Carleton UNIVERSITY

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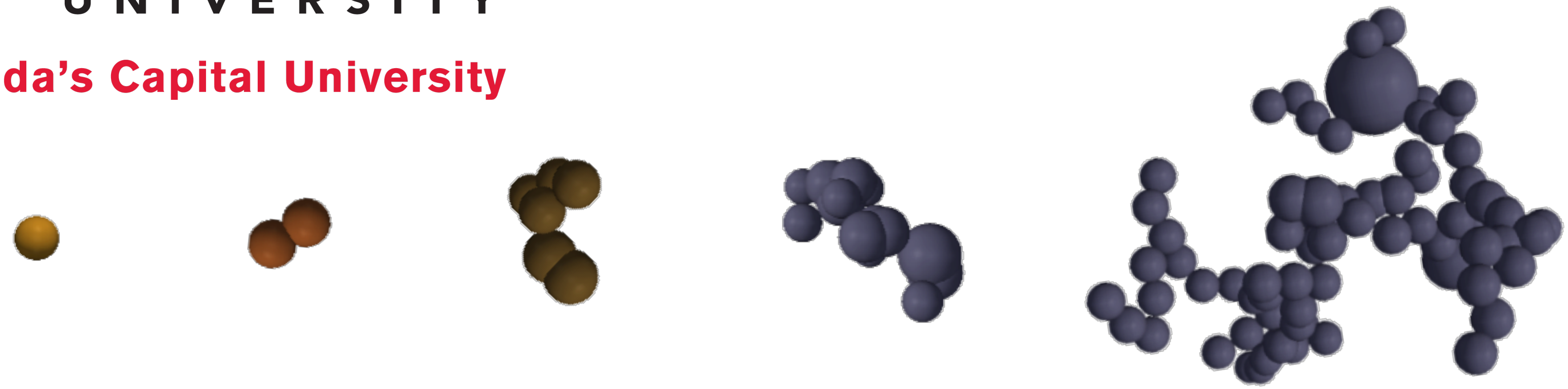


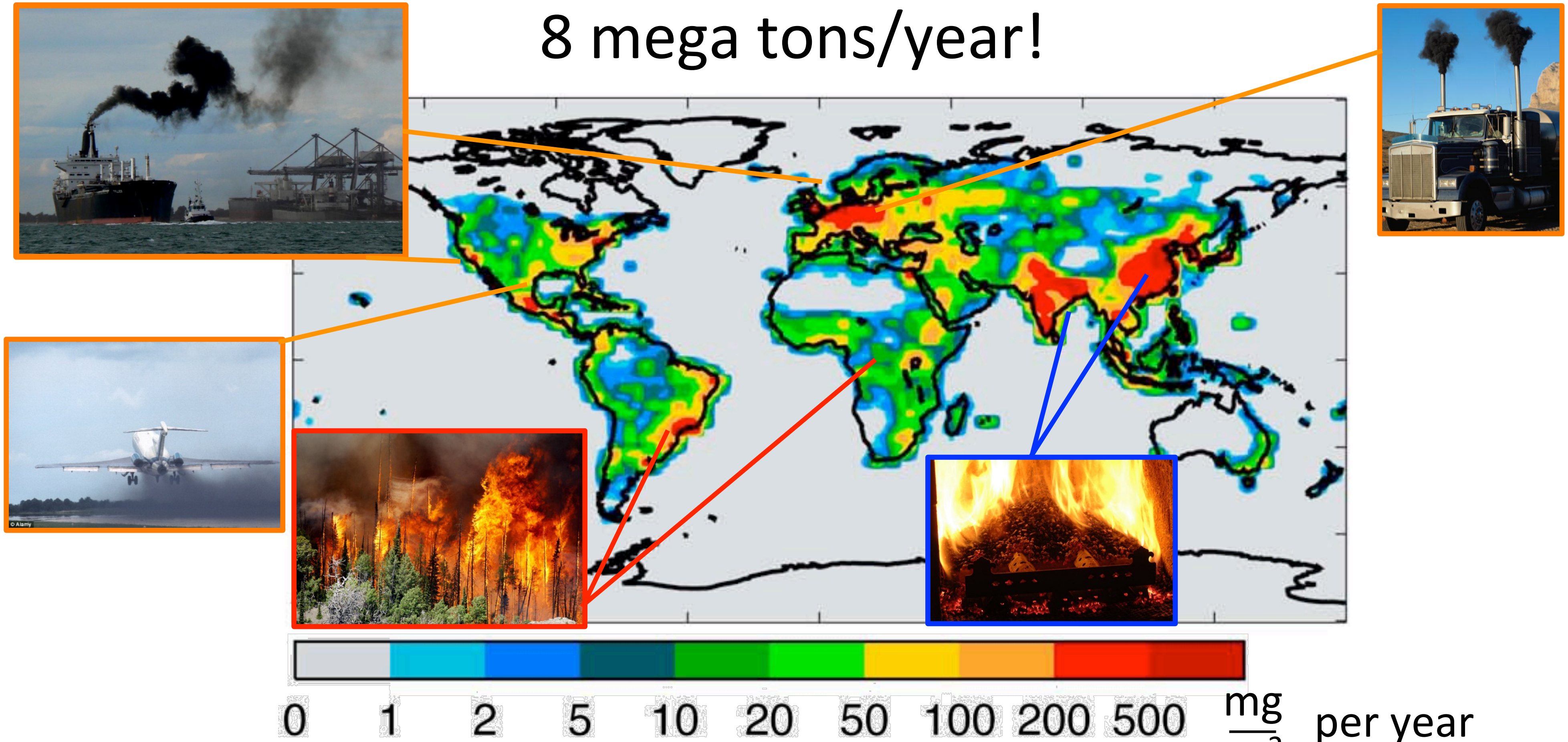
Surface Growth, Coagulation and Oxidation of Soot by a Monodisperse Population Balance Model

M. Reza Kholghy[1], Georgios A. Kelesidis[2]

1. Energy & Particle Technology Laboratory, Carleton University, Canada
2. Particle Technology Laboratory, ETH Zurich, Switzerland

Soot, the 3rd Contributor to Global Warming [1]

8 mega tons/year!



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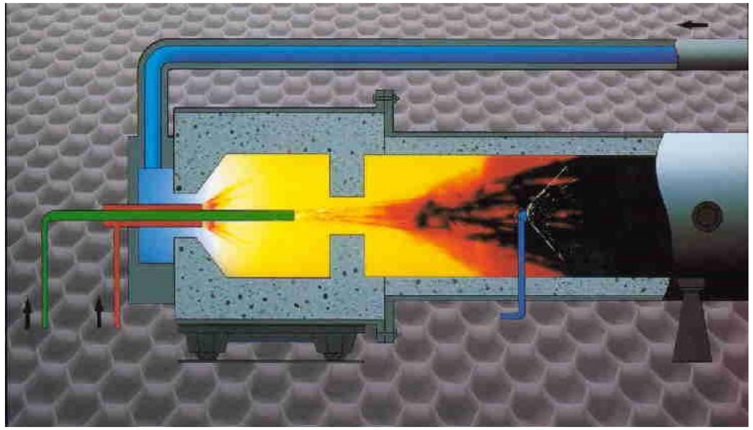
[2] Bond, T. C.; Doherty, S. J.; Fahey, D., et al. J Geophys Res 2013, 118, 5380.

Carbon Black: A $17 B Industry

15 mega tons/year! [2]

[1]

Lamp Black Process
China, 2000 BC

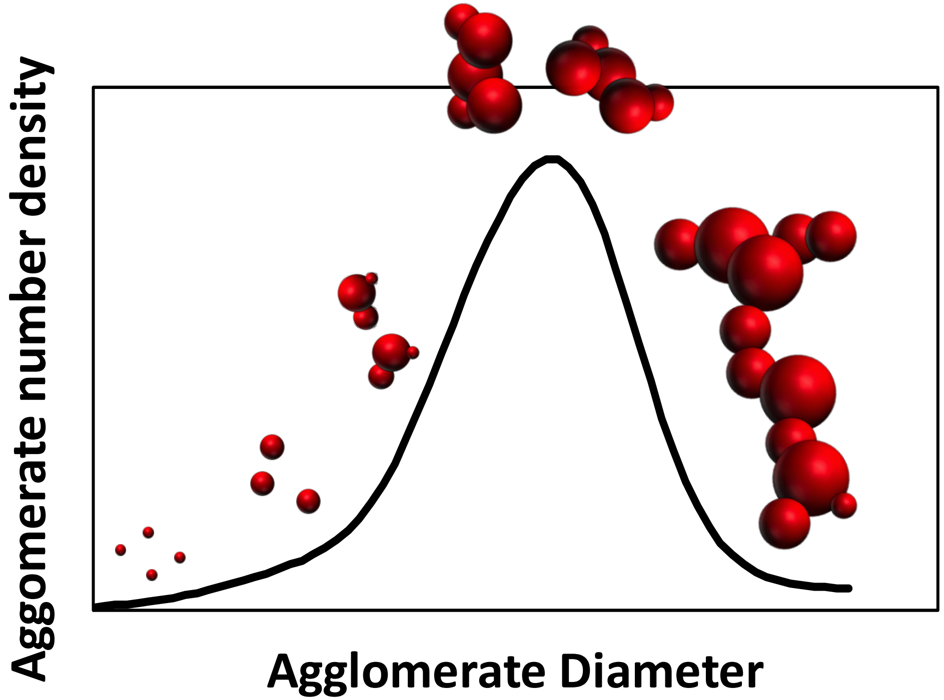


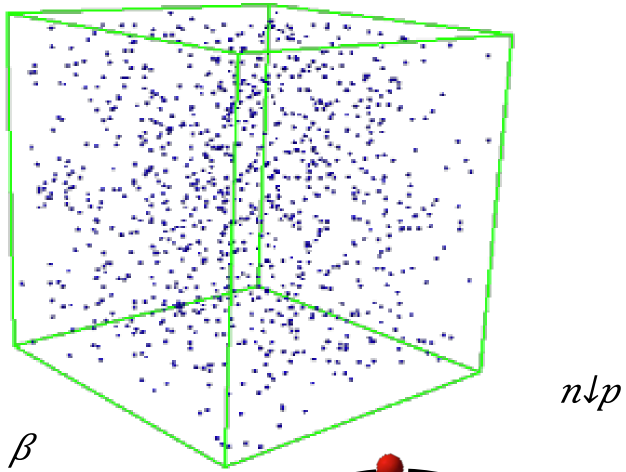
Furnace Process
only ~50% yield!!

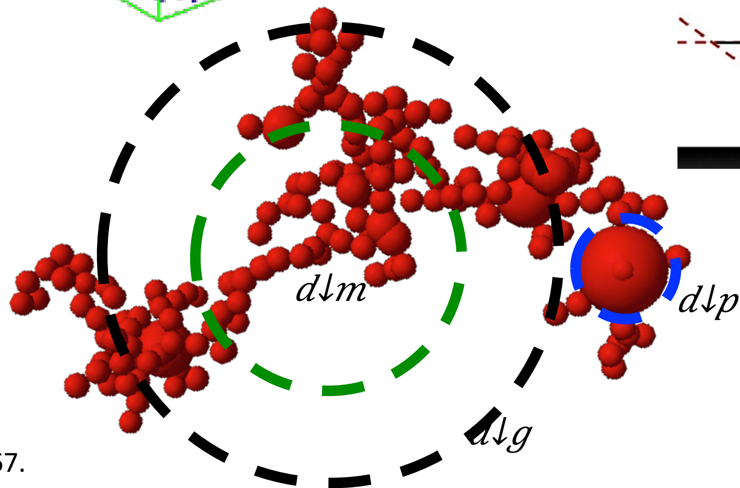
[1] G. D. Ulrich, 1984, *Chem. Eng. News* **62**, 22.
[2] Robertson, C.G. and Hardman, N.J., 2021. *Polymers*, *13*,538.

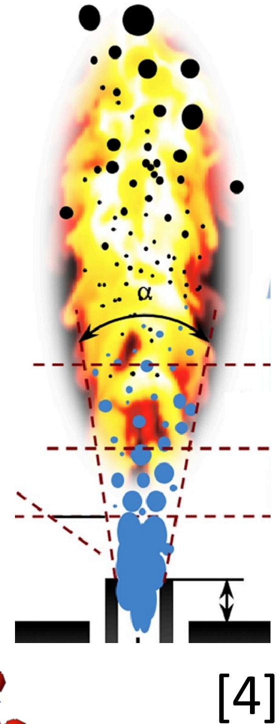
Particle Morphology & Size Distribution

Discrete Element Modeling (DEM) [1-3]









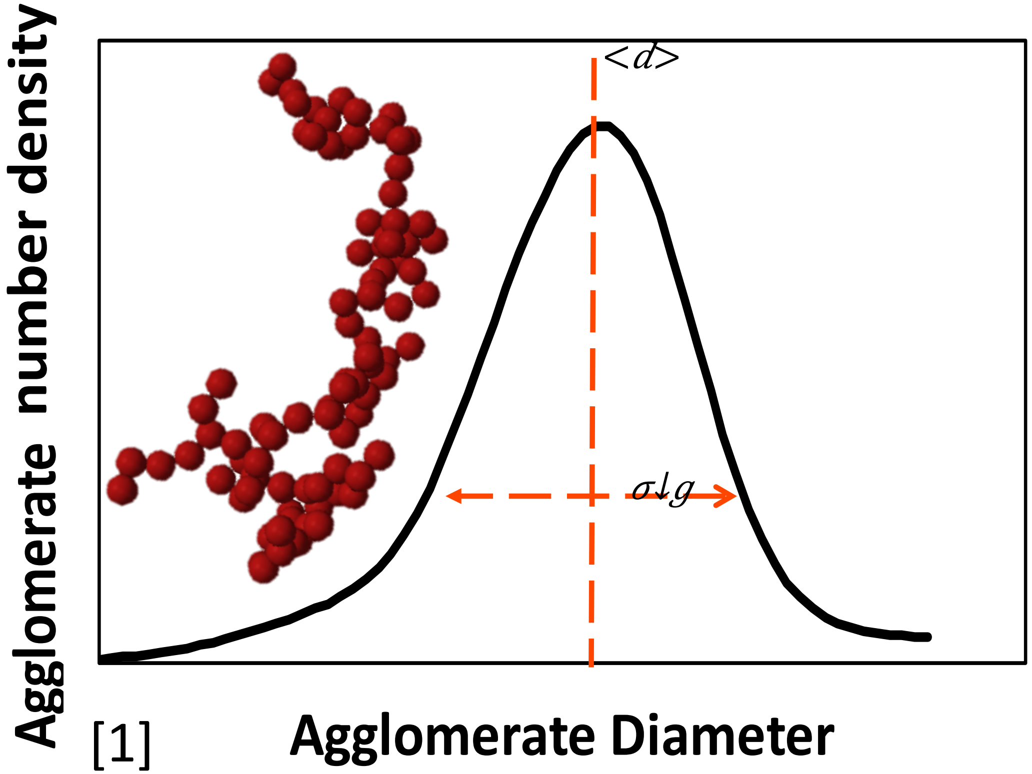
[1] Kelesidis GA, Goudeli E, Pratsinis SE, *Carbon* **121**, (2017) 527-535.
[2] Goudeli G, Eggersdorfer ML, Pratsinis SE, *Langmuir.*, **32**, **(**2016) 9276-9285.
[3] Eggersdorfer ML, Kadau D, Herrmann HJ, Pratsinis SE, *Langmuir*, **27**, **(**2011) 6358-6367.
[4] Rittler, A., Deng, L., Wlokas, I. and Kempf, A.M., 36 (2017). *P Combust Institute*, *36*, 1077-1087.

