# Improved Accuracy and Convergence of Discretized Population Balance of Lister et al.

Ed J. W. Wynn
Dept. of Chemical Engineering, University of Cambridge, Cambridge CB2 3RA, U.K.

The discretized population balance of Litster et al. (1995) is here reappraised and improved, resulting in a correction to the previously published version. Results from the new and old versions are compared. In the cases of two differing versions, the new one converges more readily and is generally more accurate.

Table 1 in Litster et al. (1995) was produced by finding the specific values for $q = 1, 2, 3, 4$ and deducing by inspecting the general case. A more rigorous derivation, using properties of the size discretization, is presented here. It is shown that the new derivation conflicts with the pattern deduced by inspection. Table 1 in Litster et al. (1995) is therefore wrong, and the table in this work should be substituted for it. Other instances of the same error in the original work are presented in corrected form.

Let $S_p$ be defined such that the volume $v = (v_i - v_{i-p})$ falls into the $(i - S_p)$th interval. (It is shown below that $S_p$ does not depend on $i$; this is a consequence of the fractal nature of the geometric discretization. It does depend on $q$.) Apart from $S_p$, the notation is the same as that in Litster et al. (1995), so that $v_i \equiv 2^{i/q}$ and the $i$th interval is defined as $2^{i/q} < v \leq 2^{(i+1)/q}$. So, the definition of $S_p$ can be written as

$$v_{i-S_p} < v_i - v_{i-p} \leq v_{i-S_p+1} \tag{1}$$

The second symbols are $\leq$'s, so that $S_p$ is defined when $(v_i - v_{i-p})$ is exactly equal to a $v_j$. (This is the case for $p = q$; since $v_i/v_{i-q} = 2^{q/q} = 2$, it follows that $v_i - v_{i-q} = v_{i-q}$.) In these cases, $(v_i - v_{i-p})$ will be deemed to fall into the lower interval that it delimits. For example, $S_q$ will equal $q+1$. Equation 1 can be rewritten as

$$2^{(i-S_p)/q} < 2^{i/q} - 2^{(i-p)/q} \leq 2^{(i-S_p+1)/q} \tag{2}$$

Taking logarithms and rearranging

$$S_p > \frac{-q\ln(1-2^{-p/q})}{\ln 2} \geq S_p - 1 \tag{3}$$

The definition of $S_p$ makes it an integer, and so from the second inequality we deduce that

$$S_p = \mathrm{Int}\left[1 - \frac{q\ln(1-2^{-p/q})}{\ln 2}\right] \tag{4}$$

where Int$[x]$ subtracts the fractional part (if any) from $x$.

The new numbers will first be used to deduce the limits of so-called Type 4 interactions. In these interactions, particles in intervals $i$ and $j$ aggregate, and some of the resulting particles are larger than $v_{i+1}$. These interactions are one type of death from the $i$th interval. Not all of the particles in the $j$th interval are large enough to send any $i$th-interval particle to a larger interval, though, and this distinguishes Type 4 interactions from Type 5.

From the definition of $S_p$ it follows that in the $(i+1-S_1)$th interval, some—but not all—of the particles are large enough to form an aggregate larger than $v_{i+1}$ on aggregating with a particle of volume $v_i$. Particles in lower intervals will be large enough to form aggregates larger than $v_{i+1}$ with the largest particles in the $i$th interval. When an $i$th-interval particle aggregates with any particle in an interval higher than the $(i+1 - S_1)$th, the result will always be larger than $v_{i+1}$. Therefore, Type 4 death occurs with intervals $i$ and $j$, where $1 \leq j \leq (i - S_1 + 1)$, and Type 5 death occurs with $(i - S_1 + 2) \leq j \leq \infty$.

Type 1 birth is when some, but not all, aggregation events between particles in the $(i-p)$th and $j$th intervals result in an $i$th-interval particle. The combination of the smallest particles in both of the intervals is not large enough, but that of the largest is. Therefore, for Type 1 birth with intervals $(i-p)$ and $j$, $j \leq i - S_p$, but $j \geq i - S_{p-1}$.

Type 3 birth is the opposite: the combination of the smallest particles in both of the intervals is small enough to be in the $i$th interval, but that of the largest is greater than $v_{i+1}$. Thus, for Type 3 birth, $j \leq i + 1 - S_{p+1}$ but $j \geq i + 1 - S_p$. Type 2 birth, in which all aggregation events between particles in the $(i-p)$th and $j$th intervals result in an $i$th-interval particle, is possible only when $p = q$ and $j = i - q$, as is stated in the original work.

