Dynamics of Soot Mobility Size during Agglomeration & Surface Growth

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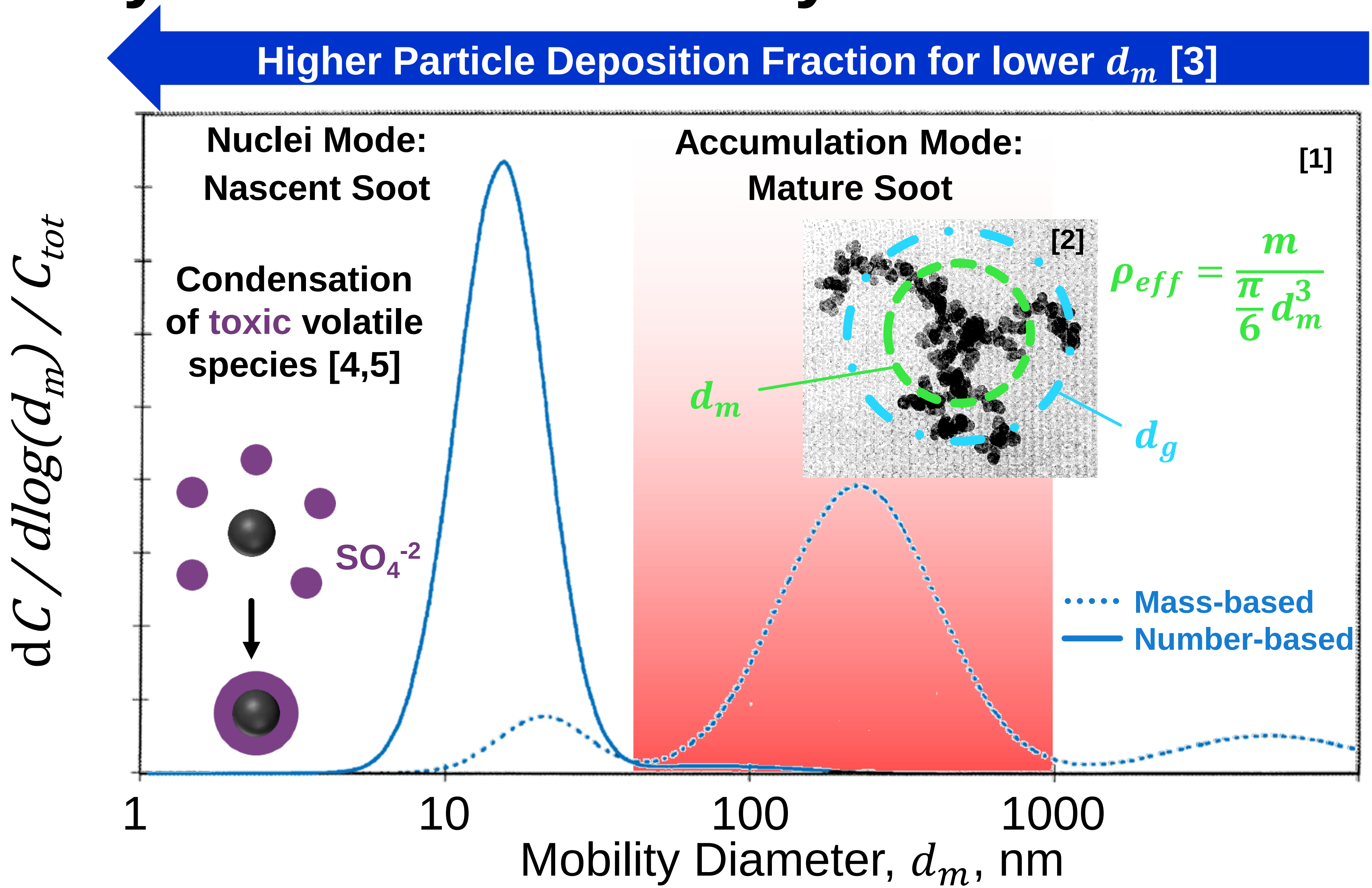
Why care about mobility size?



[1] Kittelson DB. (1998) *J. Aerosol Sci.* **29**, 575. modified

[2] Koylu UO, Faeth GM, Farias TL, Carvalho MG. (2007) *Combust. Flame* **100**, 621.

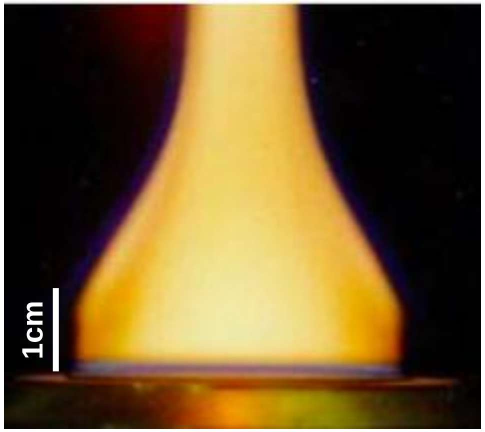
[3] Rissler J, Swietlicki E, Bengtsson A, Boman C, Pagels J, Sandström T, Blomberg A, Löndahl J. (2012) *J. Aerosol Sci.* **48,** 18.

[4] De Filippo A, Maricq MM. (2008) *Env. Sci. Technol.* **42,** 7957.

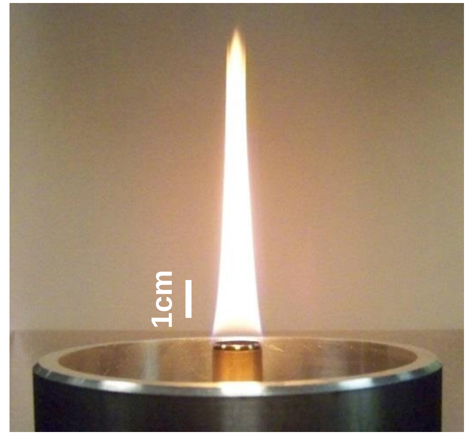
[5] Pedata P, Stoeger T, Zimmermann R, Peters A, Oberdörster G, D´Anna A, (2015) *Part. Fibre Toxicol*. **12**, 1.