Particle Morphology & Size Distribution

$dN/dt = -1/2\, \beta N^2$

[2]

$m = k\, d^{D_f}$

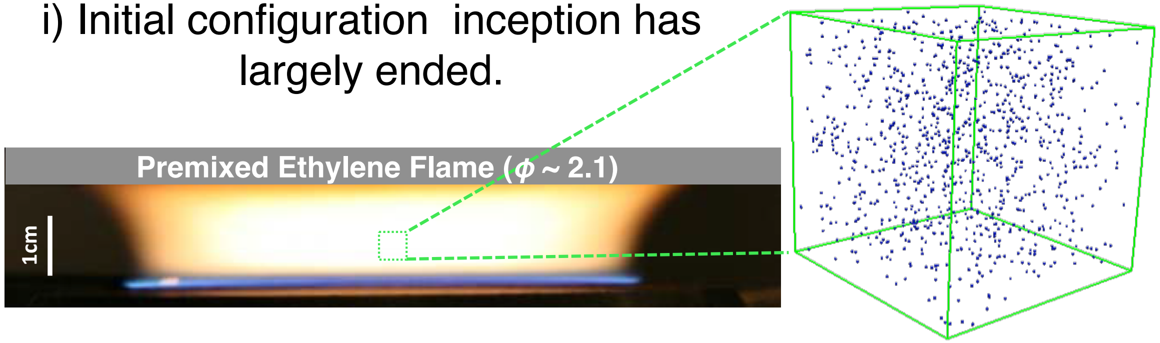


[1]

[1] Lai, F.S., Friedlander, S.K., Pich, J. and Hidy, G.M., 39, (1972) *Journal of Colloid and Interface Science*, 395-405.
[2] Kruis, F.E., Kusters, K.A., Pratsinis, S.E. and Scarlett, B., **19**, (1993) 514-526.

Soot Dynamics by Discrete Element Modeling (DEM)

i) Initial configuration inception has largely ended.



T = 1830 K

$d_{m,o}$ = 2 nm

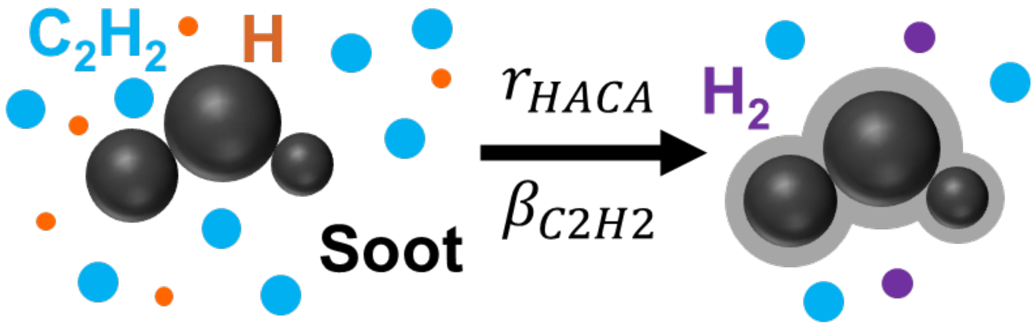
$N_{tot,o}$ = 4.5·10^{16} m^{-3}

[1,2]

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

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

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



[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] Saggese C, Ferrario S, Camacho J, Cuoci A, Frassoldati A, Ranzi E, Wang H, Faravelli T. Wang H. (2015) *Combust. Flame* **162**, 3356.

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

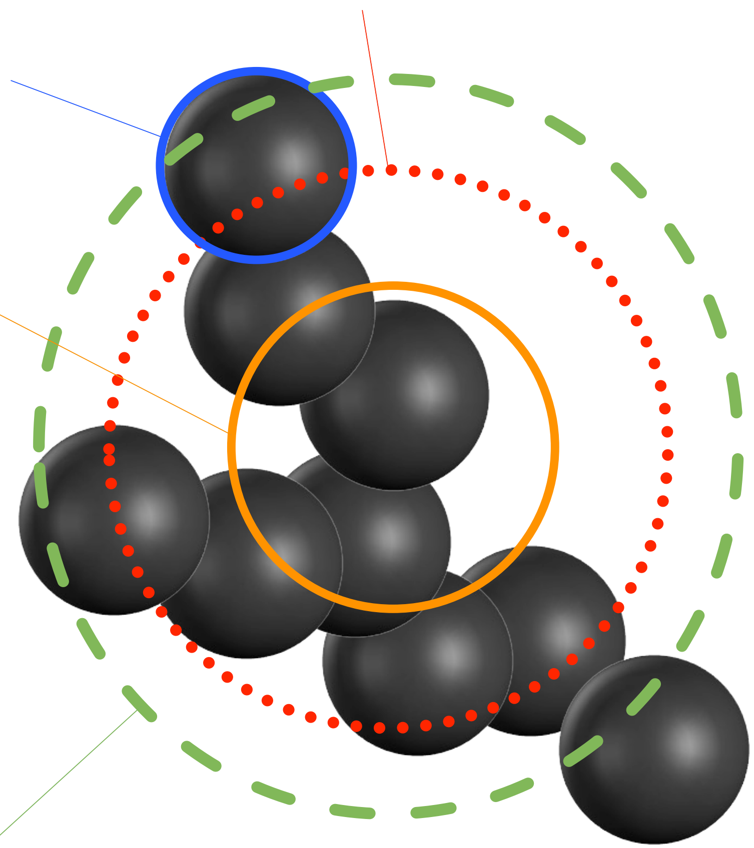
Monodisperse Population Balance Model (MPBM)

$d_p = 6M/\rho A$ $\quad$ $d_m = d_p n_p^{0.45}$

Coagulation

$dN/dt = -1/2\, \beta_p N^2$

$d_v = \sqrt[3]{6M/\rho N \pi}$



Surface Growth

Oxidation

$dM/dt = 2 MW_C \gamma \beta_{C_2H_2} [C_2H_2] N - \omega_{O_2} A$

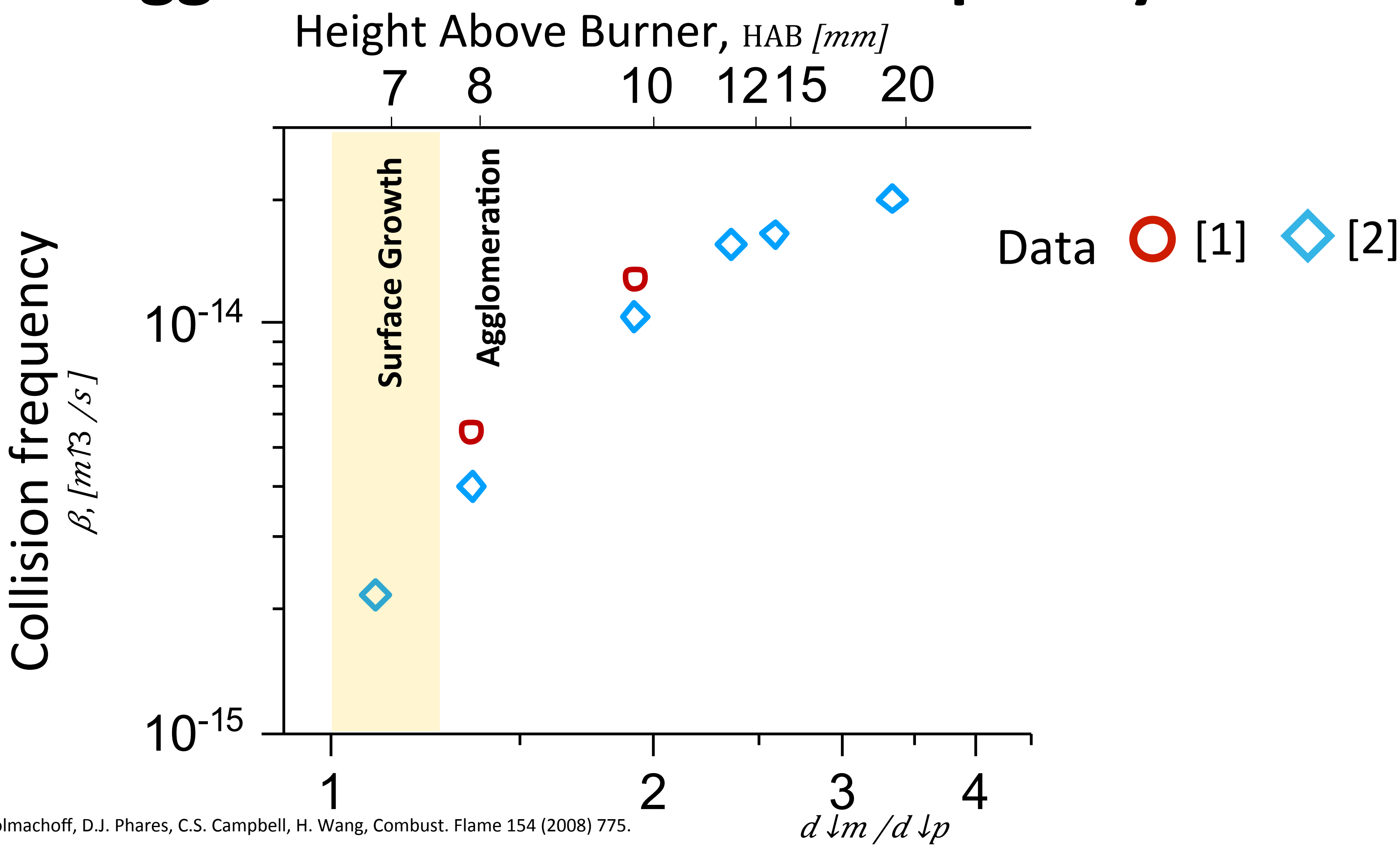
$n_p = 6M/\rho N \pi d_p^3$

$dA/dt = 4/\rho d_p \; dm/dt$

$d_g = d_m / (n_p^{-0.2} + 0.4)$

[1] Kholghy, M.R. and Kelesidis, G.A., 2021. *Combustion Flame*, *227*.

Agglomerate Collision Frequency



[1] A.D. Abid, N. Heinz, E.D. Tolmachoff, D.J. Phares, C.S. Campbell, H. Wang, Combust. Flame 154 (2008) 775.

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

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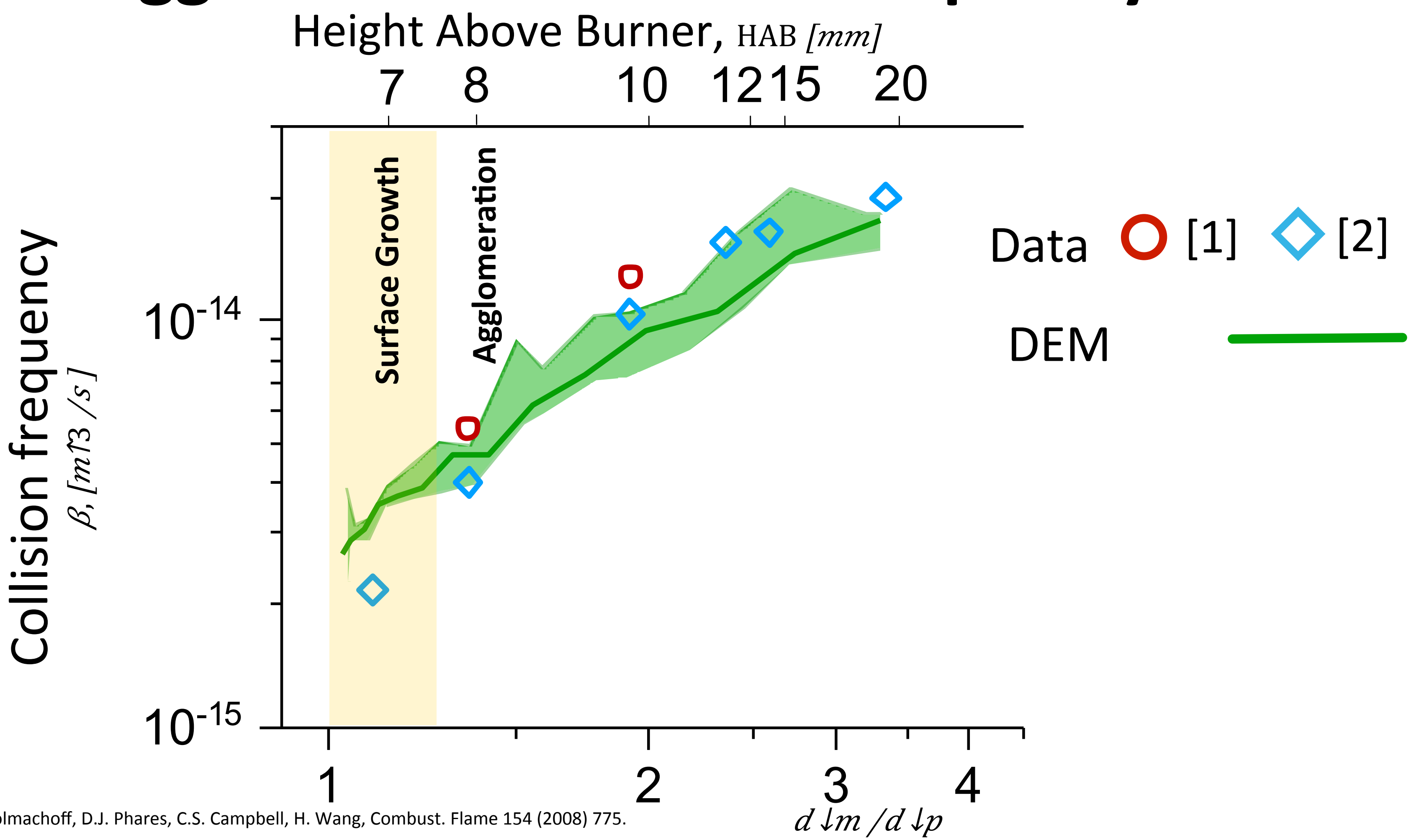

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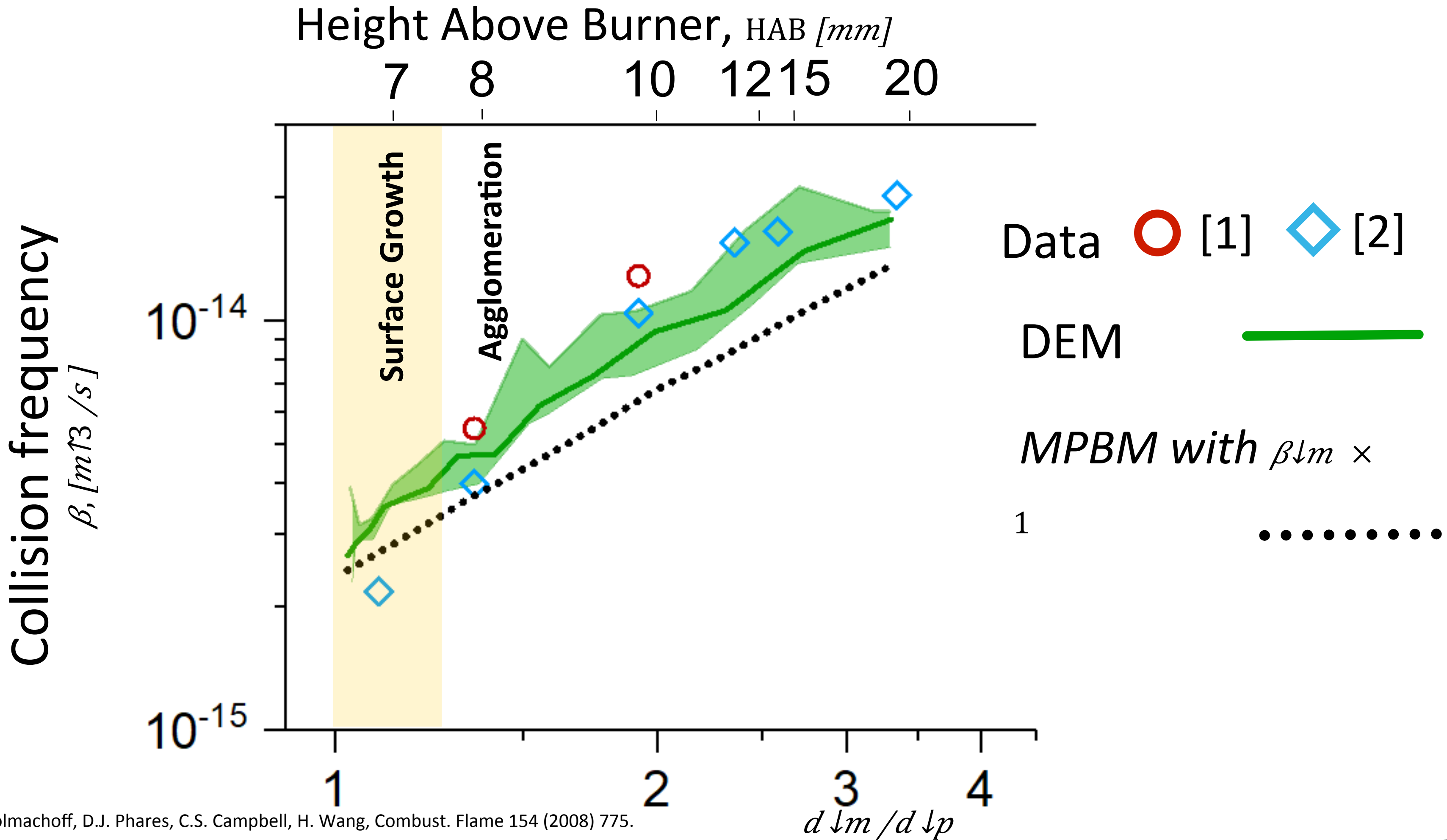