The new, general expressions for birth and death terms are reproduced in the corrected table, Table 1. Specific values are included for $q = 1, 2, 3, 4$; these agree with those originally stated. Once a specific pairing has been identified as an interaction of whatever type, the derivation for the relevant

**Table 1. Interactions that Add to (Types 1, 2 and 3) and Remove from (Types 4 and 5) the Number of Particles in the $i$th Size Interval**

| | Size Interval 1 | Size Interval 2 | | | | |
|---|---|---|---|---|---|---|
| $q$ | | Type 1 (Birth) | Type 2 (Birth) | Type 3 (Birth) | Type 4 (Death) | Type 5 (Death) |
| 1 | $i$ | — | — | — | $1 \le j \le i-1$ | $i \le j \le \infty$ |
| | $i-1$ | $1 \le j \le i-2$ | $i-1$ | — | — | — |
| 2 | $i$ | — | — | — | $1 \le j \le i-3$ | $i-2 \le j \le \infty$ |
| | $i-1$ | $1 \le j \le i-4$ | — | $i-3 \le j \le i-2$ | — | — |
| | $i-2$ | $i-4 \le j \le i-3$ | $i-2$ | — | — | — |
| 3 | $i$ | — | — | — | $1 \le j \le i-6$ | $i-5 \le j \le \infty$ |
| | $i-1$ | $1 \le j \le i-7$ | — | $i-6 \le j \le i-4$ | — | — |
| | $i-2$ | $i-7 \le j \le i-5$ | — | $i-4 \le j \le i-3$ | — | — |
| | $i-3$ | $i-5 \le j \le i-4$ | $i-3$ | — | — | — |
| 4 | $i$ | — | — | — | $1 \le j \le i-10$ | $i-9 \le j \le \infty$ |
| | $i-1$ | $1 \le j \le i-11$ | — | $i-10 \le j \le i-7$ | — | — |
| | $i-2$ | $i-11 \le j \le i-8$ | — | $i-7 \le j \le i-5$ | — | — |
| | $i-3$ | $i-8 \le j \le i-6$ | — | $i-5 \le j \le i-4$ | — | — |
| | $i-4$ | $i-6 \le j \le i-5$ | $i-4$ | — | — | — |
| $q$ | $i$ | — | — | — | $1 \le j \le i-S_1+1$ | $i-S_1+2 \le j \le \infty$ |
| | $i-p; (1 \le p \le q-1)$ | $i-S_{p-1} \le j \le i-S_p$ | — | $i+1-S_p \le j \le i+1-S_{p+1}$ | — | — |
| | $i-q$ | $i-S_{q-1} \le j \le i-S_q$ | $i-q$ | — | — | — |

$K$'s continues unchanged. Therefore, only the limits of summation need changing in Eq. 35 of Litster et al. (1995), leading to the following

$$
\begin{aligned}
\left(\frac{dN_i}{dt}\right)_{agg} &= \sum_{j=1}^{i-S_1} \beta_{i-1,j} N_{i-1} N_j \frac{2^{(j-i+1)/q}}{2^{1/q}-1} \\
&+ \sum_{p=2}^{q} \sum_{j=i-S_{p-1}}^{i-S_p} \beta_{i-p,j} N_{i-p} N_j \frac{2^{(j-i+1)/q}-1+2^{-(p-1)/q}}{2^{1/q}-1} \\
&+ \frac{1}{2} \beta_{i-q,i-q} N_{i-q}^2 \\
&+ \sum_{p=1}^{q-1} \sum_{j=i+1-S_p}^{i+1-S_{p+1}} \beta_{i-p,j} N_{i-p} N_j \frac{-2^{(j-i)/q}+2^{1/q}-2^{-p/q}}{2^{1/q}-1} \\
&- \sum_{j=1}^{i-S_1+1} \beta_{i,j} N_i N_j \frac{2^{(j-i)/q}}{2^{1/q}-1} \\
&- \sum_{j=i-S_1+2}^{\infty} \beta_{i,j} N_i N_j
\end{aligned} \tag{5}
$$

The original equations and table are correct for $q \le 4$, which is normally satisfactory, but if a finer discretization is needed, Eq. 5 should be used.