Studying Soot Formation in Flames

Free Premixed and Diffusion flames:

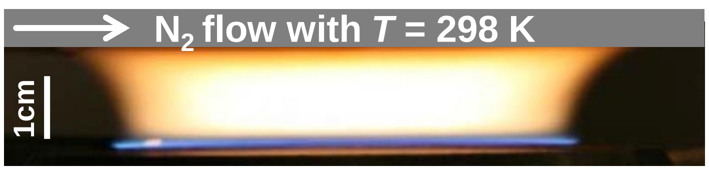


McKenna Burner [1]

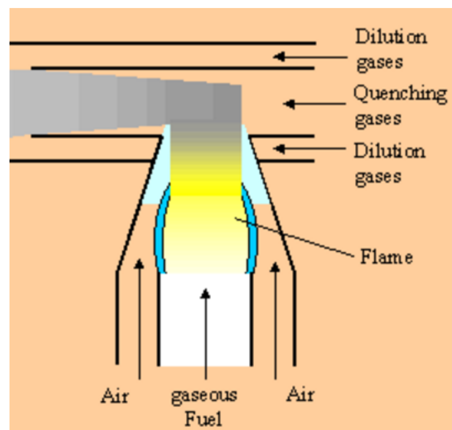


Gülder Burner [2]

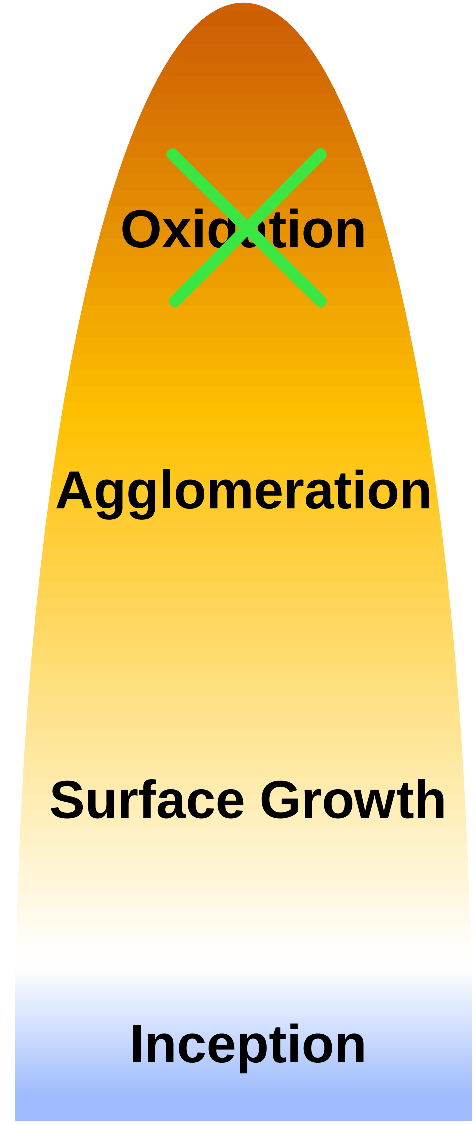
Quenched flames:



Burner-Stabilized Stagnation flame [3]



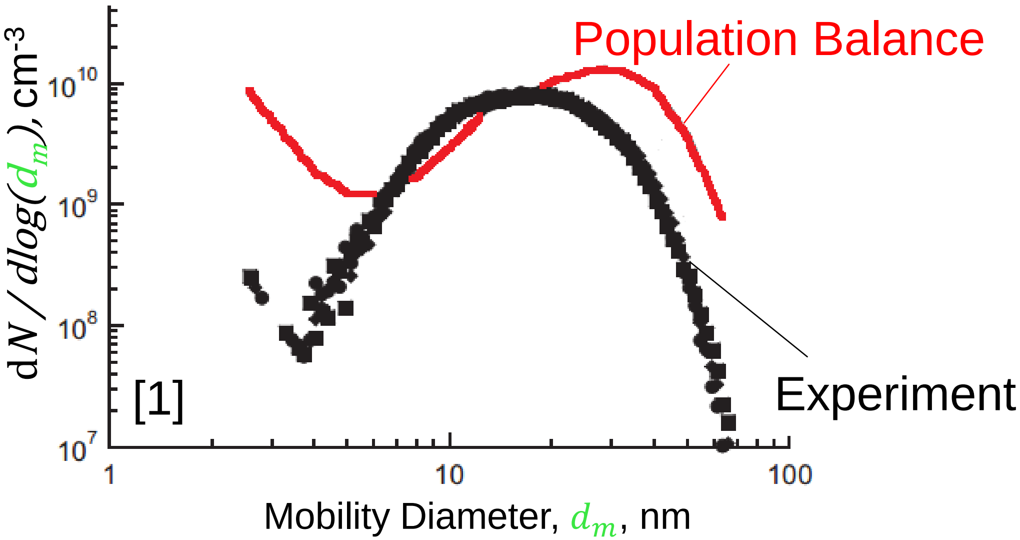
CAST Soot Generator [4]

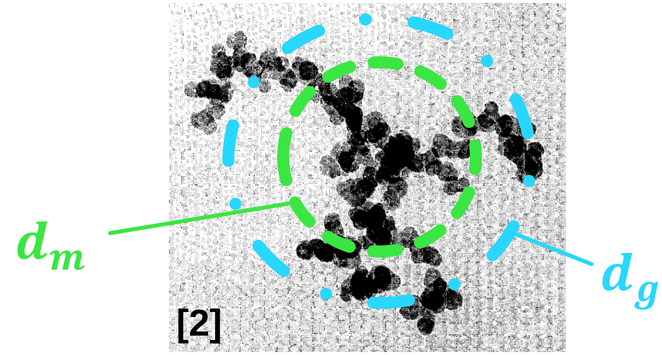


Better Modeling?

[1] www.flatflame.com/
[2] combustion.mie.utoronto.ca/
[3] Camacho J, Liu C, Gu C, Lin H, Huang Z, Tang Q, You X, Saggese C, Li Y, Jung H, Deng L, Wlokas I, Wang H. (2015) *Combust. Flame* **162**, 3810.
[4] www.sootgenerator.com/

Modeling of Soot Mobility Size





d_m = **Const** · d_g

Need for: $d_m = f\,(n_p, d_p)$

Agglomerates:

Sorensen [3], transition regime

$$\frac{d_m}{d_p} = \begin{cases} n_p^{0.46} & , n_p \leq 100 \\ \left(10^{-1.02 Kn^{-0.43}+0.92}\right) n_p^{0.51 Kn^{-0.43}} & , n_p > 100 \end{cases}$$

Goal:

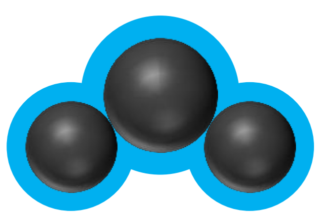
New d_m relationship for:

i) **Surface Growth/ Aggregation**

ii) **PP Size Distribution**

Aggregates?

