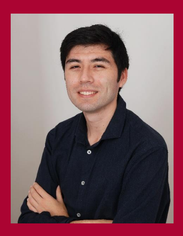
Approximating the van der Waals interaction potentials between agglomerates of nanoparticles



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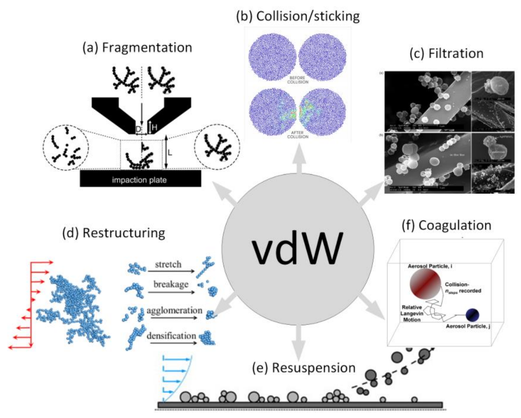
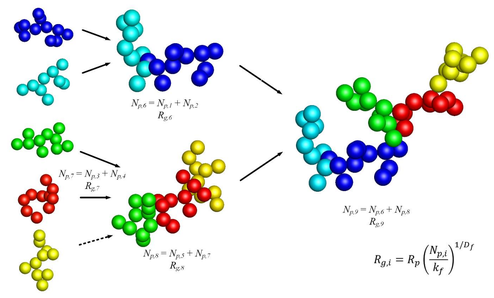
Motivation

Van der Waals interaction forces play an important role on different aerosol processes including: (a) nanoparticle fragmentation[1], (b) collision and sticking[2], (c) filtration[3], (d) restructuring[4], (e) resuspension[5], and (f) coagulation[6].

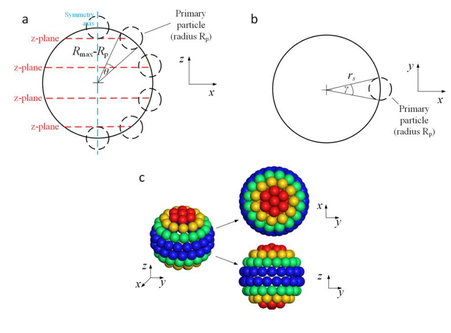


Aggregates generation

Using a modified version of FracVAL[7],



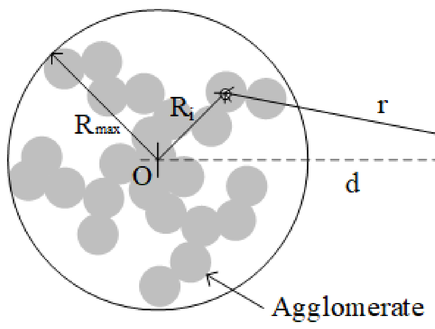
DLCA: $D_f = 1.78$ and $k_f = 1.40$
BLCA: $D_f = 1.89$ and $k_f = 1.36$



Hollow raspberry-like:
$D_f \to 2$ when $N_p \gg 1$

Calculation of interaction potentials

Agglomerate-molecule



Sphere-molecule potential:

$$W_{\mathrm{sm}}(d) = -\frac{4\pi R_p^3}{3}\left[\frac{C\rho}{(d-R_p)^3(d+R_p)^3}\right]$$

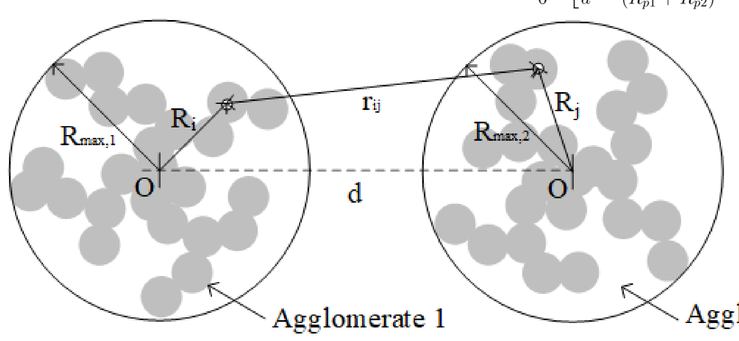
Total agglomerate-molecule interaction,

$$W_{\mathrm{Agg-Mol}}(d) = \left\langle \sum_{i=1}^{N_p} W_{\mathrm{sm}}(r_i) \right\rangle$$