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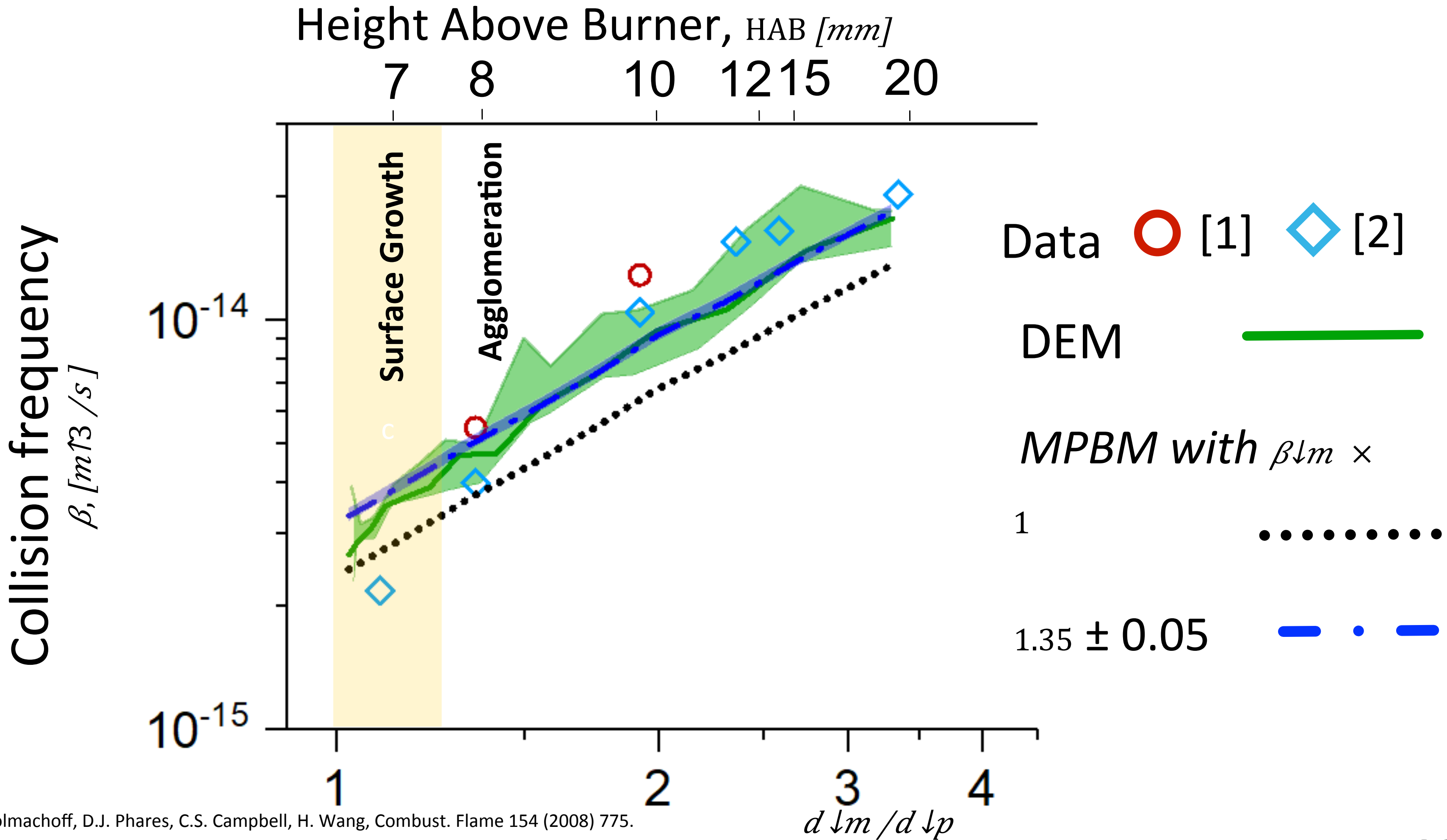

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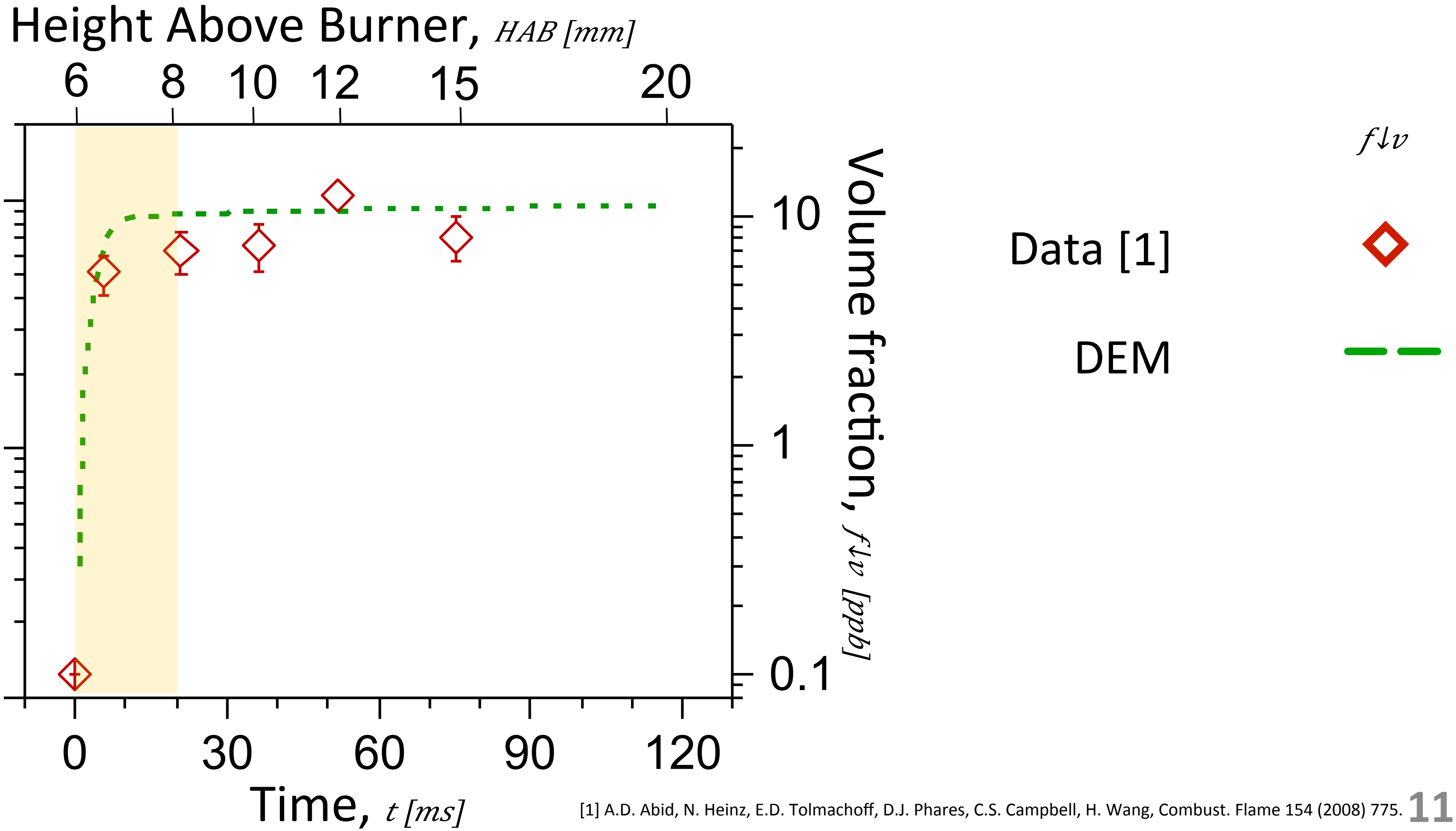
Soot Volume Fraction and Number Density



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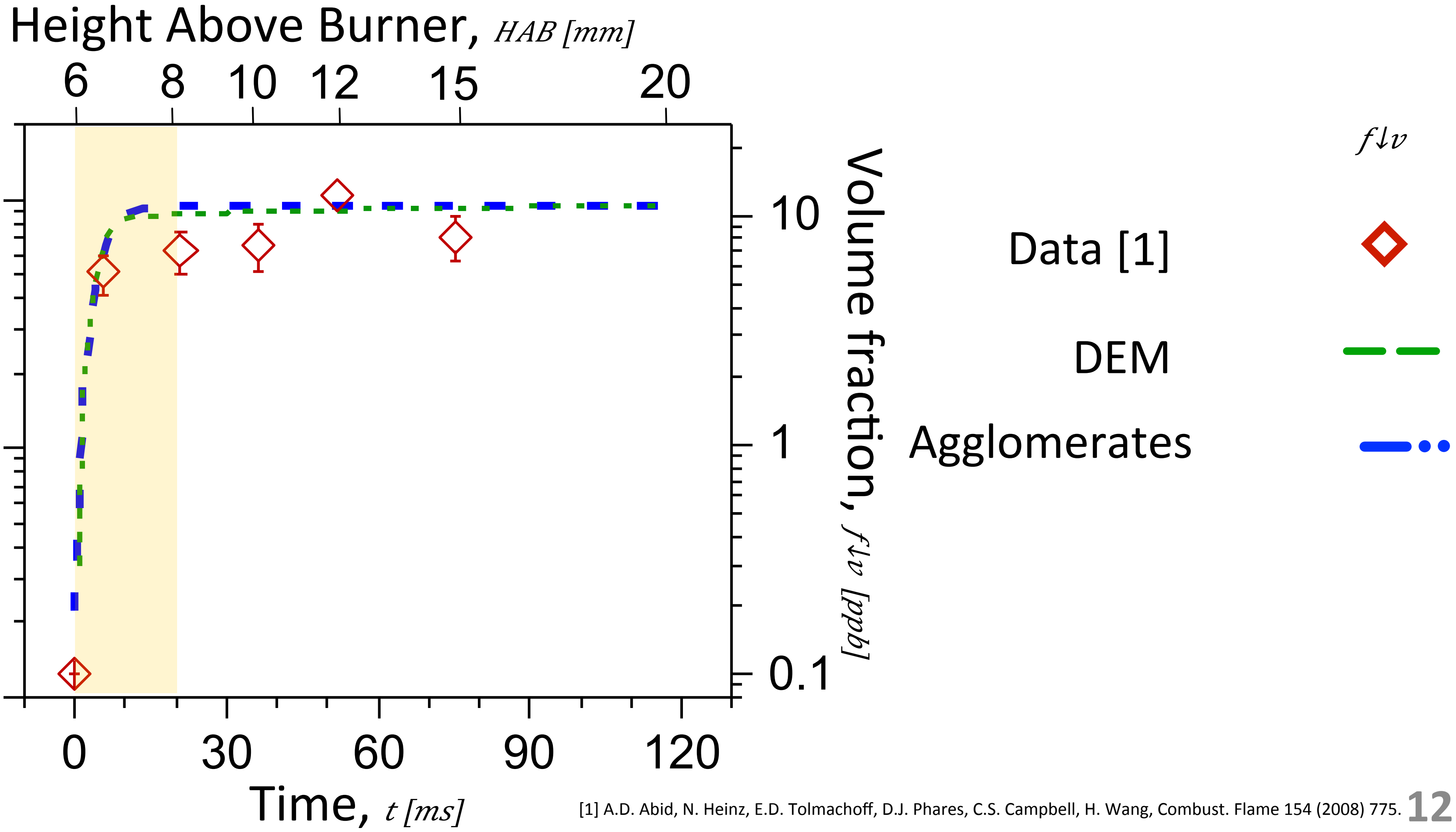

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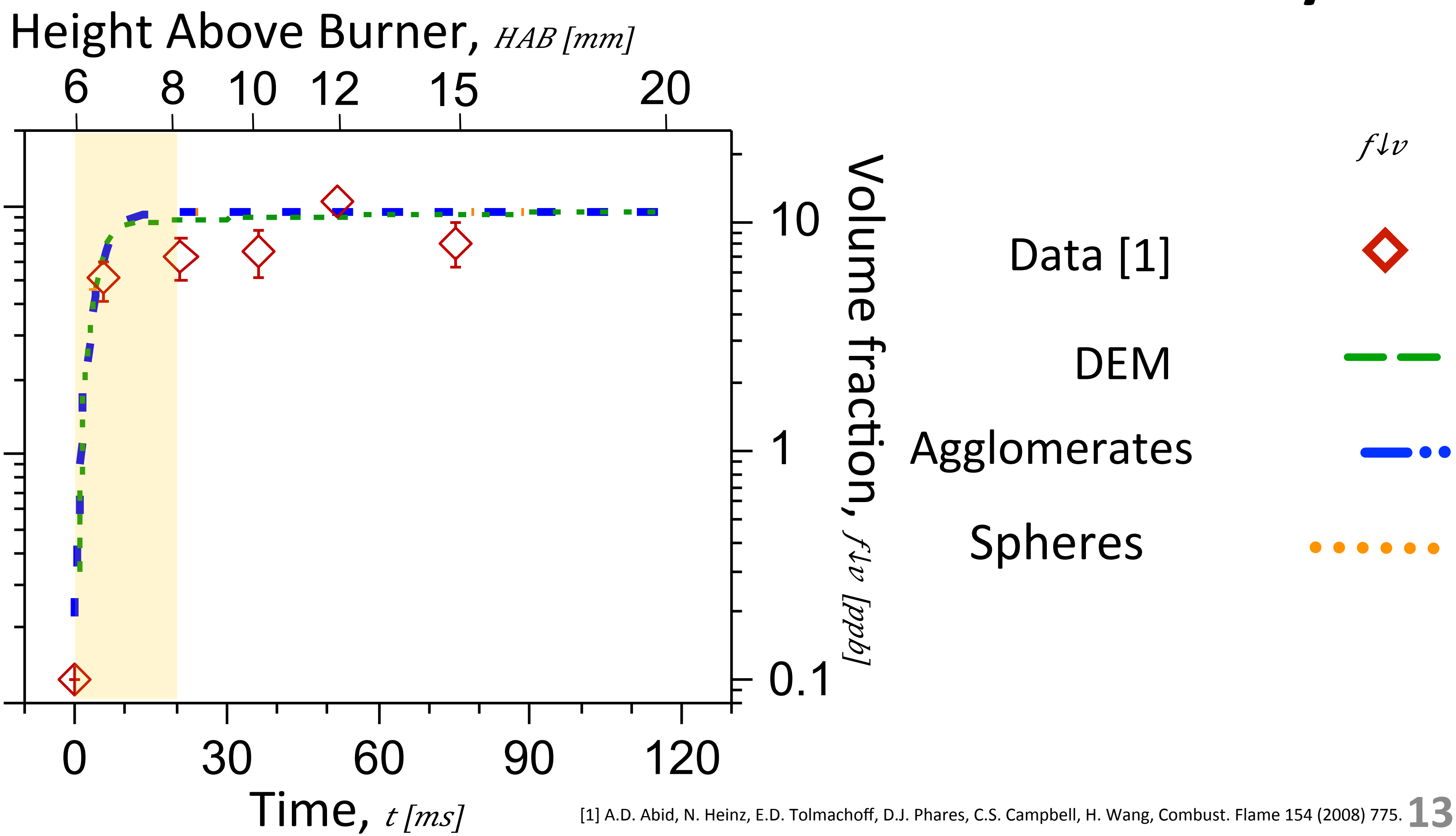