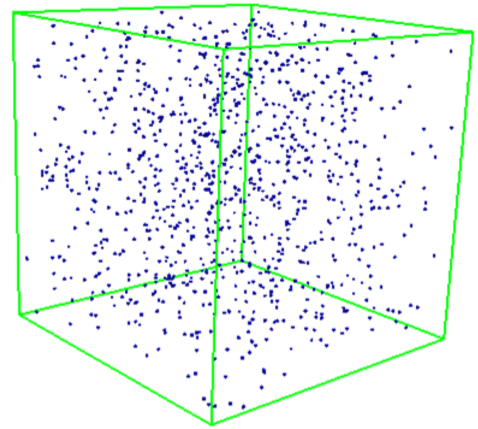
Polydisperse PPs?



[1] Saggese C, Ferrario S, Camacho J, Cuoci A, Frassoldati A, Ranzi E, Wang H, Faravelli T. Wang H. (2015) *Combust. Flame* **162**, 3356.
[2] Koylu UO, Faeth GM, Farias TL, Carvalho MG. (2007) *Combust. Flame* **100**, 621.
[3] Sorensen CM. *Aerosol Sci. Tech.* (2011) 45, 765.

Soot Dynamics by Mesoscale Simulations

i) Initial Configuration
after **Inception** primarily stops [1,2]:



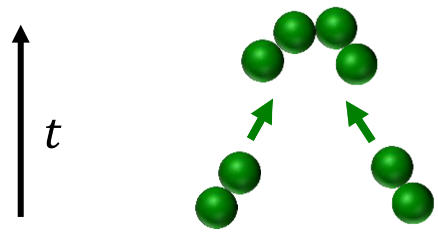
T = 1830 K

$d_{m,o}$ = 2 nm

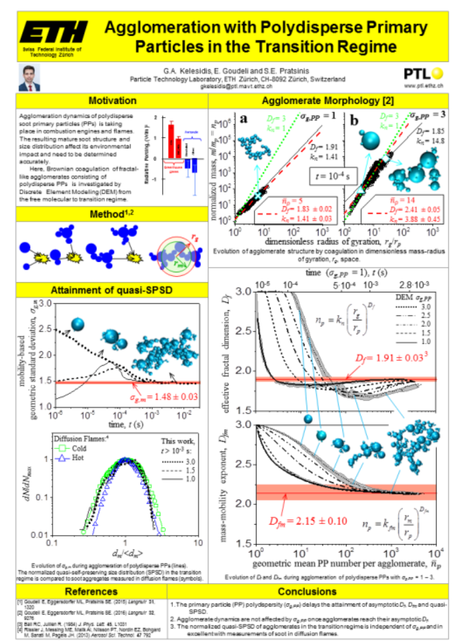
$N_{tot,o}$ = 4.5·10^{16} m^{-3}

[1,2]

ii) Discrete Element Modeling (DEM)
of **Particle Motion** and **Agglomeration** [3]



Poster Session
Today, 15.20-16.30:



[1] Abid AD, Heinz N, Tolmachoff ED, Phares DJ, Campbell CS, Wang H. (2008) *Combust. Flame* **154**, 775.

[2] Camacho J, Liu C, Gu C, Lin H, Huang Z, Tang Q, You X, Saggese C, Li Y, Jung H, Deng L, Wlokas I, Wang H. (2015) *Combust. Flame* **162**, 3810.

[3] Goudeli E, Eggersdorfer ML, Pratsinis SE. (2015) *Langmuir* **31**,1320.

[4] Appel J, Bockhorn H, Frenklach M. (2000) *Combust. Flame* **121**, 122.

[5] Friedlander SK. (2000) Smoke, Dust, and Haze: Fundamentals of Aerosol Dynamics. Oxford University Press, New York.

[6] Kelesidis GA, Goudeli E, Pratsinis SE. (2017) *Proc. Combust. Inst*. **36**, 29.

Soot Dynamics by Mesoscale Simulations

i) Initial Configuration
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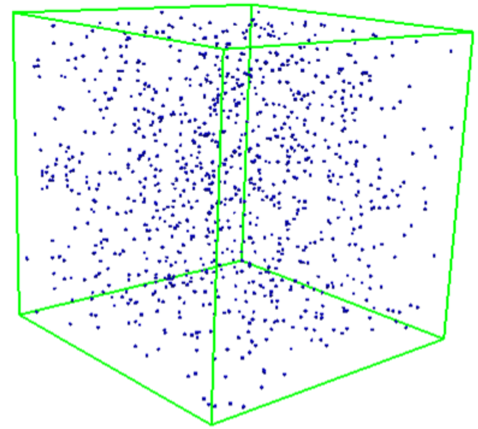

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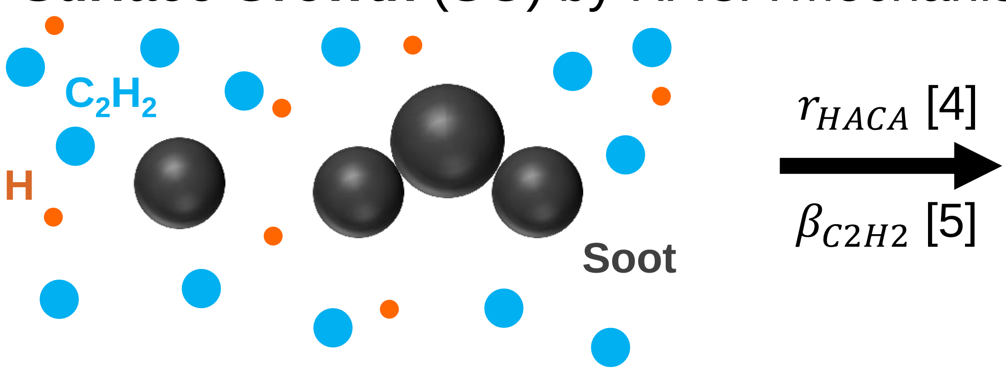
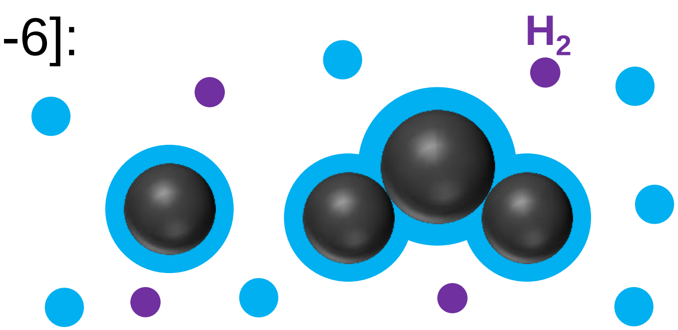
[1,2]

ii) Discrete Element Modeling (DEM)
of **Particle Motion** and **Agglomeration** [3]

iii) **Surface Growth** (SG) by HACA mechanism [4-6]:





Mass Balance
for each C_2H_2 reaction:

$$\pi \frac{d^3_{p,new}}{6} \rho_{soot} = \pi \frac{d^3_{p,old}}{6} \rho_{soot} + m_{2c}$$

[1] Abid AD, Heinz N, Tolmachoff ED, Phares DJ, Campbell CS, Wang H. (2008) *Combust. Flame* **154**, 775.
[2] Camacho J, Liu C, Gu C, Lin H, Huang Z, Tang Q, You X, Saggese C, Li Y, Jung H, Deng L, Wlokas I, Wang H. (2015) *Combust. Flame* **162**, 3810.
[3] Goudeli E, Eggersdorfer ML, Pratsinis SE. (2015) *Langmuir* **31**,1320.
[4] Appel J, Bockhorn H, Frenklach M. (2000) *Combust. Flame* **121**, 122.
[5] Friedlander SK. (2000) Smoke, Dust, and Haze: Fundamentals of Aerosol Dynamics. Oxford University Press, New York.
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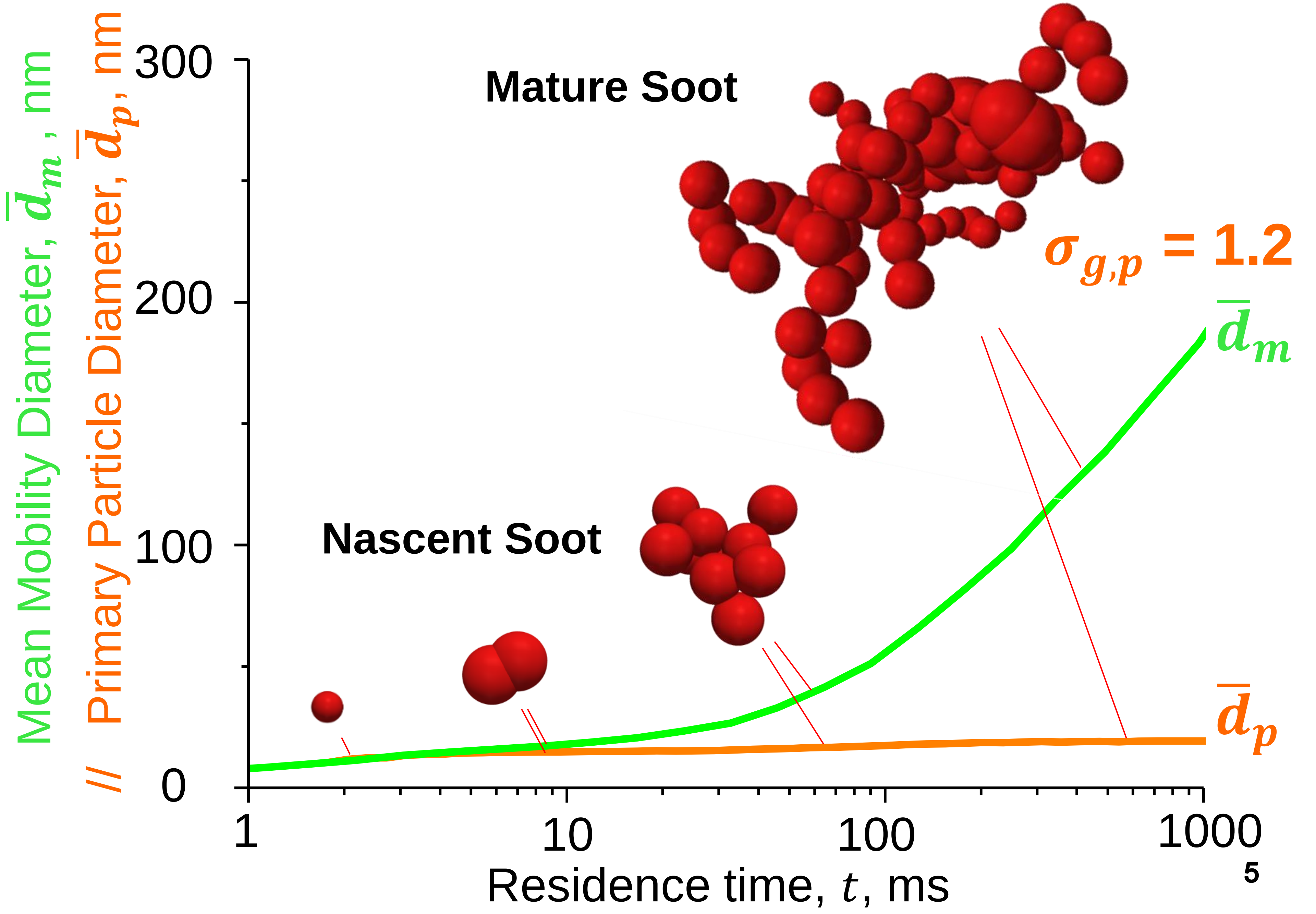
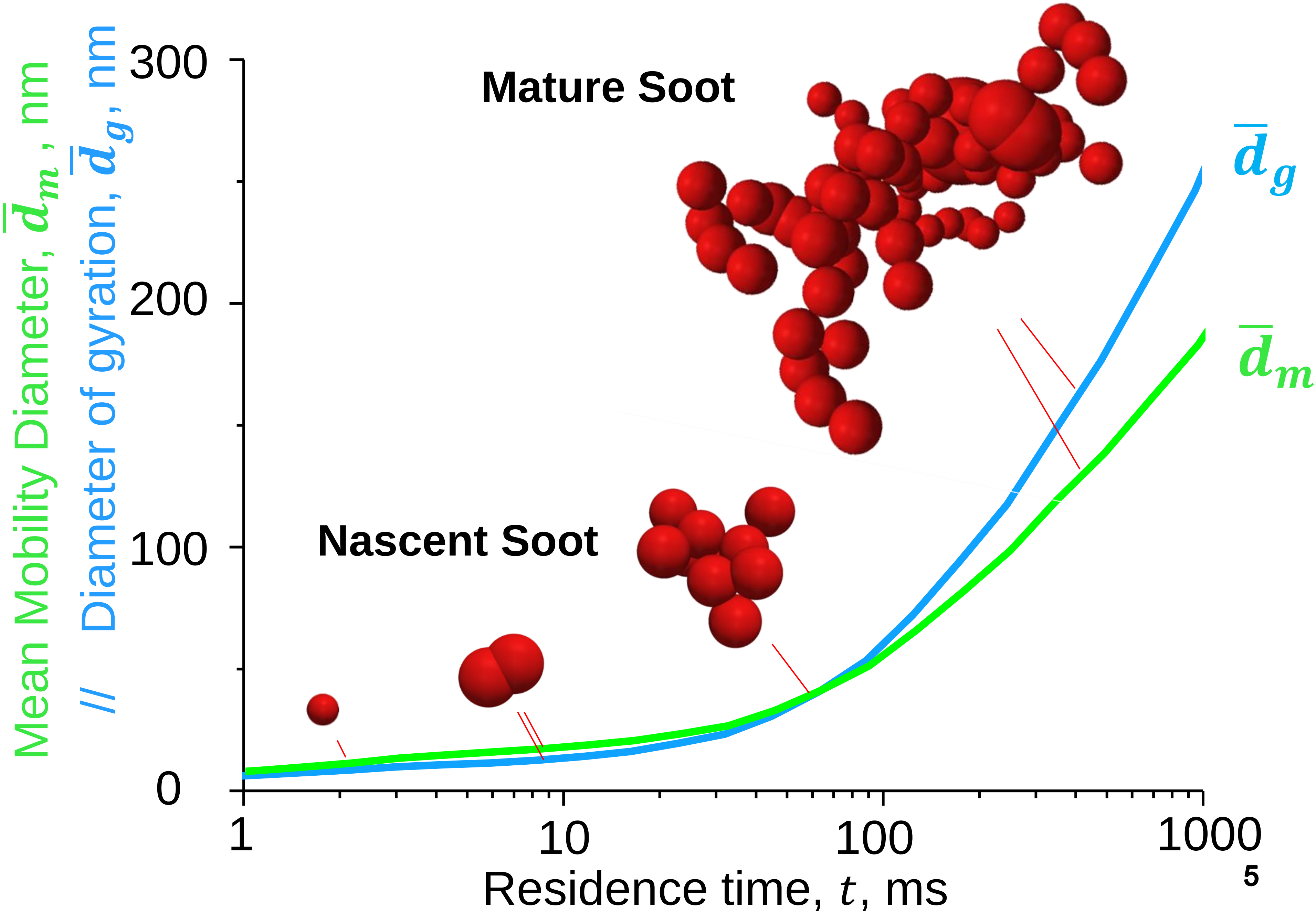
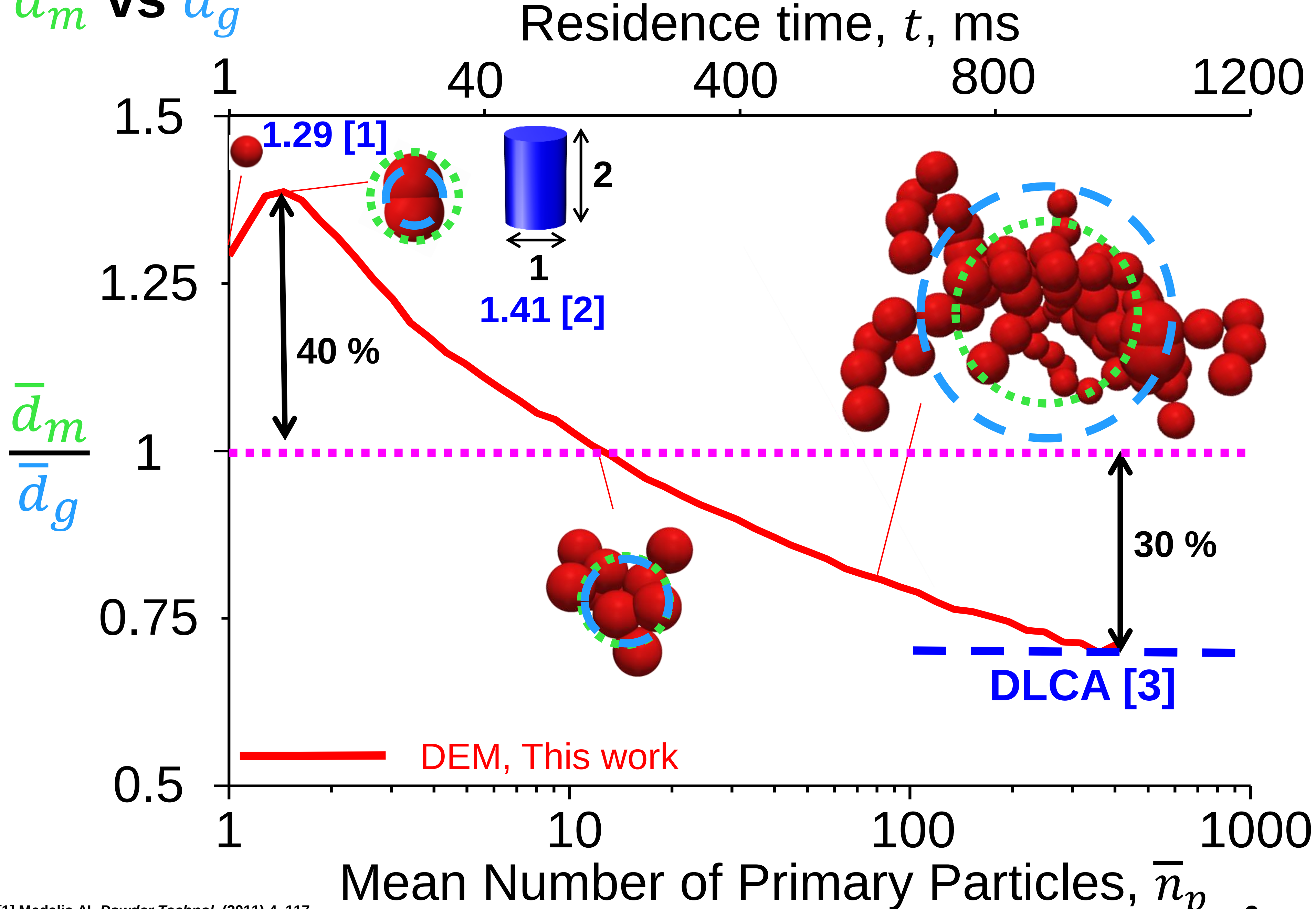
Soot Aggregation Dynamics by DEM



