# Comparison of discretisation methods to solve a population balance model of activated sludge flocculation including aggregation and breakage

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**Abstract**. Population Balance Models (PBMs) can be used to describe time evolutions of distributions of properties of individuals. In this study a PBM for activated sludge flocculation including aggregation and breakage processes was investigated. The PBM is an integro-differential equation and does not have an analytical solution. One possibility to solve the equation at relatively low computational cost is by using discretisation. Two different discretisation techniques, the fixed pivot and the moving pivot, were compared using geometric grids with different coarseness. Simulations were performed for three different processes: (1) pure aggregation, (2) pure breakage and (3) combined aggregation/breakage. For pure aggregation, results showed that the fixed pivot overestimates the large particle sizes when using coarse grids since grid refinement results in a downward trend. The estimates of the moving pivot technique show even lower estimates for the large particle sizes, with a small upward trend for finer grids. The latter suggests that these predictions are closer to the pseudo-analytical solution. For the pure breakage case it was found that for the moving pivot predictions collapsed onto one curve. Due to the specific breakage case a fixed pivot with a specific grid also collapsed onto that curve. Grid refinement for the fixed pivot case, however, resulted in overestimations. Overall, the moving pivot is found to be superior since it produces more accurate estimates even for coarse grids. The latter implies lower computational load.

## 1. Introduction

A Population Balance Model (PBM) can be used to describe the time evolution of one or more property distributions of individuals of a population. The type of model was presented in the late seventies [1], but applications were limited due to a lack of computational power. Since the latter has significantly increased, the popularity of PBM increased which is reflected by an increase in the number of studies using this type of models. Applications can be found in different scientific areas dealing with a „population“ of individuals such as e.g. crystallization, flocculation, flotation, polymerization, precipitation,… Typically one is interested in describing the evolution of the distribution of a population property. The goal is either to improve the understanding of certain phenomena or to predict the evolution of the distribution in order to control certain processes. An example of the type of data that can be described by a PBM (taken from a biological flocculation experiment using activated sludge [2]) is shown in Figure 1.
The format of the PBM depends on the process under study. The population balance equation in its most general (multi-dimensional) format looks like [3] (Ramkrishna, 2000):

$$\frac{\partial}{\partial t} f(x,t) + \nabla_x \cdot \dot{X} f(x,t) = h(x,t) \quad (1)$$

where x is a vector of properties, f(x,t) is the joint property distribution function, $\dot{X}$ is a vector containing the time derivatives of x and h(x,t) represents the birth and death of individuals typically occurring through aggregation and breakage. The next sections will deal with the description of the model structure, two solution methods of these type of equation at hand through discretisation and, finally, a comparison of these two techniques.

## 2. Description of the model

In the application under study, activated sludge flocculation, the individuals are activated sludge flocs, the property vector x is chosen to be the floc size (one-dimensional PBM) expressed as volume and the distribution f(x,t) is chosen to be the number distribution. Since the model will be used to describe data of relatively short flocculation experiments, biological floc growth is not considered allowing to leave out the second term in eq 1 since $\dot{X}$ becomes zero. The function h(x,t) consists of birth and death terms for both aggregation and breakage. Note that the latter function typically consists of 4 terms: 2 for aggregation (birth and death) and 2 for breakage (birth and death).

Most aggregation models are based on the „integral“ Smoluchowski equation [4]:

$$h(x,t)_{agg} = \frac{1}{2}\int_0^x \beta(x-x',x')f(x-x',t)f(x',t)dx' - f(x,t)\int_0^\infty \beta(x,x')f(x',t)dx' \quad (2)$$

where β is the aggregation frequency function, often referred to as the *aggregation kernel*.
The first term on the right hand side of eq 2 expresses the increase in flocs of size x by aggregation of two smaller flocs (x-x' and x') whose total volume is equal to the volume of a floc of size x (aggregation birth). The second term on the right hand side of eq 2 describes the loss of flocs of size x due to their aggregation with flocs of any other size (aggregation death).

