Coagulation of fractal-like aerosols in the transition regime

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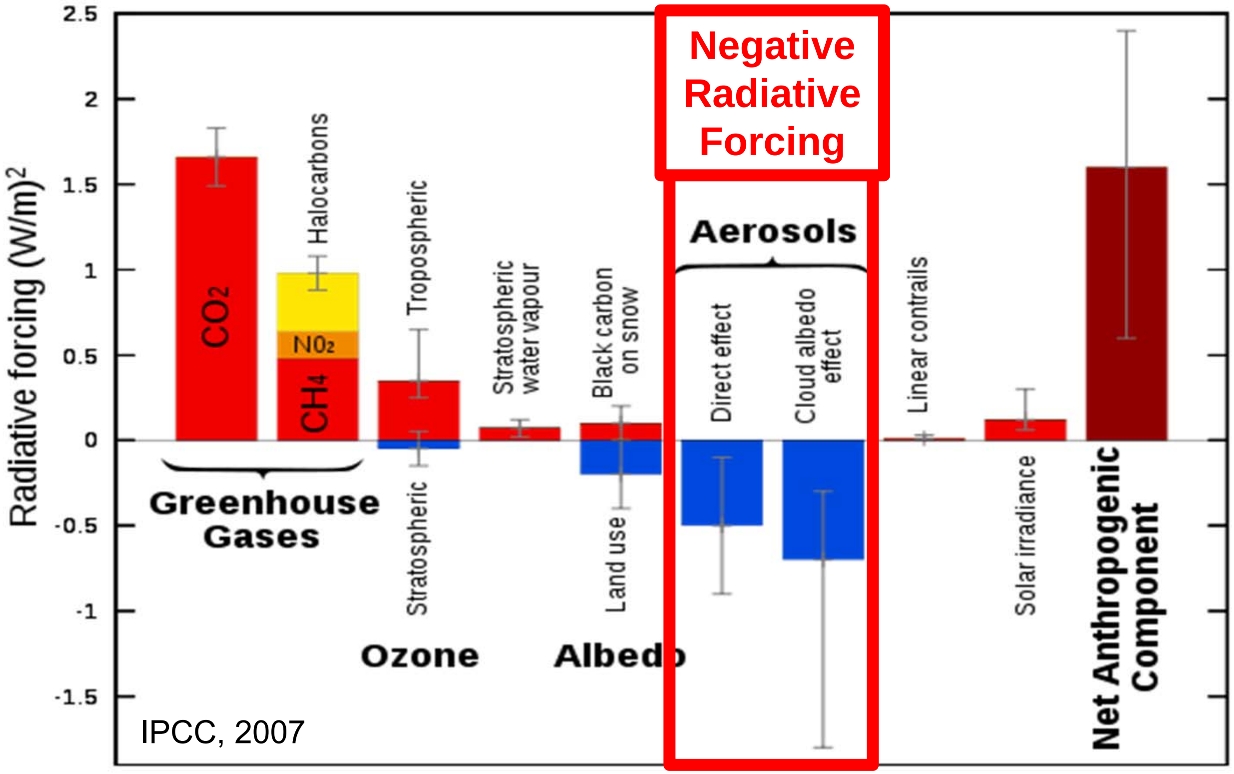
Aerosols

