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Discussions

A new model for the simplification of particle counting data

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Abstract

This paper proposes a three-parameter mathematical model to describe the particle size distribution in a water sample. The proposed model offers some conceptual advantages over two other models reported on previously, and also provides a better fit to the particle counting data obtained from 321 water samples taken over three years at a large South Africa water utility. By using the data from raw water samples taken from a moderately turbid, large surface impoundment, as well as samples from the same water after treatment, typical ranges of the model parameters are presented for both raw and treated water. Once calibrated, the model allows the calculation of total particle number and volumes over any randomly selected size interval of interest.

1 Introduction

The potential of particle counters to provide a detailed description of the numbers and sizes of particles in a suspension is often not fully realised. The counters produce a count and the size for each of numerous channels, and the real meaning of the analysis is often obscured by a sheer weight of numbers. A method is required to compact the multitude of numbers from every count to as few as possible parameters to offer a reliable description of the particle size distribution. Such models have been proposed and used in the past. It is the objective of this paper to propose the use of a new, improved model and to demonstrate its utility to analyse and compare large particle counting data sets.

The commonly used power law is simply a straight line defining the normalised particle counts N (y-axis) in terms of the geometric mean size d of each counting channel (x-axis) on a log-log plane. The conceptual weaknesses of the power law had been pointed out earlier – at small particle sizes, the particle number tends to infinity; at large sizes, the particle volume tends to infinity (Wilczak et al., 1992). The model and its calibration equations are, for n channels:

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$$N = A \cdot d^{\beta}$$

$$\begin{bmatrix} \ln A \\ \beta \end{bmatrix} = \begin{bmatrix} n & \sum \ln d \\ \sum \ln d & \sum (\ln d)^2 \end{bmatrix}^{-1} \cdot \begin{bmatrix} \sum \ln N \\ \sum \{(\ln N)\ (\ln d)\} \end{bmatrix} \quad (1)$$

To rectify the weaknesses of the power law, a variable-β model was proposed in conceptual form with no calibration data (Lawler, 1997). On a log-log plane, the variable-β model plots as an inverted parabola, centred about an axis at $d = 1$ µm. The variable-β model and its calibration equations are, for n channels:

$$N = A \cdot d^{\beta \ln d}$$

$$\begin{bmatrix} \ln A \\ \beta \end{bmatrix} = \begin{bmatrix} n & \sum (\ln d)^2 \\ \sum (\ln d)^2 & \sum (\ln d)^4 \end{bmatrix}^{-1} \cdot \begin{bmatrix} \sum \ln N \\ \sum \{(\ln N)\ (\ln d)^2\} \end{bmatrix} \quad (2)$$

The variable-β model was calibrated and compared to the power law in an exhaustive study which used the particle counts from 1432 water samples, ranging from raw surface water to treated drinking water, including samples from the intermediate treatment steps (Ceronio and Haarhoff, 2005). It was conclusively demonstrated that the variable-β model provided a better fit than the power law.

2 A refinement of the variable-β model

Despite the improved fit provided by the variable-β model, it was pointed out that the variable-β model has an important limitation (Ceronio and Haarhoff, 2005). Regardless of the values of A and β, the maximum N would always be found at a size of $d =$ 1 µm, regardless of the nature of the suspension. To remove this limitation, a further conceptual improvement was offered, without any further development or validation.

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The suggested three-parameter model is called the Ceronio model in this paper and plots as an inverted parabola on a log-log plane, without any constraints on the position of the vertical axis. The Ceronio model and its calibration equations are, for n channels:

$$N = A \cdot d^{\beta \ln d + C}$$

$$\begin{bmatrix} \ln A \\ \beta \\ C \end{bmatrix} = \begin{bmatrix} n & \sum(\ln d)^2 & \sum \ln d \\ \sum(\ln d)^2 & \sum(\ln d)^4 & \sum(\ln d)^3 \\ \sum \ln d & \sum(\ln d)^3 & \sum(\ln d)^2 \end{bmatrix}^{-1} \cdot \begin{bmatrix} \sum \ln N \\ \sum\{(\ln N)\,(\ln d)^2\} \\ \sum\{(\ln N)\,(\ln d)\} \end{bmatrix} \tag{3}$$

It is noted in passing that the first matrix on the right-hand side of the calibration equations (for all the models above) is a function of the channel settings of the particle counter only, without being affected by the counts. The onerous inversion of the matrix has therefore only to be performed once for every instrument setting. The Fig. 1 illustrates the three models fitted to a randomly selected particle count.

