T31.00004 :
Relating the aerosol particle structure to the particle transport properties using ultra small angle X-ray scattering

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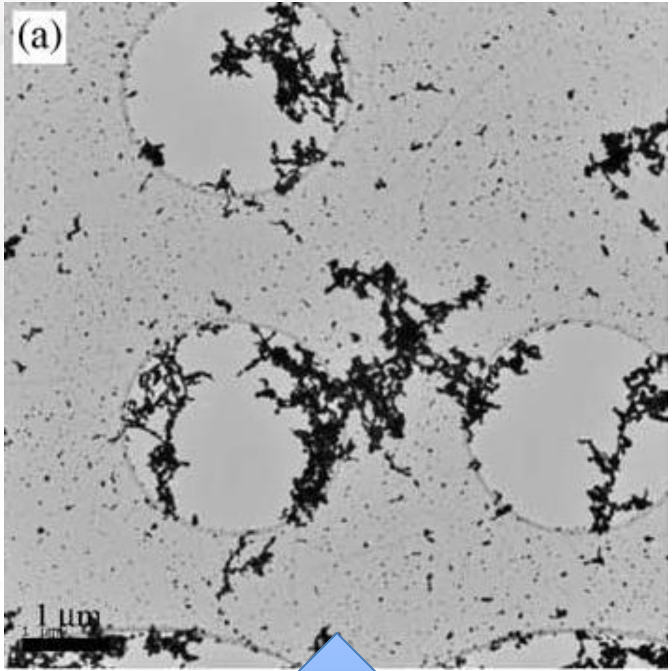
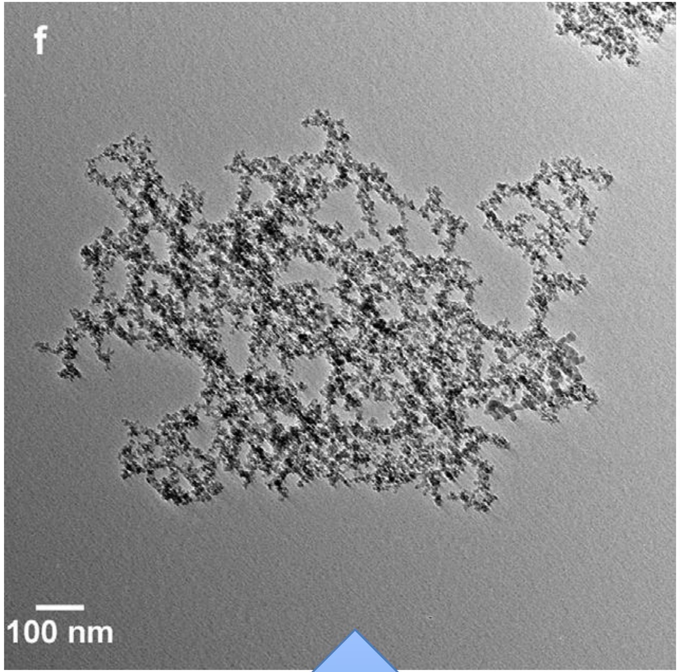
Problem statement

- Particulate aerosols pose health risks
- Often aerosol particles have a fractal like morphology
- How is the fractal structure related to particle transport (aerodynamic size) ?

Image taken from - https://www.thesweeper.com/osha-approved-sweepers accessed 1st March 2022