Radiative Forcing - Emissions

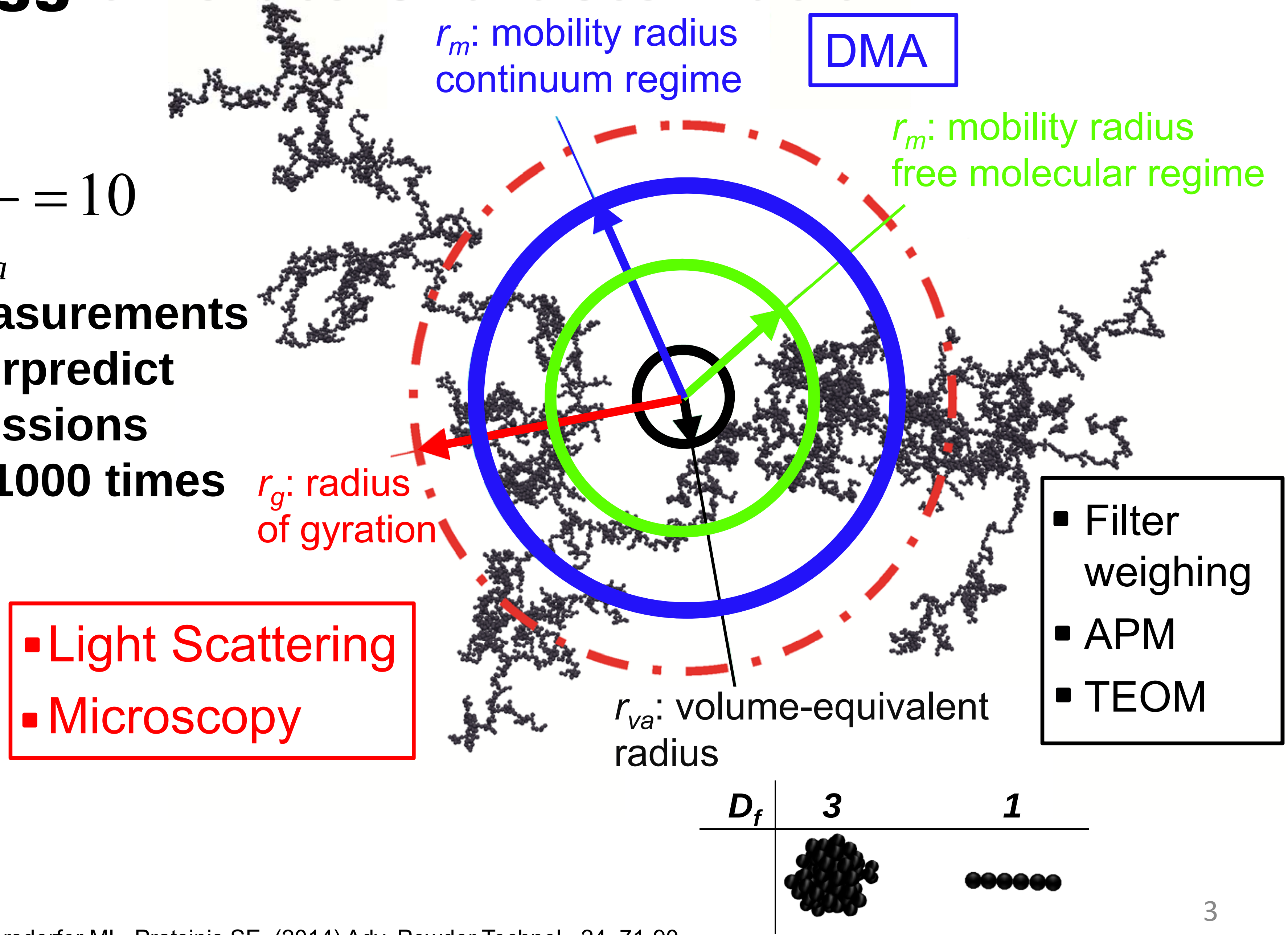


- Larger error bar than greenhouse gases
- Impact in global radiation budget by absorbing & scattering light
- Investigate & regulate emissions from aerosol measurements

Agglomerate Characterization

$$\frac{r_g}{r_{va}} = 10$$

measurements overpredict emissions by 1000 times



1. Eggersdorfer ML, Pratsinis SE. (2014) Adv. Powder Technol., 24, 71-90.

Goal:

Understanding agglomerate

- Structure (relate to agglomerate mass)
- Dynamics

in the *free molecular*, *transition* and *continuum* regime of aged aerosols in the atmosphere

Motivation:

- Connect emissions to aerosol size measurements

$$r_{va} \leftrightarrow r_g,\ r_m$$

- Facilitate understanding of aerosol contribution in climate forcing (minimize hopefully error bar)

Previous Work

- Brownian coagulation of *spheres*[1,2]

- *Non-spherical* particles

  determination of evolving structure[3,4,5]

  collisional growth and dynamics[6]

  on-line measurements of agglomerate size and structure[7,8]

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2. Buesser B, Heine MC, Pratsinis SE (2009), *J. Aerosol Sci.,* **40**, 89-100.
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5. Eggerdorfer ML, Kadau D, Herrmann HJ, Pratsinis SE (2011), *Langmuir,* **27**, 6358-6367.
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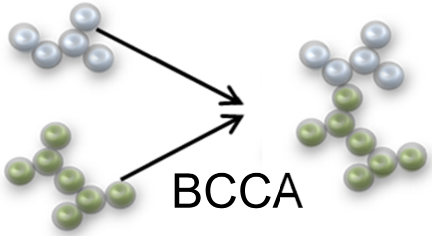
Free molecular regime: Event-driven method [1]

