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On a new family of sectional methods for the solution of the coagulation population balance

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Abstract

Sectional (zero order) methods constitute a very important class of methods for the solution of the population balance equation offering distinct advantages compared to their competitors, namely, higher order and moment methods. For the last ten years a particular sectional method, the so called fixed pivot technique [1] has been the most extensively used in the scientific community for the solution of the coagulation equation because it offers arbitrary grid choice and conservation of two moments of the particle size distribution. Very recently, a new method (called cell average technique [2]) has been developed which gives more accurate results than the fixed point technique. In the present work, the extension of this new method in order to conserve three moments is attempted. A stable algorithm for the solution of the coagulation equation is developed. The new method allows improved computation of moments of practical interest.

Keywords: Coagulation equation, population balance, sectional methods.

1. Introduction

Coagulation is a very important phenomenon for several processes of technological as well as of fundamental scientific interest. This phenomenon

alone or in combination with other particle level phenomena as fragmentation, growth-dissolution, particle size domain diffusion etc, concerns several scientific disciplines. For example, regarding industrial aerosol processes, coagulation is an important step for nanoparticle production whereas regarding atmospheric aerosols it influences the evolution of particles morphology in atmosphere. In atmospheric sciences, it is related to rain formation and in astrophysics it concerns the first steps in planet formation. Other processes where coagulation is of paramount importance are the crystallization, precipitation, pelletization and granulation. The dynamics of a particle population undergoing coagulation is described by the coagulation equation that belongs to the more general class of the population balance equations. The coagulation equation is a non-linear partial integro-differential equation and its numerical solution is by far no trivial. This is the primary reason for the development of so many methods for its solution, obtaining from various scientific disciplines.

2. Problem Statement, background

The well known coagulation population balance is a non-linear integrodifferential equation of the form:

$$\frac{\partial f(x,t)}{\partial t} = \frac{1}{2}\int_0^x K(y, x-y) f(y,t) f(x-y,t) dy - f(x,t)\int_0^\infty K(x,y) f(y,t) dy \qquad (1)$$

where t is the time, x is the particle volume, f(x,t) is the number concentration density function and K(x,y) the coagulation frequency between two particles with sizes x,y respectively. The above equation must be solved for the evolution of the particle size distribution (PSD) having as initial condition a given PSD $f(x,0)=f_o(x)$. There are several approaches to the solution of the equation (1). At the one limit the so-called higher order methods ensures high accuracy requiring large computational effort and at the other limit the moments methods requires a small computational effort offering questinable (problem dependent) accuracy. The golden section between the two approaches bridging their accuracy and computational requirements are the sectional methods.

The sectional methods developed before 1996 had several important disadvantages: many of them conserved only one integral property of the particles [3], others were designed only for a specified grid type [4,5] or they were very complicated (discrete sectional methods [6]). Several reviews on those methods exist in the literature. The major step to change the situation was made in [1] with the development of the fixed pivot technique (FPT). This technique conserves two integral properties and allows a quite arbitrary grid in a very simple and straightforward way. This method is nowadays the most widespread one and it is considered the state of the art on the subject. Of course, other sectional methods have been proposed through these years but they cannot

compete the generality and robustness of the fixed pivot technique. Yet, there is a weak point in the technique: the prediction of the second moment of the PSD is very poor. Actually, it is much worse than that given by the moment methods having fewer degrees of freedom. The next major step in the development of sectional methods was the recent cell average technique (CAT) [2]. This method has all the advantages of the fixed pivot technique but in addition gives satisfactory predictions for the moments of the distribution. A further improvement of the cell average techique (called extended cell average technique ECAT) is attempted in the present work by requiring three moments conservation during the coagulation event between particles. This choice permits improved computation of the higher moments of the distribution.