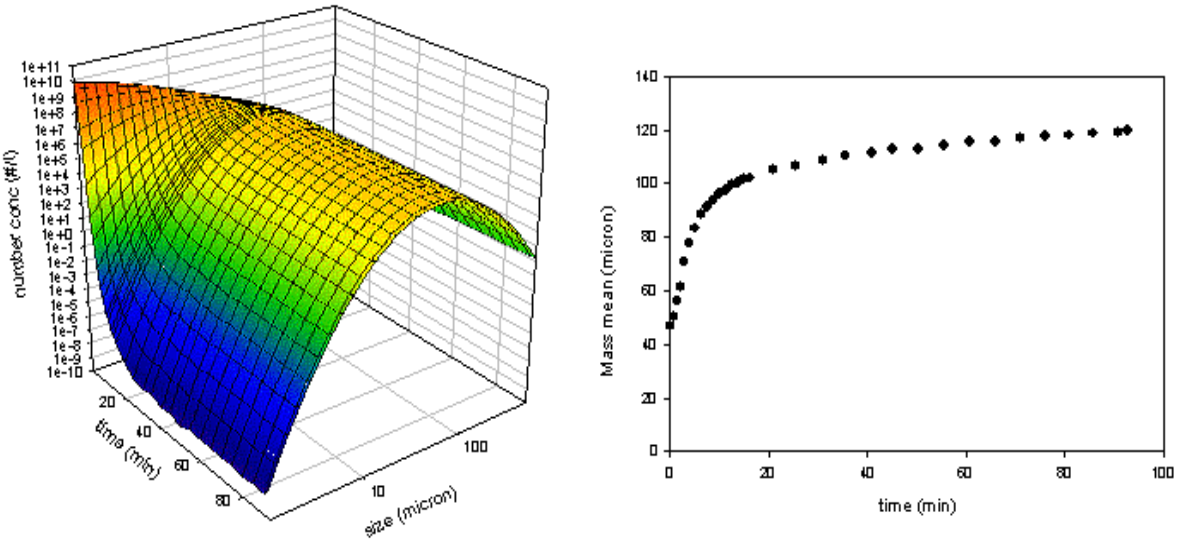


**Figure 1** - *Example of the type of data that can be modelled using a PBM: time evolution of size distribution (left) and the mass mean derived from the distributions (right) (taken from [2])*

In fact, in a PBM describing flocculation, the aggregation kernel β expresses the number of collisions that occur and can be interpreted as a description of the transport of the particles towards each other. Typically, the aggregation kernel is a function of the volume of the colliding particles. The aggregation kernel used in this study is a so-called „sum kernel“ (since it is function of the sum of the particles' volumes) and looks like [5]:

$$\beta(i,j) = 0.31\,G\left(v_i^{1/3} + v_j^{1/3}\right)^3 \quad (3)$$

where G is the average velocity gradient and $v_i$ is the volume of particle i. It describes orthokinetic flocculation.
Often a factor α is added to eq 2 to correct for hydrodynamic and/or electrostatic interactions. α can be a constant or depends on properties of the particles [6].

Breakage models are typically expressed as

$$h(x,t)_{break} = \int_x^\infty n(x)\Gamma(x',x)S(x')f(x',t)dx' - S(x)f(x,t) \quad (4)$$

where n(x) is the average number of daughter particles that are formed per event, Γ is the daughter distribution function and S the breakage rate or *breakage kernel*. The first term on the right hand side of eq 4 expresses the increase in flocs of size x by breakup of larger flocs (breakage birth). The second term on the right hand side of eq 4 expresses the loss of flocs of size x due to breakage (breakage death). In literature, binary breakage is often used, making n(x) equal to 2. The daugter distribution function can either be discrete or continuous function. In this study it was assumed that particles break up into 2 daughter particles with equal volumes. The breakage kernel is function of the particle volume. Some studies relate the breakage kernel to the turbulence regime leading to complex functionals [7,8]. The breakage kernel in this study was chosen as [9]:

$$S(i) = A\,v_i^a \quad (5)$$

where A is the breakage rate and a is a constant.

Combining eq 1-5 results in an integro-differential equation that rarely has an analytical solution (depending on aggregation and breakage functions used). Hence, other techniques need to be applied to solve the equation like e.g. successive approximations, Laplace transforms, weighted residuals,

discretisation or Monte Carlo simulations. An overview of different techniques used to obtain approximate solutions for PBMs can be found in [3]. This paper will use discretisation techniques to solve the population balance model.
When discretising the property vector x, the integrals present in eq 2 and 4 become summations and the integro–differential equation is converted into a set of ordinary differential equations that can be solved simultaneously using a time-integration algorithm. However, accurate solutions need a fine grid which implies a high computational load. If an accurate solution of the complete distribution is needed, one is to use a fine grid and the coarseness will determine the accuracy of the solution. If one is interested in accurate estimates of certain properties of the distribution, other techniques can be used that were developed in order to decrease the computational load while still assuring the conservation of at least 2 integral properties of x (e.g. numbers and mass). These techniques will be discussed in more detail in the following sections.