Agglomerate-agglomerate

Sphere-sphere potential:

$$W_{\mathrm{ss}}(d) = -\frac{A_{\mathrm{Ham}}}{6}\left[\frac{2R_{p1}R_{p2}}{d^2-(R_{p1}+R_{p2})^2} + \frac{2R_{p1}R_{p2}}{d^2-(R_{p1}-R_{p2})^2} + \log\left(\frac{d^2-(R_{p1}+R_{p2})^2}{d^2-(R_{p1}-R_{p2})^2}\right)\right]$$

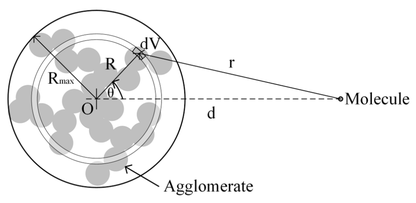


Total agglomerate-agglomerate interaction,

$$W_{\mathrm{Agg-Agg}}(d) = \left\langle \sum_{i=1}^{N_{p,1}} \sum_{j=1}^{N_{p,2}} W_{\mathrm{ss}}(r_{ij}) \right\rangle$$

Coarse-grained models

Agglomerate-molecule



The total interaction energy agglomerate-molecule,

$$W(d) = \int_{V_a} w(r)\rho dV_a$$

Morphological characterization of agglomerates,

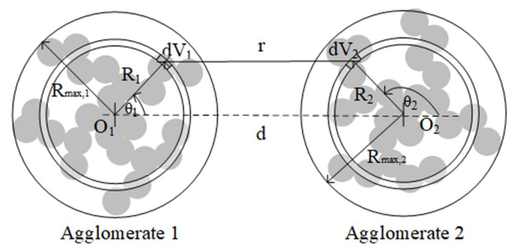
$$\frac{V_a(r)}{V_p} = \varphi\left(\frac{r}{R_p}\right)^{D_f}$$

For fractal-like agglomerates with fractal dimension $D_f \in [1,3]$ and packing factor φ

Van der Waals interaction energy,
$w(r) = C/r^6$

Model	Equation
Volume-equivalent sphere	$W(d) = -\varphi\frac{4\pi R_v^3}{3}\left[\frac{C\rho}{(d-R_v)^3(d+R_v)^3}\right]$
No cut-off	$W(d) = -\frac{\pi C\rho\varphi D_f}{6dR_p^{D_f-3}}\int_0^{R_{\max}} R^{D_f-2}\left[(d-R)^{-4}-(d+R)^{-4}\right]dR$
With cut-off	$W(d) = -\frac{2^{D_f+2}\pi C\rho\varphi D_f}{3dR_p^{D_f-3}}\int_0^{R_{\max}} R^{D_f-2}\exp(-(R/\xi')^{\gamma})\left[(d-R)^{-4}-(d+R)^{-4}\right]dR$
Proposed model (params α_1, α_2)	$W(d) = -\alpha_1\frac{R_p\pi C\rho\varphi}{9d^4}\left[\frac{1}{(1+R_{\max}/d)^{D_f+\alpha_2}}+\frac{1}{(1-R_{\max}/d)^{D_f+\alpha_2}}-2\right]$

Agglomerate-agglomerate



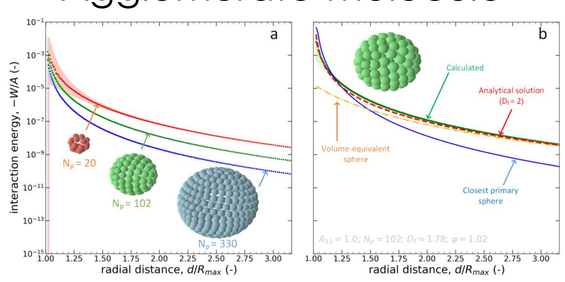
The total interaction energy agglomerate-agglomerate,