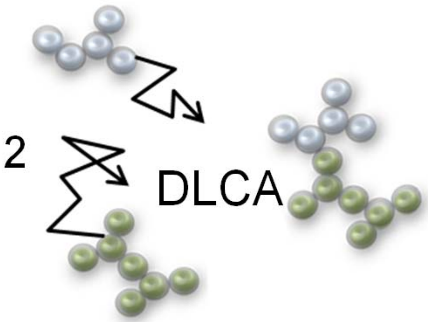
SiO$_2$ particles (like fly ash)
T = 27 ^{o}C

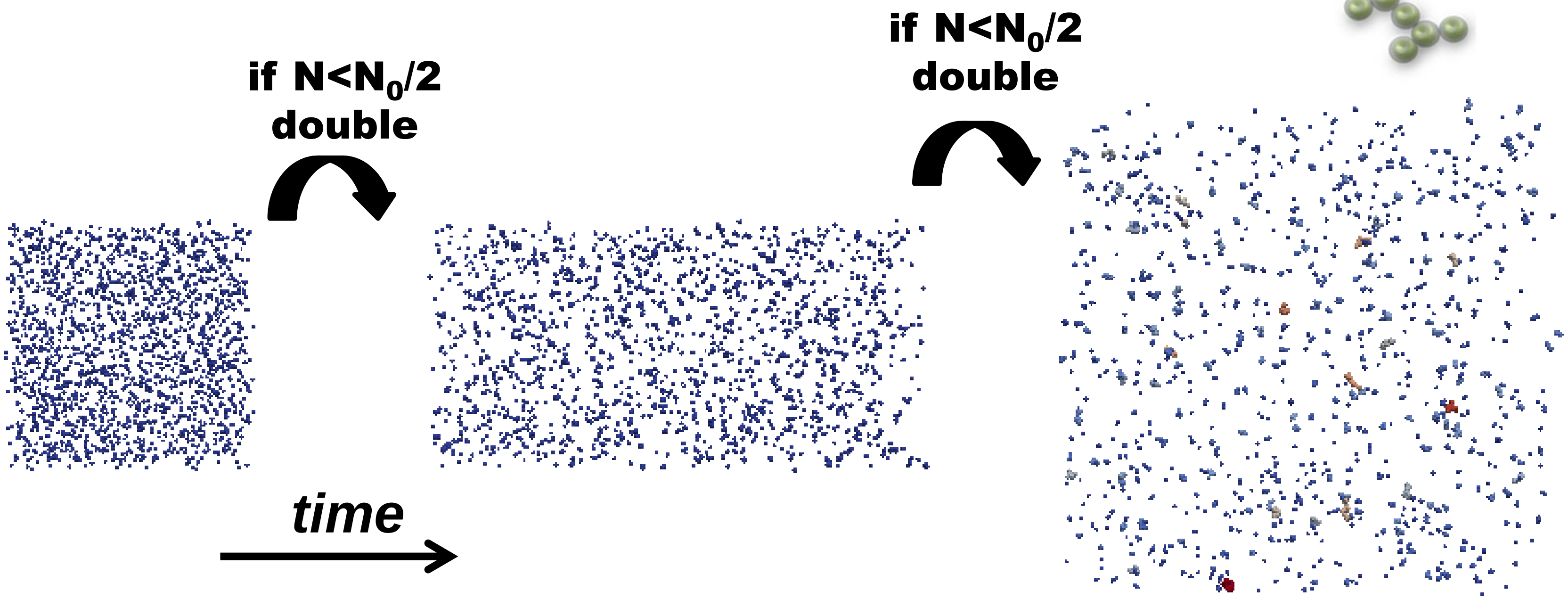
Ballistic trajectories:



$$\bar{u}_p = \sqrt{\frac{8k_BT}{\pi m_p}}$$

Continuum regime: Langevin Dynamics [2]





