Monitoring of Particle Size Distribution Using Lasentec FBRM

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You are all familiar with the measurement principle of the FBRM. Nevertheless, this gives a good introduction to my talk as the data provided by the instrument represents a chord length distribution.

**Focused Beam Reflectance Measurement (FBRM)**

- **Motivation**
- **CLD Model**
- **Inverse Methods**
- **Results**
- **Conclusions**
This chord length distribution (CLD) provides a wonderful tool in many applications (e.g., for batch-to-batch consistency tests). But for a combination of the measurement and particle population models, the CLD is not well suited. And apart from this, everyone might be interested in what the particle size distribution (PSD) that one is usually more familiar with might look like. In this work we developed a tool to calculate PSDs from CLD data.
This constitutes an inverse problem and therefore this goal is achieved in two steps: First, a CLD model is developed that describes the CLD of single particles and particle populations. Second, inverse methods are used to restore PSDs on the basis of the given model.

Before explaining this concept in detail, as an introduction I would like to directly start with some examples of measured CLD data and the calculated PSDs.
Let me start with a very simple example. We might measure with the FBRM a monomodal population of ceramic spheres in water. The concentration of the solid particles is 30 Vol% and we use a measurement time of five minutes. We obtain the result shown in this graph. On the right there is the characteristic peak with a tail to the left of the CLD corresponding to the spheres. On the left we see counts caused by the surface properties of the particles.
Some Examples

- Ceramic spheres in water, sieved, 450 - 560 µm

Choosing a measurement time of two seconds, the distribution is more scattered, as less counts are used to calculate this normalized distribution. This results in the fact that statistical error increases with the number of counts per measurement.
Some Examples

This is shown on the right-hand side where the error norm is given for increasing counts per measurement. As seen in the distributions, the error norm decreases with, for example, higher measurement times.

- Ceramic spheres in water, sieved, 450 - 560 μm

CLD error norm
Some Examples

- Ceramic spheres in water, sieved, 450 - 560 µm

**CLD**

**error norm**

- Measurement time: 2 seconds
- Measurement time: 5 minutes

**Motivation**  **CLD Model**  **Inverse Methods**  **Results**  **Conclusions**
Some Examples

- Ceramic spheres in water, sieved, 450 - 560 µm

The inversion methods to calculate the PSD from CLD data are based on error analysis. Therefore, the calculated PSDs from these CLDs look rather similar.
Some Examples

Here the volume-weighted PSDs corresponding to the CLDs on the left are given. The peak of the PSDs lie in the range of 450 µm, as specified by the sieves. Some of you might use a laser diffractor particle sizer like the Malvern or the Sympatec. Based on the information of the volume-weighted PSD, we can compare the PSDs.

• Ceramic spheres in water, sieved, 450 - 560 µm
Some Examples

- Ceramic spheres in water, sieved, 450 - 560 µm
- Comparison with Laser diffractor

The blue distribution measured by the laser diffractor shows a high agreement with the calculated PSDs.

Motivation  CLD Model  Inverse Methods  Results  Conclusions
Some Examples

• Acetaminophen crystals in toluene

In a second example, the CLD of acetaminophen (drug) crystals is given. The measurement time was 30 seconds, but the concentration was only at about 1Vol%.
Some Examples

- Acetominophen crystals in toluene

The calculated PSD in its length-weighted form is given on the right-hand side with a significant peak on the right and a rather small peak on the left. As these particles are non-spherical and I am not an expert in laser diffractors, I compare this data with data obtained with an image analysis of PVM pictures.
Some Examples

- Acetaminophen crystals in toluene
- Comparison with PVM - image analysis

The red length-weighted PSD obtained by the image analysis data shows a peak close to the one of the calculated PSD. Nevertheless, the fine particles seem to be less than given by the FBRM. After this introduction I would like to explain this method of calculating PSDs from CLD data.
This explanation of the method will be divided into four main parts. In the first part, the CLD model will be explained. In the second part, the inverse methods used in this work to restore the PSDs from CLD data are shown. Then, results using simulated and real data will be presented. Finally, I will come back to the measured examples introduced before.
Let me start with the chord length distribution model.