### 3. The fixed pivot approach

Several authors have proposed methods to solve a population balance equation numerically using a reduced number of equations by applying discretisation. This reduction implies that the accuracy of the solution deteriorates. In some cases, however, one is not interested in an accurate solution of the complete distribution, but only the conservation of certain properties (e.g. number or mass conservation). Batterham et al. [12] used a geometric grid ($v_{i+1} = 2v_i$, with v the floc volume) to solve a pure aggregation population balance model conserving mass only. Hounslow et al. [13] used a similar grid and developed a set of equations conserving both numbers and mass for pure aggregation systems. Litster et al. [14] generalised Hounslow's technique for other geometric grids ($v_{i+1} = r.v_i$, where r=1/q and q is a positive integer) again for pure aggregation. Finally, Hill and Ng [15] developed a similar technique for pure breakage problems. The main disadvantage of these different methods is that they can only be used for one or a limited number of geometric grids and that the conservation of distribution properties is restricted to numbers and mass. When another grid is to be used and the properties of interest are different, new equations need to be derived from scratch.
In order to solve this problem, Kumar and Ramkrishna [10] proposed a framework that allowed to conserve any 2 chosen integral properties of the distribution. Moreover, the developed numerical technique can be used for any arbitrarily chosen grid. The main difficulty that arises and that needs to be overcome is that particles can be formed (through either aggregation or breakage) whose property x does not coincide with one of the existing grid points or *pivots*. 2 property balances are used to reallocate these particles to the adjoining pivots (schematically shown in Figure 2, left). In that way 2 arbitrarily chosen properties of the distribution can be conserved.

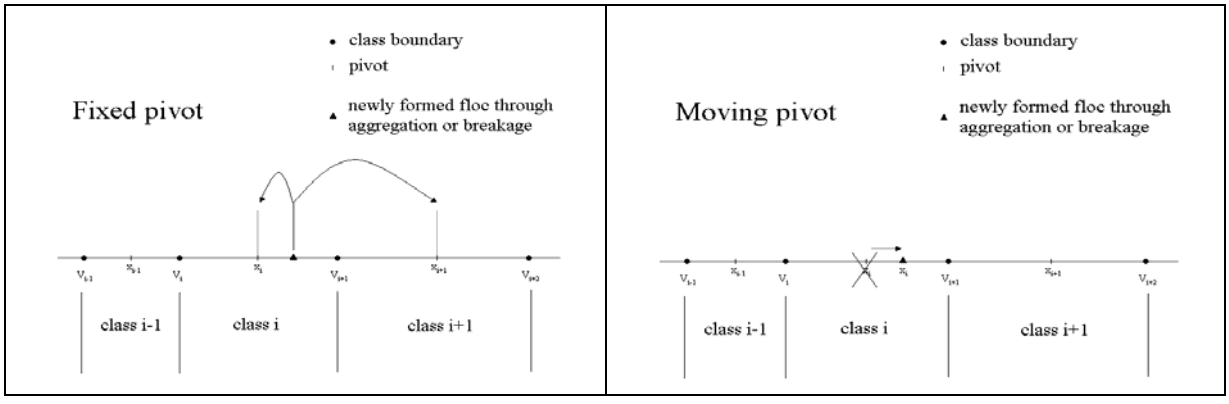


**Figure 2 -** *Schematical representation of how the different techniques deal with newly formed particles that do not coincide with an existing pivot: (left) the fixed pivot, (right) the moving pivot*

