Evolution of soot particle morphology in a diluted laminar co-flow ethylene diffusion flame

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- CARES, Nanyang Technological University

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The Need to Consider Soot

Want to reduce emissions =>

Needs models with predictive capability

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PM & PN Emissions

HISTORY OF EURO EMISSIONS STANDARDS

DIESEL PASSENGER CARS

Introduction dates			Petrol		Diesel		Petrol & Diesel
Euro standard	New approvals	All new registrations	NOx (g/km)	Mass of particles (g/km)	NOx (g/km)	Mass of particles (g/km	Number of ultra-fine particles per km
Euro 1	1 July 1992	31 December 1992	0.97 [1]	-	0.97 [1]	0.14	-
Euro 2	1 January 1996	1 January 1997	0.5 [1]	-	0.9 [1]	0.1	-
Euro 3	1 January 2000	1 January 2001	0.15	-	0.5	0.05	-
Euro 4	1 January 2005	1 January 2006	0.08	-	0.25	0.025	-
Euro 5	1 September 2009	1 January 2011	0.06	0.0045 [2]	0.18	0.0045	6×10^{11} [3]
Euro 6	1 September 2014	1 September 2015	0.06	0.0045 [2]	0.08	0.0045	6×10^{11} [4] [5]

(1) Expressed as HC+NOx.
(2) Applicable to direct injection petrol engines.
(3) Applicable to diesel engines only.
(4) Limit of 6×10^{12} in the case of direct injection petrol engines.
(5) Common limit of 6×10^{11} for direct injection petrol engines and diesel engines from September 2017/September 2018.

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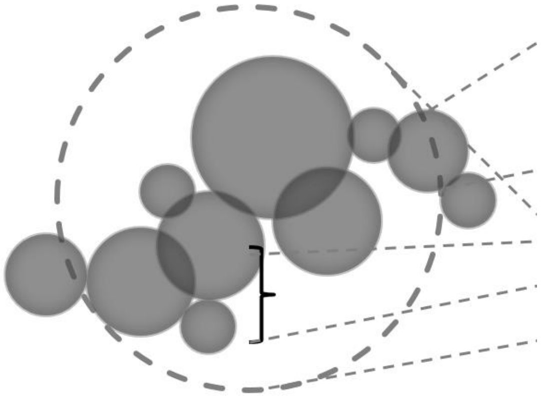
Particle Size Distributions



- Aggregate Size Distributions (ASD)
- Primary Particle Size Distributions (PPSD)
- PPSD affects ASD[1,2]
- Literature models not adequate[2]
- Cambridge model can describe ASD and PPSD

- Initial experimental results and model performance assessment
  - Experiments = Cambridge CARES
  - Modeling = CoFlame (UofT,Ryerson,UBC,NRC), DPM (Cambridge)

[1]Heine et al, Aerosol Science, 2007
[2]Menz & Kraft, Aerosol Sci. & Tech., 2013

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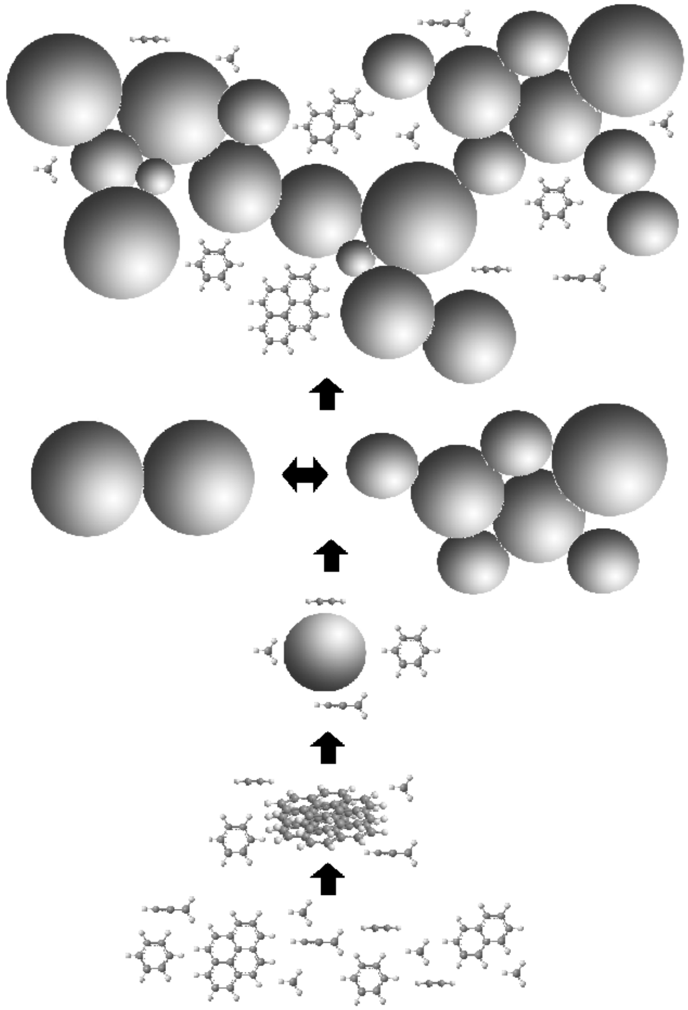
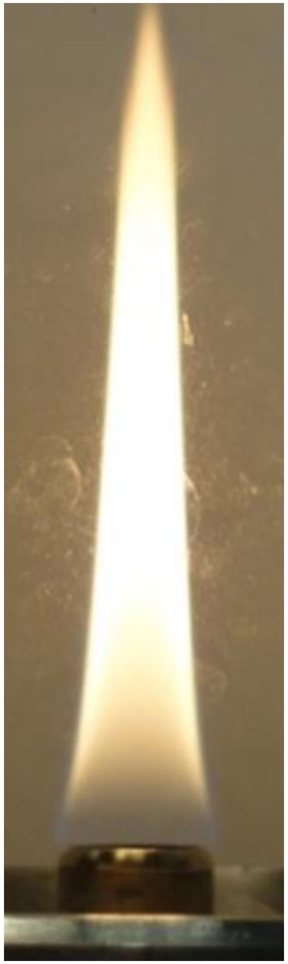
Soot Formation in Flames





