\tau_g = 1$ and $\tau_a=10^2$, $\tau_g = 10$). Finally, in Fig. 4, the MC calculated distribution is compared with the analytical distribution for the case of combined linear particle growth ($G(V) = G_0V$) and exponential particle nucleation ($S(V,t) = (N_{0s}/V_{0s})\exp(-V/V_{0s})$). It is important to point out that, to the best of our knowledge, it is the first time that MC results are reported for such long aggregation and growth times.

It is evident that for the cases studied, there is an excellent agreement between the MC calculated distributions and their corresponding moments with the analytical solutions. Furthermore, the computational requirement of the method is substantially low (see Table 1). Finally, it should be noted that, in all cases, the distributions calculated by the MC algorithm were the outcome of a single simulation run.

Numerical solution of the bi-variate PBE.

Detailed numerical simulations were carried out for several batch particulate processes undergoing particle aggregation and growth, where analytical solutions of the bi-variate PBE were available (Gelbard and Seinfeld, 1978). The initial number density function, n(v, x, 0), was assumed to follow an exponential dependence with respect to the particle volume, $n(V, x, 0) = (N_0 / (V_0 x_0)) \exp(-V / V_0) \exp(-x / x_0)$.

Figs. 5, 6 and 7 depict the contour plots for the cases of constant particle aggregation ($\beta(V,U,x,z) = \beta_0$), constant particle growth ($G_V(V,x) = G_x(V,x) = G_0$) and linear particle growth rates ($G_V(V,x) = G_0V$, $G_x(V,x) = G_0x$), respectively. Finally, Fig. 8 depicts the MC and analytical contour plots for the case of combined constant particle aggregation ($\beta(V,U,x,z) = \beta_0$) and linear particle growth ($G_V(V,x) = G_0V$, $G_x(V,x) = G_0x$). It is apparent that there is a very good agreement between the MC calculated distributions and the analytical solutions. Furthermore, the leading moments of the distribution are calculated by the MC method with good accuracy.

The above comparisons showed that the developed MC algorithm was capable of predicting the dynamic evolution of the uni-variate and bi-variate PSDs, as well as the leading moments of the distributions, with high accuracy, having, at the same time, low computational requirements. The accuracy of the method can be furthermore improved via the use of a larger sample population, which will lead to higher computational requirements and extended simulation times.



Figure 1: Comparison of dynamic PSDs for constant particle aggregation



Figure 3: Comparison of dynamic PSDs for combined constant particle aggregation and constant particle growth



Figure 5: Comparison of dynamic bivariate PSDs for constant particle aggregation ($\tau_a = 1$); a) analytical solution, b) MC simulation



Figure 2: Comparison of dynamic PSDs for sum particle aggregation



Figure 4: Comparison of dynamic PSDs for combined linear particle growth and exponential particle nucleation



Figure 6: Comparison of dynamic bivariate PSDs for constant particle growth

 $(\tau_g = 1);$ a) analytical solution, b) MC simulation



Figure 7: Comparison of dynamic bivariate PSDs for linear particle growth ($\tau_g = 3$); a) analytical solution, b) MC simulation



Figure 8: Comparison of dynamic bivariate PSDs for combined constant particle aggregation ($\tau_a = 1$) and linear particle growth ($\tau_g = 1$); a) analytical solution, b) MC simulation

Table 1	• Simulation	times	and	percent	errors	in	the	MC	calculated	zeroth	and	first	order	moments	of	the
distribution for various batch particulate processes.																

Case	Aggregation kernel	Growth rate model	Time, τ_{α}	Time, τ_g	m ₀	m ₁	Error in m ₀	Error in m ₁	CPU time, sec
1.1	βο	-	10 ³	0	1.9959 10 ⁻²	1.000579	0.00 %	0.06 %	3.1
1.2	βο	-	10 ⁶	0	1.9999 10 ⁻⁶	9.9797 10 ⁻¹	0.00 %	0.20 %	6.7
2.1	$\beta_0(V+U)$	-	3	0	4.9700 10 ⁻²	1.0005796	0.17 %	0.06 %	10. 7
2.2	$\beta_0(V+U)$	-	6	0	2.4701 10-3	1.0005796	0.35 %	0.06 %	137.1
3.1	βο	G_{0}	100	1	1.9608 10 ⁻²	1.0792141	0.00 %	0.05 %	305.0
3.2	βo	G_{0}	100	10	1.9608 10 ⁻²	1.7869251	0.00 %	0.03 %	301.2
4.1 ^a	-	G_0V	0	1	100.1775	19.78475	0.18 %	0.58 %	247.4
4.2 ^a	-	G_0V	0	10	100.1775	43549.85	0.18 %	1.14 %	247.5
Case	Aggregation kernel	Growth rate model	Time, τ_{α}	Time, $ au_{g}$	m ₀₀	m ₁₀ =m ₀₁	Error in m ₀₀	Error in m ₁₀	CPU time, sec
5	βο	-	1	0	0.666706	1.0629667	0.00 %	6.3 %	1182
6	-	G_{0}	0	1	1	2.062966	0.00 %	3.15 %	94.9
7	-	G_0V	0	3	1	21.350258	0.00 %	6.29 %	1354
8	β ₀	G_0V	1	1	0.666706	2.889443	0.00 %	6.58 %	1662

^aCombined with exponential nucleation.

Litterature

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