• Chord length distribution model
  – CLD of a single particle
  – CLD of a particle population
  – Discrete description

• Inverse Methods

• Results

• Conclusions
• **3-dimensional geometric approach**
  – accounting for 2-D projections of all 3-D orientations

We compute the chord length distribution of a particle by regarding all of its 3-D orientations. Then, the chords of the corresponding 2-D projection are summed up to the CLD of the particle.
3-dimensional geometric approach
– accounting for 2-D projections of all 3-D orientations

Within the model, the shape of the particle is described by the general ellipsoid equation given here. This is a 4-parameter description with $a$, $b$, and $c$ being the half axes of the particle and the exponent $k$ describing the sphericity of the particle. In the following slides, three examples of CLDs of single particles will be presented.
The first example is a sphere, with \( a = b = c \) and \( k = 2 \). The graph shows the value of the logarithmic chord length distribution over the chord length ranging from 1 \( \mu \)m to 1 mm. In the case of a sphere, the CLD shows a characteristic peak at the diameter of the sphere.
Motivation

CLD Model

Inverse Methods

Results

Conclusions

For a needle as shown on the right side, the picture looks different. The exponent $k=10$ describes an almost cuboid shape as you can see on the left side. The CLD consists of two peaks, with the less significant one at higher chord lengths referring to the length of the needle.

$\begin{align*}
a=b=c, & \quad k=2 \\
3a=3b=c, & \quad k=10
\end{align*}$
In the last example, the CLD of an octahedron is given as the blue curve. It shows a monomodal, but very broad, chord length distribution. How can we now calculate the CLD of a particle population? Regarding the shapes, it is already obvious that for a relation of the CLD to a PSD the characteristic size within the particle size distribution has to be defined. In these three examples we have given the CLDs of particles with the same characteristic length of 200 µm: The diameter (in the case of the sphere), the length of the needle (in the case of the needle), and the diameter of a sphere having the same volume as the octahedron (in the case of the octahedron). As discussed in the following slides, this is one of the points to be fixed when calculating the CLD out of a particle size distribution.
Therefore, let us fix the shape of the particles in the population (here the sphere) and let us fix the characteristic length of this shape (here the diameter of the sphere).
Then, as already seen, we can calculate the CLD of this particle with a characteristic size L. Let us call it $q_p(s,L)$. 

$q_p(s,L=20\mu m)$
And we can calculate $q_p$ for a particle with a different characteristic size $L$. 

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CLD model - particle population
The CLD q of this particle population is given by the superposition of the two single-particle CLDs. What was shown here in the simple example can be formulated generally in an integral equation. Discretizing the integral equation leads to a linear matrix equation of the form $q = An + e$. $q$ is the measured CLD data vector, $A$ is the CLD PSD model matrix based on the single particles CLDs $q_p$ as given in the integral formulation. $e$ is the error vector. And $n$ is the PSD vector to be determined. Although the equation looks rather simple, it is not straightforward to solve the equation for $n$. In fact, it comes out that the problem is ill-posed for most of the particle shapes. This means that it is difficult to obtain a feasible solution for $n$. Therefore, in the following slides we present the inverse methods we used to solve this restoration problem.
CLD model - particle population

- **integral formulation**

\[ q(s) = \int_{0}^{\infty} q_p(s, L) n(L) \, dL + e \]

- **matrix formulation**

\[ q = A n + e \]

Measured CLD data

- **Motivation**
- **CLD Model**
- **Inverse Methods**
- **Results**
- **Conclusions**
CLD model - particle population

- integral formulation

\[ q(s) = \int_{0}^{\infty} q_p(s, L) n(L) \, dL + e \]

- matrix formulation

\[ q = A n + e \]

Motivation | CLD Model | Inverse Methods | Results | Conclusions
--- | --- | --- | --- | ---

measured CLD-PSD model matrix

CLD data

[Graph showing CLD data and matrix formulation]
CLD model - particle population

- integral formulation

\[ q(s) = \int_{0}^{\infty} q_p(s, L) n(L) \, dL + e \]

- matrix formulation

\[ q = A n + e \]

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CLD-PSD model error vector measured CLD data matrix
- integral formulation

\[ q(s) = \int_{0}^{\infty} q_p(s, L) n(L) \, dL + e \]

- matrix formulation

\[ q = An + e \]
Outline

- Chord length distribution model

- Inverse Methods
  - Tikhonov regularization
  - Projections onto convex sets (POCS)

- Results

- Conclusions

These two methods are the Tikhonov regularization, a very well-known and established way of solving ill-posed problems, and the method of projections onto convex sets (POCS), which has been used mainly in image restoration. These methods will be presented in the following slides.
In the Tikhonov regularization, not only the residual $q - A n$ is minimized like in the least squares solution, but as well a second term that introduces a constraint on the solution of $n$. The physical grounds of this constraint are given by the matrix operator $B$. The weighting between the minimization of the residual and the a priori constraint is given by lambda. A typical representation of the solutions can be seen on the right side. The euclidian norm of the residual is given on the y-axis, the norm of the a priori constraint is given on the x-axis.