$$W(d) = \int_{V_2}\int_{V_1} w(r)\rho_1\rho_2 dV_1\, dV_2$$

Model	Equation
Volume-equivalent sphere	$W(d) = -\frac{A_{\mathrm{Ham}}}{6}\left[\frac{2R_{v1}R_{v2}}{d^2-(R_{v1}+R_{v2})^2}+\frac{2R_{v1}R_{v2}}{d^2-(R_{v1}-R_{v2})^2}+\log\left(\frac{d^2-(R_{v1}+R_{v2})^2}{d^2-(R_{v1}-R_{v2})^2}\right)\right]$
Rmax-Sphere/Volume pondered	$W_{ve}(d) = -\left(\frac{R_v}{R_{\max}}\right)^6\frac{A_{\mathrm{Ham}}}{6}\left[\frac{2R_{\max,1}R_{\max,2}}{d^2-(R_{\max,1}+R_{\max,2})^2}+\frac{2R_{\max,1}R_{\max,2}}{d^2-(R_{\max,1}-R_{\max,2})^2}+\log\left(\frac{d^2-(R_{\max,1}+R_{\max,2})^2}{d^2-(R_{\max,1}-R_{\max,2})^2}\right)\right]$
Babick *et al.* [17]	$W(d) = -A_{\mathrm{Ham}}\frac{\bar{\varphi}}{27}\left(\frac{3D_{\max}^2}{d^2}-\frac{16D_{\max}^2}{4d^2-D_{\max}^2}+\frac{D_{\max}^2}{d^2-D_{\max}^2}\right)$, $\bar{\varphi} = N_p\left(\frac{R_p}{R_{\max}}\right)^3$
Proposed model (params x, α)	$W(d) = -\frac{(D_{v1}D_{v2})^3A_{\mathrm{Ham}}}{9x^6}\left(\frac{(x/d)^6}{\left(1-(x/d)^{D_f+\alpha}\right)\left(4-(x/d)^{D_f+\alpha}\right)}\right)$, $D_f = \frac{2D_{f1}D_{f2}}{D_{f1}+D_{f2}}$

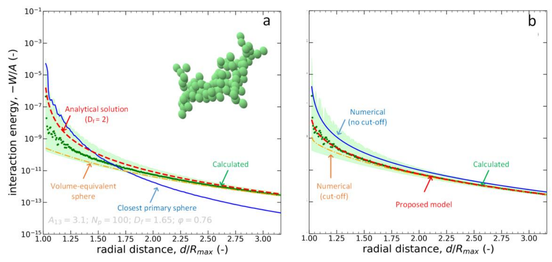
Results

Agglomerate-molecule

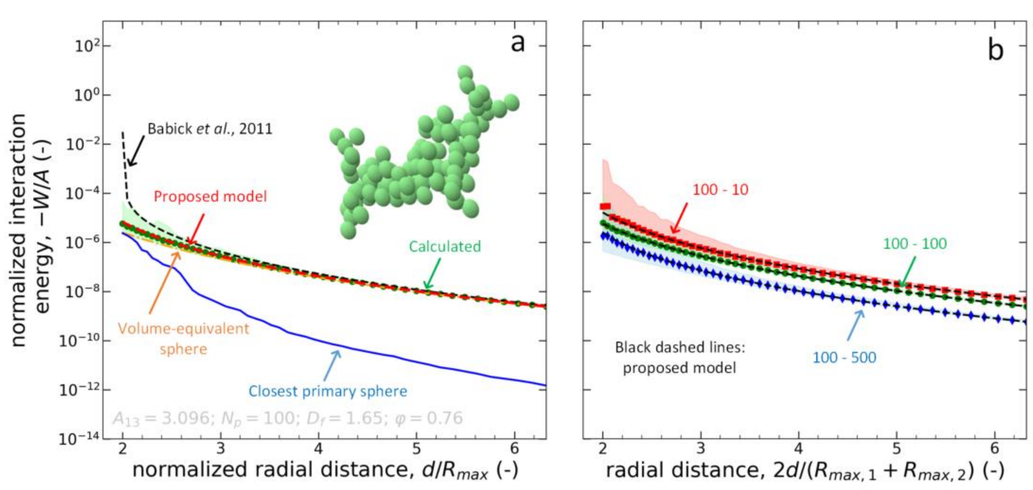


The raspberry-like agglomerate and molecule interaction is predicted by an analytical expression derived in this work.

Different models are compared and a simple semi-analytical is proposed for fractal-like agglomerates such as DLCA and BLCA.



Agglomerate-agglomerate



Conclusions

- A new **analytical model** is proposed for predicting the agglomerate-molecule vdW interactions with integer fractal dimension.
- Simple **semi-analytical** models are proposed for predicting non-integer fractal dimension agglomerate-molecule and agglomerate-agglomerate vdW potentials.

References

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