1. Allen MP, & Tildesley DJ. (1991). Computer Simulation of Liquids, Oxford University Press, New York.
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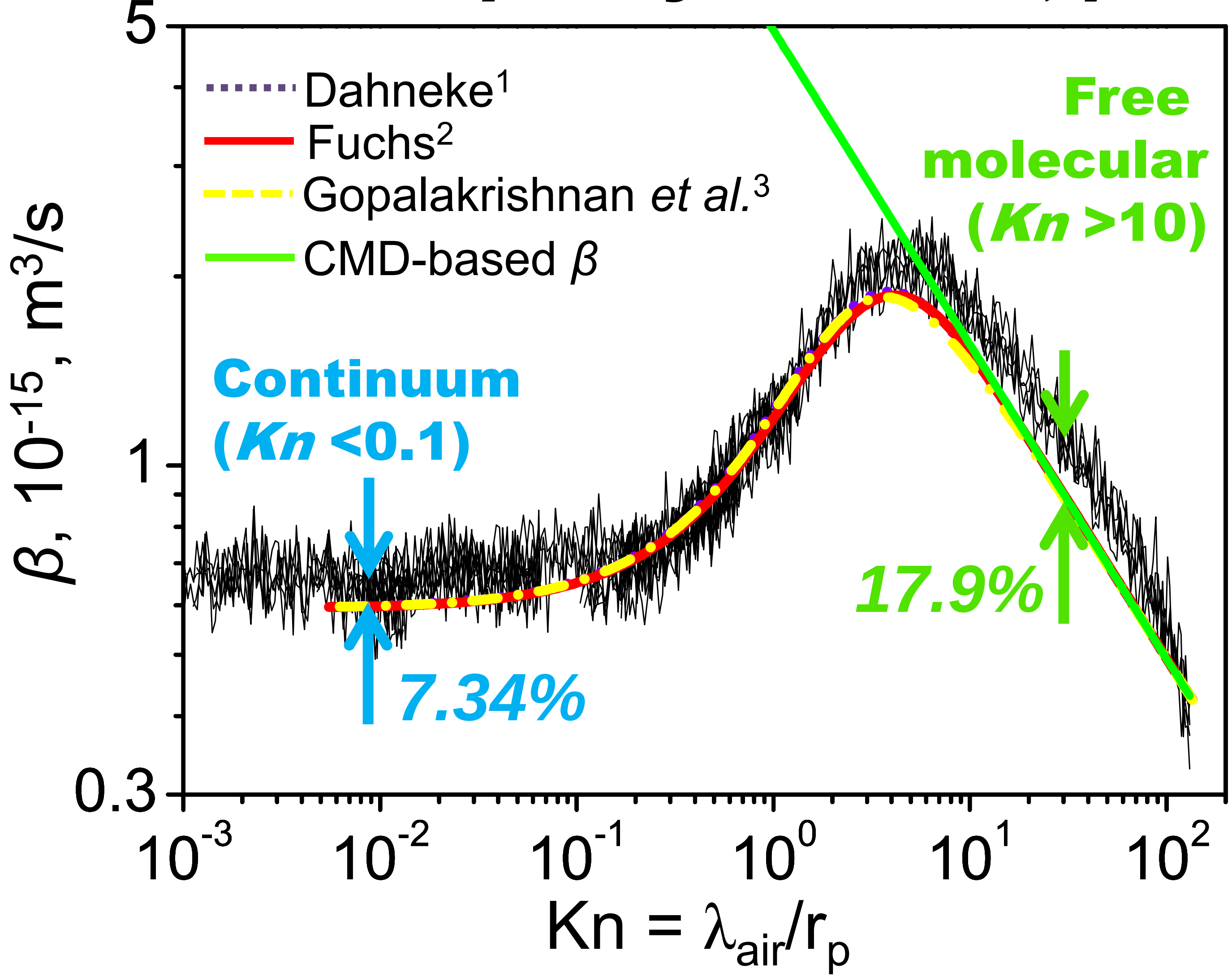
Validation – Full Coalescence

Collision Frequency Function, β



Enhancement due to *polydispersity* & *attainment of self-preserving size distribution*