Once the models are calibrated, they can be used to rapidly obtain any desired property of the suspension. To obtain the total number of particles in any random size interval between d_1 and d_2, using the Ceronio model for illustration:

$$\#d_1, d_2 = A \int_{d_1}^{d_2} d^{\beta \cdot \ln d + C} \cdot dd \tag{4}$$

The corresponding total particle volume (assuming the particles to be spheres) in any random size interval between d_1 and d_2 is calculated with:

$$V_{d_1, d_2} = \frac{\pi A}{6} \int_{d_1}^{d_2} d^{\beta \cdot \ln d + C + 3} \cdot dd \tag{5}$$

The power of the Ceronio model lies predominantly in its ability to model suspensions where the maximum normalised counts deviate from $d = 1\,\mu\text{m}$. The diameter where the normalised count reaches a maximum is provided by:

$$d_{\max} = e^{-C/2\beta} \tag{6}$$

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3 Particle counting data

Rand Water is a large water supply utility supplying about 3.7 million $m^3\,day^{-1}$ to a population of roughly 11 million people in the Gauteng Province, as well as parts of the Mpumalanga, Free State and North West provinces of South Africa. Its primary water source is Vaal Dam, an impoundment of 2536 million m^3. Raw water is conveyed from the Vaal Dam by channel and pipes to two treatment plants – Zuikerbosch and Vereeniging. At Zuikerbosch, the bulk of the raw water is first retained in a large balancing tank before it proceeds to treatment in the larger systems; at Vereeniging there is no balancing tank and the water is treated directly upon arrival. Particle counting is done on samples of the raw water entering both treatment systems, and at numerous points on the treated water leaving the plants. This paper utilises the counts for four sampling positions, namely the two raw water sampling points (ZB Raw and VR Raw) and two selected points on the treated water (pipelines B10 and A20, henceforth labelled ZB Final and VR Final), yielding a total of 321 samples. The data used was collected at roughly fortnightly intervals from August 2006 to September 2009, covering slightly more than three years.

The particle counter used was a PAMAS 3116 FM with 16 channels, covering the range from 1 µm upwards. The channels used are separated at 1; 2; 3; 4; 5; 6; 7; 8; 10; 15; 20; 25; 30; 40; 50, and 100 µm. From these channel boundaries, the geometric mean of each channel was calculated to obtain the "*d*" required for the calibration matrices provided earlier. From the differential counts in each channel, the normalised counts were calculated by dividing them by the width of each channel, to obtain the "*N*" in the calibration matrices. The d- and N-values were used for further analysis.

For both the raw and treated water samples, there were very few counts in the higher size ranges. A necessary data screening step was to eliminate those larger channels which returned zero values, therefore not contributing to a meaningful fit of the data. The results are shown in Table 1.

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The channels below the line in Table 1 were eliminated from further consideration, based on the large percentage of samples having zero particle counts. There were therefore $15-4=11$ data points available for each calibration. After accounting for the three parameters in the Ceronio model, this left $11-3=8$ degrees of freedom, which is considered adequate for the purpose of reliable model calibration. The few zero counts in channel 11 were replaced by values of "1" to prevent the calibration procedure from trying to take the logarithm of zero.

4 Comparison of the Ceronio and variable-β model

Both the Ceronio and variable-β models were calibrated for each of the 321 samples. The goodness of fit for each sample was determined from the sum of squares SS, i.e. the sum of the squared differences between the logarithm of the actual count and logarithm of the modelled count. Figures 2 and 3 below show the cumulative distributions for the SS for the Zuikerbosch and Vereeniging samples, respectively.

The Figs. 2 and 3 clearly show the improvement in fit brought about by the Ceronio model. The sums of squares were reduced by 30 to 40 % in all cases, the improvement thus being about constant for both treatment plants, and for both raw and treated water.

5 Typical parameter values for the Ceronio model

Although the Ceronio model provided the best fit, some of the samples included in Figs. 2 and 3 were not modelled very accurately, as evidenced by the large sum of squares. The data was filtered in a further step to include only those samples which could be modelled within a sum of squares of 2. This filtering step removed 56 (17 %) samples from the data set, about evenly spread amongst the four sampling positions, which left 265 samples (VG Raw: $n=65$; VG Final: $n=67$; ZB Raw: $n=69$; ZB Final: $n=64$). The parameter values of these samples were used to determine the cumulative distributions for the four sampling points discussed below.