Varying the regularization parameter lambda, one observes solutions on the given line. Approximating lambda to 0 leads to the least squares solution, approximating lambda to infinity leads to solutions with a high residual. If the error $e$ is known, then lambda can be chosen such that residual and error norm are equal. If not, then a value of lambda can be chosen based on the curvature of this line. Once the value of lambda is fixed, a direct solution of $n$ can be obtained using the regularized solutions here.
Inverse Methods \( q = A n + e \)

- **Tikhonov Regularization**

\[
\|q - An\|^2 + \lambda^2 \|Bn\|^2 \rightarrow \text{min}
\]

- B: matrix operator
  - based on physical reasoning
- \( \lambda \): regularization parameter
Inverse Methods \( q = A n + e \)

- **Tikhonov Regularization**

\[
\|q - An\|^2 + \lambda^2 \|Bn\|^2 \rightarrow \min
\]

- \( B \): matrix operator
  - based on physical reasoning
- \( \lambda \): regularization parameter

Motivation  CLD Model  Inverse Methods  Results  Conclusions
Inverse Methods  \( q = A n + e \)

- **Tikhonov Regularization**

\[
\|q - An\|^2 + \lambda^2 \|Bn\|^2 \rightarrow \min
\]

- \( B \): matrix operator
  - based on physical reasoning
- \( \lambda \): regularization parameter

Motivation  CLD Model  **Inverse Methods**  Results  Conclusions
Inverse Methods $q = A\ n + e$

- **Tikhonov Regularization**

$$\left\| q - A\ n \right\|^2 + \lambda^2 \left\| B\ n \right\|^2 \rightarrow \min$$

$B$: matrix operator
- based on physical reasoning

$\lambda$: regularization parameter

regularized equations

$$n = (A^T A + \lambda B^T B)^{-1} A^T q$$

Motivation  CLD Model  **Inverse Methods**  Results  Conclusions
An alternative method to solve the restoration problem is the method of projections onto convex sets (POCS). The method can be illustrated as follows: The solution is found by defining a consistent set of constraints $C_1$, $C_2$, and so on. These constraints are defined in such a way that the solution lies in the intersection of these constraints. Then, projection operators $P_1$, $P_2$, etc., can be defined and the iteration given in the equation below converges to a point on the boundary of the intersection as illustrated here. Some possible constraints formulated in the convex sets framework are introduced in the following slide.
Inverse Methods \( q = A n + e \)

- Projections onto Convex Sets (POCS)
  - set of consistent constraints
  - solution fullfills all constraints, i.e. \( \in C_o \)
Inverse Methods \( q = A n + e \)

- **Projections onto Convex Sets (POCS)**
  - set of consistent constraints
  - solution fullfills all constraints, i.e. \( \in C_o \)
  - Projection operators \( P_1, P_2, \ldots, P_m \)
  - \( n^{k+1} = (P_1P_2\ldots P_m)n^k \)
    converges to boundary of \( C_o \)
Inverse Methods \( q = A n + e \)

- **Projections onto Convex Sets (POCS)**
  - set of consistent constraints
  - solution fullfills all constraints, i.e. \( \in C_o \)
  - Projection operators \( P_1, P_2, \ldots P_m \)
  - \( n^{k+1} = (P_1P_2\ldots P_m)n^k \)
  - converges to boundary of \( C_o \)

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\( C_1 \) \( C_2 \) \( C_3 \) starting value

exact solution
Inverse Methods  \( q = A n + e \)

- **Projections onto Convex Sets (POCS)**
  - set of consistent constraints
  - solution fulfills all constraints, i.e. \( \in C_o \)
  - Projection operators \( P_1, P_2, \ldots P_m \)
  - \( n^{k+1} = (P_1P_2\ldots P_m)n^k \)
    converges to boundary of \( C_o \)
Inverse Methods \( q = A n + e \)