The set of equations needed to conserve both mass and numbers is given by [10]:

$$\frac{dN_i}{dt} = \sum_{\substack{j,k \\ x_{i-1} \le (x_j + x_k) \le x_{i+1}}}^{j \ge k} [1 - \frac{1}{2}\delta_{j,k}]\eta_i \beta_{x_j, x_k} N_j N_k - N_i \sum_k \beta_{x_i, x_k} N_k + \sum_{\substack{k \\ j \ge i}} n_{i,k} S(x_i) N_j - S(x_i) N_i \qquad (6)$$

where

$$\eta_i = \begin{cases} \dfrac{x_{i+1} - (x_j + x_k)}{x_{i+1} - x_i} & x_i \le (x_j + x_k) \le x_{i+1} \\ \dfrac{(x_j + x_k) - x_{i-1}}{x_i - x_{i-1}} & x_{i-1} \le (x_j + x_k) \le x_i \end{cases} \quad and \quad n_{i,k} = \int_{x_i}^{x_{i+1}} \frac{x_{i+1} - v}{x_{i+1} - x_i} \Gamma(v, x_k) dv + \int_{x_{i-1}}^{x_i} \frac{v - x_{i-1}}{x_i - x_{i-1}} \Gamma(v, x_k) dv \quad (7)$$

where $\Gamma(v,x_k)$ represents the breakage distribution function which describes the probability that a daughter particle of size v is formed from the breaking of a particle of size $x_k$. In this study the latter was chosen to be 1 if $v=x_k/2$ and 0 in all other cases.

Eq 6 consists of 4 terms. The first is the aggregation birth term and contains a factor η (eq 7) responsible for the reallocation of the formed particles to the adjoining pivots if they do not coincide with a pivot. If they do coincide with a pivot, η becomes 1. Important here is to note that the summation is performed for aggregated particles that have a volume between the pivots $x_{i-1}$ and $x_{i+1}$. The second term describes the loss of particles due to aggregation (aggregation death) and does not require any reallocation since particles only disappear and are not formed. Term three (breakage birth) does require a factor for reallocation ($n_{i,k}$) based on the breakage distribution function (eq 7). The fourth term describes the loss of particles due to breakup (breakage death) and since no particles are formed during this process this term also does not require any reallocation. Note that eq 6 and 7 are the simplified equations that can only be used to conserve numbers and mass and will, hence, yield identical results as the ones derived by Hounslow et al. [13] when a geometrical grid with factor 2 (volume-based) is used. The advantage of the fixed pivot technique is its generality in terms of the properties to be conserved and the grid choice. For the general equations of the fixed pivot technique, the reader is referred to the literature [2,10].

The developers of the fixed pivot technique performed a study [10] in which they compared their technique with an analytical solution (meaning their population balance model had a rather simple structure with regard to aggregation and breakage kernels) to check the performance of the technique and this for a pure breakup, a pure aggregation and a combined aggregation/breakage case. For the pure breakup case, the technique was found to produce accurate predictions even when using coarse grids. The predictions for the cases involving aggregation (pure aggregation and the combined case) suffered from severe overpredictions in the large particle size range. By using a finer grid the degree of overprediction was reduced. The reason of this overprediction was addressed to steep nonlinear gradients in the number density functions. The problem was tackled by the moving pivot technique described in the next section.

## 4. The moving pivot approach

In order to overcome the problem of steep nonlinear gradients that may occur in the number density functions leading to overprediction in the large particle size range, Kumar and Ramkrishna [11] proposed the so-called *moving pivot* technique. This technique accounts for the evolving non-uniformity of the distribution in each interval as a result of breakage and aggregation events by allowing a varying pivot location (Figure 2, right). The other features (arbitrary choice of grid and integral properties to be conserved) were also maintained. For the derivation of the equations, the reader is referred to the literature [2,11]. The equations conserving numbers and mass are given below:

$$\begin{aligned} \frac{dN_i}{dt} &= \sum_{\substack{j,k \\ v_i \le (x_j + x_k) \le v_{i+1}}}^{j \ge k} [1 - \frac{1}{2}\delta_{j,k}] \beta_{x_j, x_k} N_j N_k - N_i \sum \beta_{x_i, x_k} N_k + \sum_{j \ge i} S(x_i) N_j \overline{B}_{i,j}^{(1)} - S(x_i) N_i \\ \frac{dx_i}{dt} &= \frac{1}{N_i} \sum_{\substack{j,k \\ v_i \le (x_j + x_k) \le v_{i+1}}}^{j \ge k} [1 - \frac{1}{2}\delta_{j,k}] [(x_j + x_k) - x_i] \beta_{x_j, x_k} N_j N_k - \frac{1}{N_i} \sum_{j \ge i} S(x_i) N_j [\overline{B}_{i,j}^{(v)} - x_i \overline{B}_{i,j}^{(1)}] \end{aligned} \quad (8)$$

where

$$\overline{B}_{i,j}^{(1)} = \int_{v_i}^{v_{i+1}} \Gamma(v, x_j) dv \qquad \overline{B}_{i,j}^{(v)} = \int_{v_i}^{v_{i+1}} v \Gamma(v, x_j) dv \quad (9)$$