Parameter A determines the height of the size distribution, as shown in Fig. 4. As expected for a surface water impoundment subject to sharp seasonal turbidity variations, this parameter covers a broad range. The value of A corresponds directly to the normalised count at $d = 1\,\mu m$. From Fig. 5, the two raw water samples had A-values about two orders of magnitude higher than the final treated water samples.

Parameter β, as shown on Fig. 6 below, determines the curvature of the size distribution. The interesting observation from Fig. 7 is that the cumulative distributions for the raw and treated waters are not different. Using the 10th and 90th percentiles as guidelines, the range of β was from -1.4 to -0.5.

Parameter C moves the size distribution from left to right, as shown in Fig. 8 below. Figure 9 indicates that the range of C is between -1.5 to $+1.5$. The C-values of the raw water samples lie consistently to the left of the C-value of the treated water samples, indicating that the raw waters had relatively more small particles than the treated water samples. To show this more clearly, the cumulative distribution of d_{max}, as calculated with Eq. (6), is shown in Fig. 10. The median value for the raw water samples is at $0.8\,\mu m$. This raw water is flocculated in the treatment plant to move d_{max} to a significantly higher value (not directly measured in this study), after which the treatment process removes the bulk of the particles. We know from fundamental filtration theory that particles at $d = 1\,\mu m$ are the most difficult to remove, explaining why the median value for the treated water samples is at $d_{max} = 1.0\,\mu m$, the point where the Ceronio model collapses into the simpler variable-β model. Figure 10 also shows that d_{max} is not constant, but varies quite a bit. For treated water, using the 10th and 90th percentiles, d_{max} varies from 0.3 to $1.7\,\mu m$, emphasising the weakness of the variable-β model, which forces d_{max} to be $1\,\mu m$.

The smallest particles that could be counted, due to the technological limitations of the particle counter, are in the interval between 1 and $2\,\mu m$, which are characterised by a mean particle diameter of $1.4\,\mu m$. This means that the values for d_{max} are mostly just smaller that the smallest particles that can actually be counted, with no actual data points to validate the shape and position of the apex of the predicted particle count.

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This is an unfortunate limitation, which of course applies equally to the validation of the variable-β and Ceronio models. This implies that, until this validation can be done by including smaller particles, not too much weight should be placed to the exact value of d_{max}. For other purposes, which usually deal with particles larger than 1 µm, the better fit of the Ceronio model cannot be faulted.

6 Examples of the model application

Although the objective of this paper is to demonstrate the benefits of the Ceronio model rather than to adjudicate the performance of a specific treatment plant, the following analysis is offered as an example of how the model can be used to turn particle numbers into more tangible physical parameters.

The total number of particles between 2 and 10 µm was calculated for each count, using the model parameters and the four-point Simpson's rule. The corresponding cumulative distributions are shown in Fig. 11.

Why use the values calculated from the model, rather than using the particle count directly without any modelling? The first reason is that the model is calibrated from all the channels, providing a more robust distribution than could be obtained from fewer values which might include some outliers. Secondly, when using the particle counts directly, the size range have to coincide with the channel settings of the instrument – a limitation which does not exist when using a calibrated model.

7 Conclusions

Particle counters produce many numbers for every sample, which are not easily interpreted. Mathematical models present a way to compress this data into two or three model parameters, which are much more amenable to analysis. This paper reviewed two previously published models and proposed a third model, demonstrating that the

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proposed model offers both conceptual advantages and better fits than the earlier models, using 321 water samples from a large water utility in South Africa. Typical ranges of the model parameters were established for both raw surface water and treated drinking water. Once the model parameters are established, numerical integration allows the calculation of the total particle number and volume over any random size interval.

References

Ceronio, A. D. and Haarhoff, J.: An improvement on the power law for the description of particle size distribution in potable water treatment, Water Res., 39, 305–313, 2005.

Lawler, D. F.: Particle size distributions in treatment processes: theory and practice, in: Proceedings of the Fourth International Conference: The role of particle characteristics in separation processes, IAWQ-IWSA Joint Specialist Group on Particle Separation, Jeruslaem, 29–30 October 1996, 1997.

Wilczak, A., Howe, E. W., Aleta, E. M., and Lee, R. G.: How pre-oxidation affects particle removal during clarification and filtration, Journal of the American Water Works Association, 94, 85–94, 1992.

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Table 1. Percentage of samples that recorded zero counts in the channels indicated.