## Example

The Case Study II of the Litster et al. was reconsidered using the original and the corrected versions. This case is size-independent aggregation only in a CST, with a feed having an exponential PSD (with respect to volume). The chosen value of $I_{agg}$ was 0.994, as in the original case study.

As mentioned above, the two versions are identical for $q \le 4$. Beyond that, the comparison can be made in Figures 1 and 2. Figure 1 shows the effect of increasing $q$ on the error in the sixth moment; it therefore corresponds to part of Figure 10 in the original work. It can be seen that the original version is initially better than the corrected version; it seems that the error noted above initially cancels out some intrinsic numerical errors in the method.

Figure 2 plots the root-mean-square (RMS) error in the individual values of the discretized PSD, normalized by dividing by the average value. This clearly shows that the original version is flawed; as $q$ increases, the original version becomes worse whereas the corrected version improves uniformly. The results of Litster et al. (1995) are generally restricted to $q \le 6$, where differences between the original and the corrected versions are not significant. Those results may

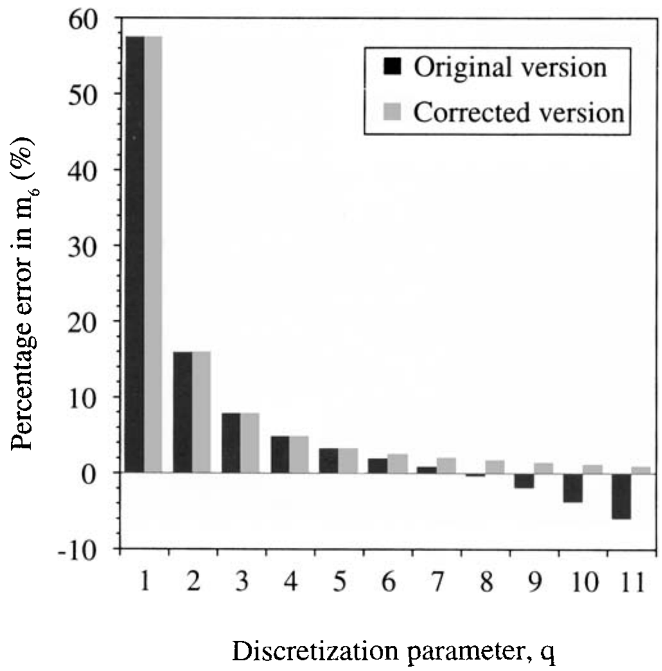


**Figure 1. Error in sixth moment against $q$.**

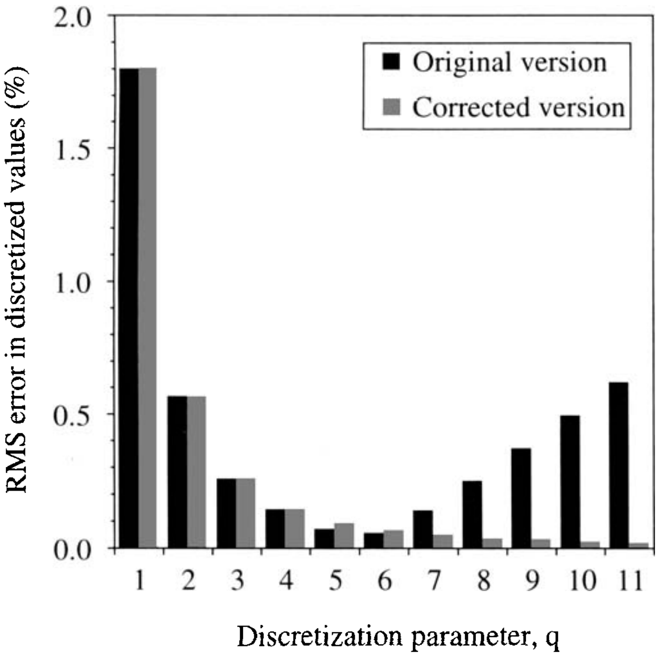


**Figure 2. RMS error in discretized values against *q*.**

therefore be taken as representative of the method, corrected or uncorrected.

When implemented, the corrected version converged much more stably than the original. The corrected version always gave positive values of the number density, while the original did not. In some instances, the corrected version required more CPU time than the original, probably because it made consistent improvements with each iteration while the original did not. It is worthwhile to note that the errors in moments can be significant even when the errors in individual data points are small; the corrected version's estimates of the sixth moment in Figure 1 are based on accurate values. The errors that remain are due to the discretization.

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## Literature Cited

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