Computers and Chemical Engineering 96 (2017) 33–41

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

Numerical solution of the population balance equation using an efficiently modified cell average technique

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ARTICLE INFO

Article history:
Received 23 August 2016
Received in revised form 12 October 2016
Accepted 22 October 2016
Available online 26 October 2016

Keywords:
mCAT
Pivot-based technique
Population balance equation
Region of high amount of time

ABSTRACT

In order to increase the accuracy of the modified cell average technique (mCAT) alongside the zeroth and first moments and increase the speed of the technique, a new supplemental solver has been developed in the region of high amount time, a region where the ratio of the zeroth moment to the initial zeroth moment ($\mu_0(t)/\mu_0(0)$) is too small or too large depending on the process and the amount of error is high there. The solver is conceptually easy to understand and straightforward for programming. A number of analytically solved problems were simulated by incorporating this solver into the mCAT and the results were compared with the previous solver. Significant improvements for different phenomenon especially the aggregation related systems were observed.

1. Introduction

Solving the populations balance equation, because of its vast applications in diverse processes, has been a great concern for the researchers. This equation, even in its most simple form, has a non-linear integro-differential nature that makes it intractable to analyze. Another difficulty in solving the PBE numerically is the scarcity of the number of analytically-solved problems that the numerical methods refer to. Most methods are divided into these categories: the pivot-based techniques (Kumar and Ramkrishna, 1996; Kostoglou, 2007; Kumar et al., 2008; Mostafaei et al., 2015), the finite element and finite volume methods (John et al., 2009; Qamar et al., 2009; Ahmeda et al., 2013; Kumar and Kumar, 2013), the Monte Carlo simulation (Lin et al., 2002; Zhao et al., 2007; Xu et al., 2014) and the method of moments (Marchisio and Fox, 2005; Yuan et al., 2012; Bruns and Ezekoye, 2012; Santos et al., 2013). The present method is, in fact, a modified cell average technique which is a fixed-pivot technique (FPT) and a continuation of the previous one (Mostafaei et al., 2015). The problem with most the PBE solvers including modified cell average technique (Mostafaei et al., 2015) and its predecessors cell average technique (Kumar et al., 2008) and FPT (Kumar and Ramkrishna, 1996) is that they cannot be used in high amount of time, because modeling of this region is hard due to its unique condition. For example, in this region the degree of aggregation is high and that is why a little deviance from the actual values may lead to a large error. In the previous work by the authors, a supplemental solver (Fig. 1) was introduced to increase the accuracy of the method by stretching the grid in order to lower the accumulation at the last point. This solver was successful for moderately high amount time, but not in very high amount of time where the accumulation at the lowest part of the internal coordination or the highest part, depending on the process, is high. A new supplemental solver has been incorporated. The goal here is to predict the density function and its zeroth and first moments in this region.

2. Mathematical description

2.1. The source of errors

A population balance equation (PBE) which describes a one-dimensional batch type process reads (Ramkrishna, 2000):

$$\frac{\partial f(x,t)}{\partial t} + \frac{\partial (G(x,t)f(x,t))}{\partial x} = B_{agg} + B_{break} - D_{agg} - D_{break}, \quad (1a)$$

where the birth and death terms are:

$$B_{agg} = \frac{1}{2}\int_0^x \beta(u, x-u, t) f(u,t) f(x-u,t)\, du, \quad (1b)$$

$$D_{agg} = f(x,t)\int_0^\infty \beta(u,x,t) f(u,t)\, du, \quad (1c)$$

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http://dx.doi.org/10.1016/j.compchemeng.2016.10.012
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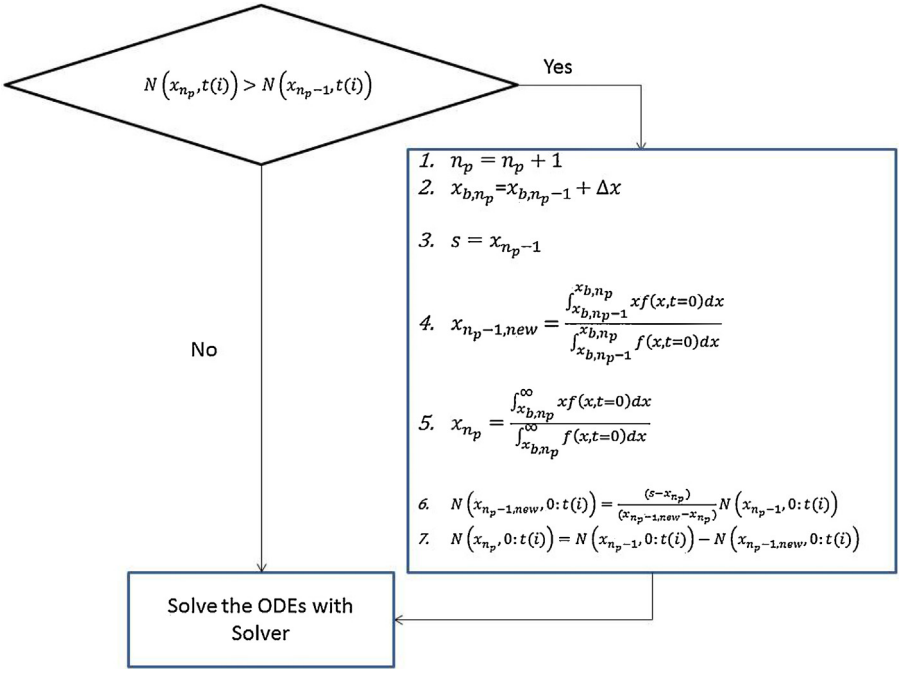

Fig. 1. mCAT supplemental solver algorithm presented in Mostafaei et al. (2015).

$$B_{break} = 2\int_0^{\infty} S(u,t)f(u,t)P(x|u,t)\,du, \tag{1d}$$

$$D_{break} = S(x,t)f(x,t). \tag{1e}$$

The f is the density function, G is the growth term, β donates the coagulation kernel, and functions S and P are the selection function and the breakage probability density function respectively.