Channel	d_{min}	d_{max}	ZB Raw	ZB Final	VR Raw	VR Final
9	10	15	0 %	0 %	0 %	0 %
10	15	20	0 %	0 %	0 %	0 %
11	20	25	6 %	14 %	16 %	9 %
12	25	30	37 %	44 %	46 %	38 %
13	30	40	52 %	46 %	64 %	46 %
14	40	50	87 %	71 %	86 %	78 %
15	50	100	92 %	88 %	93 %	86 %

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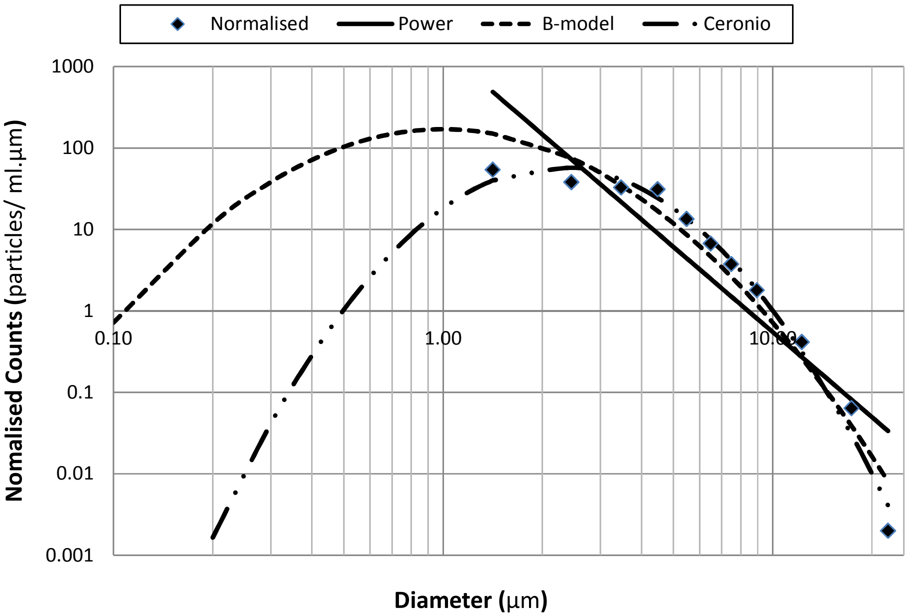

Fig. 1. The power law, the variable-β model and the Ceronio model, fitted to the same particle count.

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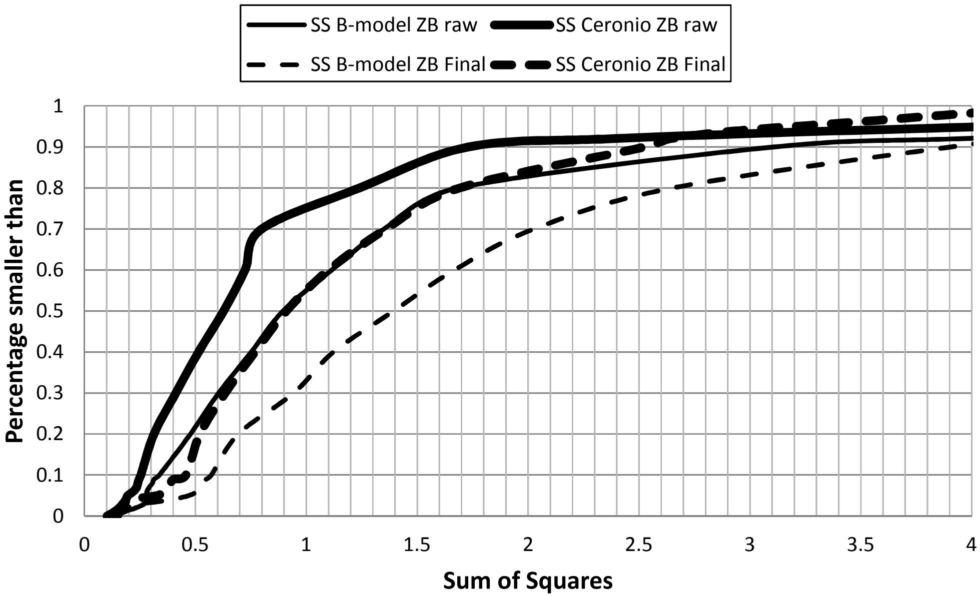

Fig. 2. Cumulative sum of square counts for the ZB treatment plant.