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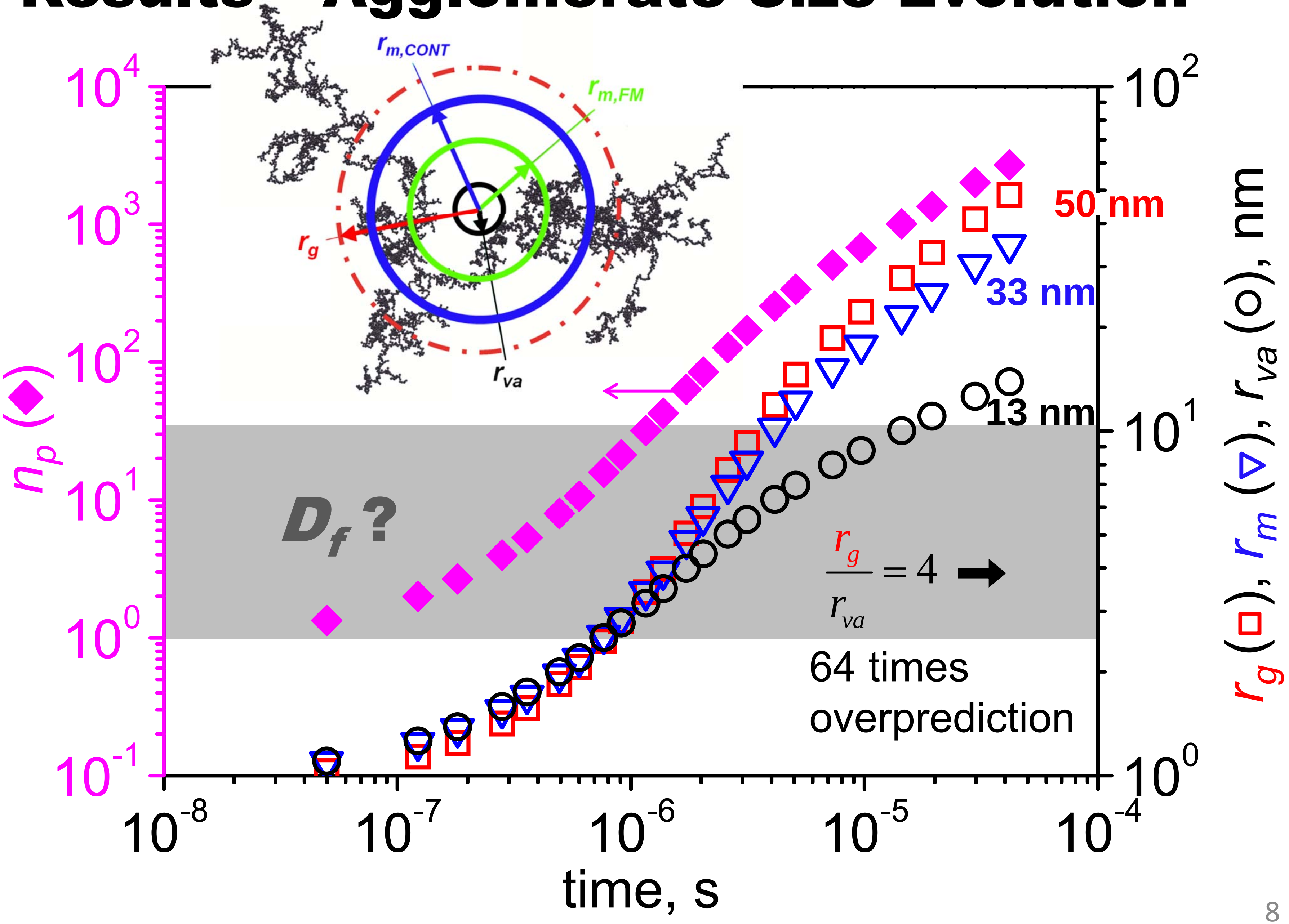
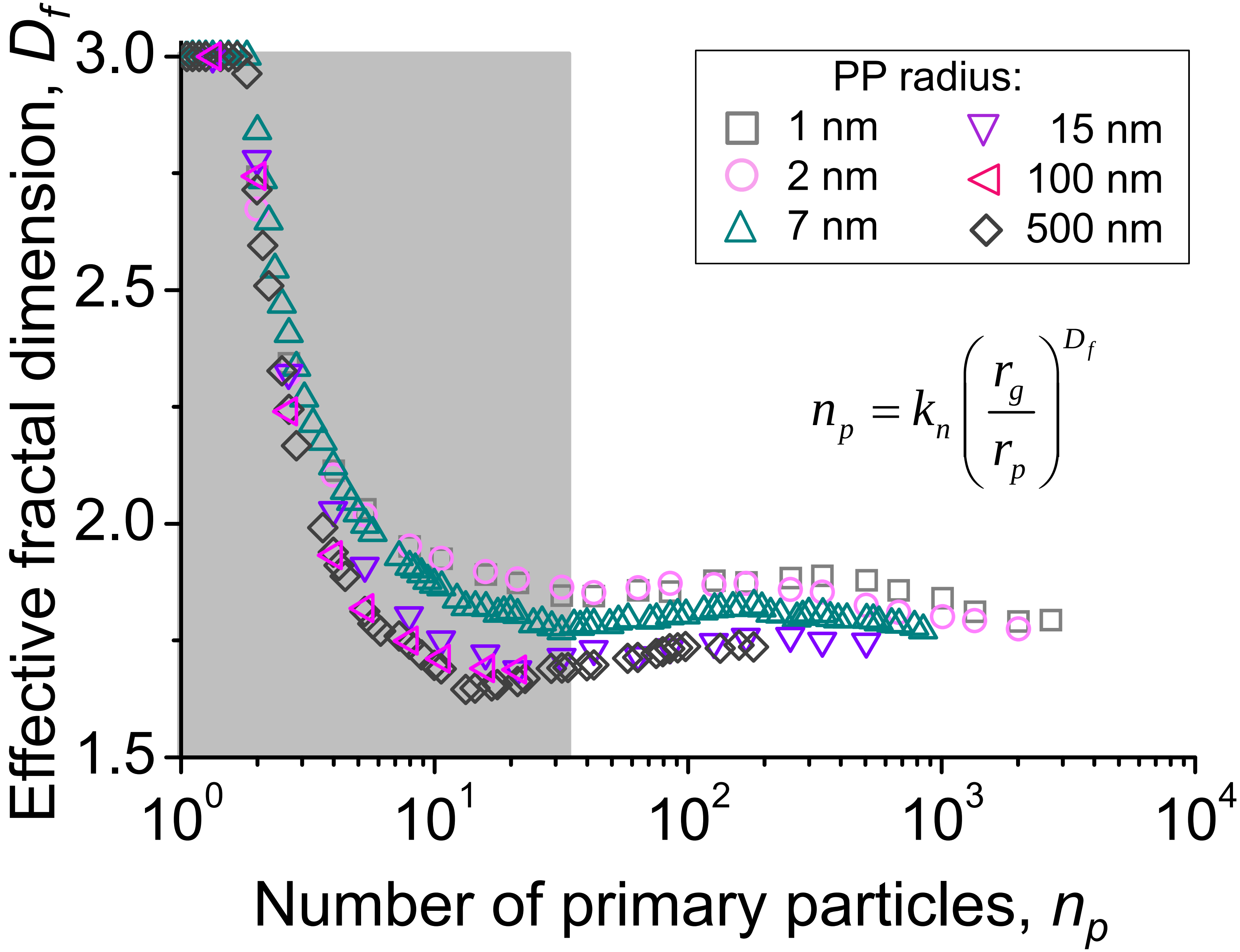
Results – Agglomerate Size Evolution

