Supporting Information

Predicting average void fraction and void fraction uncertainty in fixed beds of poly-lobed particles

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Appendix S1: Standard Deviation Calculation

In this work, the simulations and measurements are deterministic and accurate. The resulting void fraction is different each time the same simulation is performed again as the particles are inserted with different (random) orientations and positions. The average void fraction thus ought to be treated as a random variable. In this work we are interested in comparing the effects of shape on the void fraction. Thus we must be able to quantify how much of the differences between two simulations with different shapes are due to the shape or to the loading procedure.

By definition, the **uncertainty** is the value I so that 95% of the random values of the void fraction will be within $\pm I$ of the average . With a Gaussian probability law, this definition is equivalent to $I = 1.96\sigma$ which is classically simplified to $I = 2\sigma$. In mathematical terms, 95% of the area under the Gaussian probability curve is within average $\pm I$. In our study, the effect of particle position and orientation is estimated by repeating the simulations and estimating the standard deviation.

The standard deviation of the sum or difference of two independent Gaussian random variables is given by $\sigma_{X-Y} = \sigma_{X+Y} = \sqrt{\sigma_1^2 + \sigma_2^2}$, yielding $\sigma_{X-Y} = \sigma_{X+Y} = \sigma_X\sqrt{2}$ when $X1$ and $X2$ follow a Gaussian probability law with standard deviation σ_X. The effect of insertion window size is estimated using the difference between two simulations, hence the introduction of a $\sqrt{2}$ in the calculations.