The mCAT introduced in Mostafaei et al. (2015) is a sectional method in which the whole internal dimension (here volume) is divided into a finite number of cells. Then, by concentrating all particles of each cell in a specific point that is called the representative point, the density function can be rewritten like the following form:

$$f(x,t) = \sum_{i=1}^{n_p} N_i(t)\delta(x - x_i), \tag{2}$$

where n_p is the number of cells, δ is the Dirac delta function, and both N_i and x_i are the number of particles and representative point of the ith cell respectively. By replacing above equation in population balance equation in a specific cell and integrating it with counting on the migrating particles which come from and go to the adjacent cells, the discretized formula can be reached:

$$\frac{dN_i}{dt} = -\frac{\lambda_i}{x_{i+1} - x_i} + B_i - D_i, \qquad i = 1, \tag{3a}$$

$$\frac{dN_i}{dt} = \frac{\lambda_{i-1}}{x_i - x_{i-1}} - \frac{\lambda_i}{x_{i+1} - x_i} + B_i - D_i, \qquad i = 2, \ldots, n_p - 1 \tag{3b}$$

$$\frac{dN_i}{dt} = \frac{\lambda_{i-1}}{x_i - x_{i-1}} + B_i - D_i, \qquad i = n_p. \tag{3c}$$

The B_i and D_i are the birth rate and death rate of particles in the ith cell and λ is a variable called the kernel of the discretized equation. This set of equations preserves the zeroth moment but for the first moment to be preserved, an equality should be fulfilled:

$$x_{n_p}B_{n_p}(t) + \sum_{i=1}^{n_p-1}(\lambda_i(t) + x_iB_i(t)) = \int_0^{\infty} x(B_{agg} + B_{break})\,dx. \tag{4}$$

However, as discussed in Mostafaei et al. (2015), for a fixed grid (or a grid that is only dependent on the growth term), this equality cannot be maintained otherwise the density function in some cells becomes negative which is meaningless and undesirable. So, the source of errors lies in the incapability to keep both these conditions. For the aggregation process, this shows itself as an accumulation at last points. To alleviate this problem in the last paper, a solver was introduced such that if the condition would be fulfilled, then based on preserving both moments, a new cell would be added to the system of equations (Mostafaei et al., 2015) (Fig. 1). This method was effective for relatively high amount of times but in very high times, the solver would lose its role. The error increases and the solver becomes time-consuming. A solver that is based on the mCAT method, very fast in terms of computation, much more precise than previous methods such as CAT, FPT or mCAT is proposed here.

2.2. Processes

As mentioned above, the burden of computation of density function and preserving the first moment cannot just be put on the kernel of the discretized equation (λ), so the only factor aside from the kernel that is part of the system of equation and has a direct effect on the computation is the grid, specifically the representative points. Therefore, the focus of the new supplemental solver lies in these points and their connection with the system of equations, type of process and specially the first moment.

Consider a system with all major processes in it (Eq. (1)). Then, by multiplying both sides by variable x and integrating it through the whole part of internal dimension, the rate of first moment can be achieved:

$$\frac{d\mu_1}{dt} = \int_0^{\infty} G(x,t)f(x,t)\,dx + \int_0^{\infty} x(B_{agg} + B_{break})\,dx - \int_0^{\infty} x(D_{agg} + D_{break})\,dx \tag{5}$$

substituting Eq. (2) in Eq. (5), we obtain:

$$\frac{d\mu_1}{dt} = \sum_{i=1}^{n_p} N_i(t)G(x_i,t) + \sum_{i=1}^{n_p}(V_i'(t) + x_iB_i(t)) - \sum_{i=1}^{n_p} x_iD_i(t) \tag{6}$$

where variable V_i' is called *the difference volume flux* and defined as:

$$V_i' = \int_{x_{b,i}}^{x_{b,i+1}} (x - x_i)(\mathrm{B_{agg}} + \mathrm{B_{break}})\,dx. \tag{7}$$

In Eq. (3), by multiplying each equation with its own representative point and then adding up all equations, the result would be:

$$\sum_{i=1}^{n_p} x_i\frac{dN_i}{dt} = x_{n_p}B_{n_p}(t) + \sum_{i=1}^{n_p-1}(\lambda_i(t) + x_iB_i(t)) - \sum_{i=1}^{n_p} x_iD_i(t). \tag{8}$$

Eq. (8) can be rewritten as:

$$\frac{d(\sum_{i=1}^{n_p} x_iN_i)}{dt} - \sum_{i=1}^{n_p} N_i(t)\frac{dx_i}{dt} = x_{n_p}B_{n_p}(t) + \sum_{i=1}^{n_p-1}(\lambda_i(t) + x_iB_i(t)) - \sum_{i=1}^{n_p} x_iD_i(t). \tag{9}$$

The first term at the left side of Eq. (9) is the rate of first moment. So if this term would be kept at the right side, then the reorganized equation would be:

$$\frac{d\mu_1}{dt} = \sum_{i=1}^{n_p} N_i(t)\frac{dx_i}{dt} + x_{n_p}B_{n_p}(t) + \sum_{i=1}^{n_p-1}(\lambda_i(t) + x_iB_i(t)) - \sum_{i=1}^{n_p} x_iD_i(t) \tag{10}$$

by putting both the right sides of Eqs. (6) and (10) in one side and omitting the unnecessary parts, we would have:

$$\sum_{i=1}^{n_p} N_i(t)\left[\frac{dx_i}{dt} - G(x_i,t)\right] + \sum_{i=1}^{n_p-1}\lambda_i = \sum_{i=1}^{n_p} V_i'. \tag{11}$$

This formula is the basis of the new supplemental solver which will be discussed deeply in the following sections.