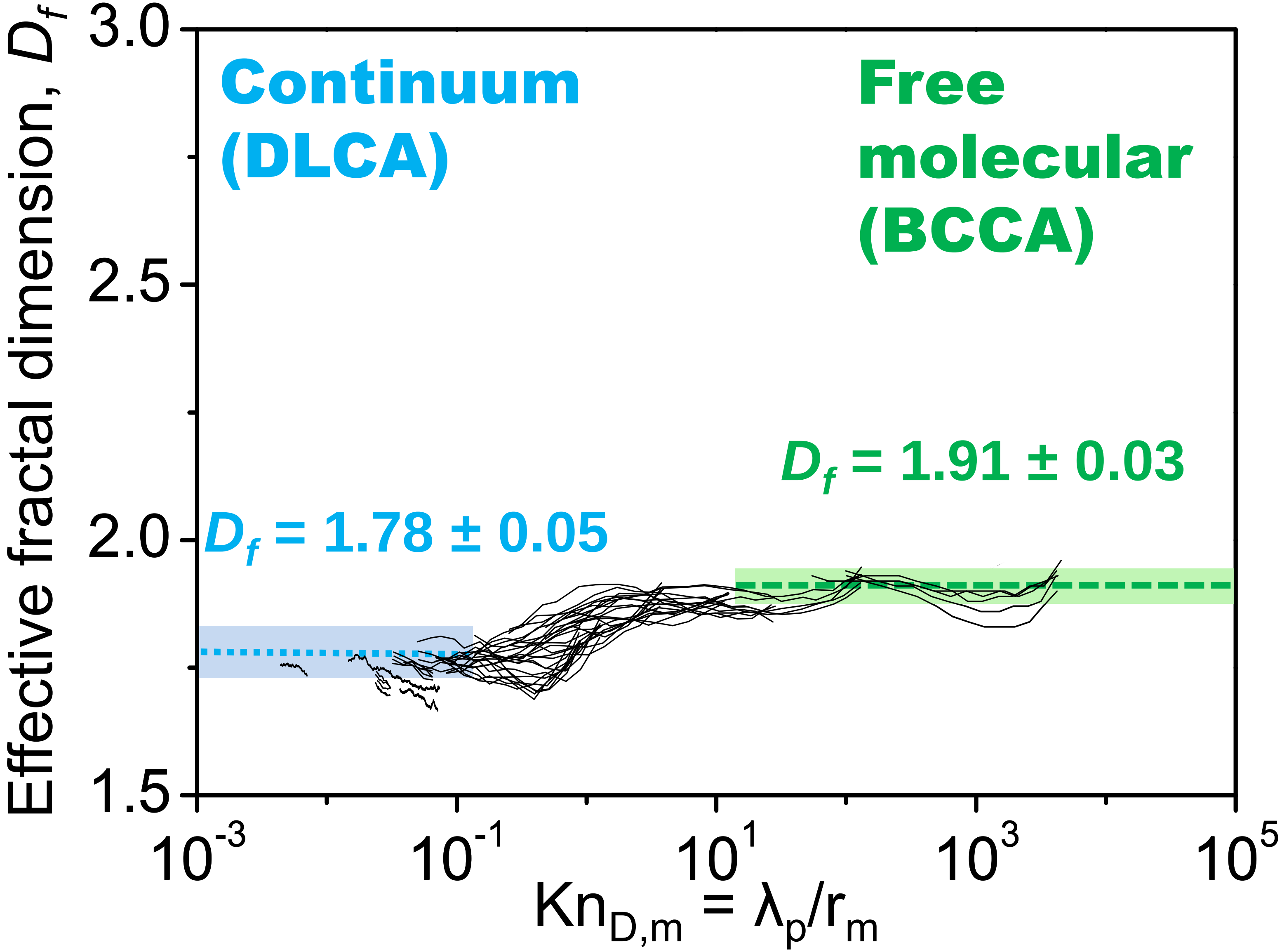


1. Eggersdorfer ML, Pratsinis SE. (2014) Adv. Powder Technol., 24, 71-90.

Results – Agglomerate Structure Evolution