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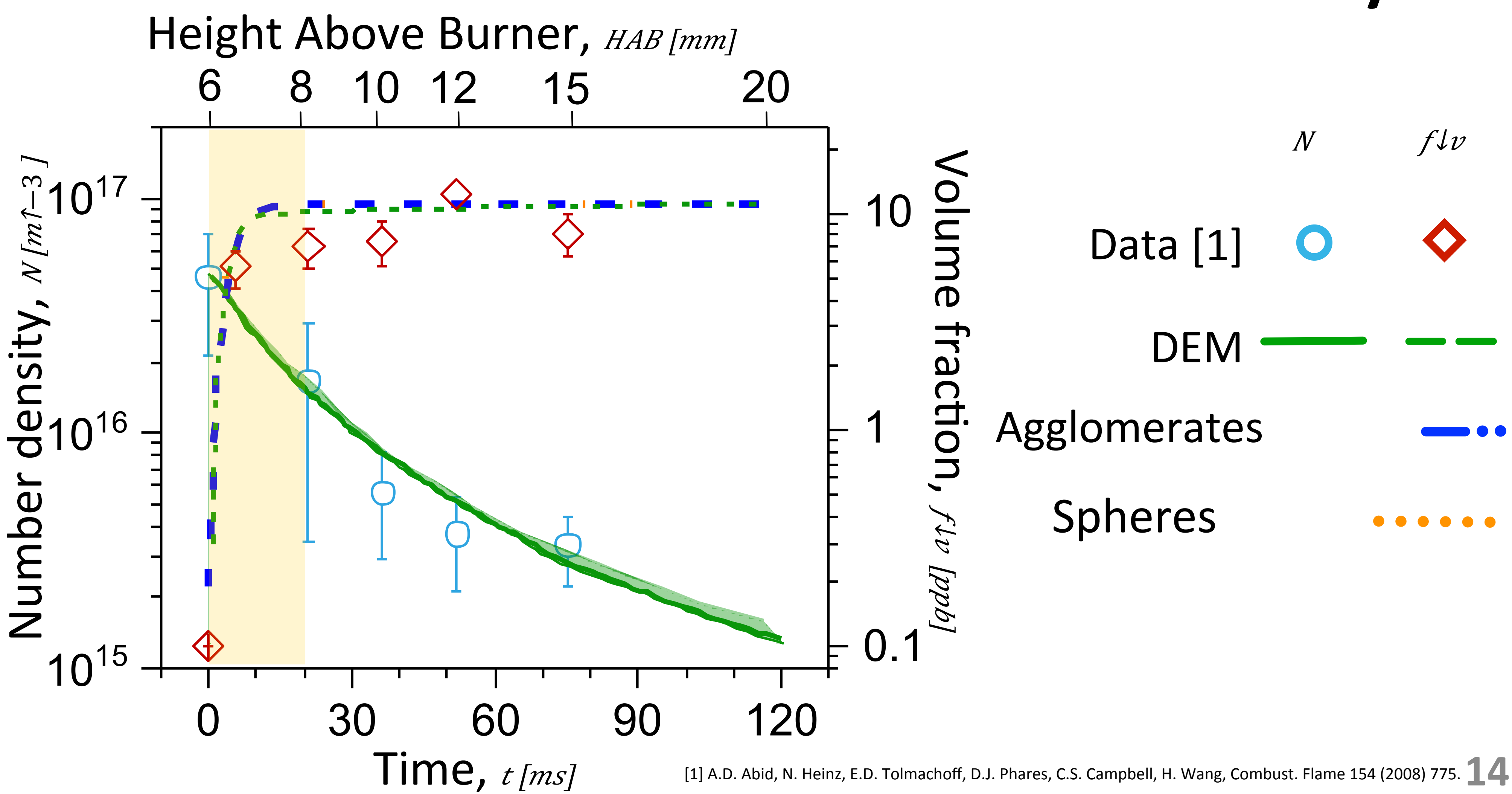

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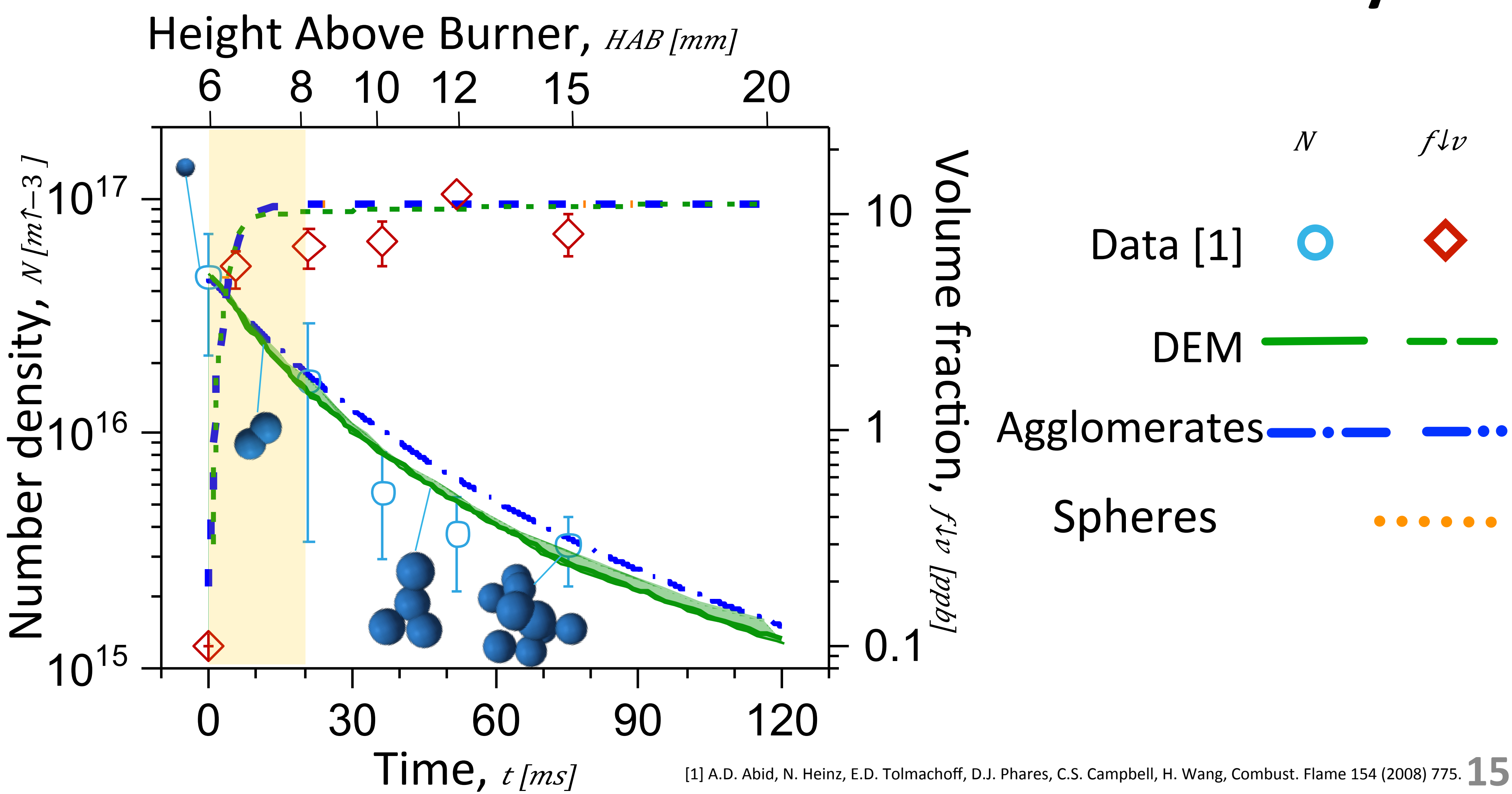

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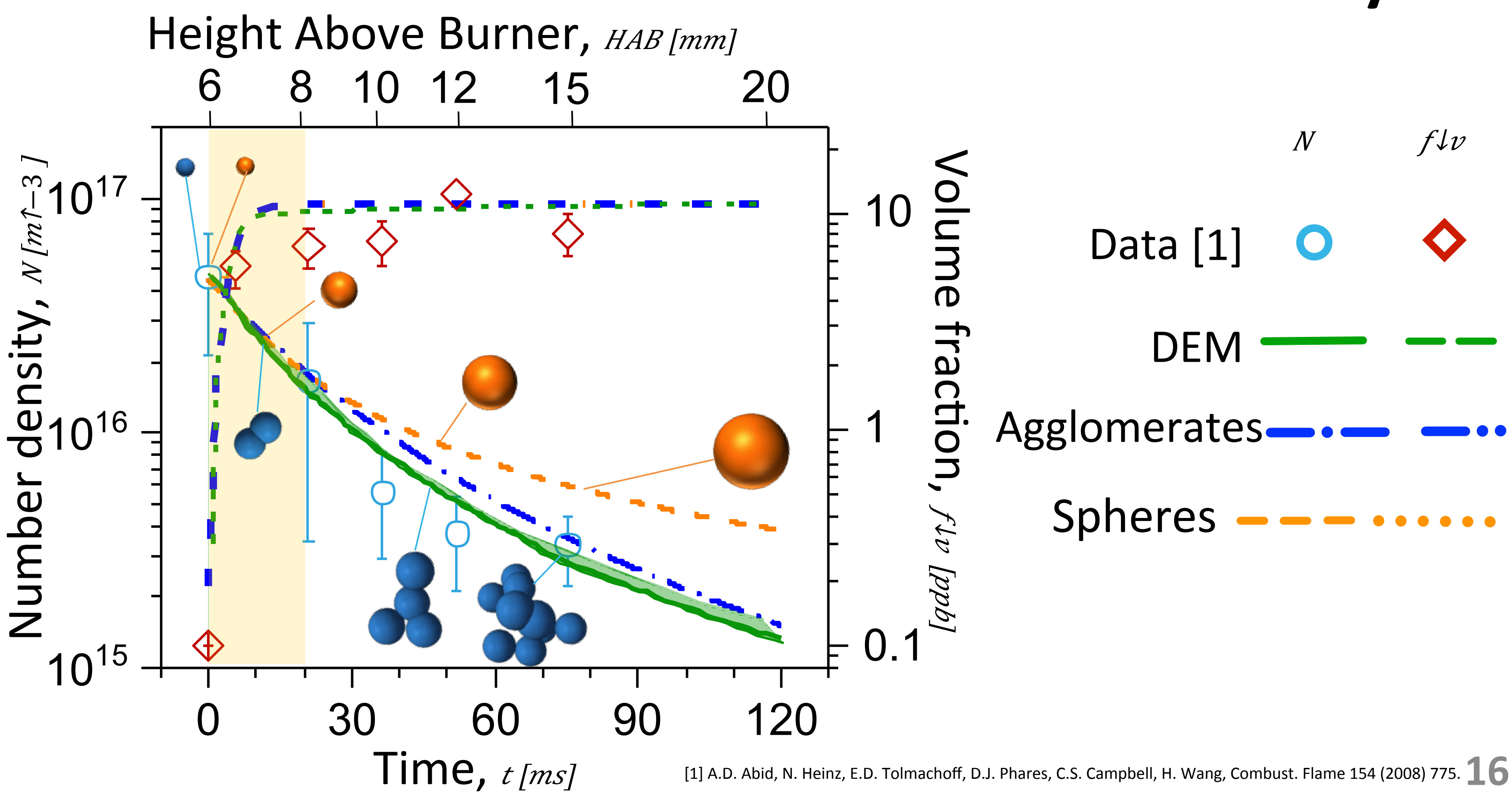

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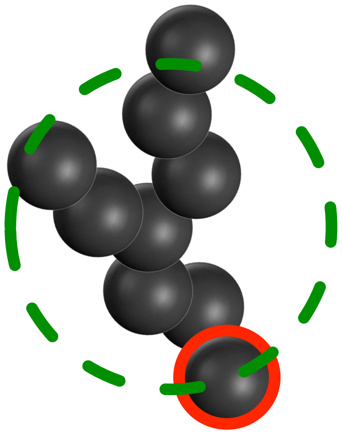
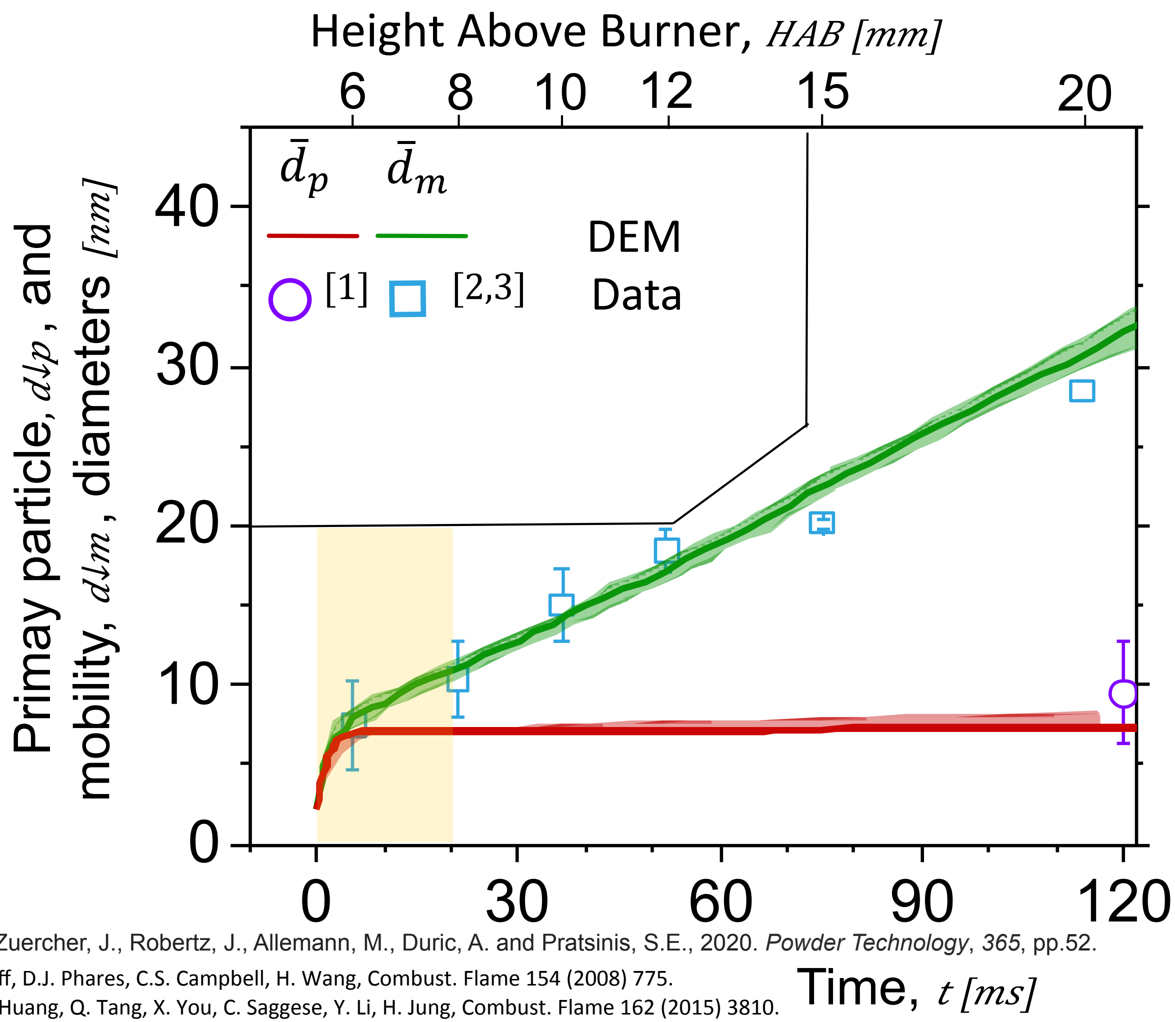
Evolution of d_p and d_m





[1] Kelesidis, G.A., Kholghy, M.R., Zuercher, J., Robertz, J., Allemann, M., Duric, A. and Pratsinis, S.E., 2020. *Powder Technology*, *365*, pp.52.

[2] A.D. Abid, N. Heinz, E.D. Tolmachoff, D.J. Phares, C.S. Campbell, H. Wang, Combust. Flame 154 (2008) 775.