The first equation in eq 8 describes the time variation of $N_i$ and looks similar to the one of the fixed pivot method. It also contains 4 terms (aggregation birth/death and breakage birth/death). However, the first and the third term are different compared to eq 6. The difference in the first term is the fact that the summation now involves aggregated particles that are formed between the class boundaries $v_i$ and $v_{i+1}$ (and not between pivots as was the case in the fixed pivot approach). A similar difference occurs in the third term where the integrals (eq 9) have different integration limits as the ones for $n_{i,k}$ (eq 7). A closer look at the second equation in eq 8 reveals that only 2 terms are responsible for changing the pivots $x_i$, one for aggregation birth and one for breakage birth. In fact, the equation is nothing but a determination of the

average diameter (in this case volume) of every size class when new particles are born into them. In this way, the pivots are allowed to move inside the class boundaries depending on the amount and the volume of particles that are born into the class through either aggregation or breakage.
The technique was compared with the fixed pivot technique, but only for its additional features [11]. It was found that the moving pivot technique did not overpredict in the large particle size range, but instead a small underestimation was observed. However, the results for the moving pivot technique were much closer to the analytical solution compared to the fixed pivot technique with exactly the same grid. Further refinement of the grid improved the accuracy of the solution.

## 5. Numerical results

In this study the objective was to compare solutions of the PBM described in section 2 and to determine the optimal solution method and grid coarseness, both accounting for accuracy of the solution and the required calculation time. Three different cases were investigated: (1) pure aggregation, (2) pure breakage and (3) combined aggregation/breakage. Unlike [10,11], no analytical solution of the PBE was available. Both solution methods described in sections 3 and 4 were implemented in the modelling and simulation platform WEST that was used to perform all simulations [16].

*Simulation conditions*

The distribution properties to be conserved were chosen to be numbers and mass (resp. 0th and 3rd moment of the distribution). Different geometrical grids were used ($v_{i+1} = s.v_i$ , with s ranging between 1.3-2). The lower boundary of the size range was chosen to be 0.6μm since single bacterial cells making up the floc have a diameter of about 1μm. The upper boundary of the size range was chosen to be the upper limit of the class of which the pivot did not exceed 800μm. This resulted in a number of classes ranging from 31 for the case where s=2 up to 82 classes for the case where s=1.3. As initial condition, a floc monodispersion of diameter 5.5μm with a total volume of 5.9E+10 $\mu m^3$ was chosen.
The initial condition was different for the different grid/solution method combinations. When using a fixed pivot technique, the pivots, in between which the monodisperse diameter was situated, were detected and the mass and numbers were reallocated to these adjoining pivots conserving both mass and numbers of the monodispersion. All other Ni values were set to zero. When using the moving pivot technique, the class containing the monodisperse diameter was given 5.5μm as pivotal size and was filled with 6.77E+8 flocs as initial $N_i$. All other pivots were chosen to be the class centers and $N_i$'s were set equal to zero. Parameters $\alpha$ and A were chosen as 0.1 and 5000 respectively (or set respectively to zero for the pure aggregation and pure breakage cases), which corresponds to moderate aggregation and breakage. During all simulations the 3rd moment of the distribution was monitored in order to check for mass losses. No significant mass losses were observed during all simulations (<1E-3 %).
Numerical results are presented in terms of cumulative oversize numbers (CON) as function of the floc volume, which is defined as:

$$CON(v,t) = \int_{v}^{\infty} n(v',t)dv' \tag{10}$$

Such a plot emphasises the predictions for number density in the large particle size tail of the distribution and the 0th moment of the size distribution (total numbers) in one single plot. To emphasise the predictions in the small particle size tail, the cumulative undersize numbers (CUN) can be used, which is similar except for the different integration boundaries:

$$CUN(v,t) = \int_{0}^{v} n(v',t)dv' \tag{11}$$

*Pure aggregation and pure breakage simulations*

First, simulations using either the fixed or moving pivot approach were performed for pure aggregation and pure breakage processes. Results are shown in Figure 3 for pure aggregation (A=0) at t=23s and in Figure 4 for pure breakage ($\alpha$=0) at t=10s. These time instants were chosen in order to still be able to observe the moving front. Since no steady state will be reached for pure aggregation and pure breakage, the front disappears after a while and all volume will be concentrated in the largest size class for pure aggregation and in the first size class for pure breakage.