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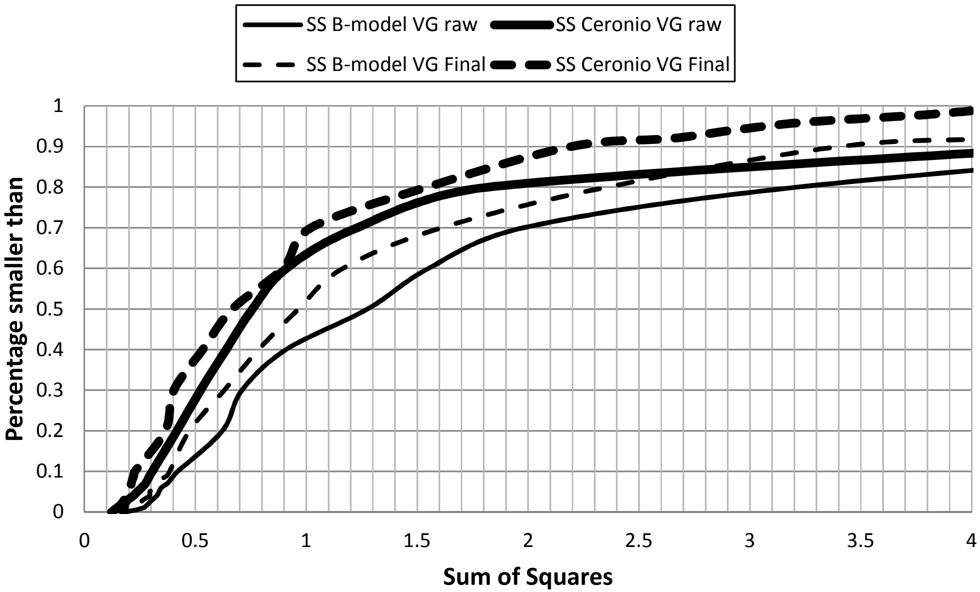

Fig. 3. Cumulative sum of square counts for the VG treatment plant.

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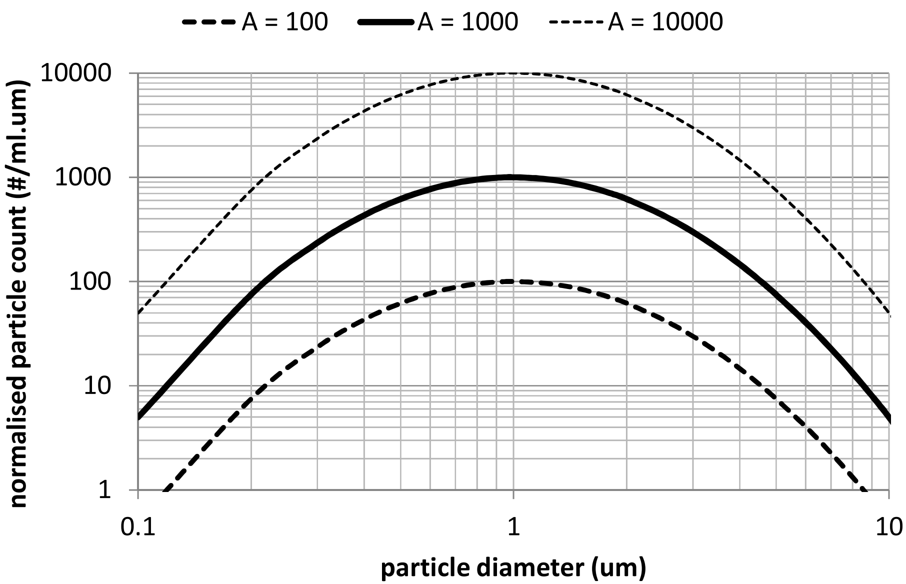

Fig. 4. The effect of model parameter A on the particle size distribution, with $\beta = -1$ and $C = 0$.