- **Projections onto Convex Sets (POCS)**
  - set of consistent constraints
  - solution fullfills all constraints, i.e. \( \in Co \)
  - Projection operators \( P_1, P_2, \ldots, P_m \)
  - \( n^{k+1} = (P_1 P_2 \ldots P_m) n^k \)
    - converges to boundary of \( Co \)
• POCS - constraints based on data and measurement error

Properties of residual \( r \equiv An - q \)  
properties of error \( e \)  

residual bounds  
error statistics  

First we regard the constraints based on data and the measurement error. The basic idea behind the formulation of these constraints is similar to the considerations in the Tikhonov regularization: The closer the properties of the residual \( r = \ldots \) to the properties of the error, the closer the obtained result is to the exact result. Therefore, bounds on the norm of the residual, the mean of the residual, or the residual at every data point can be described using error statistics like chi square or t-student distributions.
Inverse Methods \[ q = A n + e \]

- **POCS - constraints based on data and measurement error**
  
  Properties of residual \( r \equiv A n - q \) and properties of error \( e \)
  
  Residual bounds error statistics

- **POCS - a priori constraints based on physical reasoning**
  
  - Nonnegativity
  - Normalized PSD

Additionally, a priori constraints can be formulated based on physical reasoning. In our case this might be non-negativity of the PSD and constant area under the normalized PSD.
After introducing the basis of the restoration of the PSD from CLD data, I would like to show some theoretical test cases.

Motivation | CLD Model | Inverse Methods | Results | Conclusions
Let me start with a simulated test case for Tikhonov regularization.
Results - simulated CLD data

- **Tikhonov regularization - an example**
  - population of octahedra
  - CLD including gaussian error

The simulated CLD of a population of octahedra includes a gaussian error.
Results - simulated CLD data

- CLD including gaussian error

The difficulty obtaining a feasible solution is obvious in the least squares result. Setting lambda to 0, a highly scattering PSD is obtained due to the ill-posed character of the problem.
Results - simulated CLD data

• Tikhonov regularization - an example
  – population of octahedra
  - CLD including gaussian error

• $\lambda = 7900 \rightarrow$ overregularized solution

Nevertheless, setting the value of lambda to high results in a CLD that differs significantly from the original CLD.
Results - simulated CLD data

• Tikhonov regularization - an example
  – population of octahedra
  - CLD including gaussian error

  • $\lambda : 1.6$

However, the Tikhonov regularization using an optimal choice of lambda leads to a PSD very close to the original PSD given in red.
Results - simulated CLD data

- Tikhonov regularization - an example
  - population of octahedra
  - CLD including gaussian error

- $\lambda : 1.6$

And the corresponding CLD constitutes a smooth fit on the original scattered data.
Results - simulated CLD data

• Projections Onto Convex Sets - an example

The shortcomings of the method of Tikhonov regularization are obvious in a more complex example.
Results - simulated CLD data

- Projections Onto Convex Sets - an example
  - PSD using Tikhonov

The sharp peak of the PSD given here cannot be restored. Moreover, as in the earlier example, non-negative PSD values occur.
Results - simulated CLD data

• Projections Onto Convex Sets - an example
  – PSD using POCS
    • residual constraints
    • a priori constraints

Applying the method of POCS to this restoration case gives a different picture. When applying constraints on the residual and a priori constraints, the recovered CLD almost coincides with the original one. As well, the sharp peak is recovered correctly.
Results - experimental CLD data

• An example: acetaminophen crystals

After these simulated test cases I would like to come back to the example of measured CLD data as shown before. The example corresponds to the measurement of a population of acetaminophenon crystal.
Results - experimental CLD data

• An example: acetaminophen crystals

Micrographs of these crystals show a more or less perfect octahedric shape.
Results - experimental CLD data

- An example: acetaminophen crystals

- assumption: octaederic shape

Therefore, a population of octahedra was assumed.
• **Measured CLD-data**

An example of a CLD measured during a batch crystallization of acetaminophen is given here.
Results - experimental CLD data

- Tikhonov regularization

  - \( \lambda \): optimal (30.1)

Applying the method of Tikhonov regularization, a clearly bimodal PSD is obtained. The corresponding CLD is a smooth fit to the measured data.
• Projections onto Convex Sets
  – residual constraints
  – nonnegativity