3. Paper approach

3.1. Methodology

The scope of the sectional methods is to convert the integrodifferential equation (1) to a system of ordinary differential equations for the quantities N_i where following a finite volume convention it is assumed that

$$N_i = \int_{v_i}^{v_{i+1}} f(x,t)dx \tag{2}$$

The symbols $v_1,v_2,v_3\ldots$ stand for the finite volume (sectional) discretization of the particle volume domain. Each size located in a class i is automatically assigned to the pivot x_i of the class. The pivots are defined from the relation $v_i=(x_{i-1}+x_i)/2$. The rigorous mathematical developed of sectional methods for the equation (1) leads to methods capable to conserve only one integral moment of the particle size distribution as the coagulation proceeds. Only by developing heuristic methods the situation can be improved. So the fixed pivot technique shares any new particle (resulting from a coagulation event) entering the class i, to its adjacent pivots. The weights of sharing are chosen to ensure the conservation of two moments. The new idea behind the cell average technique is than the sharing procedure must be not applied to individual particles entering the section I, but to the average particle. It is not clear why this new approach leads to a large improvement of the performance of the method. The further improvement in the present approach (ECAT) lies on requiring the conservation of three moment by sharing the average entering particle in section i, among three pivots. The main difficulty of the development lies to the appropriate choice of the pivots to achieve stability of the algorithm. The number of particles entering section i per unit time can be computed in discretized form as:

$$B_i = \sum_{\substack{j,k \\ v_i \le x_j + x_k < v_{i+1}}}^{j \ge k} (1 - \frac{1}{2}\delta_{j,k}) K(x_j, x_k) N_j N_k \tag{3}$$

The corresponding mass of entering particles is computed as:

$$R_i = \sum_{\substack{j,k \\ v_i \le x_j + x_k < v_{i+1}}}^{j \ge k} (1 - \frac{1}{2}\delta_{j,k})(x_j + x_k) K(x_j, x_k) N_j N_k \tag{4}$$

The mean size of entering particles can be found simply by $\bar{\alpha}_i = R_i / B_i$ and their second moment is computed as:

$$S_i = \sum_{\substack{j,k \\ v_i \le x_j + x_k < v_{i+1}}}^{j \ge k} (1 - \frac{1}{2}\delta_{j,k})(x_j + x_k)^2 K(x_j, x_k) N_j N_k \tag{5}$$

Let us say that the zeroth, first and second moment of the particles entering (per unit of time) a section i are B,R,S respectively, their average size is $\bar{\alpha} = R / B$ and they must be shared among the pivots x,y,z. The rate of particles which must be added to pivots x,y,z are denoted as a,b,c, respectively. The point here is the computation of a,b,c having known the B,R,S,x,y,z. Equating the moments of the incoming particles with the moments of the new particles having the three pivot sizes results in the system of three equations: a+b+c=B, ax+by+cz=R, $ax^2+by^2+cz^2$=S.The above system of algebraic equations is solved analytically using the method of determinants with the Krummer's rule to give:

$$a(B,R,S,x,y,z) = \frac{Byz^2 + zS + Ry^2 - Rz^2 - Bzy^2 - Sy}{yz^2 + zx^2 + xy^2 - xz^2 - zy^2 - yx^2} \tag{6}$$

$$b(B,R,S,x,y,z) = \frac{Rz^2 + Bzx^2 + xS - Bxz^2 - zS - Rx^2}{yz^2 + zx^2 + xy^2 - xz^2 - zy^2 - yx^2} \tag{7}$$

$$c(B,R,S,x,y,z) = \frac{yS + Rx^2 + Bxy^2 - xS - y^2R - x^2yB}{yz^2 + zx^2 + xy^2 - xz^2 - zy^2 - yx^2} \tag{8}$$

The number of particles added to the pivot x_i contains contribution from the particles entering sections i-2,i-1,i,i+1. The derivation of the final system of equations for N_is is not straightforward but it will be given here in a quite compact form permitting its direct implementation to an integrator of ordinary differential equations:

$$\frac{dN_i}{dt} = a_{i+1}^{(1)}U(\bar{\alpha}_{i+1} - x_{i+1}) + b_i^{(1)}U(\bar{\alpha}_i - x_i) + c_{i-1}^{(1)}U(\bar{\alpha}_{i-1} - x_{i-1})$$
$$+a_{i+2}^{(2)}U(x_{i+2} - \bar{\alpha}_{i+2} - \varepsilon) + b_{i+1}^{(2)}U(x_i - \bar{\alpha}_i - \varepsilon) + c_i^{(2)}U(x_{i-1} - \bar{\alpha}_{i-1} - \varepsilon) \quad (9)$$
$$-N_i\sum_{k=1}^{P}K(x_i, x_k)N_k$$