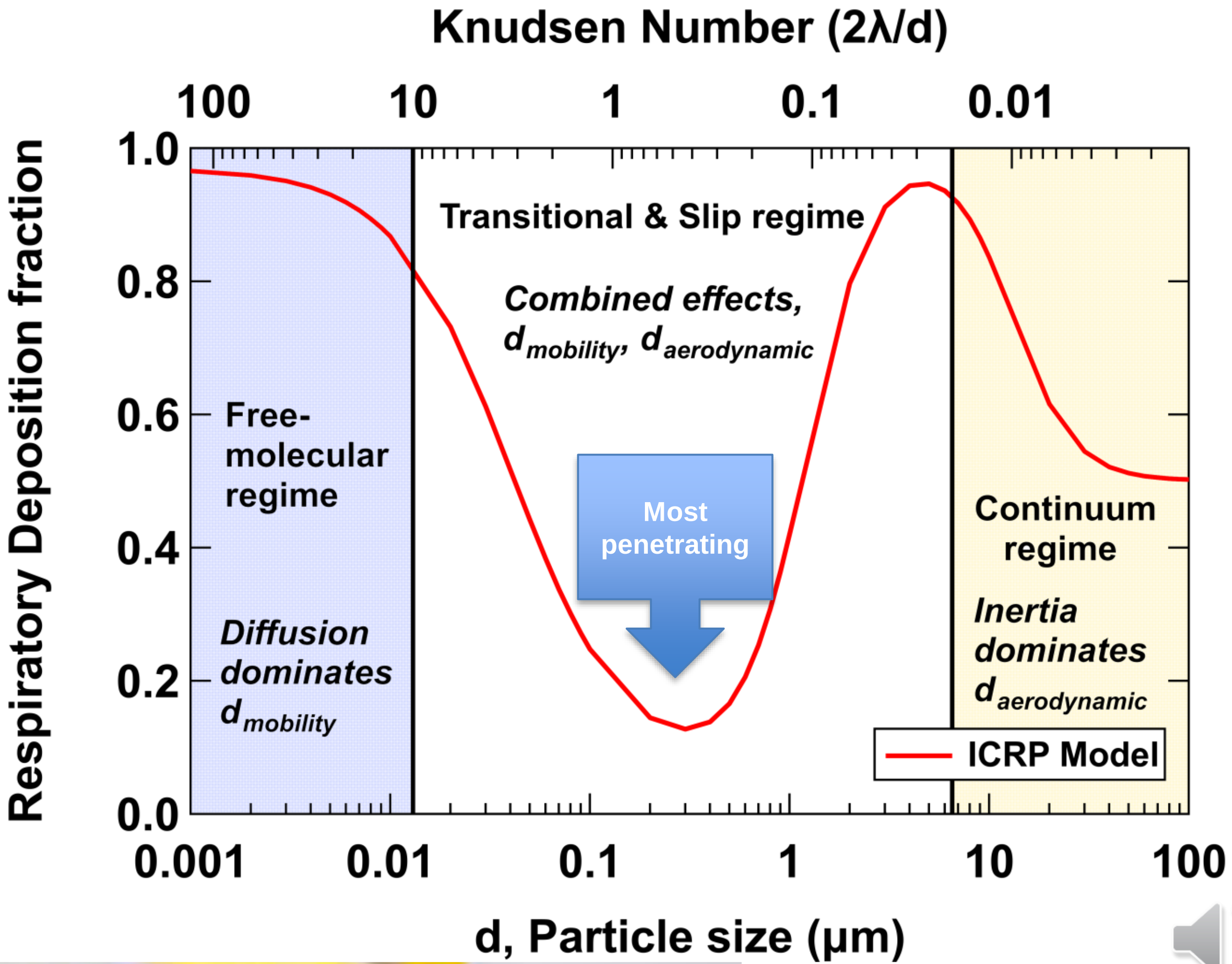
TEM Image of silver nanoaggregates[a]



TEM Image of Aerosil Fumed Silica aggregates[b]

[a]Image from Ku, B.K. and Maynard, A.D., 2006. Generation and investigation of airborne silver nanoparticles with specific size and morphology by homogeneous nucleation, coagulation and sintering. *Journal of Aerosol Science*, *37*(4), pp.452-470.

[b]Mulderig, A., Beaucage, G., Vogtt, K., Jiang, H. and Kuppa, V., 2017. Quantification of branching in fumed silica. *Journal of Aerosol Science*, *109*, pp.28-37.