When applying the POCS method, we also observe this bimodality and, of course, no negative values occur.
To summarize this method, let me come back to the first slide of this talk. A tool to restore PSD from CLD data has been developed.
This is based on a geometrical CLD model that calculates the CLD from PSDs, assuming equal shape of all particles in the population and neglecting all optical effects and the application of an inverse method. We have shown in theoretical test cases that this inverse problem can be solved.
Conclusions

- CLD + optical effects
- measurement characteristics
- no perfectly equal shapes

In the practical case, the measured CLD implies not only the information of this geometrical CLD, but it is also affected by the optics of the device and its measurement characteristics. Moreover, no perfectly equal shapes will occur. Therefore, as in every particle sizing method, the PSD is only an approximation of the real PSD. But for sure, improvements of the CLD measurement will lead to improvements of the approximated PSD. And the PSD restoration might help in finding some of the shortcomings. On the other hand, it might be possible to include some of the optical effects into the CLD model and improve the PSD estimation.

- approximation of PSD
- measurement improvements
  lead to PSD improvements

Motivation       CLD Model       Inverse Methods       Results       Conclusions
Conclusions

• CLD + optical effects
• measurement characteristics
• no perfectly equal shapes

To discuss some of these optical effects, let me come back to the example of spheres shown at the very beginning.

• geometrical CLD model
• inverse method
  • Tikhonov
  • POCS

• approximation of PSD
• measurement improvements
  lead to PSD improvements
Conclusions

- CLD + optical effects
- Measurement characteristics

Ceramic spheres in water, sieved, 450 - 560 μm

This distribution was obtained from a dispersion with 30 Vol% particles.
Conclusions

- CLD + optical effects
- measurement characteristics

Ceramic spheres in water, sieved, 450 - 560 µm

Measuring the particle for the same time of 30 seconds, but in a dispersion with only 1 Vol%, this comparison shows some features of the optical effects of the FBRM. First, the CLD scatters more as fewer counts are detected with the lower particle concentration.
• CLD + optical effects

• measurement characteristics

Ceramic spheres in water, sieved, 450 - 560 µm

Furthermore, the noise peak on the left is higher at low concentrations. Why is this? The further a particle is detected away from the probe, the higher the probability that the weaker signal coming back to the device is detected as several signals. Measurements of a single particle at defined positions in front of the probe show this effect. In the case of a low particle concentration, the particles are detected on average further away from the probe and this splitting of signals increases.
Conclusions

- Acetaminophen crystals in toluene
- Comparison with PVM - image analysis

This effect was obvious in the comparison of PSD data from acetaminophen crystals with PVM measurements shown at the beginning. The calculated PSD shows a peak at the left, although almost no particles occur in this size range.
• CLD + optical effects

• measurement characteristics

Ceramic spheres in water, sieved, 450 - 560 µm

The fact that the particles are detected at a further distance leads to another effect. At further distance from the probe window the laser beam is broader than it is very close to the window. This can lead to a longer signal being backscattered. That this effect becomes more and more important the smaller the particles is obvious when comparing the means of populations obtained with the FBRM and a laser diffractor.
Conclusions

• Ceramic spheres - Laser diffractor vs. FBRM

• comparison of the $L_{43}$

On this graph, the $L_{43}$ mean obtained with the laser diffractor is given on the right axis and the $L_{43}$ resulting from the calculated PSD is given on the left axis. One can observe that for the ceramic particle system discussed, the means correspond almost perfectly for large particle sizes. Nevertheless, for small ceramic spheres, the mean of the FBRM PSD is higher than the $L_{43}$ measured by the laser diffractor.
One can discuss which of these effects should be included by the model and which are problems of the measurement that have to be overcome. But in the end, I would like to emphasize one feature of spheres that might be nice for Lasentec users: Especially when presenting the CLD distributions in volume-weighted and logarithmic form, the PSD and the CLD are not that different (but only for spheres)!
Acknowledgements
• $q = An + e$ : Ill - or well conditioned?