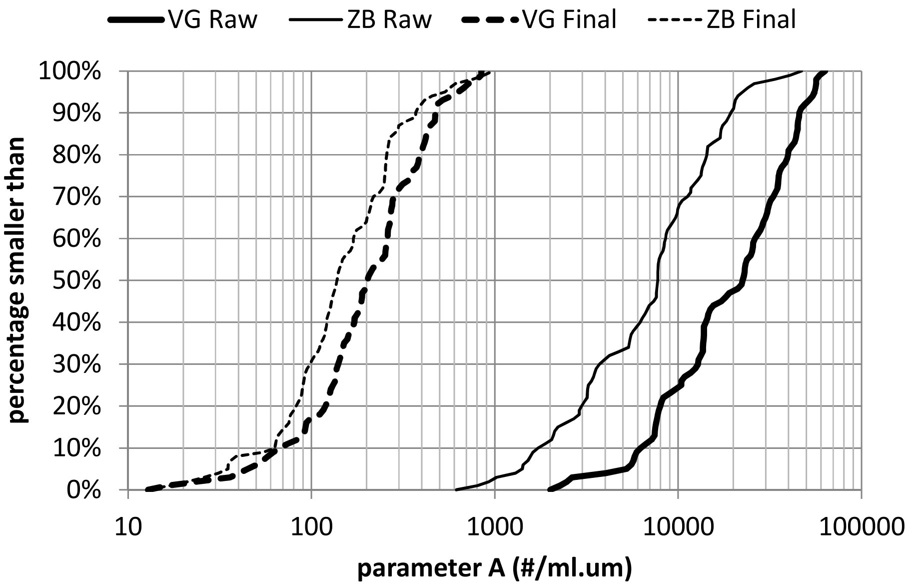

Fig. 5. The cumulative distribution of model parameter *A*.

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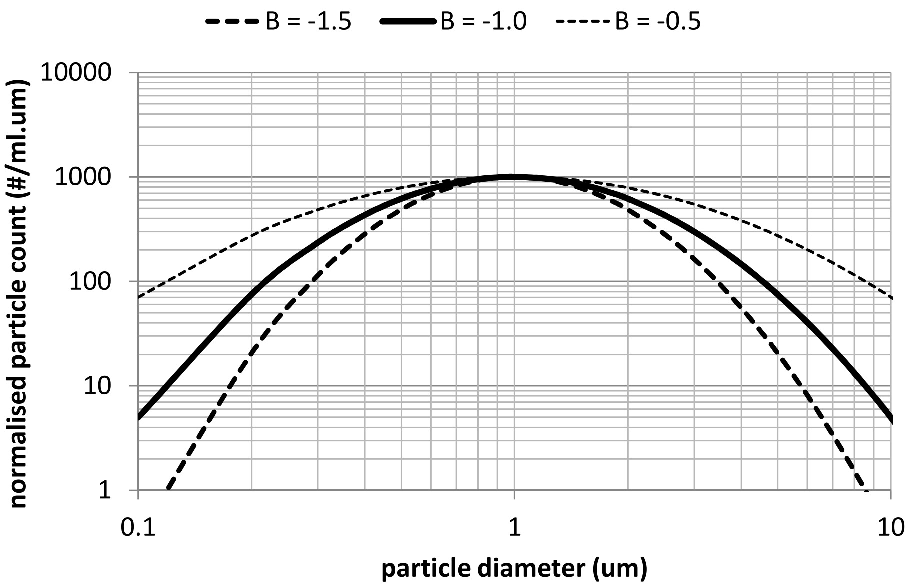

Fig. 6. The effect of model parameter β on the particle size distribution, with $A = 1000$ and $C = 0$.

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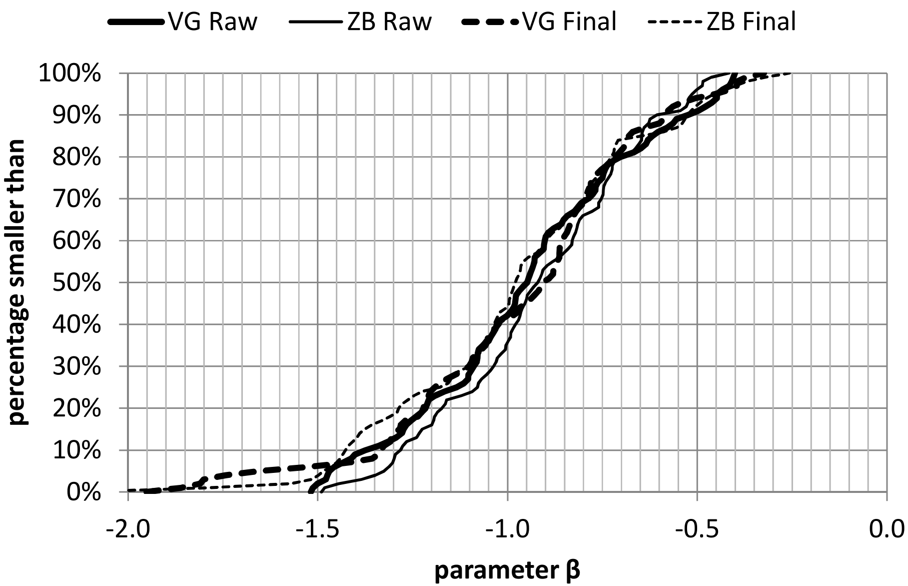

Fig. 7. The cumulative distribution of model parameter β.