2.2.1. Aggregation

A system consisting of the aggregation and growth processes is discussed here. From the previous work (Mostafaei et al., 2015):

$$\lambda_i = V_i', \qquad i = 1,\ldots,n_p - 1. \tag{12}$$

Based on this equation and Eq. (11) the following form would be obtained:

$$\sum_{i=1}^{n_p} N_i(t)\left[\frac{dx_i}{dt} - G(x_i,t)\right] = V_{n_p}' \tag{13}$$

Before dismantling the above equation, two important rules should be taken into account: first, in a system involving growth, the grid moves with respect to the growth term (Kumar and Ramkrishna, 1997) and second, a representative point must not leave its cell. At the end:

$$\frac{dx_i}{dt} = G(x_i,t), \qquad i = 1,\ldots,n_p - 1 \tag{14a}$$

$$\frac{dx_i}{dt} = G(x_i,t) + \frac{V_{n_p}'}{N_i}, \qquad i = n_p. \tag{14b}$$

These equations should be solved alongside Eq. (3). But because Eq. (14a) has a simple form, usually it can be solved analytically and that is why the only problem that can be faced from the above equations is solving the complicated Eq. (14b). Because of this problem, a new simpler formula extracted from the previous equations is introduced to lower the computational time and make the solver much more simpler. In the new formula, the variable x_{n_p} has been replaced by the first moment μ_1 and instead of solving a complicated ODE (Eq. (14a)), two easier equations would be solved. By putting the terms of Eq. (1) in Eq. (5) it can be confirmed that processes like aggregation and breakage do not have any effect on the first moment. In other words:

$$\frac{d\mu_1}{dt} = \int_0^\infty G(x,t)f(x,t)\,dx = \sum_{i=1}^{n_p} N_i(t)G(x_i,t) \tag{15}$$

also, it is known that:

$$\mu_1 = \sum_{i=1}^{n_p} x_iN_i \tag{16}$$

by rewriting this equation and consider x_{n_p} as an unknown variable, then

$$x_{n_p} = \frac{\mu_1 - \sum_{i=1}^{n_p-1} x_iN_i}{N_{n_p}} \tag{17}$$

so by putting Eq. (17) in Eq. (15), the new equation would be as follows:

$$\frac{d\mu_1}{dt} = \sum_{i=1}^{n_p-1} N_i(t)G(x_i,t) + N_{n_p}G\left(\frac{\mu_1 - \sum_{i=1}^{n_p-1} x_iN_i}{N_{n_p}}, t\right). \tag{18}$$

Through both Eqs. (17) and (18), it can be seen that they are good replacements for Eq. (14b).

In a special case where there is no growth ($G(x,t) = 0$) and the aggregation is the only process present, the right side of Eq. (18) disappears and the first moment remains constant. In this case, it is needed to use Eq. (17) which is much more simpler than Eq. (14b).

2.2.2. Breakage

The overall trend for systems involving both the breakage and growth processes is like before with a slight change which is related to the kernel of the discretized equation:

$$\sum_{i=1}^{n_p} N_i(t)\left[\frac{dx_i}{dt} - G(x_i,t)\right] = V_1'. \tag{19}$$

The important rules that were mentioned in the last part can be used here too. In other words:

$$\frac{dx_i}{dt} = G(x_i,t), \qquad i = 2,\ldots,n_p \tag{20a}$$

$$\frac{dx_i}{dt} = G(x_i,t) + \frac{V_1'}{N_i}, \qquad i = 1. \tag{20b}$$

Like the aggregation case, the complexity of Eq. (20b) might cause problem. That is why it is recommended to replace this formula with the following equations:

$$x_1 = \frac{\mu_1 - \sum_{i=2}^{n_p} x_iN_i}{N_1} \tag{21}$$

$$\frac{d\mu_1}{dt} = \sum_{i=2}^{n_p} N_i(t)G(x_i,t) + N_1G\left(\frac{\mu_1 - \sum_{i=2}^{n_p} x_iN_i}{N_1}, t\right). \tag{22}$$

Similarly, if there is no growth in the system,, then the first moment remains constant. In this case just Eq. (21) can take the place of Eq. (20b).

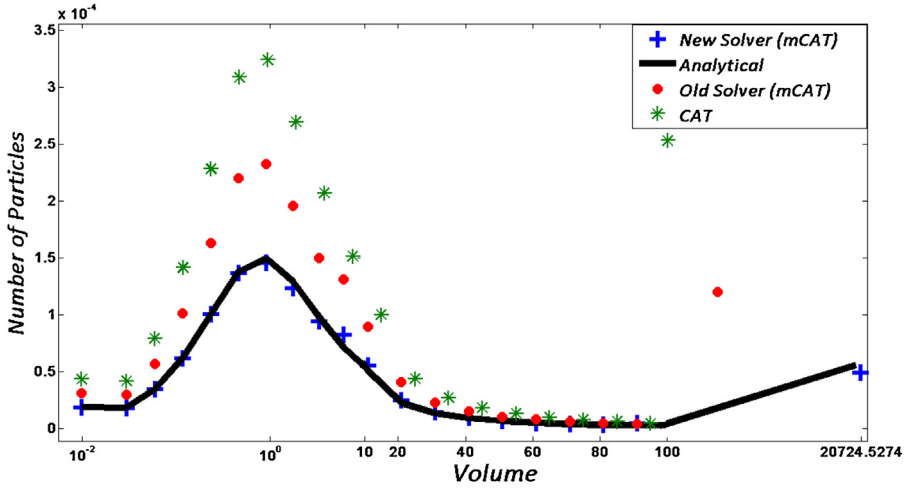

Fig. 2. Aggregation: the number of particles calculated by both the supplemental solvers of mCAT, CAT and the analytical solutions ($\mu_0(t)/\mu_0(0) = 0.001$, $\beta(x, y) = x + y$).