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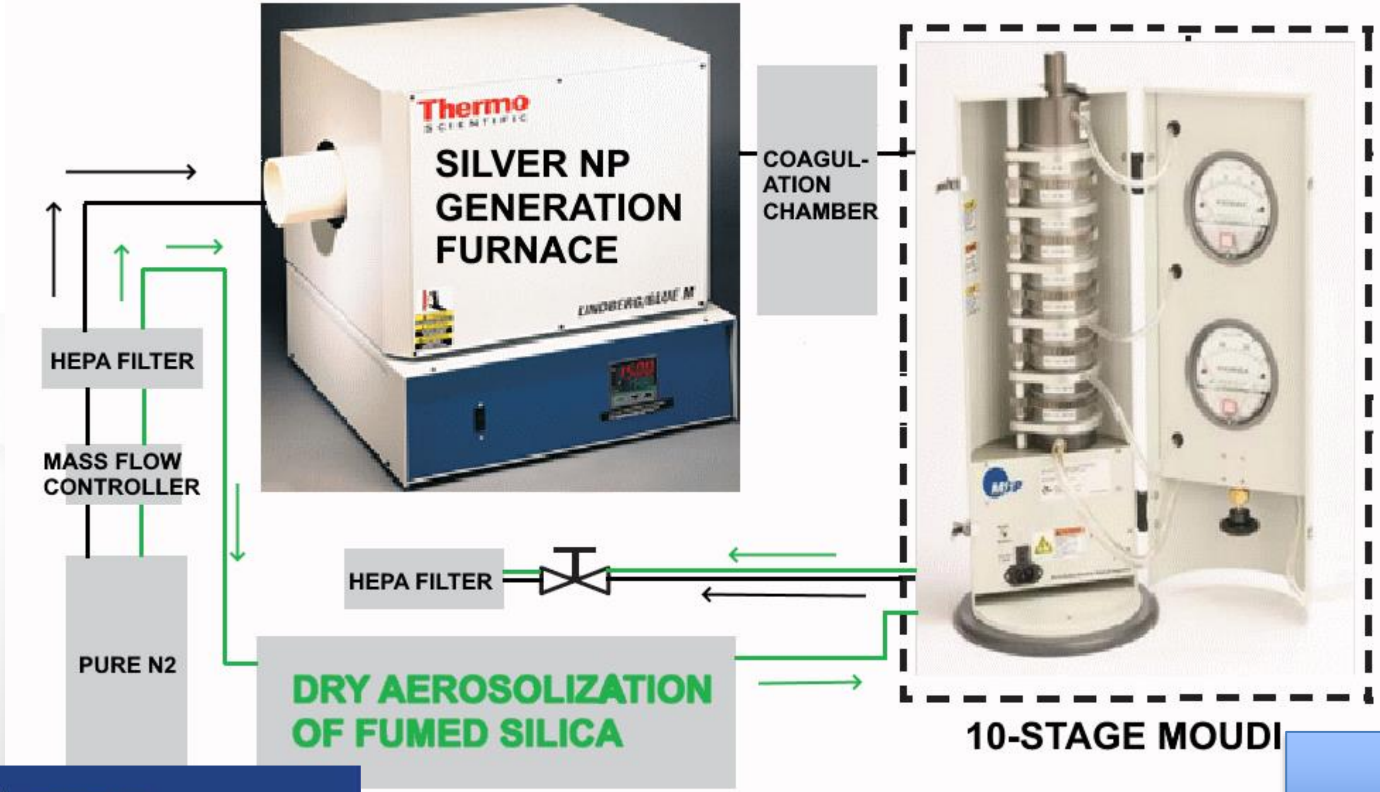
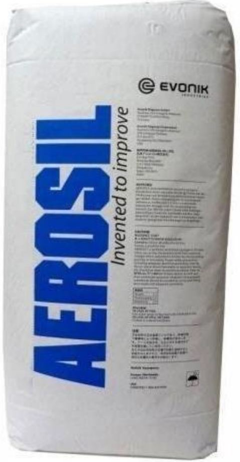
Ku et al. *Nanotechnology* 2006, 17, 3613-3621