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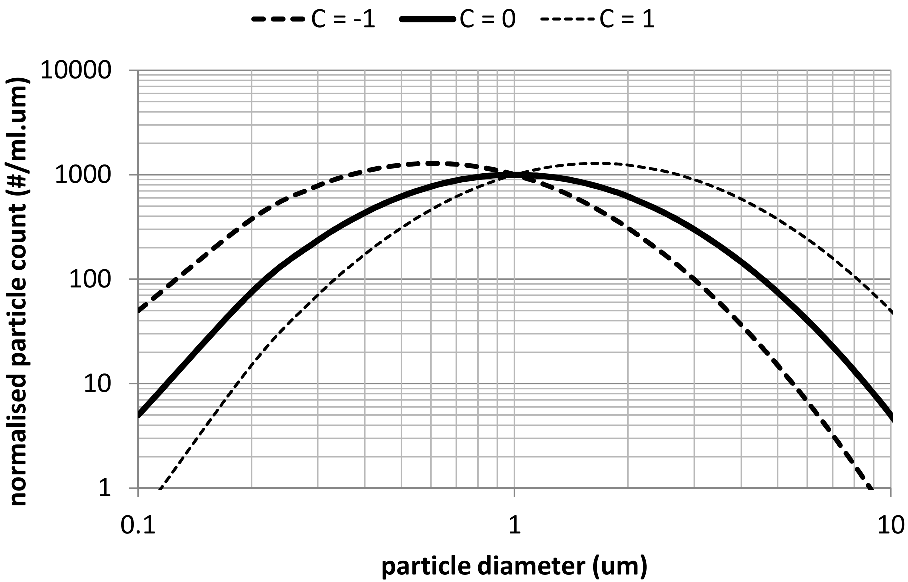

Fig. 8. The effect of model parameter C on the particle size distribution, with $A = 1000$ and $\beta = -1$.

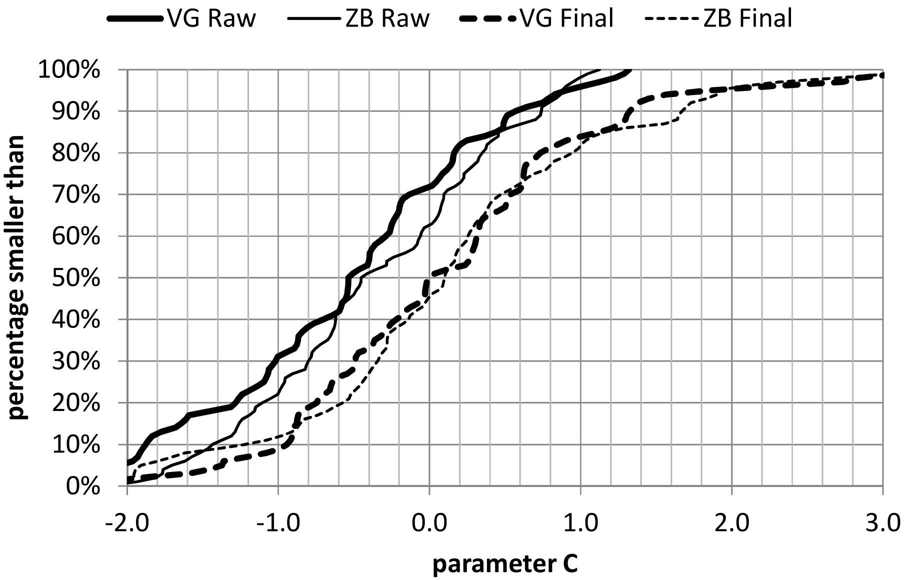

Fig. 9. The cumulative distribution of model parameter C.

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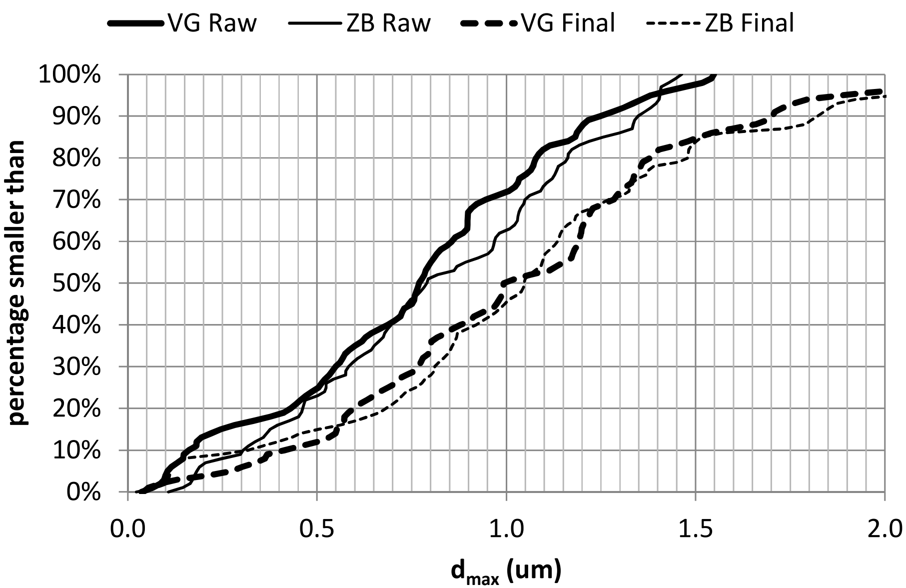