3. Results and discussion

Before analyzing the systems, an important note should be pointed out. As it is known, the reason for adding the supplemental solver to the method was to lower the error, which in case of the old solver (Fig. 1) was to add a new point to the grid by preserving both moments. But as time goes higher, the grid may stretch and the number of cells may become high, In this case, the capability to compare the old solver to the new one gets lower. For this reason, the two following equations have been introduced to make the old solver look like the new one:

$$N_{n_{p,s},new} = \sum_{n_{p,s} \le i} N_i, \tag{23a}$$

$$x_{n_{p,s},new} = \sum_{n_{p,s} \le i} (x_i N_i) / \sum_{n_{p,s} \le i} N_i, \tag{23b}$$

where the variable $n_{p,s}$ is the number of cells at start of programming which is the same as the new supplemental solver. For all methods, the half-geometric half-linear grid that was developed in the last paper (Mostafaei et al., 2015) has been put to use. The representative points, in case of the mCAT methods, have been achieved based on the formula that uses the initial particles size distribution in the last paper and for the CAT, the arithmetic mean of boundary points in each cell.

3.1. Aggregation

The system presented here is the sum kernel with an exponential function as the initial condition (see Appendix A). As it can be seen from Fig. 2, all methods predict the overall trend of the density function but the result of the new supplemental solver is much more precise than the other two solvers. This means the ability to predict the number of particles at the last point has a direct impact on the predictability of the method specially in very high amount of time when the aggregation degree is very high.

The over-prediction of the density function by the old supplemental solver of mCAT and CAT leads to the overestimating of the zeroth moment, unlike the new supplemental solver of mCAT which predicts this variable very well (Fig. 3). But for the first moment, by looking at Fig. 4, a relatively high under-prediction can be seen. This phenomenon is on the contrary of the zeroth moment which means for the first moment the effect of the last point is much higher than other points and also its effect on the zeroth moment.

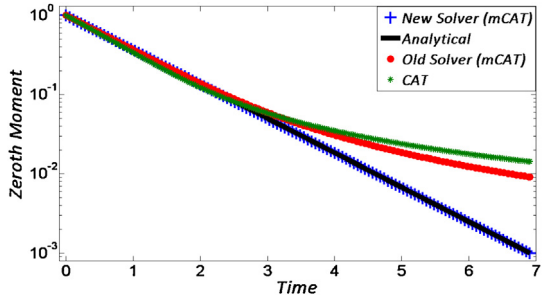

Fig. 3. Aggregation: the zeroth moment of the density function calculated by both the supplemental solvers of mCAT and CAT and their comparison with the analytical solution.

For analyzing the extent of error, the variable *Relative Accumulated Error* which is independent of number of points and process type is used.

$$RAE(t) = \frac{\sum_{i=1}^{n_p} |N_i(t) - N_{i,real}(t)|}{\mu_{0,real}(t)}. \tag{24}$$

It is obvious from Fig. 5 that the error of the new supplemental solver is much less than the old one and CAT, for instance the error of the new solver at last point is about 1/30 of the old supplemental solver's and 1/50 of the CAT. Another important fact that should be taken into account too, is the computation time. For similar methods, the one that has a lower computation time would be preferred. Fig. 6 reveals that the new supplemental solver is considerably faster than both the old one and CAT and in this factor like the previous variables the new solver is preferable.

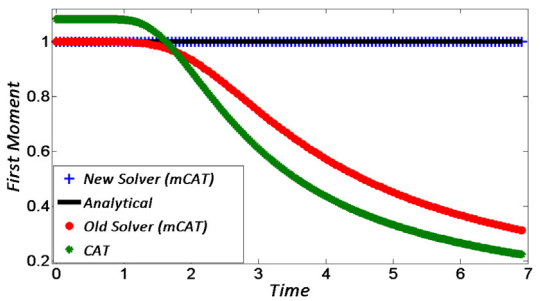

Fig. 4. Aggregation: the first moment of the density function calculated by both the supplemental solvers of mCAT and CAT and their comparison with the analytical solution.

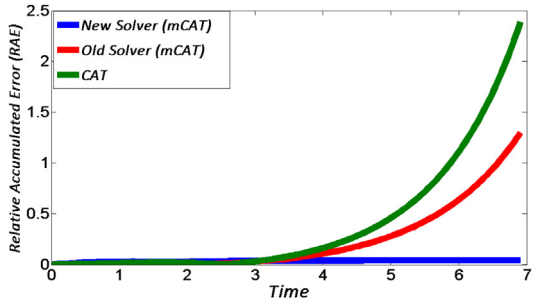

Fig. 5. Aggregation: the comparison of the relative accumulated error for both the supplemental solvers of mCAT and CAT.