Materials & Methods

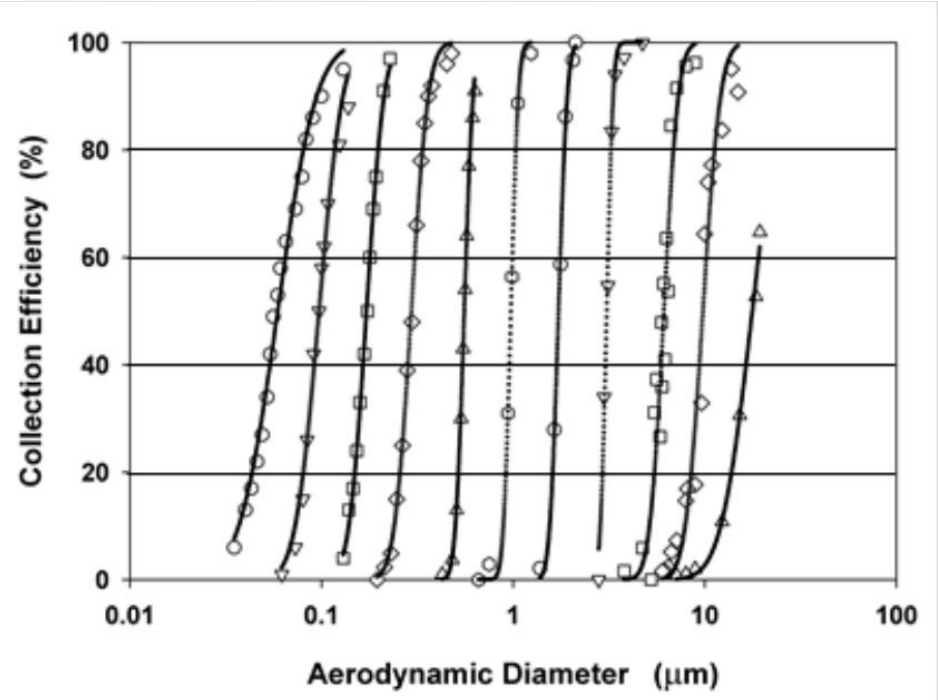




Inertial Impaction

Ku, B.K. and Maynard, A.D., 2006. Generation and investigation of airborne silver nanoparticles with specific size and morphology by homogeneous nucleation, coagulation and sintering. *Journal of Aerosol Science*, *37*(4), pp.452-470.

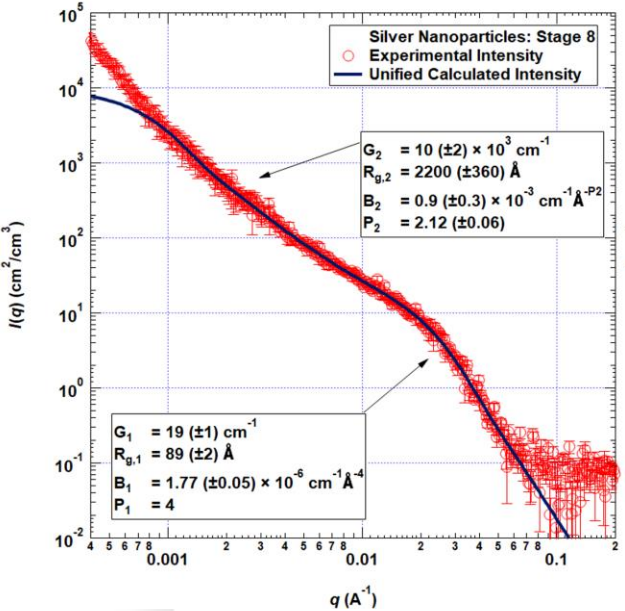
Aerodynamic size based on MOUDI

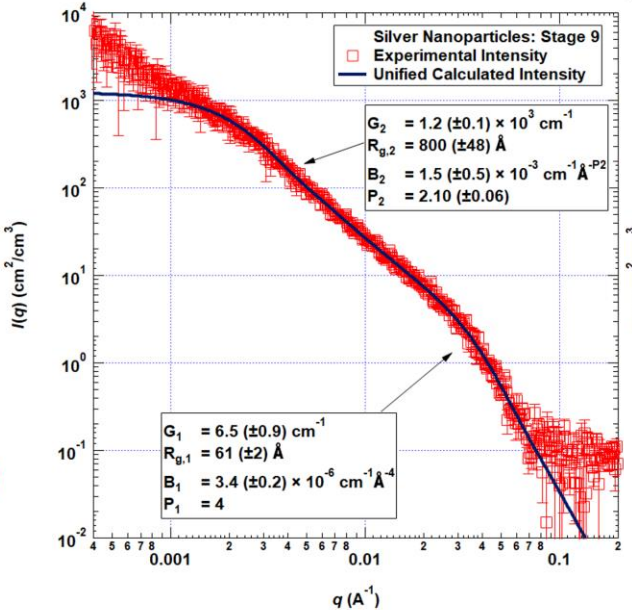


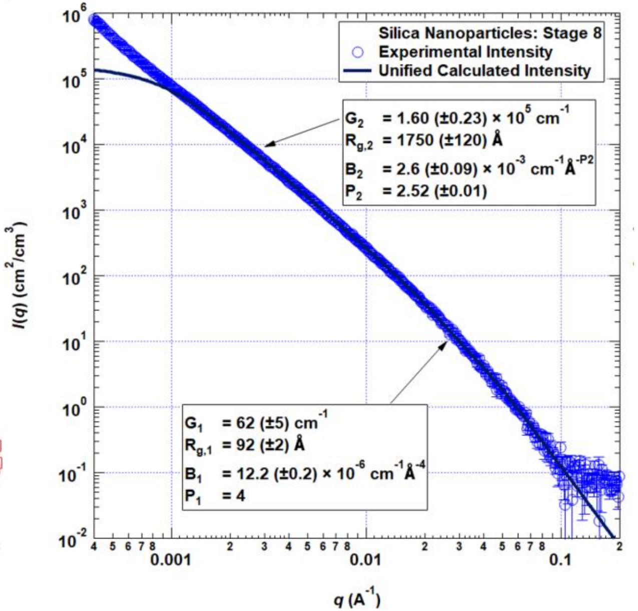
MOUDI Stage	d50, cut size (nm)	Geometric mean / Aerodynamic size (nm)
Pre	18000	-
1	10000	13416
2	5600	7483
3	3200	4233
4	1800	2400
5	1000	1342
6	560	748
7	320	423
8	180	**240**
9	100	**134**
10	56	**75**
After Filter	<56	