[3] J. Camacho, C. Liu, C. Gu, H. Lin, Z. Huang, Q. Tang, X. You, C. Saggese, Y. Li, H. Jung, Combust. Flame 162 (2015) 3810.

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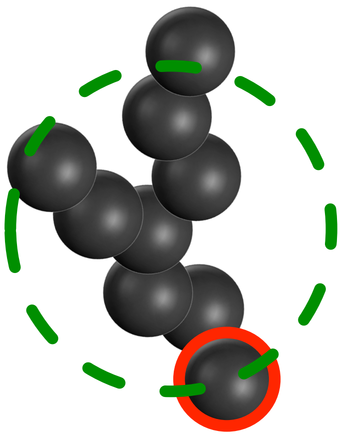

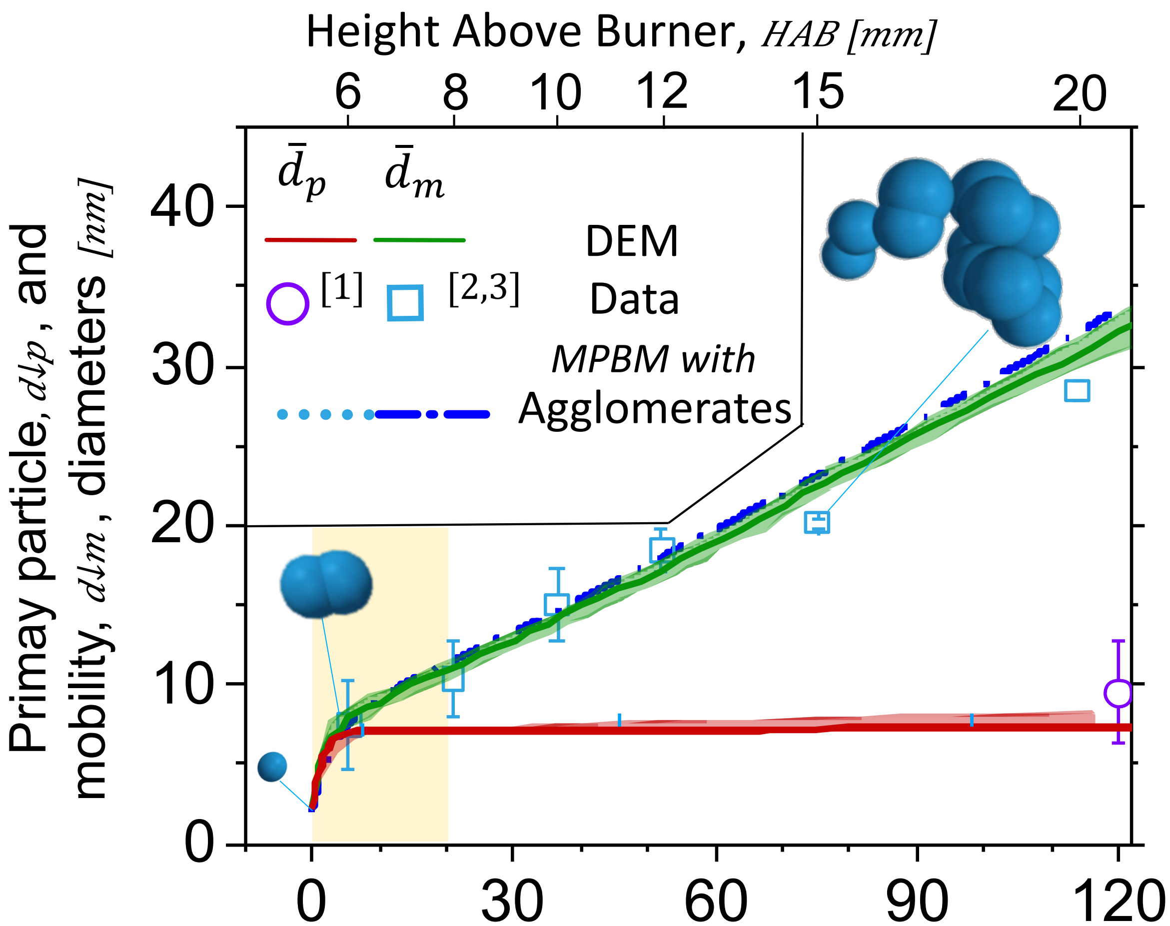

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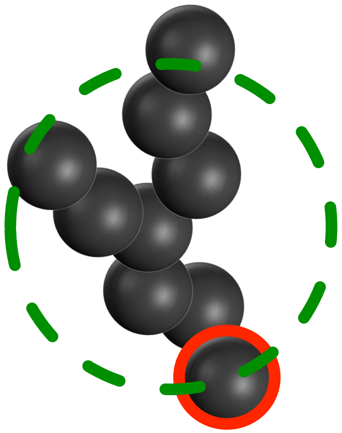

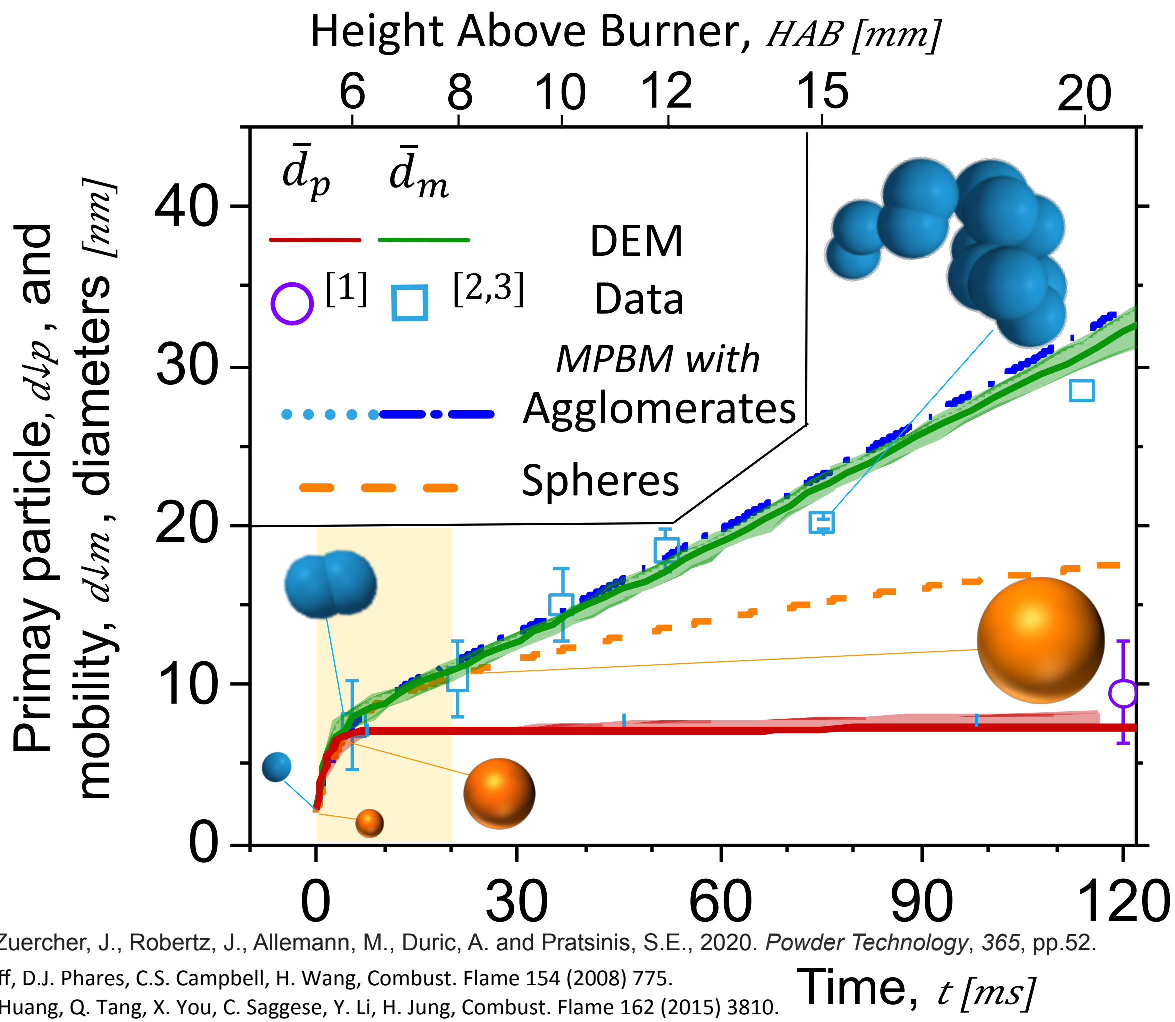

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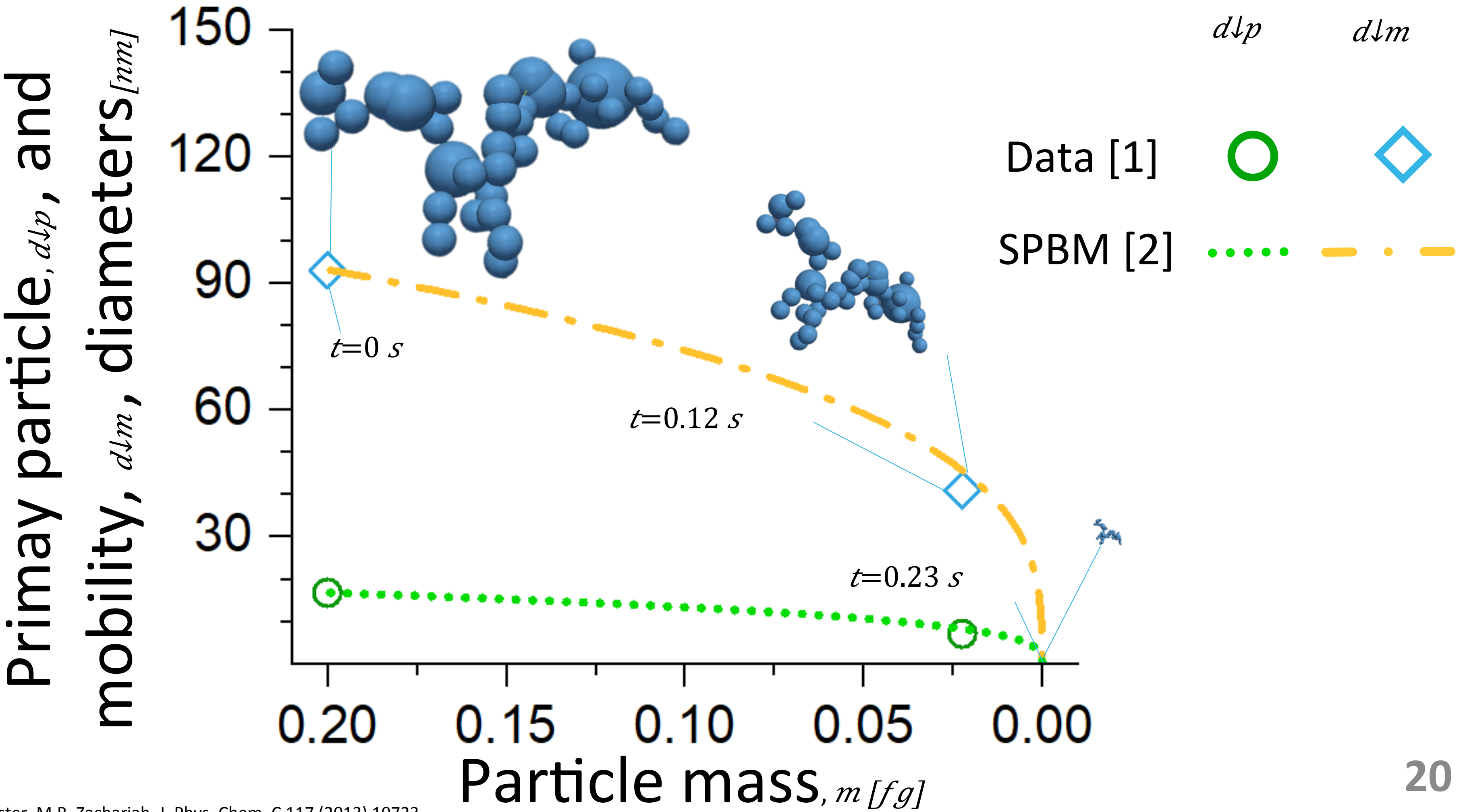
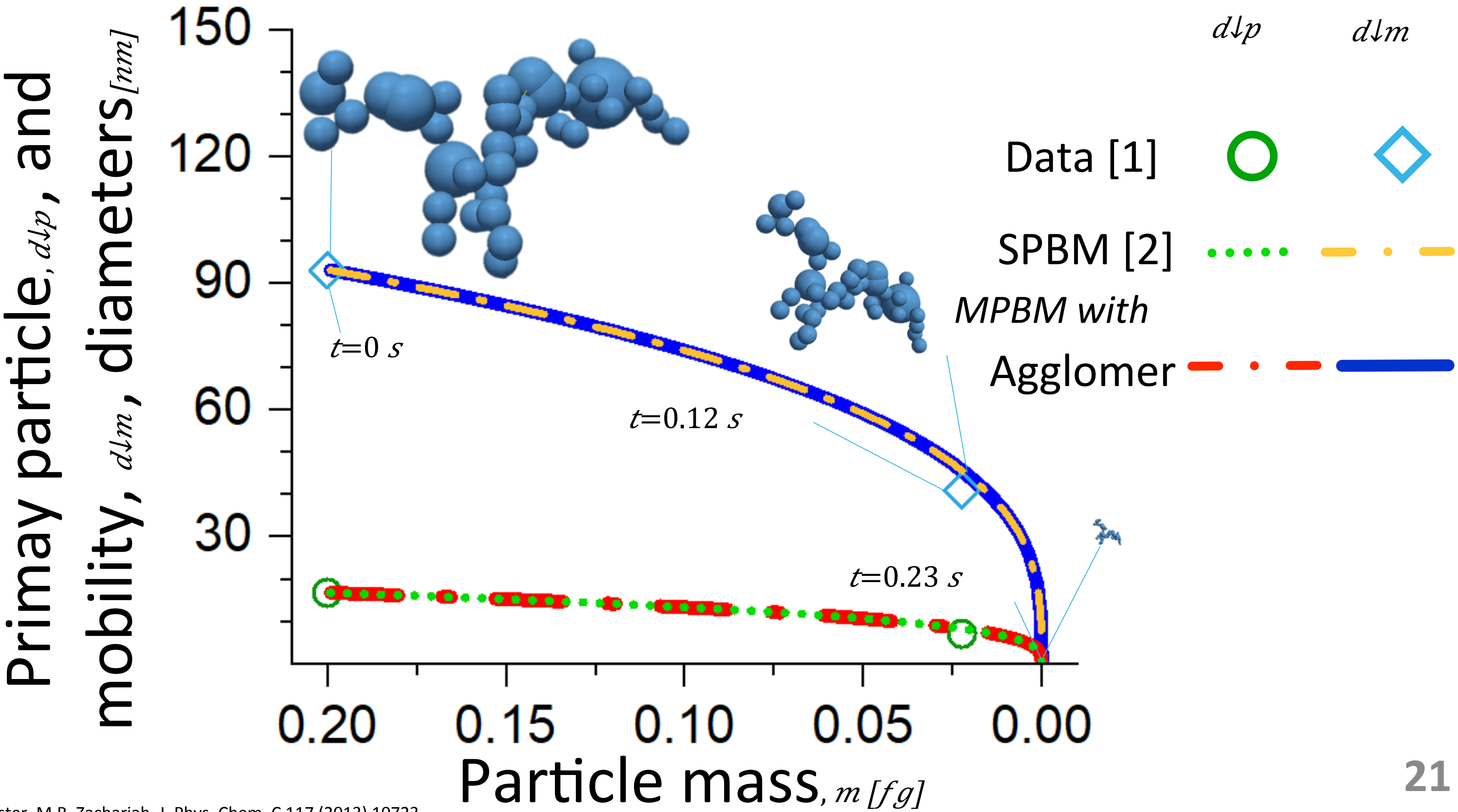
Agglomerate Surface Oxidation



[1] X. Ma, C. Zangmeister, M.R. Zachariah, J. Phys. Chem. C 117 (2013) 10723.