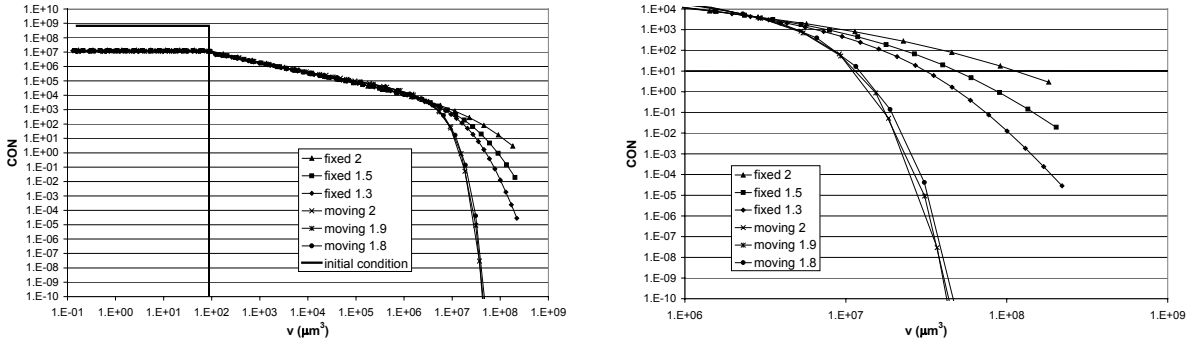


**Figure 3 –** *Predictions of the cumulative oversize numbers as function of the particle volume for pure aggregation (A=0) for t=23s: (left) complete range, (right) zoom in*

For pure aggregation, three different geometric grids were studied using the fixed pivot method (s=1.3, 1.5 and 2) and three using the moving pivot technique (s=2, 1.9 and 1.8). Both total numbers and mass were well predicted by all grid/technique combinations (mass not shown). Coarse grids tend to overpredict the large particle sizes for the fixed pivot technique. The finer the grid, the lower the prediction. The differences between the investigated grids at CON=10 are still quite large (63% for s=1.5 and 323% for s=2 using s=1.3 as reference), implying that the accuracy of the prediction can still be improved significantly by further refining the grid. Litster et al. [14] used s-values as low as 1.12 to approach an analytical solution for their case. The moving pivot technique resulted in much lower predictions of the large particle sizes compared to the fixed pivot estimates. However, the differences between the investigated grids at CON=10 are much smaller (10% for s=2 using s=1.8 as reference), implying that the accuracy cannot be improved a lot by further refining the grid and that the solution obtained can be regarded as being close to the pseudo-analytical solution. This was also observed by Kumar and Ramkrishna [11]. They compared the results with the analytical solution and found that the latter was lying in between the fixed and moving pivot prediction but closer to the latter. It can be concluded that the moving pivot technique is superior in terms of accuracy, even for coarse grids. However, it should be mentioned that the calculation load for the moving pivot is higher than the one for the fixed pivot for the same grid coarseness. Still, it is recommended to use the moving pivot technique for pure aggregation cases since coarser grids can be used that are less computation intensive than the fine grids required by the fixed pivot to obtain the same accuracy.