MSP, TSI Models 100 and 110 – MOUDI® Impactors
https://tsi.com/getmedia/771ace7e-bda8-4f34-87ed-6c872ea98deb/MSP_MOUDI_Impactors_MSP_PI-100_US-web?ext=.pdf

Ultra-small angle X-ray Scattering







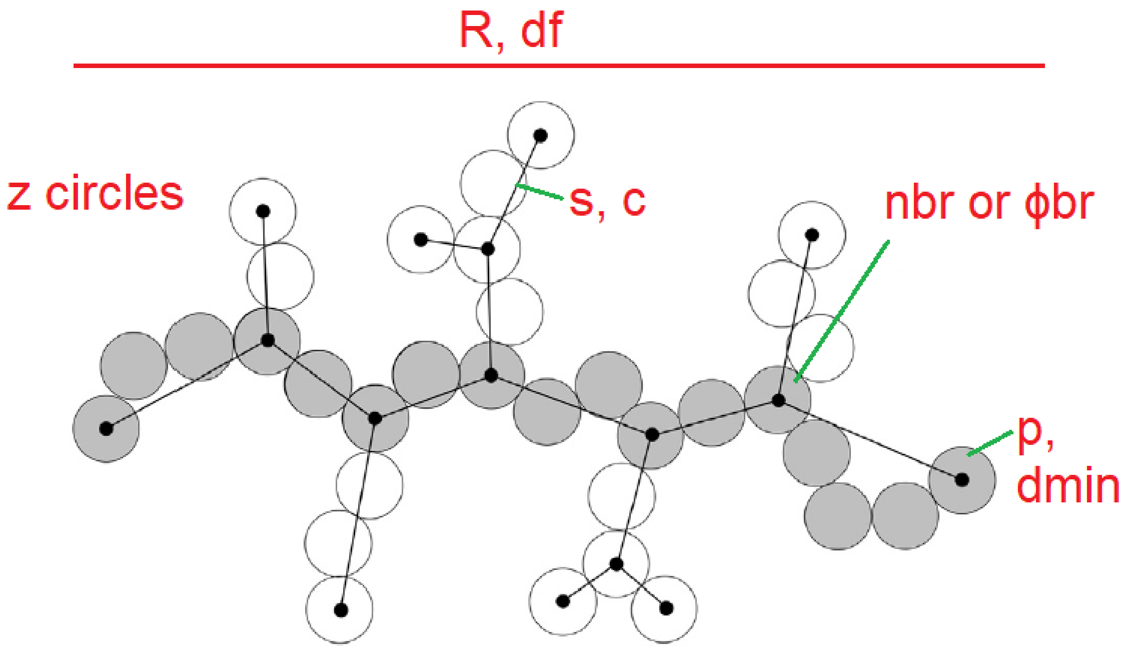
Unified Fit :

$$I(q) = \sum_{i=1}^{n} \left\{ G_i e^{-\frac{q^2 R_{g,i}^2}{3}} + e^{-\frac{q^2 R_{g,i+1}^2}{3}} B_i q^{*-P_i} \right\}; \qquad q^* = \frac{q}{\operatorname{erf}\left(\frac{1.06 q R_{g,i}}{\sqrt{3}}\right)^3} \qquad q = \frac{4\pi}{\lambda} \sin\left(\frac{\theta}{2}\right)$$

Beaucage, G. Approximations Leading to a Unified Exponential/Power-Law Approach to Small-Angle Scattering *J. Appl. Cryst.* 1995, *28* (6), 717–728.

Descriptors for aggregate simulations

Aggregate size, R
Primary particle size, d_p
Degree of aggregation, z
Short-circuit path length, p
Connective path length, s
Fractal dimension, d_f
Tortuosity, d_{min}
Connectivity, c
Branch fraction, ϕ_{br}
Branch number, n_{br}



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Beaucage, G. Determination of branch fraction and minimum dimension of mass-fractal aggregates. *Physical Review E – Statistical, Nonlinear, and Soft Matter Physics* 2004, 70, 031401-1–031401-10.
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Ramachandran, R., Beaucage, G., Kulkarni, A. S., McFaddin, D., Merrick-Mack, J., & Galiatsatos, V. Branch content of metallocene polyethylene. *Macromolecules* 2009, 42, 4746–4750.