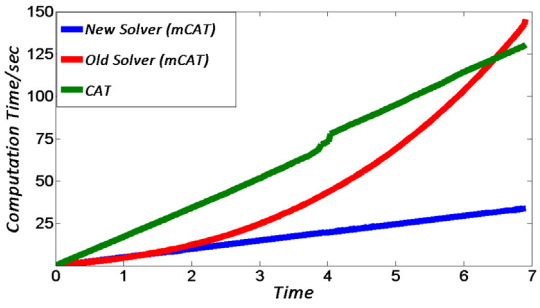

Fig. 6. Aggregation: the comparison of the computation time for both the supplemental solvers of mCAT and CAT.

3.2. Aggregation and growth

In this system a sum kernel as coagulation kernel, a linear function as growth term and an exponential function as initial condition has been chosen (see Appendix A). Fig. 7 shows the density function predicted by both the supplemental solvers of mCAT and CAT.

It can be concluded easily that the new supplemental solver is far better in predicting the density function than the old supplemental solver and CAT, however the two other techniques still can predict the general trend of the function. As it is clear from Fig. 7, the overestimation of the old supplemental solver and CAT leads to over-predicting of the zeroth moment, as shown in Fig. 8. However, based on Fig. 9, the results of the old supplemental solver and CAT for the first moment tend to drop after a specified point, which is in counterpoint to the zeroth moment and a sign that the effect of the last point on the first moment is higher than the zeroth moment. As

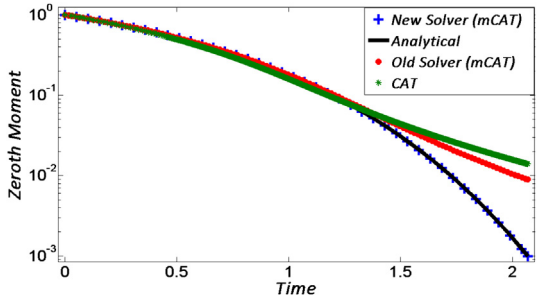

Fig. 8. Aggregation and growth: the zeroth moment of the density function calculated by both the supplemental solvers of mCAT and CAT and their comparison with the analytical solution.

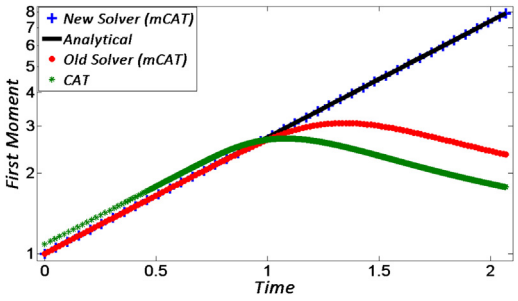

Fig. 9. Aggregation and growth: the first moment of the density function calculated by both the supplemental solvers of mCAT and CAT and their comparison with the analytical solution.

it can be seen from both these figures, the prediction of the zeroth and first moments by the new supplemental solver is very accurate.

The amount of error by each technique has been depicted in Fig. 10. Similar to the aggregation case, the new supplemental solver is by far the most accurate technique. The computation time has been presented in Fig. 11. The results show that the old supplemental solver solves the equation much longer than the new one but much faster than CAT.

3.3. Breakage

A system with a constant selection function and a step function as initial condition is chosen for this study. The details of the problem has been discussed in Appendix A. Fig. 12 depicts the density function of both the new and old supplemental solvers of mCAT and

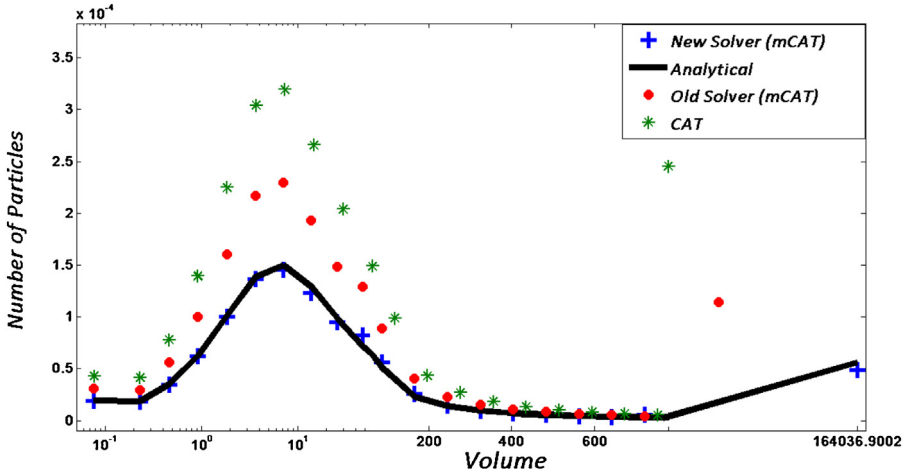

Fig. 7. Aggregation and growth: the number of particles calculated by both the supplemental solvers of mCAT, CAT and the analytical solutions ($\mu_0(t)/\mu_0(0) = 0.001$, $\beta(x, y) = x + y$ and $G(x, t) = x$).

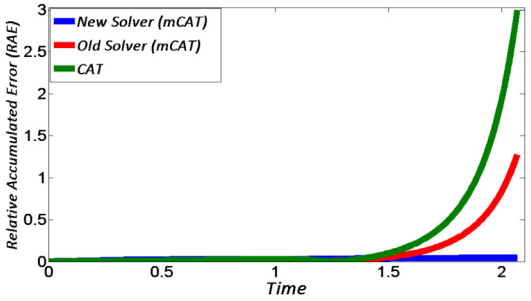

Fig. 10. Aggregation and growth: the comparison of the relative accumulated error for both the supplemental solvers of mCAT and CAT.