Results – Agglomerate Structure Evolution



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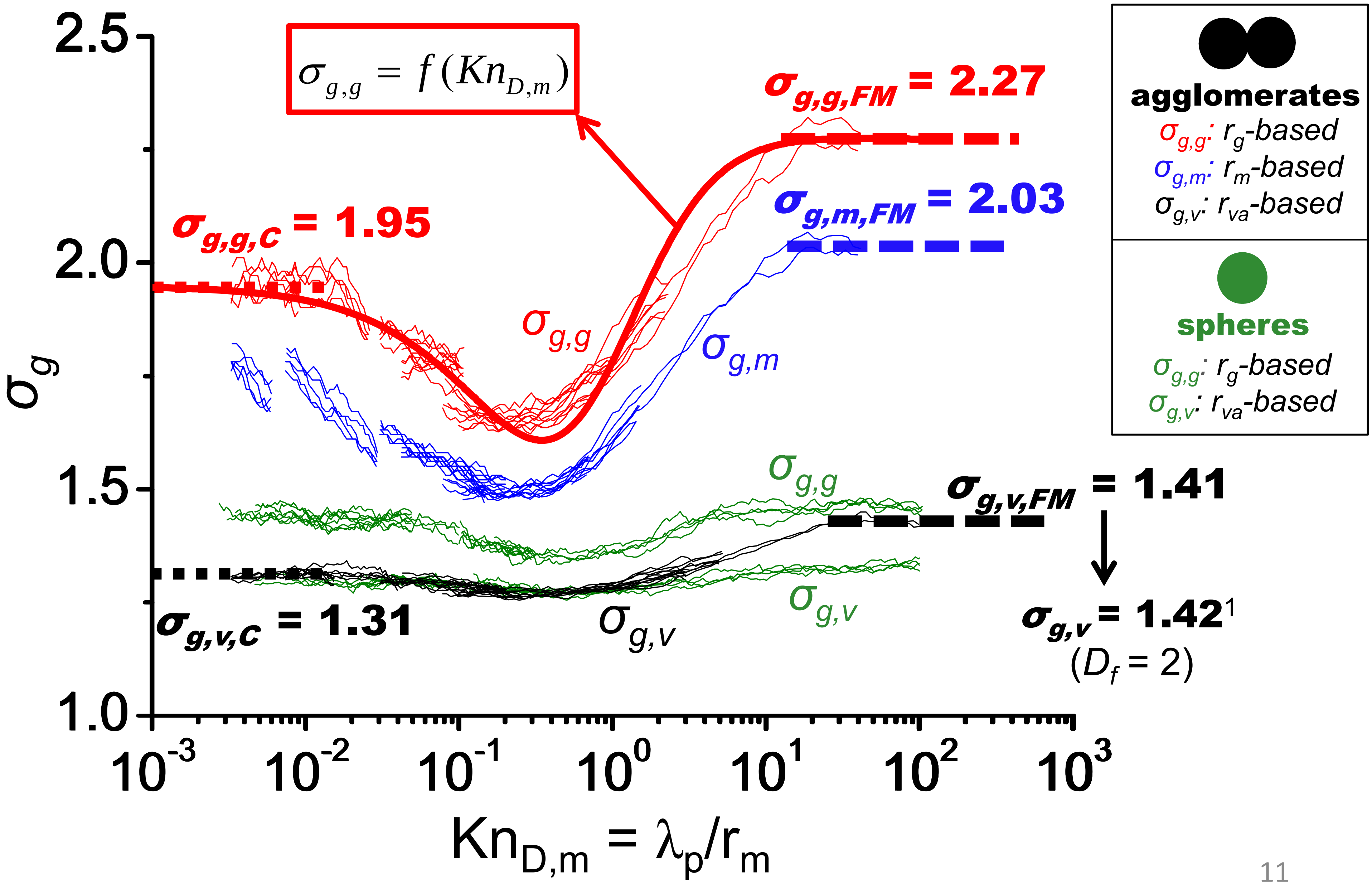
Results – Geometric Standard Deviation