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Aggregate topological parameters

Unified Fit :

$$I(q) = \sum_{i=1}^{n} \left\{ G_i e^{-\frac{q^2 R_{g,i}^2}{3}} + e^{-\frac{q^2 R_{g,i+1}^2}{3}} B_i {q^*}^{-P_i} \right\}; \qquad q^* = \frac{q}{\left(\mathrm{erf}\left(\frac{1.06 q R_{g,i}}{\sqrt{3}} \right) \right)^3} \qquad q = \frac{4\pi}{\lambda} \sin\left(\frac{\theta}{2}\right)$$

Parameters from Unified Fit used to determine topological parameters:

$$d_f = P_2; \quad z = \frac{G_1}{G_2} + 1; \quad d_{min} = \frac{B_2 R_{g,2}^{d_f}}{C_p \Gamma(d_f/2) G_2}; \quad C_p = \text{polydispersity factor}$$

$$R = \frac{R_e}{d_p} = z^{1/d_f} = p^{1/d_{min}} = s^{1/c} \qquad \phi_{br} = \frac{z - p}{p} \qquad n_{br} = \frac{z^{\left[\left(\frac{9}{4d_f} - \frac{5}{4c}\right) + \left(1 - \frac{1}{c}\right)\right]} - 1}{2}$$

Beaucage, G. Approximations Leading to a Unified Exponential/Power-Law Approach to Small-Angle Scattering *J. Appl. Cryst.* 1995, *28* (6), 717–728.

Beaucage, G. Determination of branch fraction and minimum dimension of mass-fractal aggregates. *Physical Review E – Statistical, Nonlinear, and Soft Matter Physics* 2004, 70, 031401-1–031401-10.

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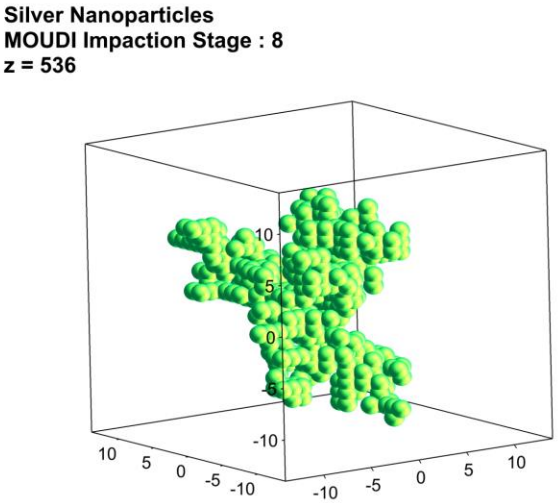
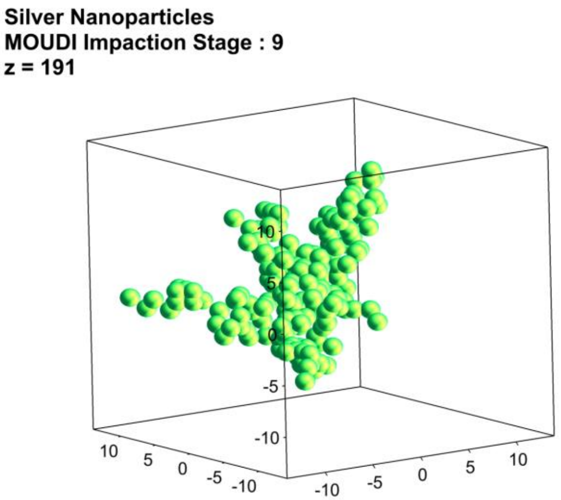
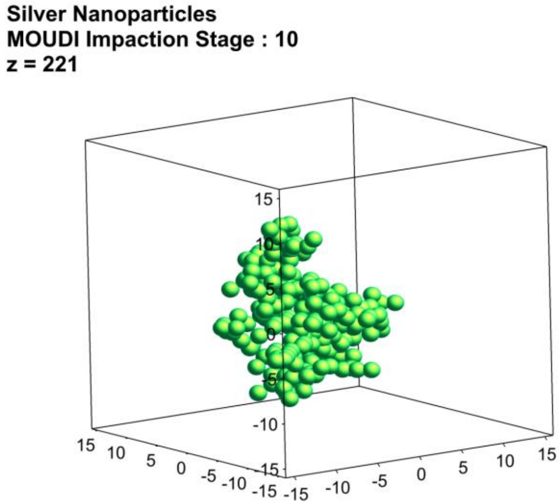
Simulated Aggregates – Silver NPs