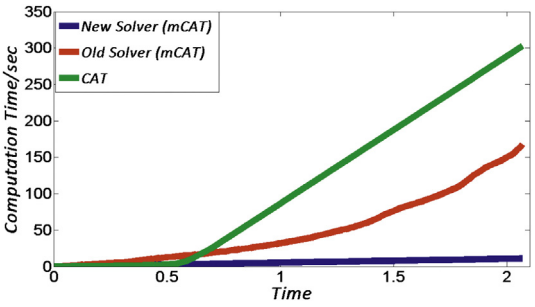

Fig. 11. Aggregation and growth: the comparison of the computation time for both the supplemental solvers of mCAT and CAT.

CAT and their comparison to the analytical solution. The results of the old supplemental solver and CAT are very different from the earlier cases in which the deviance of these two techniques from analytical solution was clear. Breakage is a linear process, a process of degree one. That is why the accumulation at first point, V'_1, which is the source of error is much smaller than its counterpart in the aggregation process, V'_{n_p}.

Fig. 12 implies that there are no deviance of the old supplemental solver and CAT from analytical for zeroth moment, as it is evident from Fig. 13. Despite of that, Fig. 14 reveals a divergence for the old solver from analytical solution. In other words, not only the number of particles are important but also the location of the representative points. Because a small difference in the first point has led to this discrepancy for the first moment, unlike the new supplemental solver which has a high level of accuracy in the prediction of these variables.

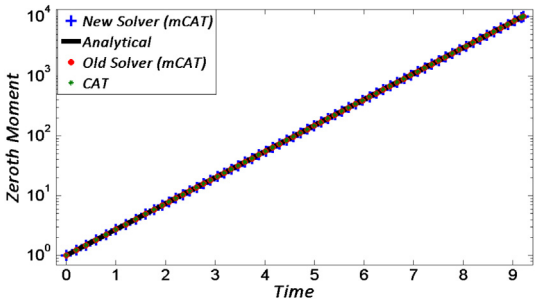

Fig. 13. Breakage: the zeroth moment of the density function calculated by both the supplemental solvers of mCAT and CAT and their comparison with the analytical solution.

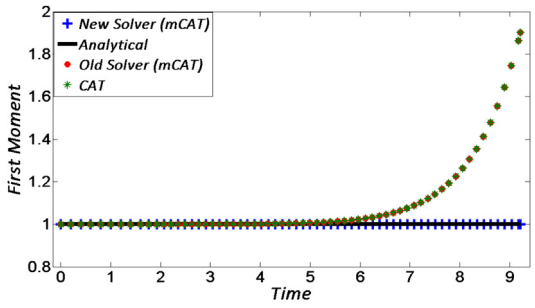

Fig. 14. Breakage: the first moment of the density function calculated by both the supplemental solvers of mCAT and CAT and their comparison with the analytical solution.

The RAE of all techniques has been shown in Fig. 15. It can be found out from this figure that all methods are very accurate however it is a little surprise that the precision of the new supplemental solver is a little lower than the other two techniques. For computation time too, the old solver is slightly faster but Fig. 16 shows that both the solvers like CAT are pretty fast. Unlike the other two cases, the aggregation-only and the aggregation and growth, in breakage the old supplemental solver of mCAT and CAT showed some improvements and in some aspects they were a little better than the new supplemental solver, however it showed a significant deviance from the actual value of first moment, something that was not seen in the new supplemental solver.

By looking closer at above figures, it can be found out the results of the old supplemental solver and CAT are the very close to each

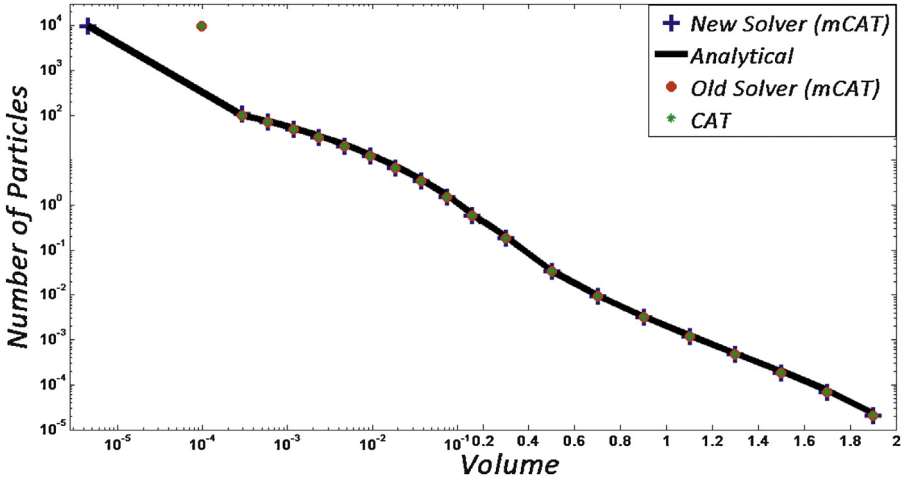

Fig. 12. Breakage: the number of particles calculated by both the supplemental solvers of mCAT, CAT and the analytical solution ($\mu_0(t)/\mu_0(0) = 10{,}000$, $S(x, t) = 1$ and $P(x|x') = 1/x'$).

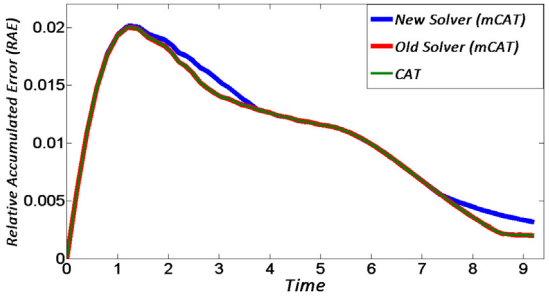

Fig. 15. Breakage: the comparison of the relative accumulated error for both the solvers.