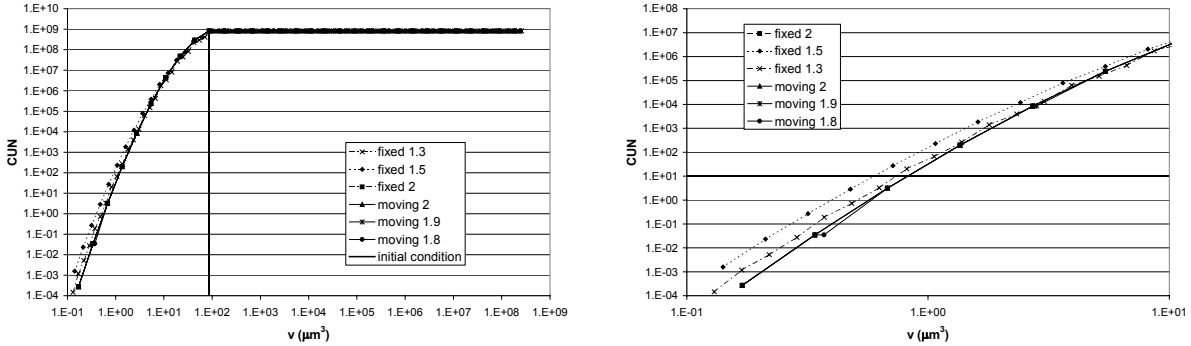


**Figure 4 -** *Predictions of the cumulative undersize numbers as function of the particle volume for pure breakage (α=0) for t=10s: (left) complete range, (right) zoom in*

For pure breakage, three grids were studied using the fixed pivot method (s=1.3, 1.5 and 2) and three using the moving pivot technique (s=2, 1.9 and 1.8). Both total numbers and mass were well predicted by all grid/technique combinations (mass not shown). For the different moving pivot grids, it can be observed that the predictions almost completely collapse onto the same curve and it can be seen that the pivots, although starting at a different value for each grid at t=0s, all move to the pivot values of the grid with s=2. Moreover, the prediction of the fixed grid for s=2 also collapses onto that same curve. For finer grids the fixed pivot yielded different results at CUN=10 (22% for s=1.5 and –0.07% for s=2 using s=1.3 as a reference). This result, strange at first sight, actually has a simple explanation. It is caused by the kind of breakage used in this study (binary breakage into equally sized daughters). If a grid with s=2 is used, a breakage event will give rise to particles of the size of the pivot of the underlying class. Therefore, no errors will be made using this kind of grid and the fixed and moving pivot technique will yield the same results. When a finer grid is used (s=1.3 and 1.5), however, the fixed pivot method is not able to correct for the fact that particles are born into smaller volumes than the pivot, resulting in overpredictions. The degree

of overprediction depends on the coarseness of the grid. The moving pivot can correct for this by moving the pivots to the same volumes as for a grid with s=2 (still remaining within their boundaries). This example shows the flexibility of the moving pivot technique. In this special case the fixed pivot technique will yield comparable results. However, for other kinds of breakage (e.g. binary breakage into unequal daughters, multiple breakage), results are expected to look similar to the aggregation results and the moving pivot will be superior. Therefore, it is recommended to use the moving pivot for pure breakage.

*Combined aggregation/breakage simulations*

Finally, the PBM was solved for the combined aggregation/breakage case. Under the conditions mentioned earlier, it took about 300s to reach a steady state. The steady state numerical results are shown in Figure 5 for CON and in Figure 6 for CUN. Total numbers and mass are estimated correctly (mass not shown). For the fixed pivot approach, the estimates for larger particle sizes are different for the investigated grids at CON=10 (33% for s=1.5 and 70% for s=2 using s=1.3 as a reference). A downward trend can clearly be observed and it is assumed that the „exact" or pseudo-analytical solution can be found by further refinement of the grid. A similar trend was observed by others [10,14].

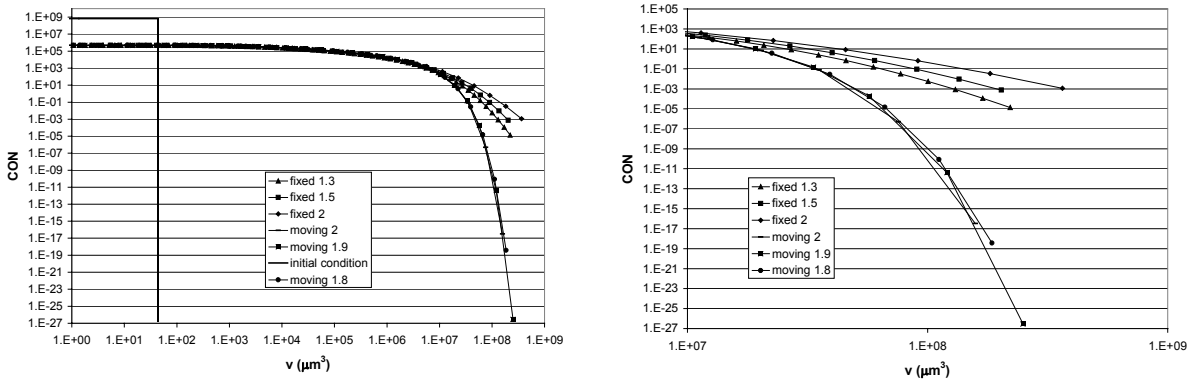


**Figure 5 –** *Steady state predictions of the cumulative oversize numbers as function of the particle volume for the fixed and moving pivot: (left) the complete volume range, (right) zoom in*