		dmin	c	df	z	p	R
Ag NP Stage 8	Unified Fit	1.8 (0.1)	1.2 (0.1)	2.1 (0.1)	540 (200)	200 (70)	19 (4)
	Simulated aggregate	1.837	1.3222	2.4289	**536**	115.9026	13.2929606
Ag NP Stage 8	Unified Fit	1.5 (0.1)	1,4 (0.1)	2.1 (0.1)	190 (30)	38 (4)	12 (2)
	Simulated aggregate	1.3867	1.4764	2.0473	**191**	35.07639	13.0066856
Ag NP Stage 8	Unified Fit	1.5 (0.2)	1.5 (0.3)	2.2 (0.2)	220 (90)	36 (10)	12 (4)
	Simulated aggregate	1.3892	1.5099	2.0975	**221**	35.70424	13.11317563

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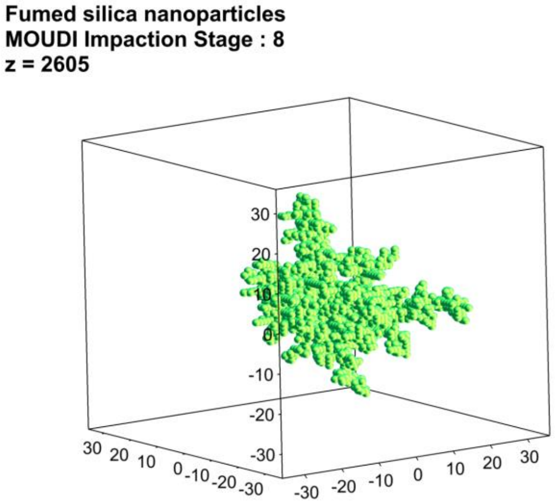
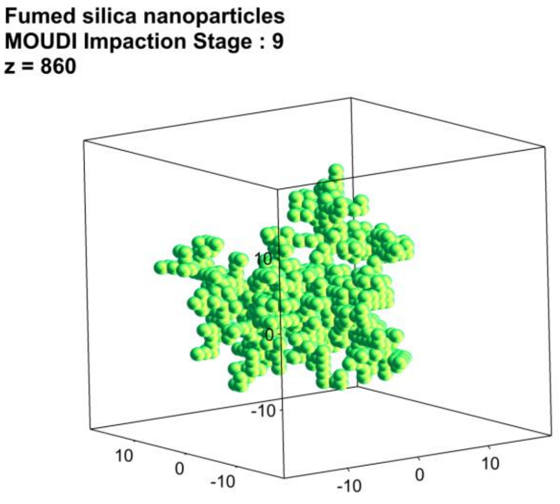
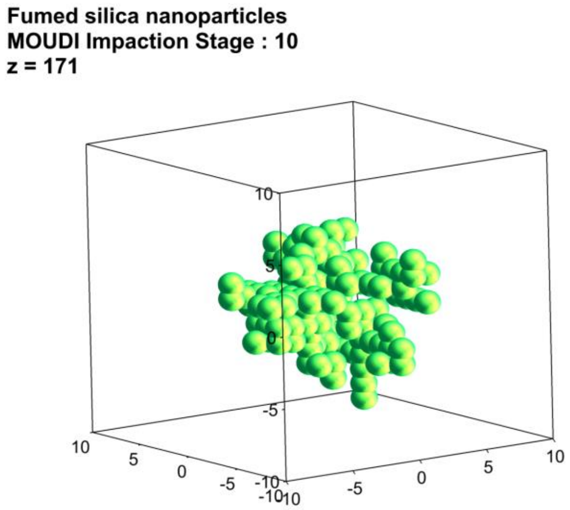
Simulated Aggregates – Fumed silica







		dmin	c	df	z	p	R
silica Stage 8	Unified Fit	1.2 (0.1)	2.1 (0.1)	2.5 (0.1)	2600 (430)	43 (4)	23 (2)
	Simulated aggregate	1.3734	1.7969	2.4679	**2605**	79.60052	24.21557965
Silica Stage 8	Unified Fit	1.9 (0.1)	1.5 (0.4)	2.9 (0.5)	860 (800)	80 (50)	9 (5)
	Simulated aggregate	1.5376	1.5973	2.456	**860**	68.73344	15.66131986
silica Stage 8	Unified Fit	1.7 (0.1)	1.8 (0.7)	3.1 (0.6)	171 (100)	18 (6)	5 (3)
	Simulated aggregate	1.6529	1.5093	2.4947	**171**	30.16506	7.854093151