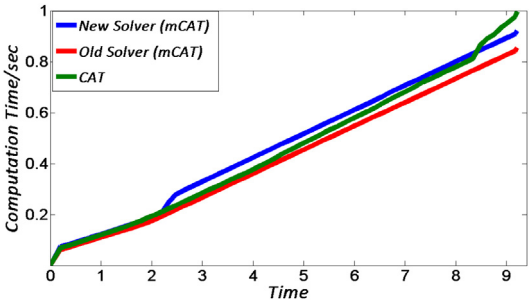

Fig. 16. Breakage: the comparison of the computation time for both the solvers.

other. The reason is, in this specific problem the representative points of both these techniques are the same and the difference volume flux of each cell for these techniques are all equals and negative. That is why the kernel of the discretized equations would be same which would lead us to the same results.

4. Conclusion

In this study, a new supplemental solver that takes the place of its predecessor at last paper (Mostafaei et al., 2015) is devised. The new solver enhanced the accuracy of the important elements of mCAT method; density function and both the zeroth and first moment at high amount time, something that was never done before for this kind of method. The supplemental solver was based on the mathematics of the mCAT method and the solver itself was dependent on the type of the process. After that even a replacement that acted as a shortcut was proposed based on the essence of the solver and nature of processes like breakage and aggregation. The results were surprising, because not only that in all cases the new supplemental solver was very accurate especially in systems involving aggregation that the error of both the old supplemental solver and CAT were very high but also the method was much faster. In other words in addition to increase the accuracy of mCAT method with this new supplemental solver, the computation time is lowered too.

Appendix A. Analytical solutions

Aggregation: With the sum kernel, $\beta(x, y) = x + y$, and an exponential initial condition, e^{-x}, the analytical solution reported by Ramkrishna (2000) is:

$$f(x,t) = e^{-t-2x+xe^{-t}}\,\frac{I_1(2x\sqrt{1-e^{-t}})}{x\sqrt{1-e^{-t}}} \tag{A.1}$$

where I_1, is the first order modified Bessel function. There is no analytical solution for integral of Eq. (A.1). So, it is recommended to solve this integral numerically. The zeroth moment too can be achieved from the PBE easily:

$$\mu_0(t) = \mu_0(0)e^{-t} \tag{A.2}$$

Aggregation and growth: Ramabhadran et al. (1976) solved the combined aggregation and growth processes with $G(x, t) = x$ and $\beta(x, y) = x + y$:

$$T = 1 - e^{-t} \tag{A.3a}$$

$$\omega = \exp\left(-\frac{T}{1-T}\right) \tag{A.3b}$$

$$f(x,t) = \frac{\omega}{x\sqrt{1-\omega}}\exp(-x(1-T)(2-\omega))I_1(2x(1-T)\sqrt{1-\omega}) \tag{A.3c}$$

there is no way to integrate Eq. (A.3c) analytically and should be integrated numerically. However, the zeroth and first moments from the population balance equation can be exploited:

$$\mu_0(t) = \mu_0(0)\omega(t) = \mu_0(0)\exp(\mu_1(0) - \mu_1(0)e^t) \tag{A.4a}$$

$$\mu_1(t) = \frac{\mu_1(0)}{1-T} = \mu_1(0)\exp(t) \tag{A.4b}$$

Breakage: The initial condition is defined as the following:

$$f(x,0) = \frac{1}{2}(1-\theta(x-2)) = \begin{cases} \frac{1}{2} & \text{if } x \le 2, \\ 0 & \text{if } x > 2. \end{cases} \tag{A.5}$$

The analytical solution of a breakage system with $S(x, t) = 1$ and $P(x|x') = \frac{1}{x'}$ based on (Ziff and McGrady, 1985) is:

$$f(x,t) = e^{-t}f(x,0) + e^{-t}\sqrt{8t}\int_0^\infty I_1(u\sqrt{8t})f(xe^{u^2},0)\,du. \tag{A.6}$$

Integrating this equation to reach $N(x_i, t)$ is not an easy task even for such a simple initial condition, however the following form can be reached:

$$N(x_i,t) = M(x_{b,i+1},t) - M(x_{b,i},t), \tag{A.7}$$

where

$$M(x,t) = \frac{xe^{-t}}{2} + e^{-t}\sqrt{8t}\int_0^{\sqrt{\ln(2/x)}} I_1(u\sqrt{8t}) \times \left(\frac{x}{2} - e^{-u^2}\right)du, \quad (x \le 2). \tag{A.8}$$

Unfortunately this equation can not be solved analytically too. Nonetheless, it can be easily confirmed that:

$$\mu_0(t) = \mu_0(0)\exp(t). \tag{A.9}$$

Appendix B. A review to the CAT and mCAT

The formulation of both the CAT (Kumar et al., 2008) and mCAT (Mostafaei et al., 2015) has been presented in this appendix. As it is known the birth and death term alongside the difference volume flux are defined as:

$$B_i = \int_{x_{b,i}}^{x_{b,i+1}} (\mathrm{B_{agg}} + \mathrm{B_{break}})\,dx. \tag{B.1}$$

$$D_i = \int_{x_{b,i}}^{x_{b,i+1}} (\mathrm{D_{agg}} + \mathrm{D_{break}})\,dx. \tag{B.2}$$

$$V_i' = \int_{x_{b,i}}^{x_{b,i+1}} (x - x_i)(\mathrm{B_{agg}} + \mathrm{B_{break}})\,dx. \tag{B.3}$$

Now these term would be achieved for the aggregation and breakage processes.