Soot Aggregation Dynamics by DEM

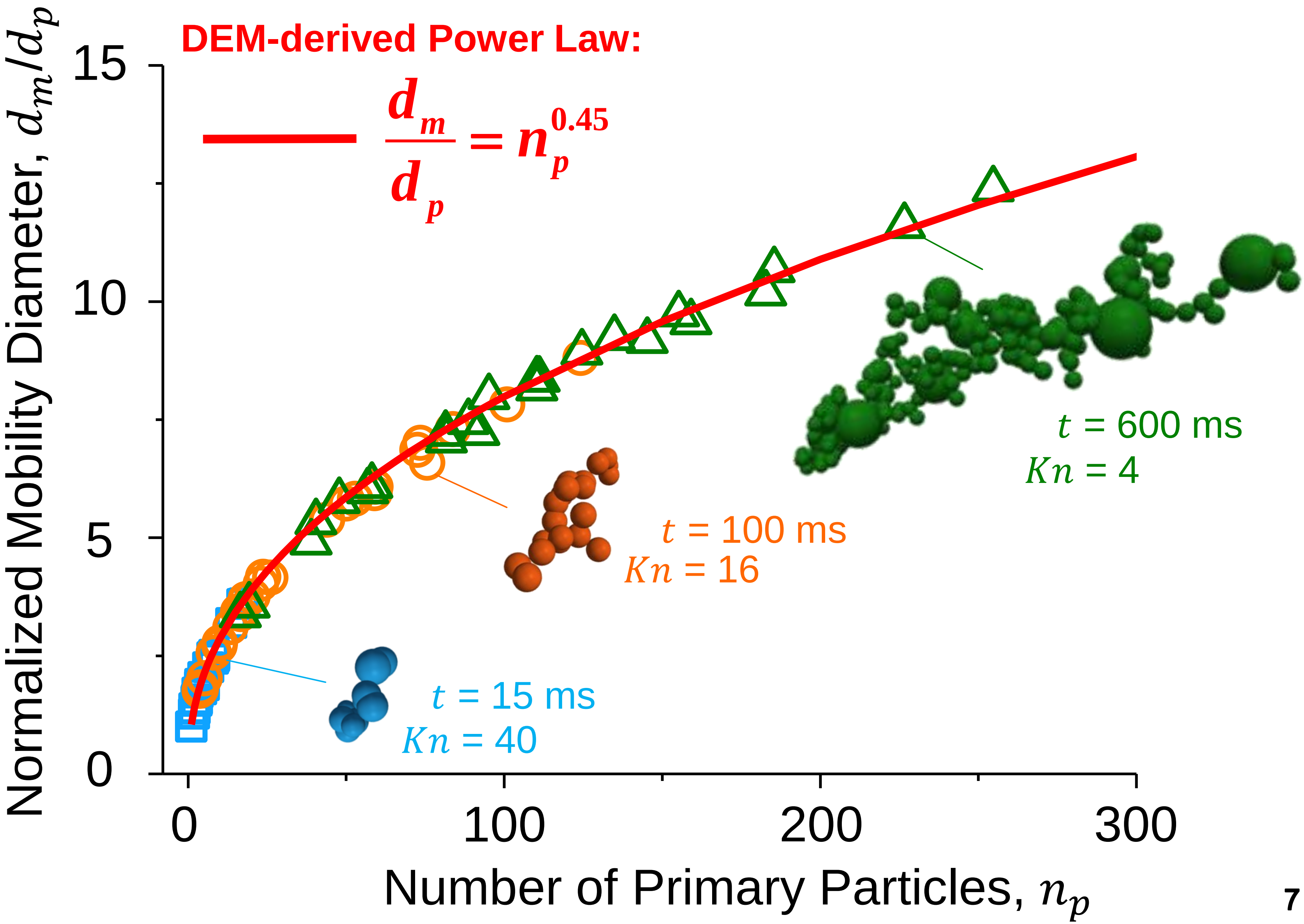


d_m vs d_g

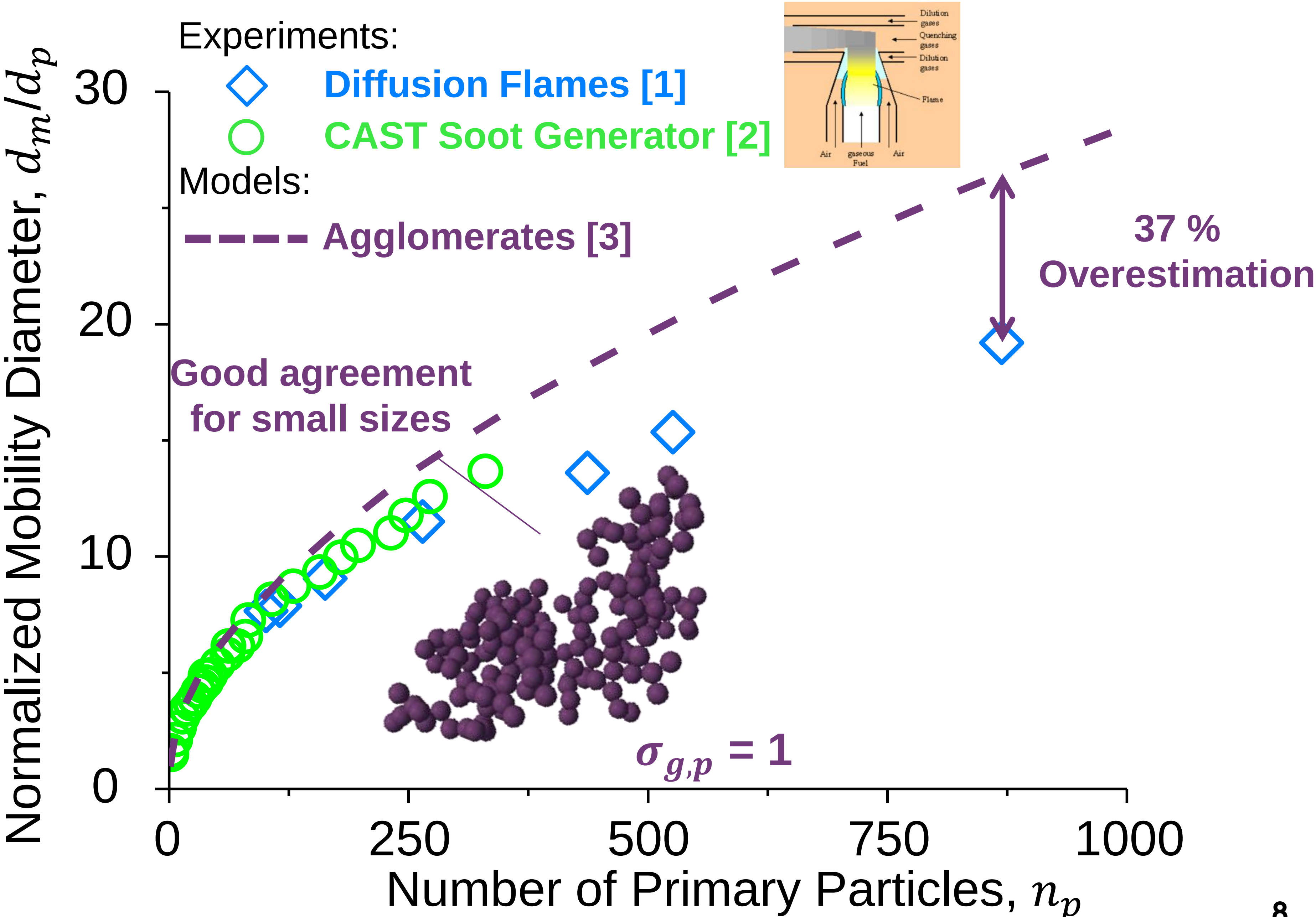


[1] Medalia AI. *Powder Technol.* (2011) 4, 117.
[2] Johnson DL, Leith D, Reist PC. *J. Aerosol Sci.* (1987) 18, 87.
[3] Wang GM, Sorensen CM. *Phys. Rev.* (1999) E60, 3036.