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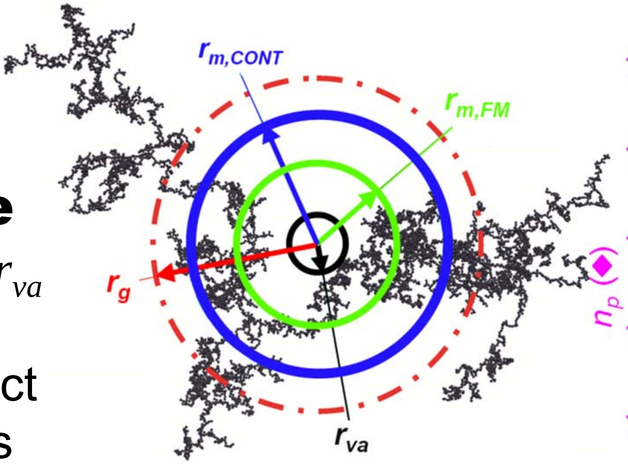
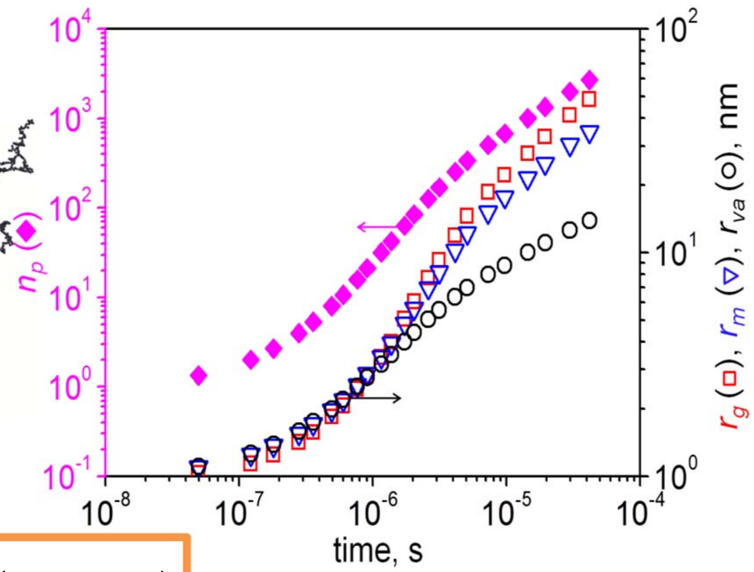
Conclusions





Agglomerate Size

For $n_p > 10 \Rightarrow r_g > r_m, r_{va}$

$$\frac{r_g}{r_{va}}, \frac{r_m}{r_{va}} > 1 \Rightarrow$$ overpredict emissions

Structure

- *Transition* regime: smooth shift of D_f $\boxed{D_f = f(Kn_{D,m})}$
- *FM* regime: $D_f = 1.91 \pm 0.03$
- *Continuum* regime: $D_f = 1.78 \pm 0.05$

D_f evolution from spherical to fractal-like structures: $\boxed{D_f = f(n_p)}$

Geometric Standard Deviation of Quasi-Self-Preserving

	Spheres		*Agglomerates*	
	FM	***Continuum***	***FM***	***Continuum***
• $\sigma_{g,v}$	1.33	1.32	1.41	1.31
• $\sigma_{g,m}$	1.46	1.44	2.03	-
• $\sigma_{g,g}$	1.46	1.44	2.27	1.95

$$\boxed{\sigma_{g,g} = f(Kn_{D,m})}$$

THANK YOU FOR YOUR ATTENTION!