Aggregation: By putting Eq. (2) in above equations for the case, the terms would be:

$$B_i = \sum_{j=1}^{i}\sum_{k=1}^{j}\frac{1}{2}(1+ne(j,k))(H(x_j+x_k-x_{b,i}) - H(x_j+x_k-x_{b,i+1}))\beta_{jk}(t)N_jN_k, \tag{B.4a}$$

$$D_i = N_i\sum_{j=1}^{n_p}\beta_{ij}(t)N_j, \tag{B.4b}$$

$$V_i' = \sum_{j=1}^{i}\sum_{k=1}^{j}\frac{1}{2}(1+ne(j,k))(H(x_j+x_k-x_{b,i}) - H(x_j+x_k-x_{b,i+1})) \times (x_j+x_k-x_{b,i})\beta_{jk}(t)N_jN_k \tag{B.4c}$$

where *ne* and *H* are the *not equal* and the *Heaviside* functions respectively as below:

$$ne(a,b) = \begin{cases} 0 & \text{if } a=b \\ 1 & \text{if } a\neq b \end{cases}$$

$$H(x) = \begin{cases} 0 & \text{if } x<0 \\ \frac{1}{2} & \text{if } x=0 \\ 1 & \text{if } x>0 \end{cases}$$

The kernel of discretized equation for both the CAT and mCAT is:

$$\lambda_i = V_i'H\left(\frac{V_i'}{B_i}\right) + V_{i+1}'H\left(-\frac{V_{i+1}'}{B_{i+1}}\right), \quad \text{for the CAT} \tag{B.5a}$$

$$\lambda_i = V_i', \quad \text{for the mCAT.} \tag{B.5b}$$

Breakage: By repeating the operation, this time for the breakage process, we have:

$$B_i = 2S(x_i,t)N_i\int_{x_{b,i}}^{x_i}P(x|x_i,t)\,dx + \sum_{k=i+1}^{n_p}2S(x_k,t)N_k\int_{x_{b,i}}^{x_{b,i+1}}P(x|x_k,t)\,dx, \tag{B.6a}$$

$$D_i = S(x_i,t)N_i, \tag{B.6b}$$

$$V_i' = 2S(x_i,t)N_i\int_{x_{b,i}}^{x_i}(x-x_i)P(x|x_i,t)\,dx + \sum_{k=i+1}^{n_p}2S(x_k,t)N_k\int_{x_{b,i}}^{x_{b,i+1}}(x-x_k)P(x|x_k,t)\,dx. \tag{B.6c}$$

The kernel for the breakage is:

$$\lambda_i = V_i'H\left(\frac{V_i'}{B_i}\right) + V_{i+1}'H\left(-\frac{V_{i+1}'}{B_{i+1}}\right), \quad \text{for the CAT} \tag{B.7a}$$

$$\lambda_i = V_{i+1}', \quad \text{for the mCAT.} \tag{B.7b}$$

Aggregation and breakage: The terms can be achieved from the above equations:

$$B_i = B_{i,agg} + B_{i,break}, \tag{B.8a}$$

$$D_i = D_{i,agg} + D_{i,break}, \tag{B.8b}$$

$$V_i' = V_{i,agg}' + V_{i,break}'. \tag{B.8c}$$

And the kernel:

$$\lambda_i = V_i'H\left(\frac{V_i'}{B_i}\right) + V_{i+1}'H\left(-\frac{V_{i+1}'}{B_{i+1}}\right), \quad \text{for the CAT} \tag{B.9a}$$

$$\lambda_i = V_{i+1,break}' + V_{i,agg}', \quad \text{for the mCAT.} \tag{B.9b}$$

Systems involving growth: For systems involving the growth process, the following solution that has been applied in both the CAT (Kumar et al., 2008) and the FPT (Kumar and Ramkrishna, 1997) methods is implemented along with above equations:

$$\frac{dx_{b,i}}{dt} = G(x_{b,i},t). \tag{B.10}$$

By combining this set of equations and the equations of representative points in the main text, the growth term will be appeared in the system of equations. As it can be seen, the growth term only interferes with grid and so the density function is indirectly dependent on the growth process.

Appendix C. Breakage and aggregation systems

Because of the complexity of the systems including both the breakage and aggregation, there is no analytical solution in the literature except on a special example (McCoy and Madras, 2003) which in it the PSD would reach a steady state after some time, thus makes it unfitted for our study which the continuous accumulation at the boundary representative points (the last point for the aggregation and the first point for the breakage) plays an important role in high amount of times. However for readers to not go through further problems, this coupled phenomena has been sufficiently described here.

Solving these kind of systems by the new supplemental solver is quite unique because of the equation they produce:

$$\sum_{i=1}^{n_p}N_i(t)\left[\frac{dx_i}{dt} - G(x_i,t)\right] = V_{n_p,agg}' + V_{1,break}'. \tag{C.1}$$

Unlike the previous sections, we cannot consider just one of the aforementioned representative points for the new supplemental solver, because based on the above equation there is no guarantee that this representative point would stay at its cell. That is why a better solution is to consider both the representative points in the formulation of the new solver. In other words:

$$\frac{dx_i}{dt} = G(x_i,t) + \frac{V_{1,break}'}{N_i}, \quad i=1 \tag{C.2a}$$

$$\frac{dx_i}{dt} = G(x_i,t), \quad i=2,\ldots,n_p-1 \tag{C.2b}$$

$$\frac{dx_i}{dt} = G(x_i,t) + \frac{V_{n_p,agg}'}{N_i}, \quad i=n_p \tag{C.2c}$$

If there is an inclination to use the alternative for the new supplemental solver that applies the first moment, it should be noticed that the first moment can only replace just one of the aforementioned points. In other words, Eq. (18) in place of Eq. (C.2c) or Eq. (22) instead of Eq. (C.2a).

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