DEM-derived distribution of d_m over n_p



Moment of Truth!



[1] Rissler J, Messing ME, Malik AI, Nilsson PT, Nordin EZ, Bohgard M, Sanati M, Pagels JH. (2013) *Aerosol Sci. Technol.* 47, 792.
[2] Yon J, Bescond A, Ouf FX. (2015) *J. Aerosol Sci.* 87, 28
[3] Sorensen CM. *Aerosol Sci. Technol.* (2011) 45, 765.

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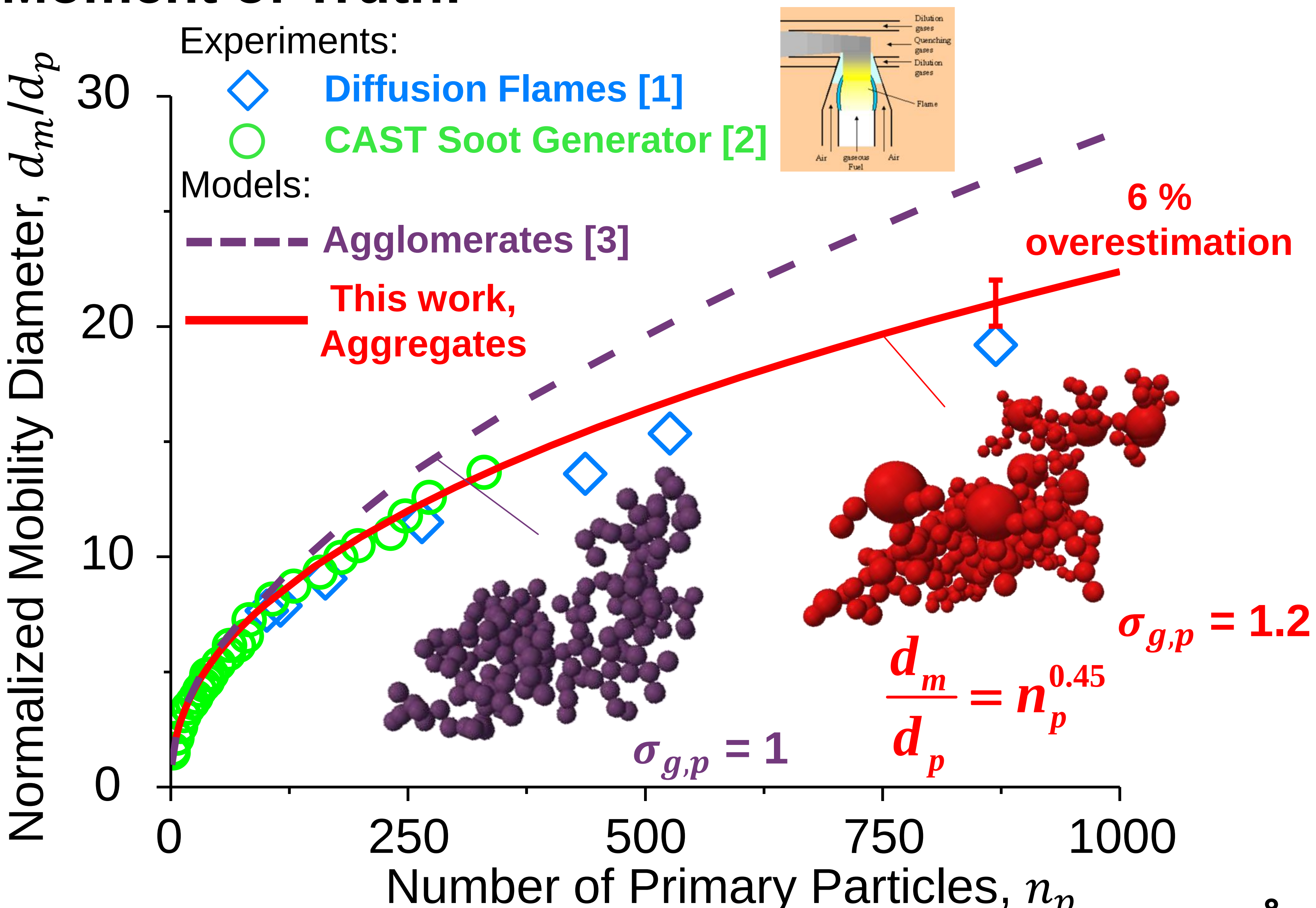

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[3] Sorensen CM. *Aerosol Sci. Technol.* (2011) 45, 765.

