Nanostrukturierte Materialien: Gesundheit, Exposition, Materialeigenschaften

Applications of a Cluster-Based Method for Analysis of Polydisperse Size Distributions Obtained by Single Particle Tracking of Nanoparticles

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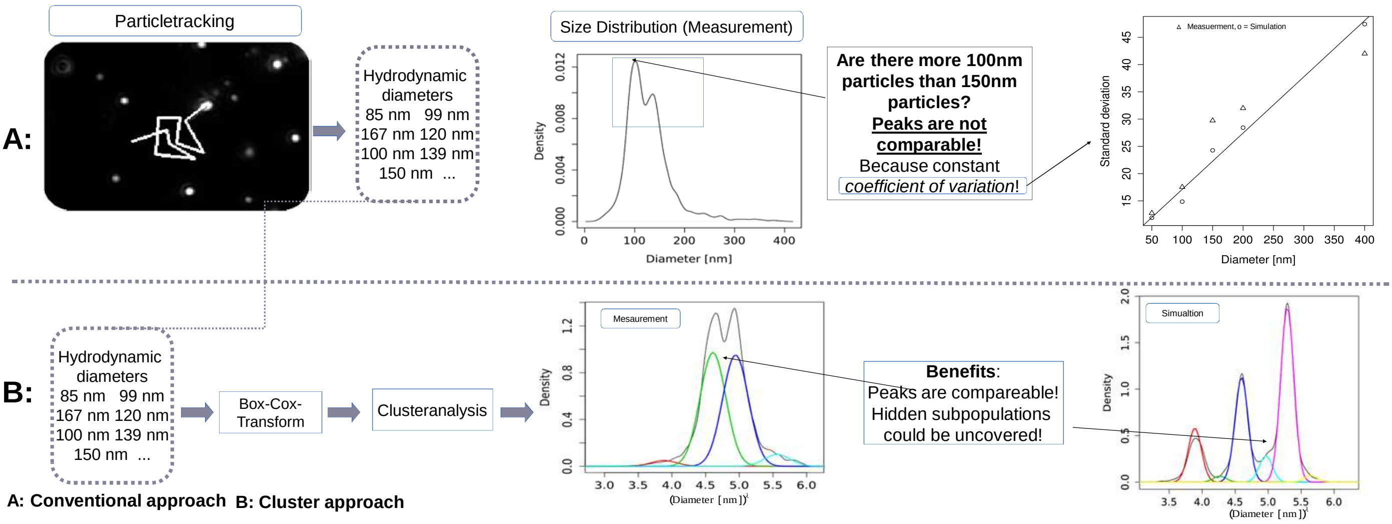
Visual Abstract



Summary

Size measurements of nanoparticles can be made by tracking single particles in Brownian motion under the microscope. The diffusion coefficient of each particle and its hydrodynamic diameter may be calculated from the trajectory, and the Stokes-Einstein-relation, respectively. This approach correctly distinguishes small and large particles and, therefore, appears suitable to characterize particles also in polydisperse suspensions. However, although much effort has been spend on optimizing the estimation of diffusion coefficients with respect to the localization error and the finite trajectory length, minor improvements have been made to correctly analyze the composition of polydisperse suspensions.
Our recent work [1] showed that analysing a polydisperse size distribution is an issue which can be successfully addressed by means of a cluster-based method. To this aim particle diameter data needed to be transformed by mathematical methods. As shown here, the Box-Cox transform led to a markedly lowered heteroscedasticity thus improving the identification of mixed particle populations. This property allowed for an automatic expectation maximization cluster analysis, which robustly segregates populations of single particle in mixed suspensions, even if the number of particle types is unknown.

The procedure appears helpful to correctly interpreting the composition of polydisperse particle suspension.

[1] Thorsten Wagner, Martin Wiemann, Inge Schmitz, and Hans-Gerd Lipinski, "A Cluster-Based Method for Improving Analysis of Polydisperse Particle Size Distributions Obtained by Nanoparticle Tracking," Journal of Nanoparticles, Vol. 2013, Article ID 936150, 9 pages, 2013. doi:10.1155/2013/936150

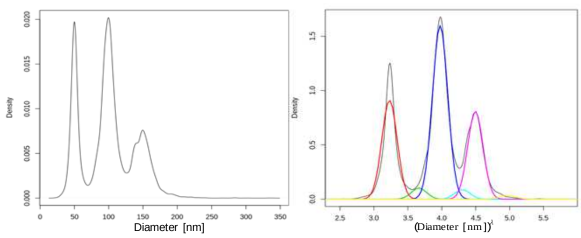
Monte Carlo Simulation

A Monte Carlo simulation was carried out to demonstrate the superiority of the cluster approach over the conventional approach (see diagrams) for a simulated particle suspension, whose compostion is shown in Table 1.

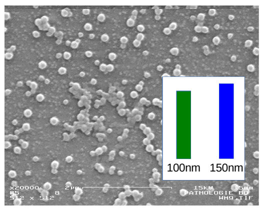
Table 1: Simulated Composition:

Diameter	Proportion
50nm	25%
100nm	50%
150nm	25%

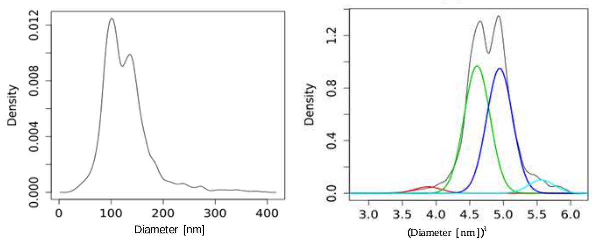
Conventional approach Cluster approach



Polystyrol nanoparticles



Conventional approach Cluster approach



We prepared a suspension of 100 nm and 150 nm polystyrene particles with equal number concentrations of both particle types, as revealed by SEM (left). While the conventional size distribution analysis overestimated the number of small particles (middle), the cluster aproach yielded largely correct results (right).

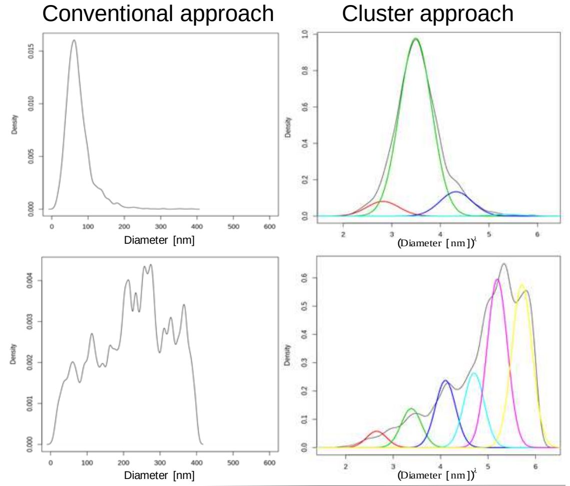
Agglomerating SiO_2-PEG nanoparticles

Pegylated SiO_2-NPs were dispersed in double distilled H_2O (upper figures). Addition of 0.3 mM phosphate buffer and 0.45% NaC led to an agglomeration within minutes (lower figures) and raised a population of agglomerated particles with a hard to interpret size distribution (lower left). Cluster analysis markedly improved the interpretability of this size distribution whose components are listed in Table 2.

Table 2: Estimated Composition:

Diameter	Proportion
25nm	4%
58nm	8%
110nm	13%
174nm	14%
242nm	31%
333nm	30%

Conventional approach Cluster approach



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