Fig. 10. The cumulative distribution of model parameter d_{max}.

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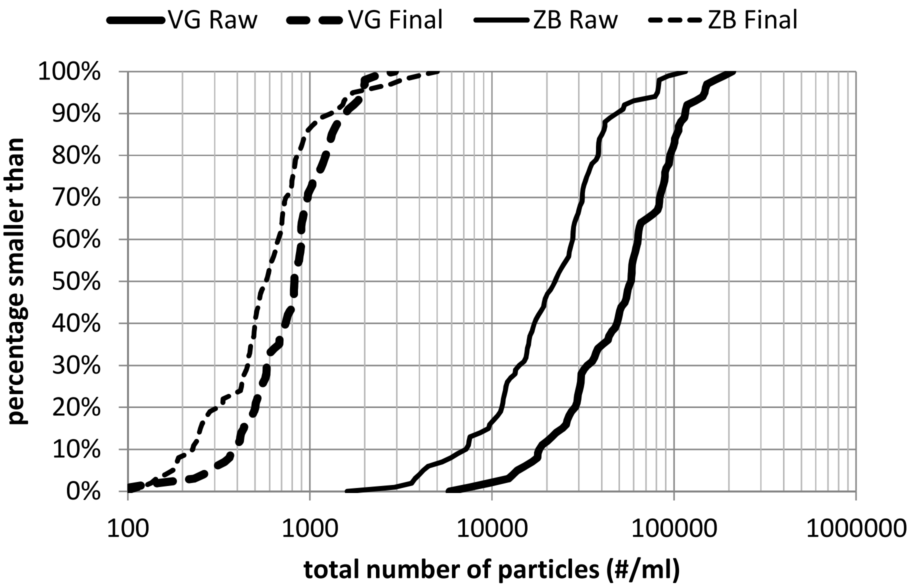

Fig. 11. The cumulative distribution of the total number of particles between 1 and 10 µm.

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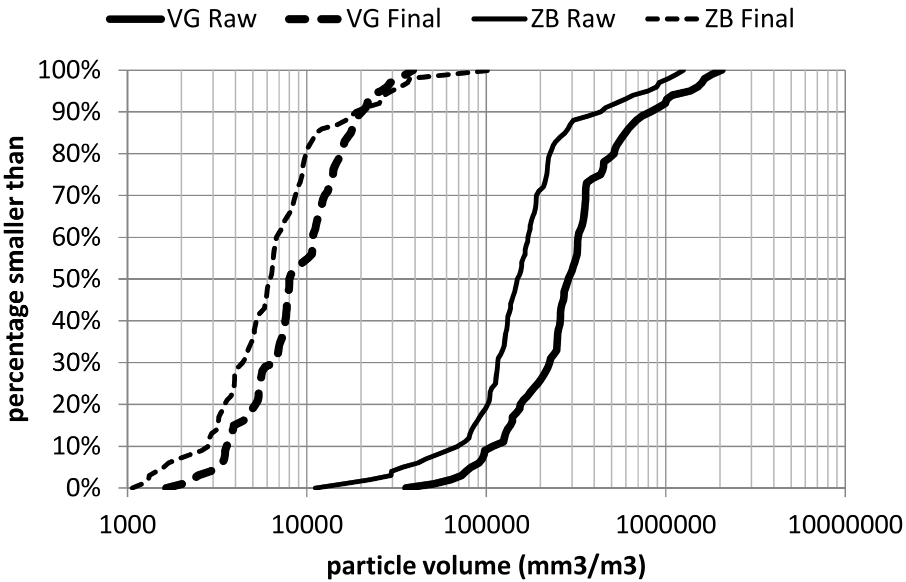

Fig. 12. The cumulative distribution of the calculated particle volume between 1 and 10 µm.

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