[2] G.A. Kelesidis, S.E. Pratsinis, Combust. Flame 209 (2019) 493.

Agglomerate Surface Oxidation



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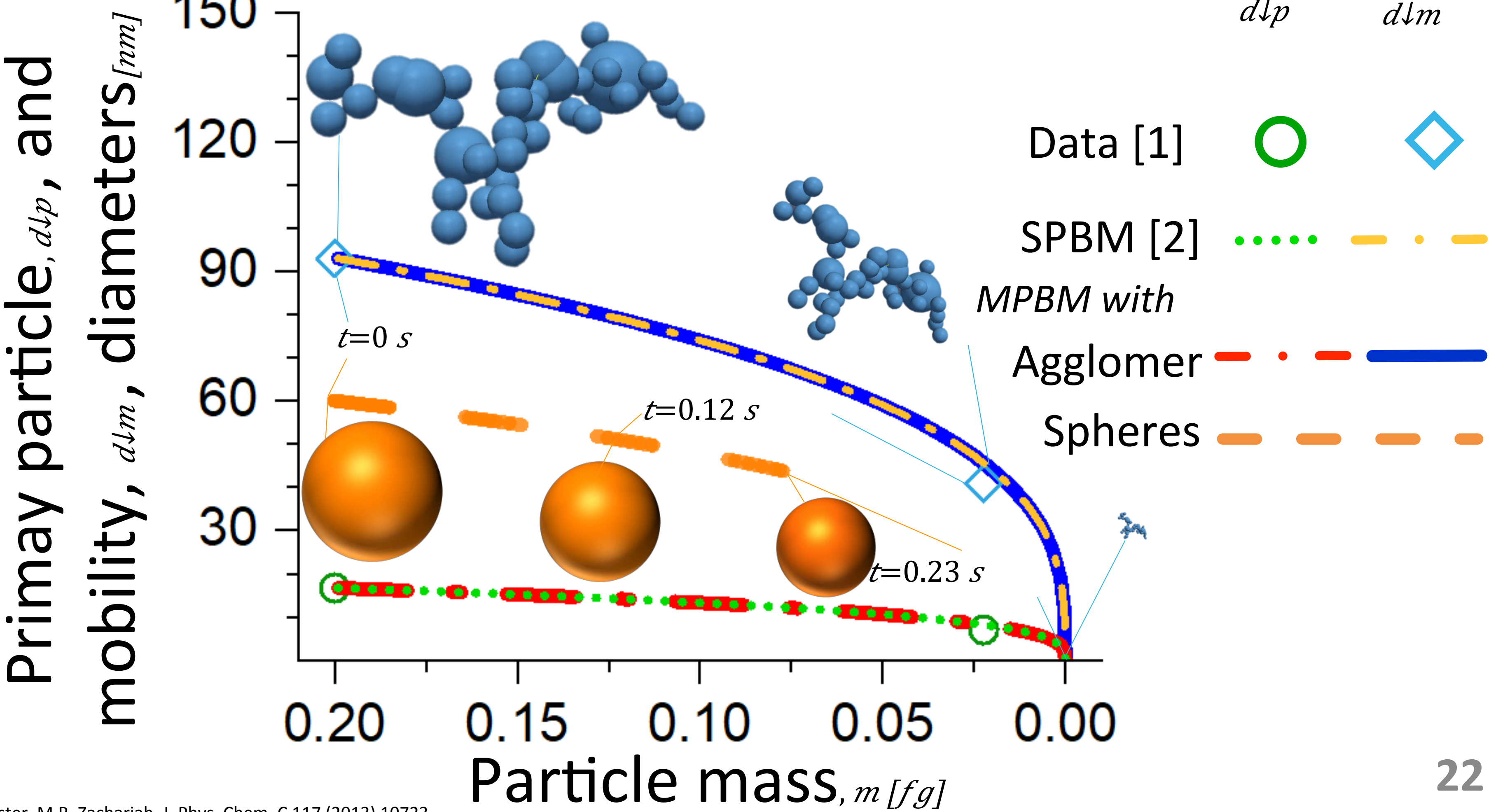

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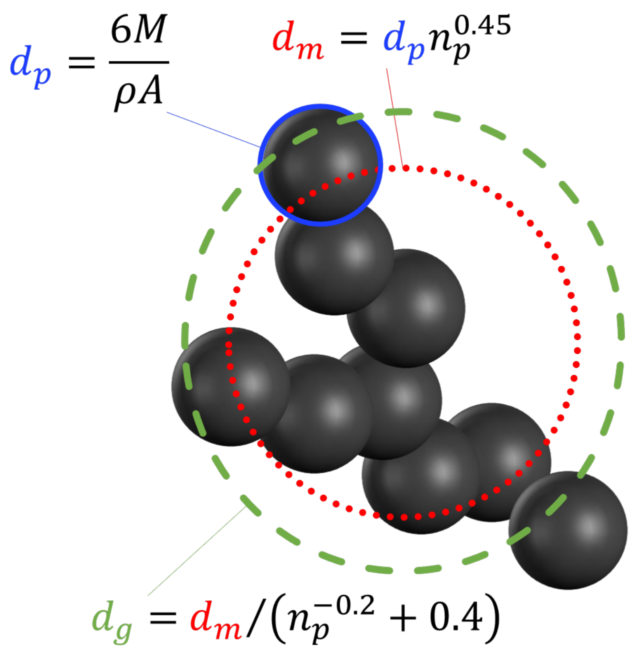
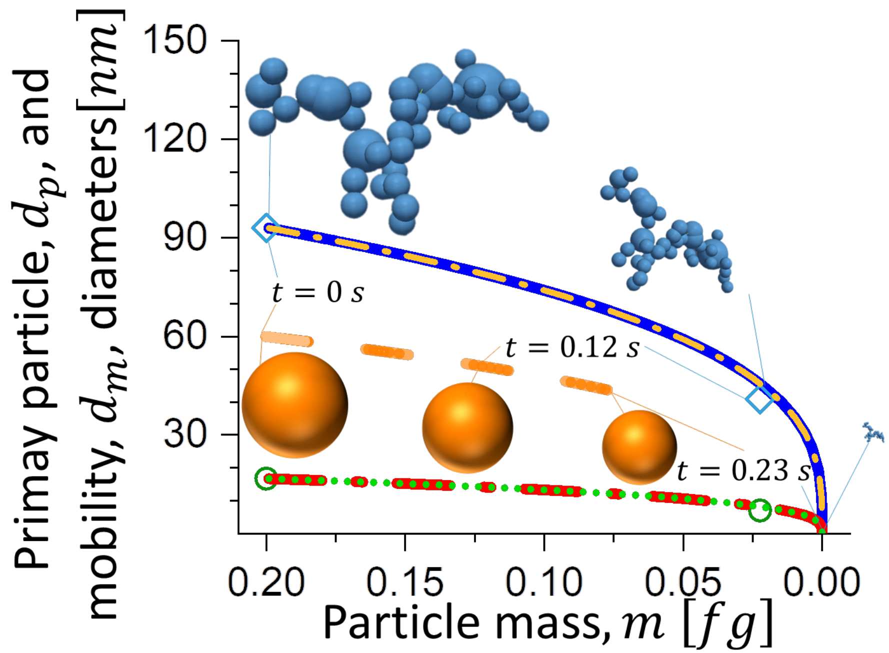
Conclusions

A simple 3-Eq model with accuracy on par with DEM by using DEM-derived power laws





Neglecting soot fractal-like structure results in significant error in predicting its coagulation & oxidation rates

Thank you for your attention

Full story in :

Kholghy, M.R. and Kelesidis, G.A., 2021. *Combustion Flame, 227*.

NSERC CRSNG

Supported by (Discovery Grant # RGPIN-2019-06330 &
Early Career Supplemental Award # DGECR-2019-00220)

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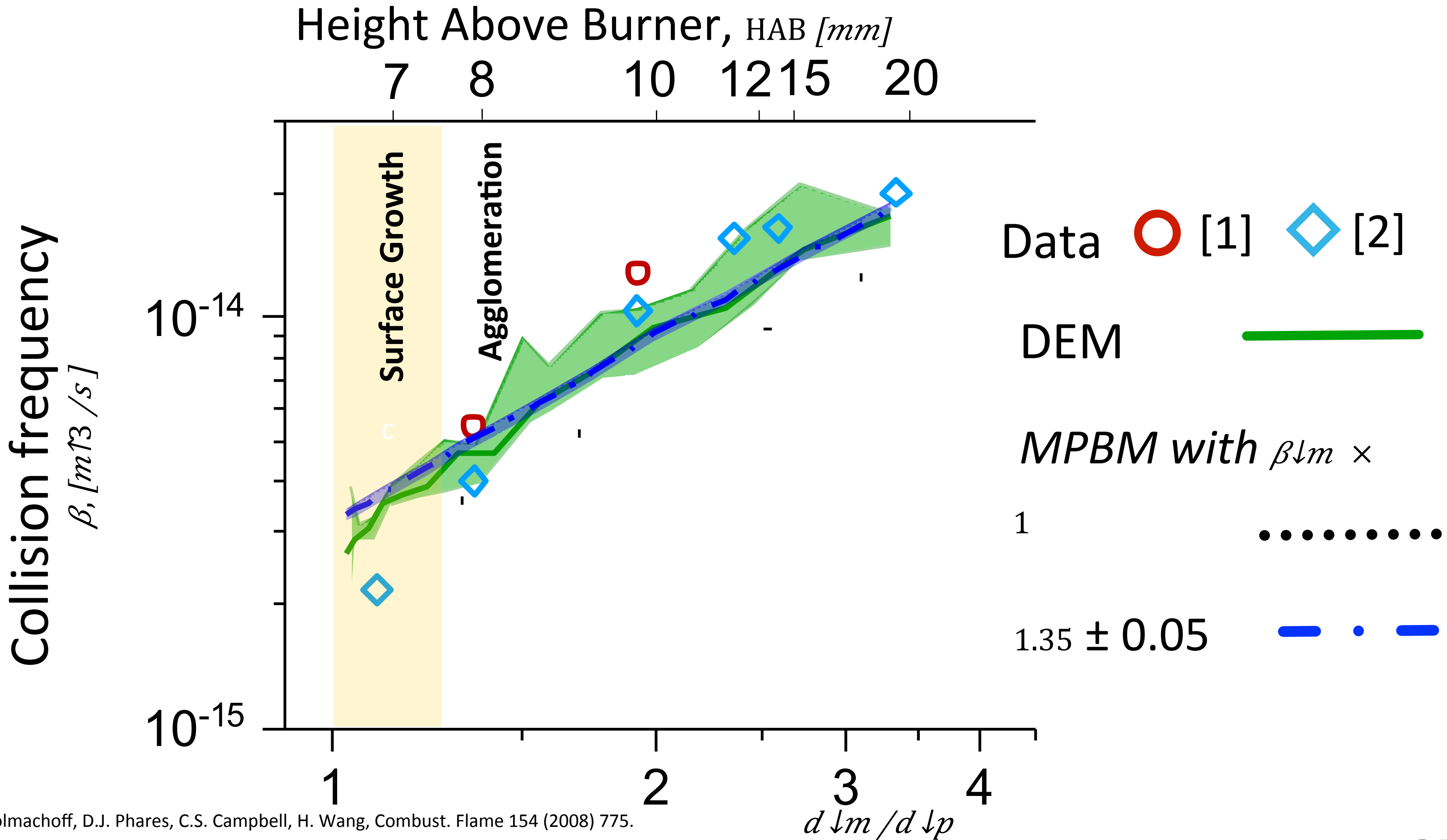
Agglomerate Collision Frequency



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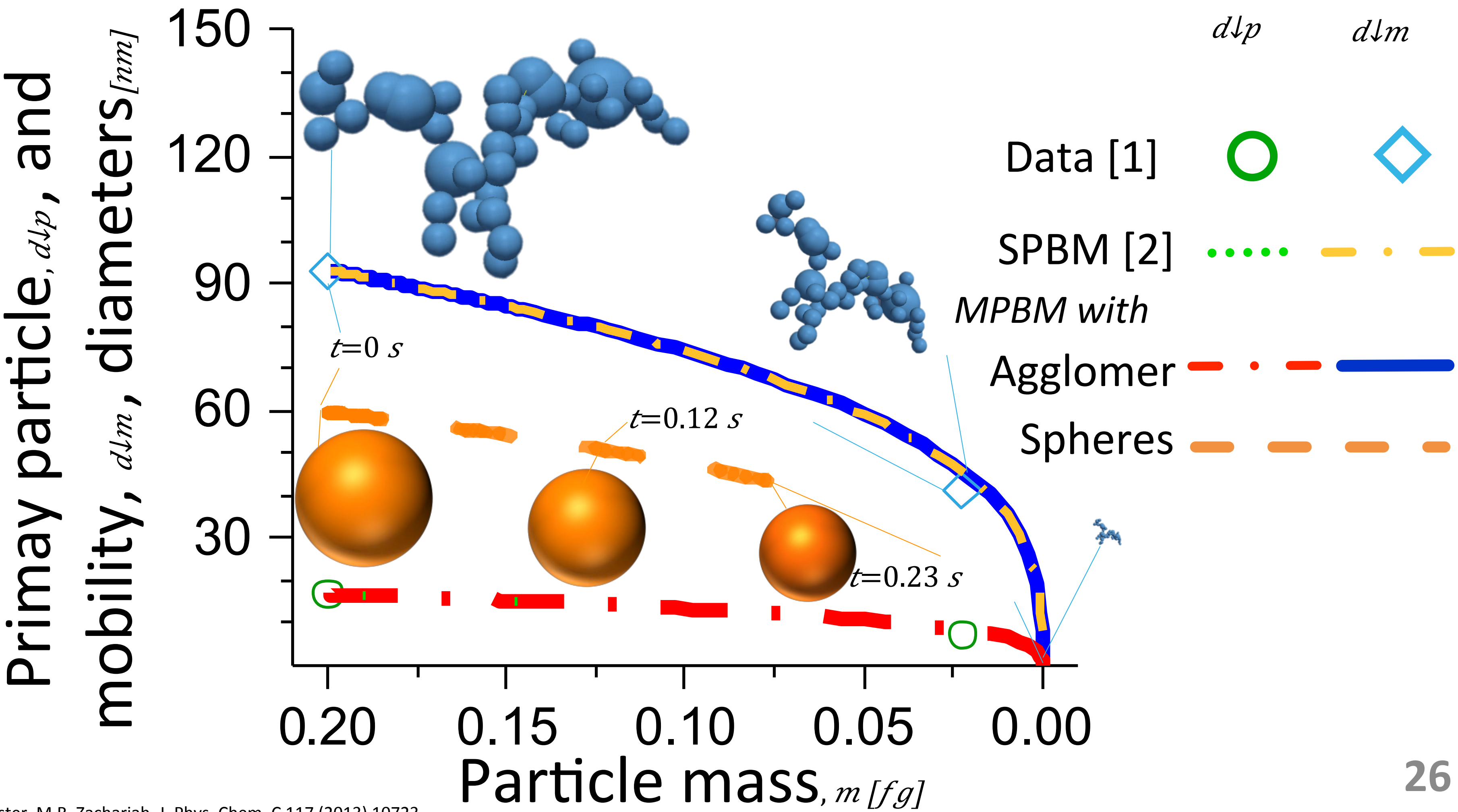
Agglomerate Surface Oxidation