where i= 1,2,3…..P, U(x) is a modified Heavyside step function defined as 1 for x≥0 and 0 for x<0. The small number ε is used to ensure that for $\bar{\alpha}_i = x_i$ the assignment will be done to pivots x_{i-1},x_i,x_{i+1}. The other coefficients in system (9) can be found as

$$a_i^{(1)} = a(B_i, R_i, S_i, x_{i-2}, x_{i-1}, x_i) \quad (10a)$$
$$b_i^{(1)} = b(B_i, R_i, S_i, x_{i-2}, x_{i-1}, x_i) \quad (10b)$$
$$c_i^{(1)} = c(B_i, R_i, S_i, x_{i-2}, x_{i-1}, x_i) \quad (10c)$$
$$a_i^{(2)} = a(B_i, R_i, S_i, x_{i-1}, x_i, x_{i+1}) \quad (10d)$$
$$b_i^{(2)} = b(B_i, R_i, S_i, x_{i-1}, x_i, x_{i+1}) \quad (10e)$$
$$c_i^{(2)} = c(B_i, R_i, S_i, x_{i-1}, x_i, x_{i+1}) \quad (10f)$$

where B_i, R_i, S_i are calculated from the equations (3), (4) and (5), respectively Also, the six-argument functions a,b,c are given by equations (6), (7) and (8) respectively

3.2. Results& discussions

In Figure 1 it is shown the dimensionless particle number concentrations N_i assigned to pivot i as computed by the three numerical methods and the analytical solution for t=98 and constant coagulation kernel. The huge improvement of CAT against FPT is obvious in Figure 1. The (artificial) long tail of PSD predicted by FPT method disappears using CAT or ECAT methods. As it can be deduced from Figure 1 the ECAT clearly improves the CAT prediction for i=10 and i=11 sections (the improvements are small since the distance from the exact result is still large). This is an expected behaviour since better handling of the second moment leads to better results for the large particles which mainly contribute to the second moments. The comparison between the numerically computed and the exact second and third moments of the PSD (constant coagulation kernel) is shown in the Figure 2. The ECAT gives the exact second moment and improved third moment with respect to the other methods.

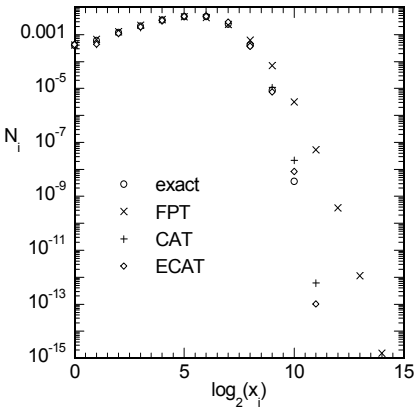

Figure 1. Exact and approximate (by FPT, CAT and ECAT) particle number concentrations N_i for constant coagulation kernel and t=98.

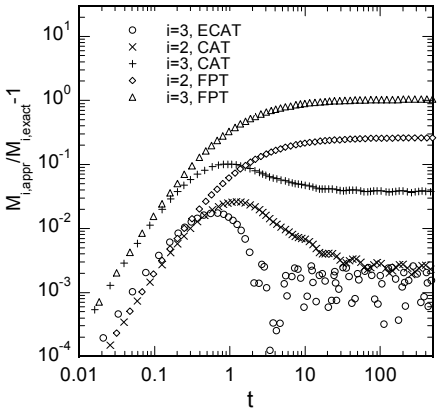

Figure 2. Evolution of the quantity $M_{i,appr}/M_{i,exact}$-1 for the three sectional methods and i=2,3 (constant coagulation kernel). For the case of ECAT and i=3 the absolute values of the above quantity are shown.

4. Conclusions/Remarks/future work

In this work a new sectional method for the solution of the coagulation equation is developed inspired by the recent cell average technique which overcomes many of the problems associated with the state of the art until today sectional techniques. More specifically, there is a radical improvement in the prediction of the evolution of the second moment of PSD and of the steep decrease of the particle number concentration for large particle sizes for the constant coagulation kernel case. The next step will be the extensive testing of the method in cases of more realistic coagulation kernels

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