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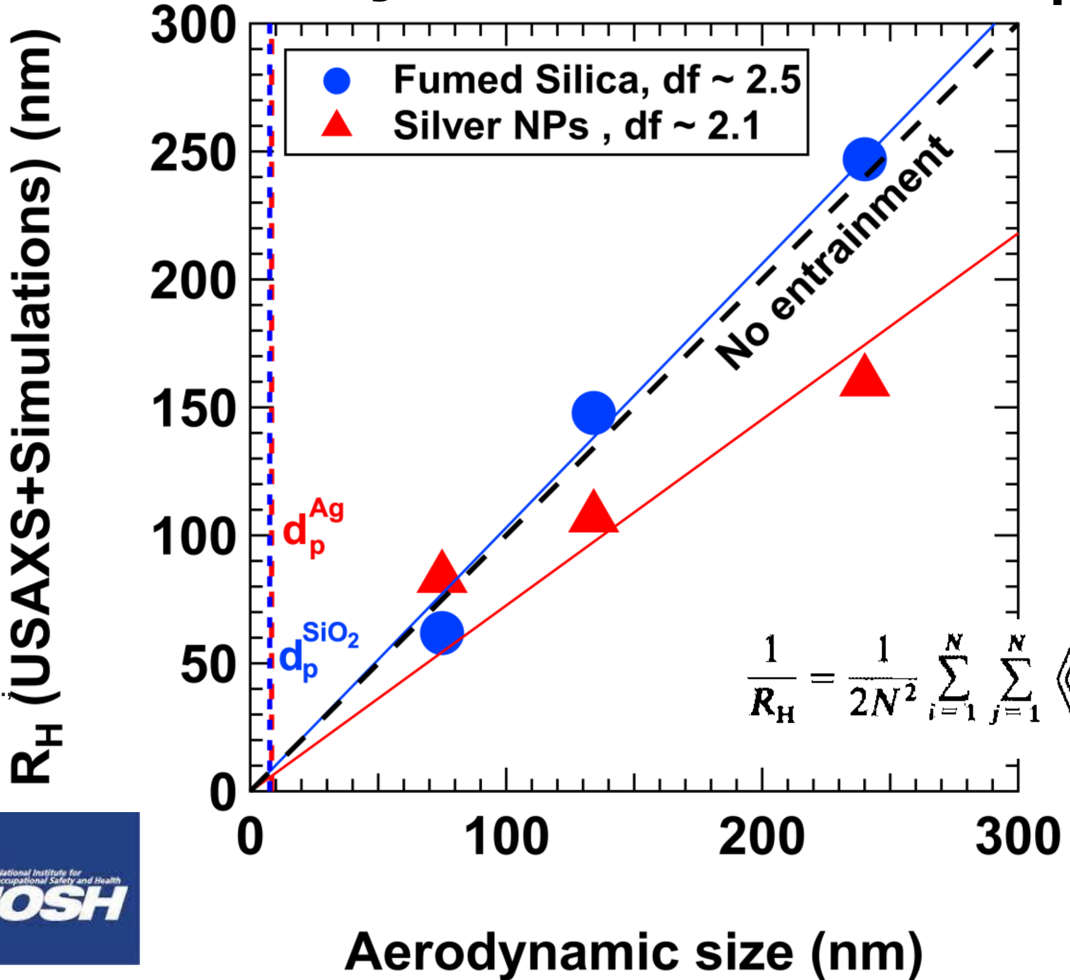
Aerodynamic size vs R_H



R_H depends on the geometrical arrangement of particles, is defined as the size of the equivalent sphere that moves with the same velocity as the cluster in a fluid

$$\frac{1}{R_H} = \frac{1}{2N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \left\langle\left\langle \frac{1}{|\vec{r}_i - \vec{r}_j|} \right\rangle\right\rangle,$$

Lattuada, M., Wu, H. and Morbidelli, M., 2003. Hydrodynamic radius of fractal clusters. *Journal of colloid and interface science*, *268*(1), pp.96-105.

Jannink, G. and Des Cloizeaux, J., 1990. Polymers in solution. *Journal of Physics: Condensed Matter*, *2*(1), p.1.

CDC Workplace Safety and Health NIOSH National Institute for Occupational Safety and Health

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Future Work

- Extend this work to chain-like particles such as carbon nanotubes
- Analyze particles with low z such as N110, N330 carbon black

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