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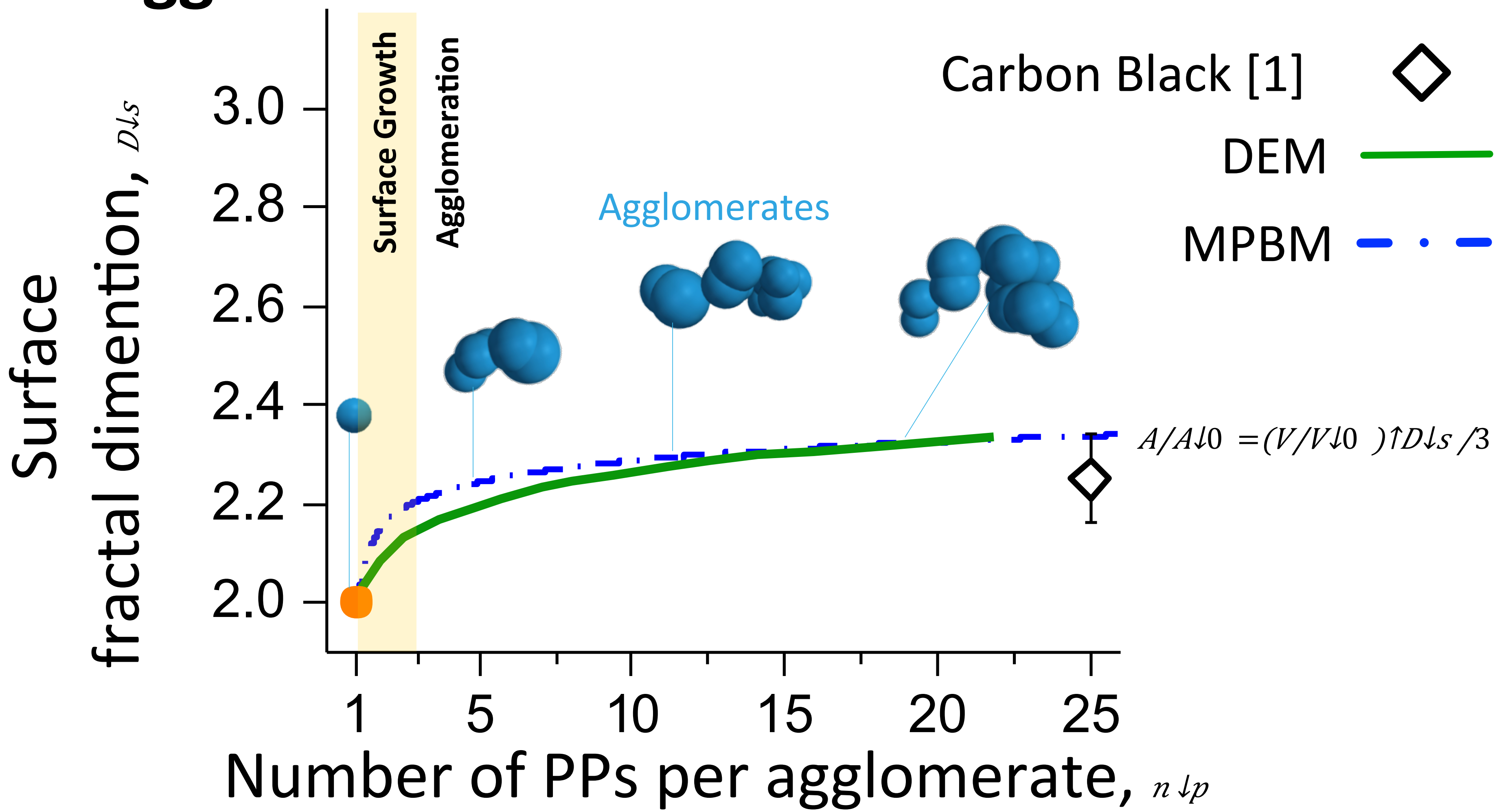
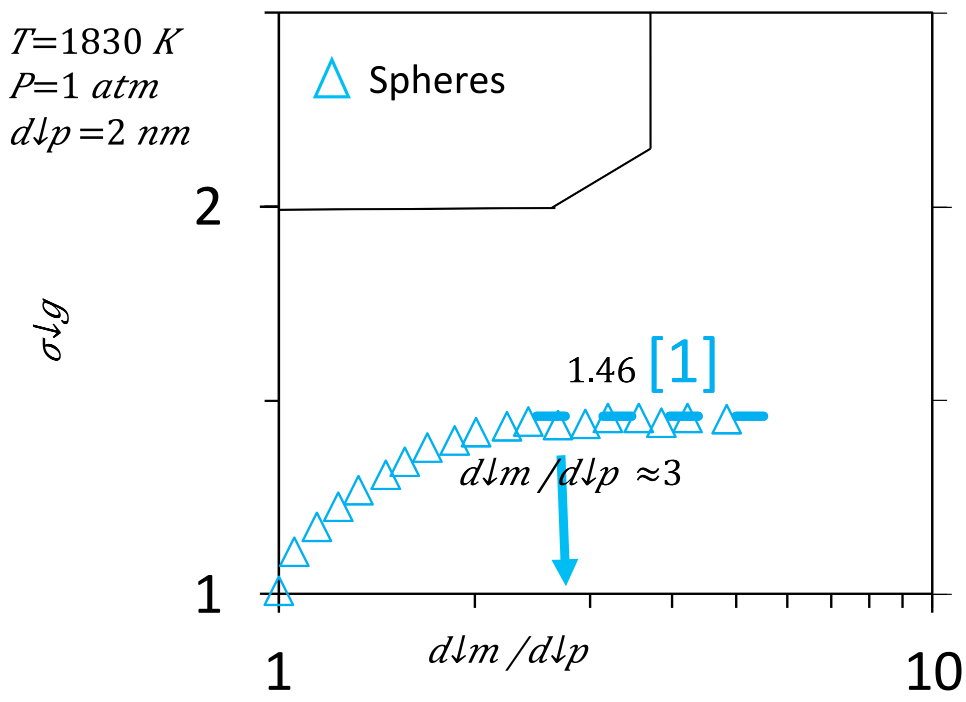
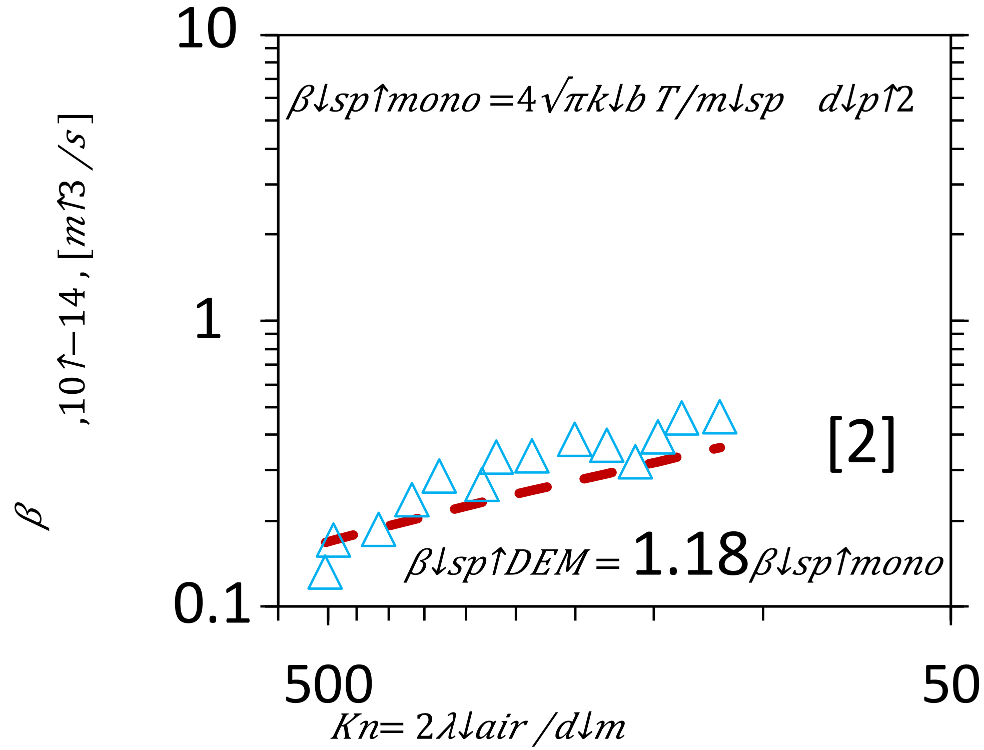
Agglomerate Surface Fractal Dimention



[1] D. Avnir, D. Farin, P. Pfeifer, Nature 308 (1984) 261.

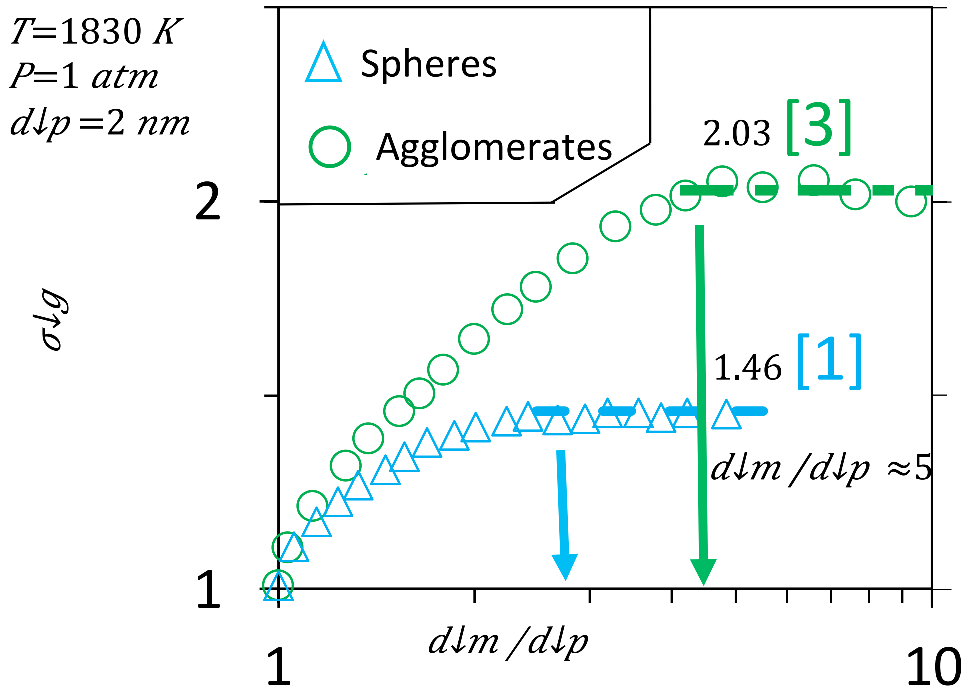
Self Preserving Size Distribution

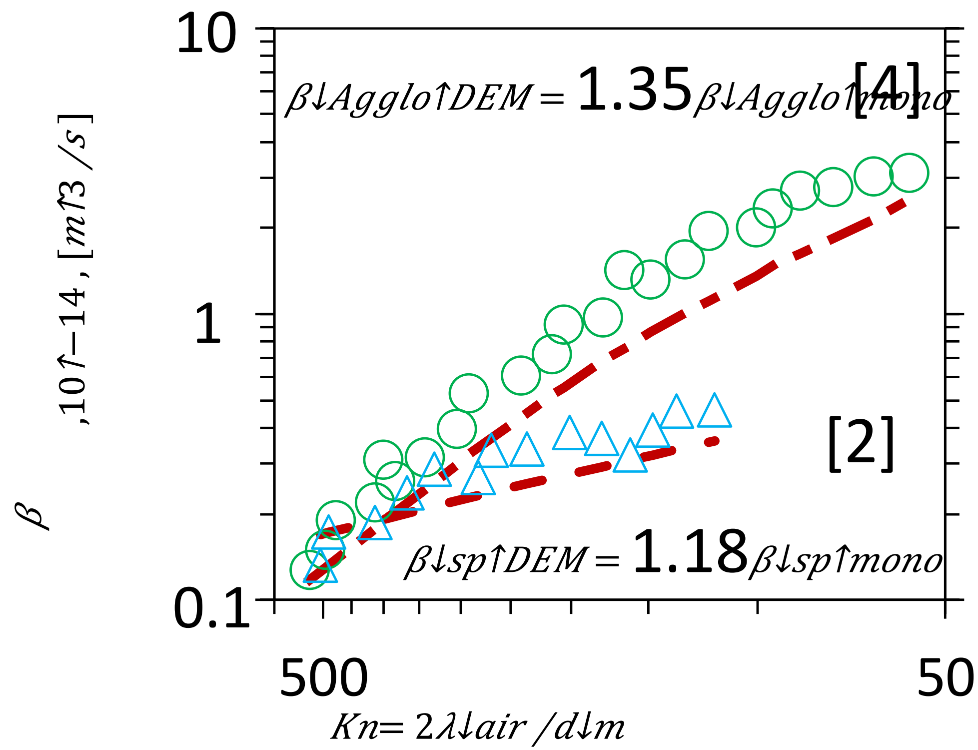




[1] Landgrebe, J.D. and Pratsinis, S.E., 139, (1990) *Journal of Colloid and Interface Science*, 63-86.
[2] Buesser B, Heine MC, Pratsinis SE.40, (2009) *J Aerosol Sci.*, (40), 89

Self Preserving Size Distribution





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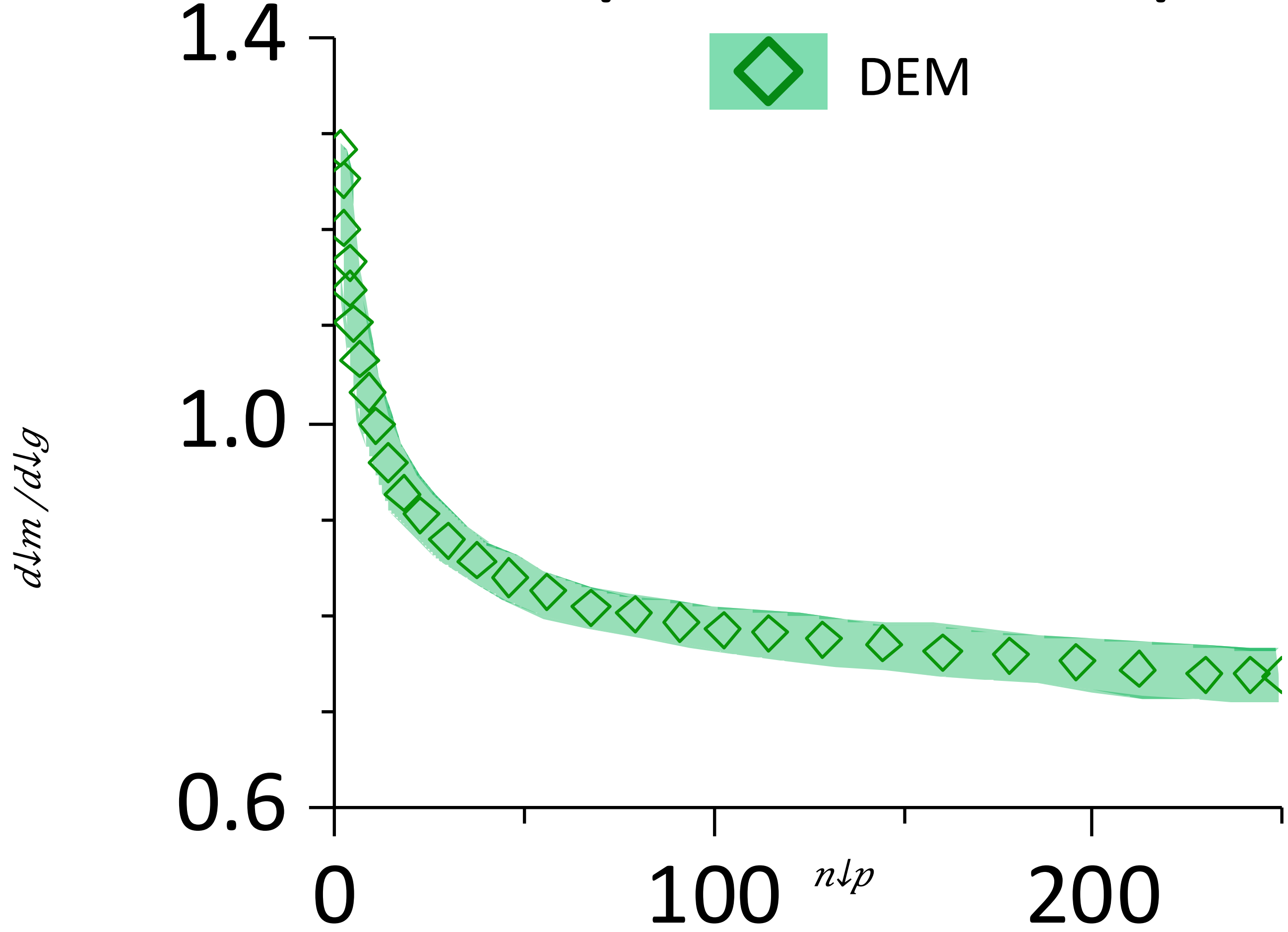
[3] Goudeli, E., Eggersdorfer, M.L. and Pratsinis, S.E., 31, (2015). *Langmuir*, 1320-1327.