Since the difference between the grids with s=1.3 and 1.5 is still rather large (33%), it is thought that the accuracy is still not very high and that further grid refinement is necessary. The moving pivot estimates are again much lower for large particle sizes. Since grid refinement does not result in large differences (<2%), the moving pivot is assumed to be closer to the pseudo-analytical solution and, hence, is superior compared to the fixed pivot.

The estimates of smaller particle sizes (Figure 6) are also different for the investigated grids. Similar results were found as the ones for the pure breakage case. However, the moving pivot estimates do not collapse as perfectly onto the same curve for all grids as well as the fixed pivot for s=2, as was the case in the pure breakage case. This is due to some inaccuracy introduced by the aggregation. In this case, it is clear that the moving pivot is again superior and will produce more accurate results.

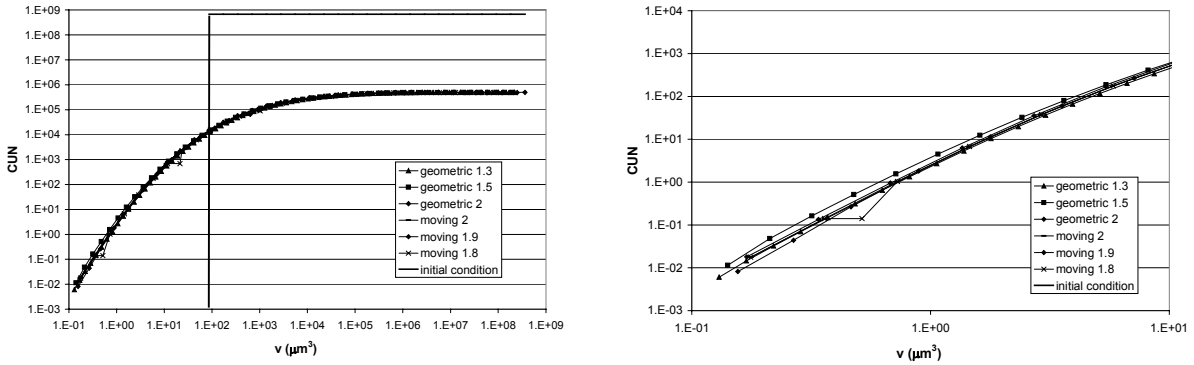


**Figure 6** - *Steady state predictions of the cumulative undersize numbers as function of the particle volume for the fixed and moving pivot: (lef) the complete volume range, (right) zoom in*

Overall, it can therefore be concluded that the moving pivot approach is superior compared to the fixed pivot method and that, even for coarse grids (s=2) and, therefore, considerably lower calculation effort, more accurate predictions can be obtained than the ones found by using the fixed pivot approach (even

when using a finer grid). Drawback of the moving pivot is, however, its longer calculation time per class considered. The differences in calculation time are, therefore, dependent on the coarseness of the grid.

## 6. Summary

Two different techniques for solving a PBM using discretisation, the fixed pivot and the moving pivot technique, were introduced. Simulations for geometric grids with different coarseness using both techniques were compared for three different processes: (1) pure aggregation, (2) pure breakage and (3) combined aggregation/breakage. The pure aggregation case revealed that the fixed pivot technique overestimates large particle sizes when using coarse grids. The moving pivot technique yielded much lower predictions, but since grid refinement caused only minor changes, it is, in agreement with literate reports, thought to be more accurate than the fixed pivot technique (even for coarse grids). In the pure breakage case, the fixed pivot technique with a specific grid was found to be adequate to produce accurate results for the specific breakage case at hand (binary breakage into equally sized daughters). For other, more general breakage cases, this will not be the case and the moving pivot is expected to be superior. The combined aggregation/breakage case revealed almost similar results compared to the pure cases. Overall, the moving pivot is found to be superior in almost all investigated cases. The only drawback is the larger computational cost. However, this is compensated since coarser grids can be used still yielding more accurate results than the fixed pivot approach.

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