$\Leftrightarrow$ analysis of $A$: condition number $\kappa = \frac{s_{\max}}{s_{\min}}$

- $\kappa \to \infty$ : $A$ has singularity
- $\kappa$ : large : $A$ is ill-posed
- $\kappa \to 1$ : $A$ is well-posed

As illustrated before, the restoration of the PSD implies to solve the linear matrix equation $q = An + e$ for $n$. The difficulty in obtaining a feasible solution for $n$ is described by the ill- or well-posedness of the problem. An analysis of this feature can be obtained by calculating the condition number of the model matrix $A$. The condition number $\kappa$ is defined by the ratio between maximum and minimum singular value. With decreasing $\kappa$, the problem becomes well-posed (i.e., it is more and more straightforward to solve the equation for $n$).

In the table shown on this slide, the values of $\kappa$ are given for different particle shapes and different ratios between CLD and PSD data points. One can observe that the values of $\kappa$ differ significantly over this range of shapes and data points. In the case of a sphere, the problem is almost well posed. Nevertheless, for different shapes, the problem is highly ill-posed. Although it is of advantage to estimate a smaller number of PSD data points from a high number of CLD data points.

<table>
<thead>
<tr>
<th>particle shape</th>
<th>sphere</th>
<th>octahedron</th>
<th>needle</th>
</tr>
</thead>
<tbody>
<tr>
<td>dim (CLD) / dim (PSD)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>360/360</td>
<td>15</td>
<td>3e+7</td>
<td>5e+5</td>
</tr>
<tr>
<td>360/90</td>
<td>6</td>
<td>1e+4</td>
<td>8e+2</td>
</tr>
<tr>
<td>90/90</td>
<td>4</td>
<td>2e+4</td>
<td>3e+5</td>
</tr>
</tbody>
</table>
Results - problem characteristics

- \( q = An + e \) : **Ill - or well conditioned?**
  - \( \kappa : large \) \( A \) is ill-posed
  - \( \kappa \rightarrow 1 \) \( A \) is well-posed

\( \kappa \rightarrow \infty \) \( A \) has singularity

\( \kappa \rightarrow \infty \) \( A \) has singularity

\( \kappa : large \) \( A \) is ill-posed

\( \kappa \rightarrow 1 \) \( A \) is well-posed

In the examples we regard ill-posed restorations of PSDs of octahedra with 90 data points from CLD raw data with 360 points.

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<td>2e+4</td>
<td>3e+5</td>
</tr>
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</table>
Q: So the error you are seeing is surface-characteristic error?

JW: On the left side of the histogram? Yes.

Q: In the separate bins of the PSD, how do you assume the distribution curves? If you have a CLD, you have to assume something about how the particles are distributed within each of the bins if you cut out the PSD.

JW: In this case, we always started with a logarithmic CLD with 360 channels and calculated a PSD with 90 logarithmic channels, where we assume that the particles have a size of the geometric mean of this interval.
Questions and Answers

Q: Do you have to know the shape of the particles?

JW: Yes, we do have to define the particle shape. By the way, this is true for every type of particle sizer. In a Laser Diffractor, usually a spherical shape is assumed.

Q: Have you tried this in a case where you have more than one kind of shape in your distribution?

JW: From a theoretical point of view, we can assume any mixture of shapes, but I would say it is better to stay with one shape in the practical case. I do not know if it is realistic to fix the distribution of shapes in the population. On the other hand, one could think of extracting particle shape information from the CLD as well.
Questions and Answers

Q: Would it be more difficult to solve if you had needles than octahedra?

JW: When we look at the model matrix A, we can get a measure for how difficult it is to get a good solution. It is much easier for a sphere than for an octahedron. It is, in some cases, more difficult for needles. So it is different for different particle shapes. This question is discussed in Slides 72 and 73.

Q: On these last slides, what is dim (CLD)/dim (PSD)?

JW: “Dim” stands for dimension. For example, estimating 90 PSD channels out of 360 CLD channels means we give more information. The problem becomes less difficult.
RB: Going back to the first slide where you have the cubes and 3-D modeling, you are going to take CLD from this particle and convert it back to a spherical equivalent diameter for your population balance. But in your population balance, are you then going to put in a shape value? Because what you have here is a particle that has a different surface area than a sphere.

JW: In the population balance it has to be the shape factor of this one.

RB: Okay, so you are using the shape factor to back out this volume. So what you are interested in is the volume, not necessarily the spherical equivalent volume, and you are putting the shape factor back in because otherwise the surface area would be wrong.

JW: When you have a special particle you always have to decide what the characteristic length of this particle is. When you have a needle, for example, it makes sense to say that the characteristic size of this needle is the length of the needle.