[4] Goudeli, E., Eggersdorfer, M.L. and Pratsinis, S.E., 32, (2016). *Langmuir*, 9276-9285.

Power laws for particle morphology



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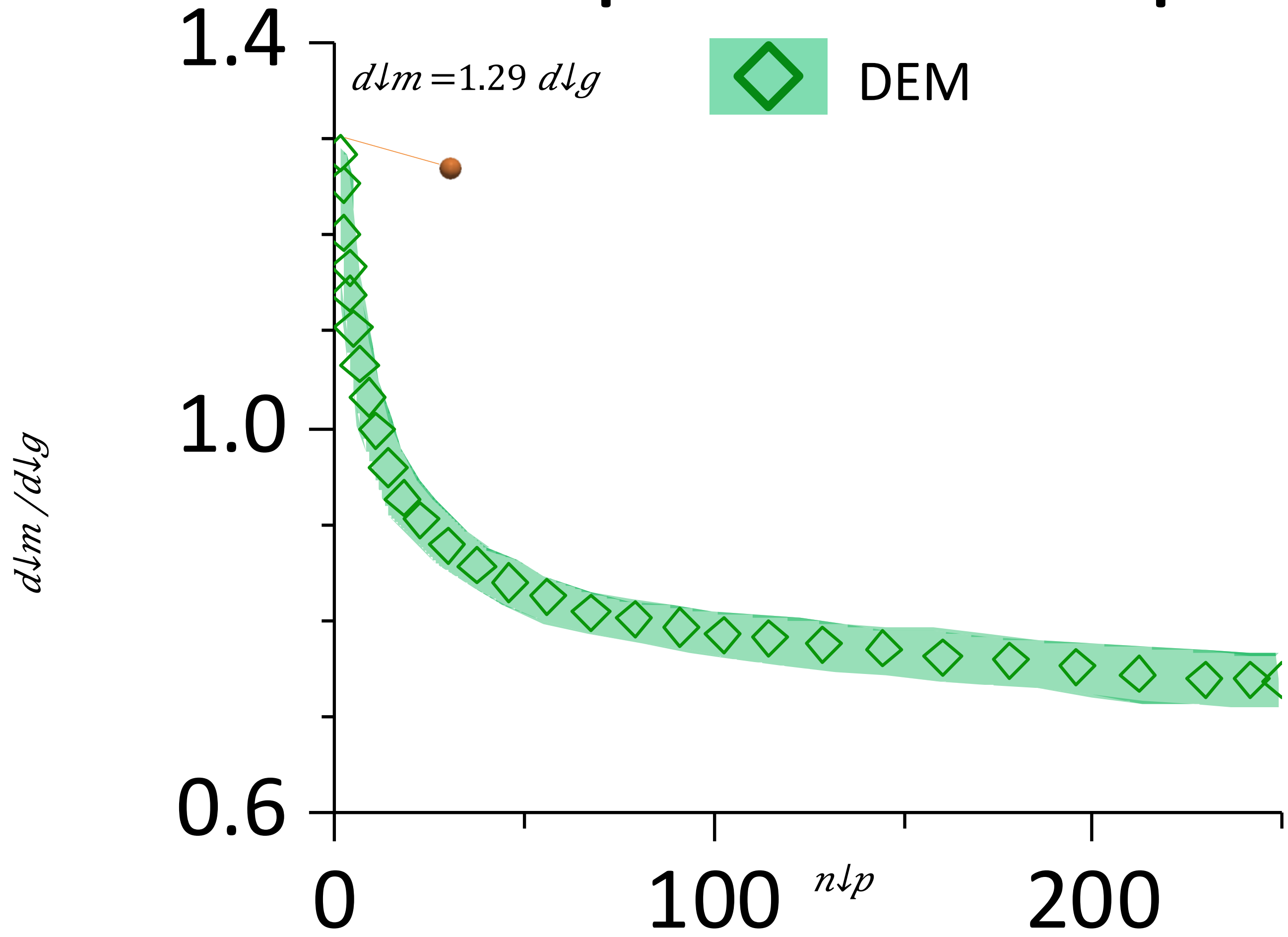
Power laws for particle morphology



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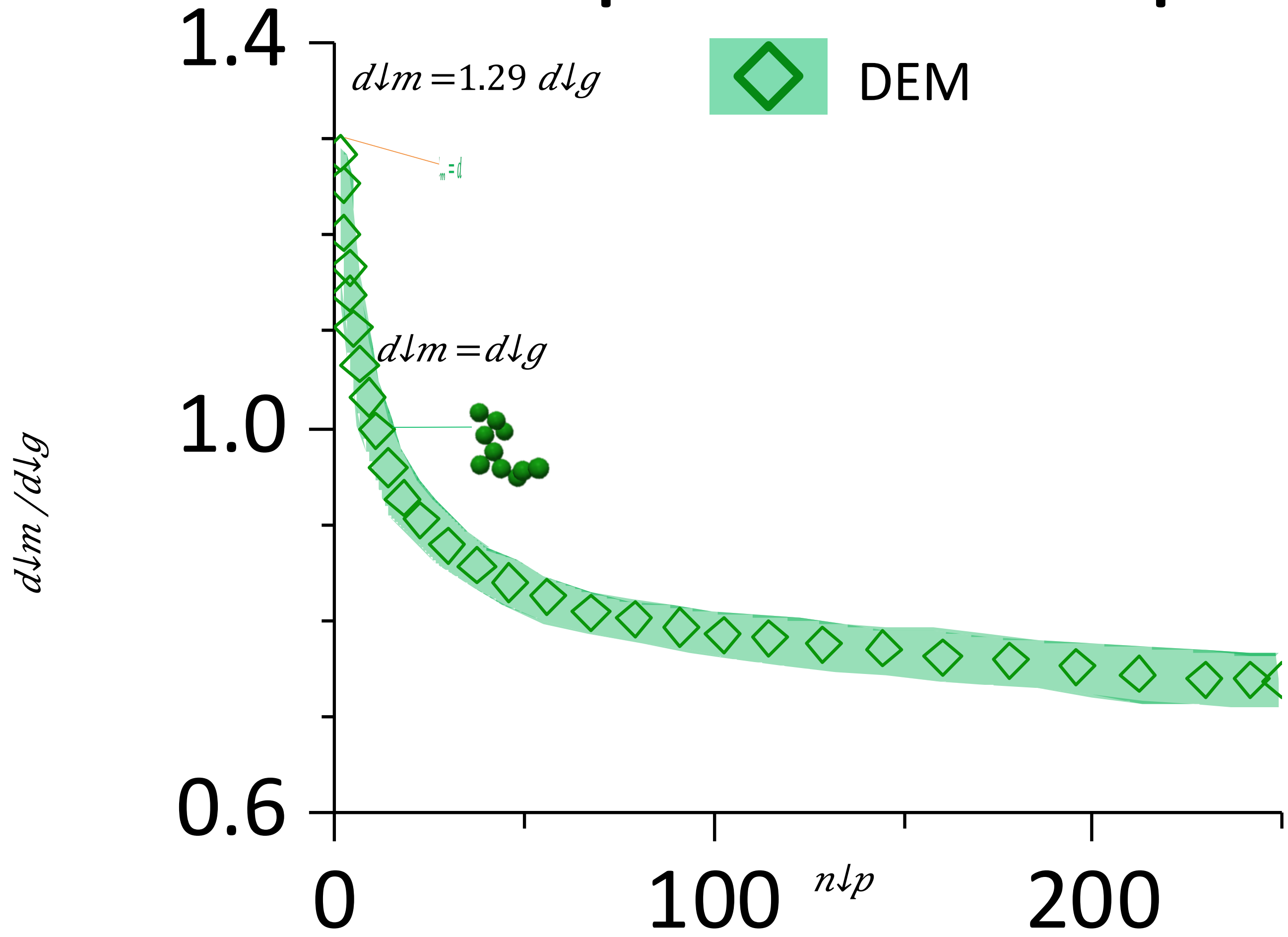
[2] Wang, G. and C. Sorensen, 1999. Physical Review E, **60**. 3036.

Power laws for particle morphology



[1] Kelesidis, G.A., Goudeli, E. and Pratsinis, S.E., 2017. *Carbon*, *121*, 527-535.
[2] Wang, G. and C. Sorensen, 1999. Physical Review E, **60**. 3036.

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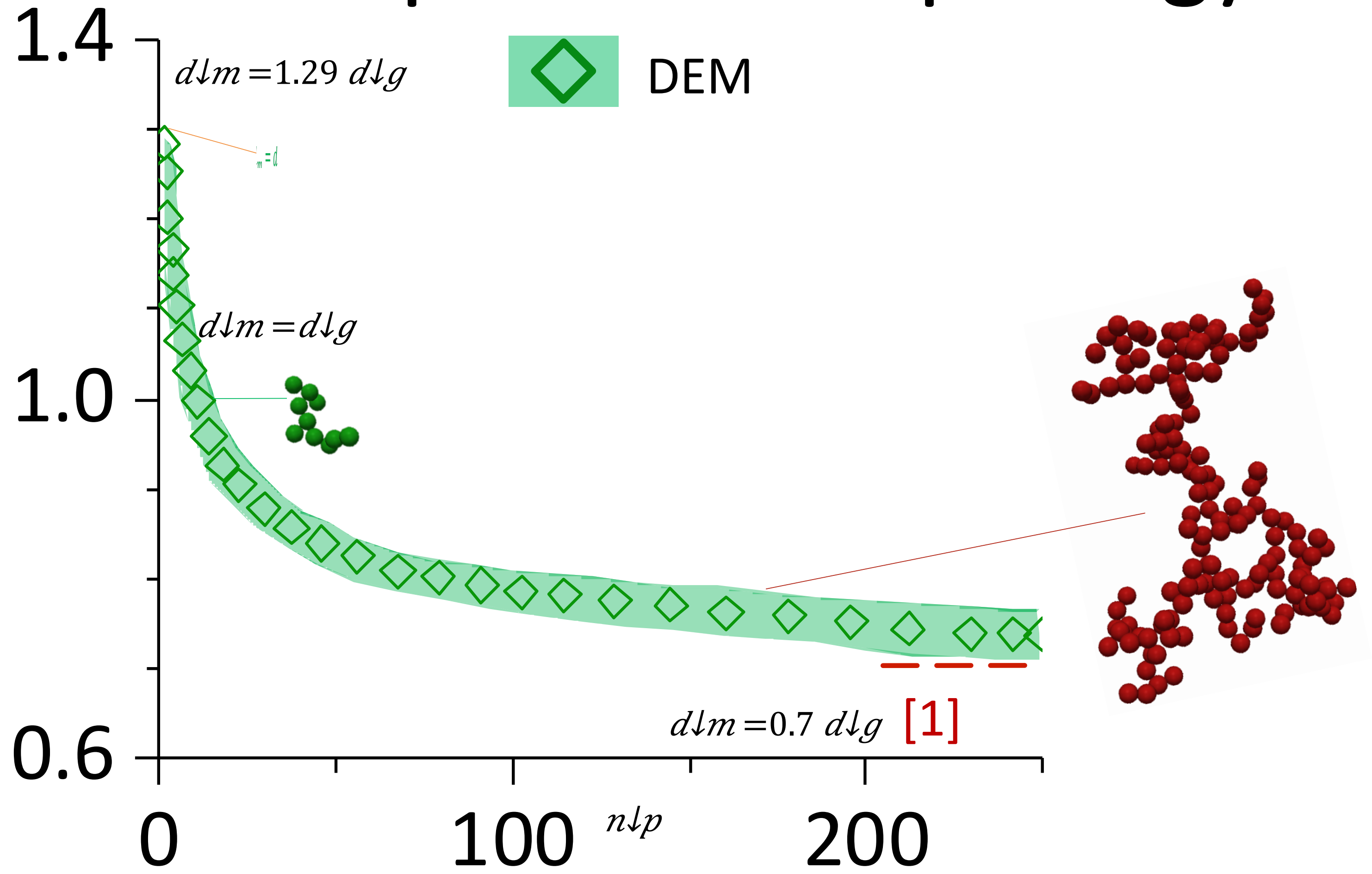

[1] Kelesidis, G.A., Goudeli, E. and Pratsinis, S.E., 2017. *Carbon*, *121*, 527-535.
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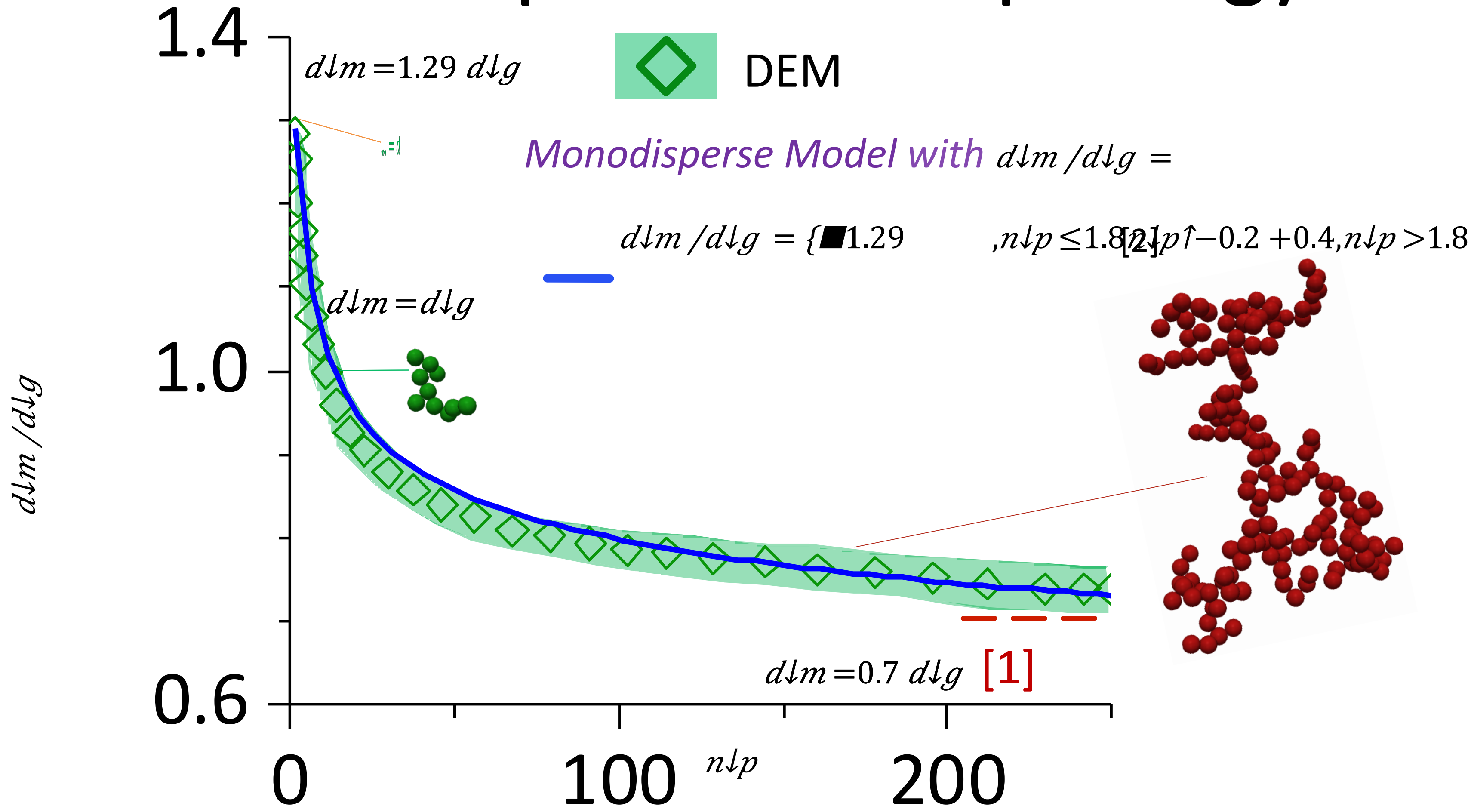

[1] Kelesidis, G.A., Goudeli, E. and Pratsinis, S.E., 2017. *Carbon*, *121*, 527-535.
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