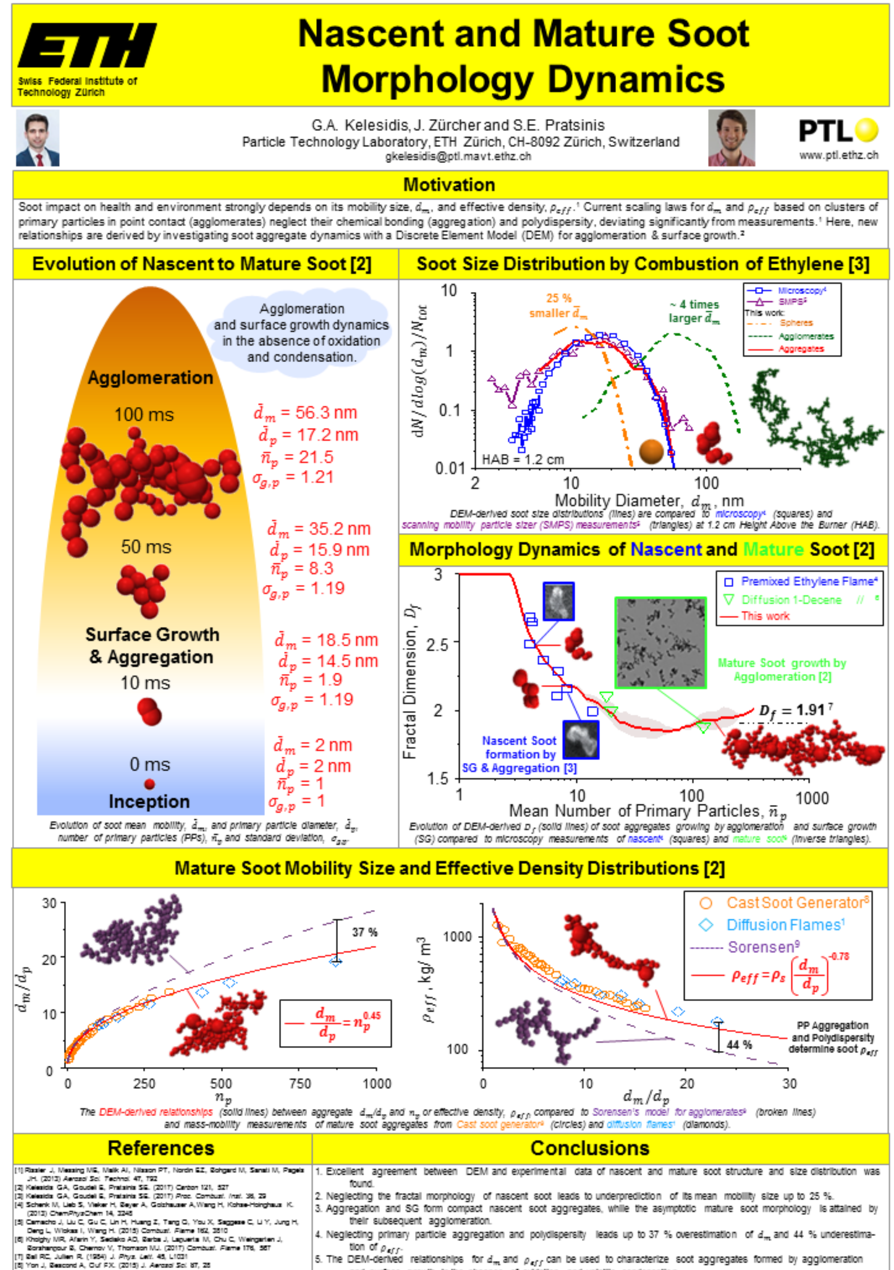
What about the Effective Density?

Scaling law accounting for PP aggregation & polydispersity:

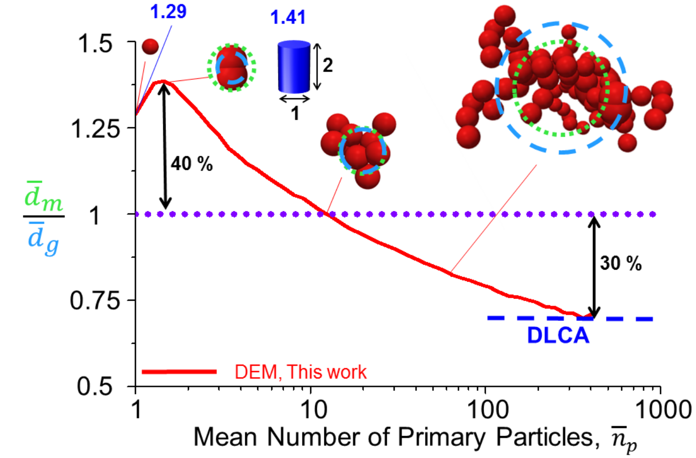
$$\frac{\rho_{eff}}{\rho_{bulk}} = \left(\frac{d_m}{d_p}\right)^{-0.78}$$

But is it any good?

Poster Session, <u>Today, 15.20-16.30</u>

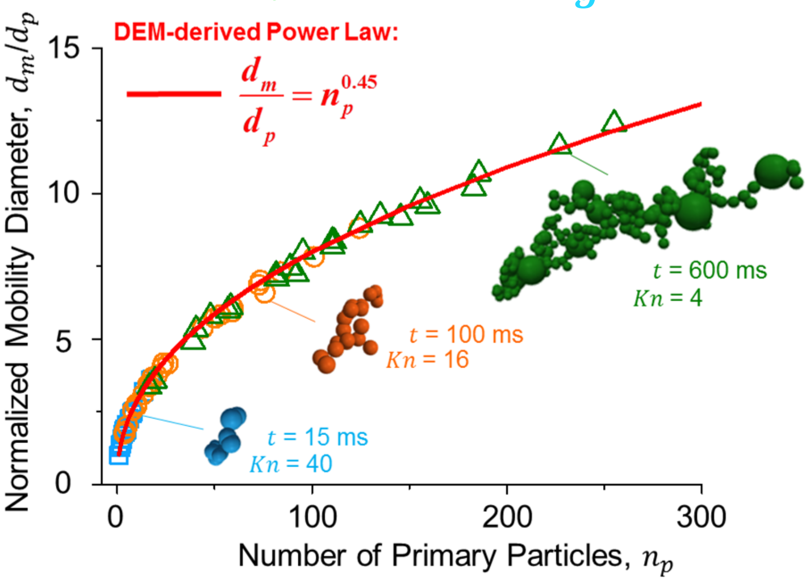


Conclusions



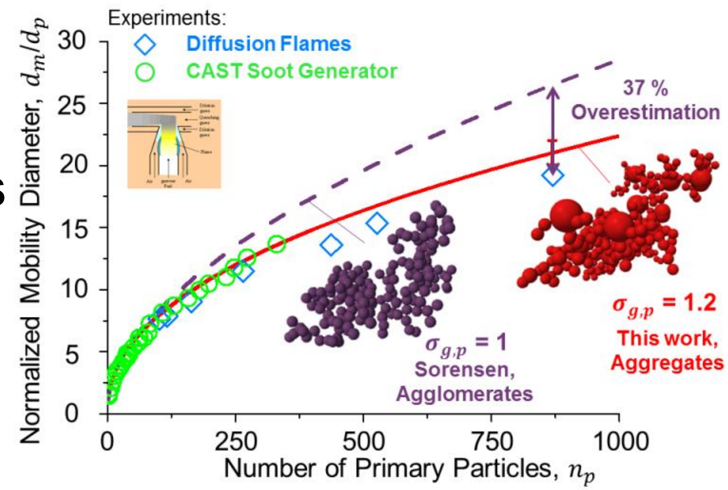
- Agglomeration & surface growth modeling reveals:

$$d_m \neq \text{Const} \cdot d_g$$



- New relationship accounting for **aggregation** and **polydispersity**:

$$\frac{d_m}{d_p} = n_p^{0.45}$$



- **Chemical Bonding of primary particles is needed for d_m!**

Thank you for your attention!

Full Story in:

Kelesidis GA, Goudeli E, Pratsinis SE,
"Morphology and Mobility Diameter of Carbonaceous Aerosols during Agglomeration & Surface Growth"
***Carbon*, 121, 527-535**