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Experimental Set-up

- CARES
- Yale burner
- Co-flow laminar diffusion flame
- Nitrogen diluted (40%) ethylene (60%) – air flame
- TEM Grid sampling (along centerline)

- Goal is full characterization

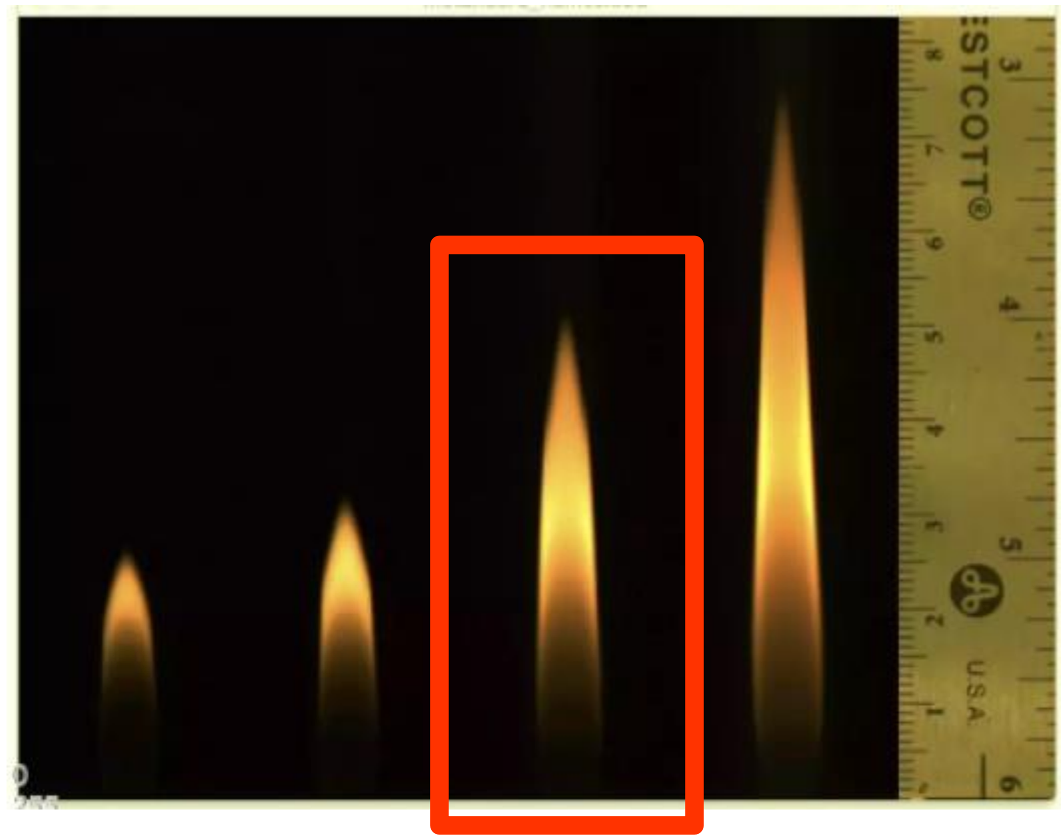

Image taken from http://guilford.eng.yale.edu/yalecoflowflames/sooting.html

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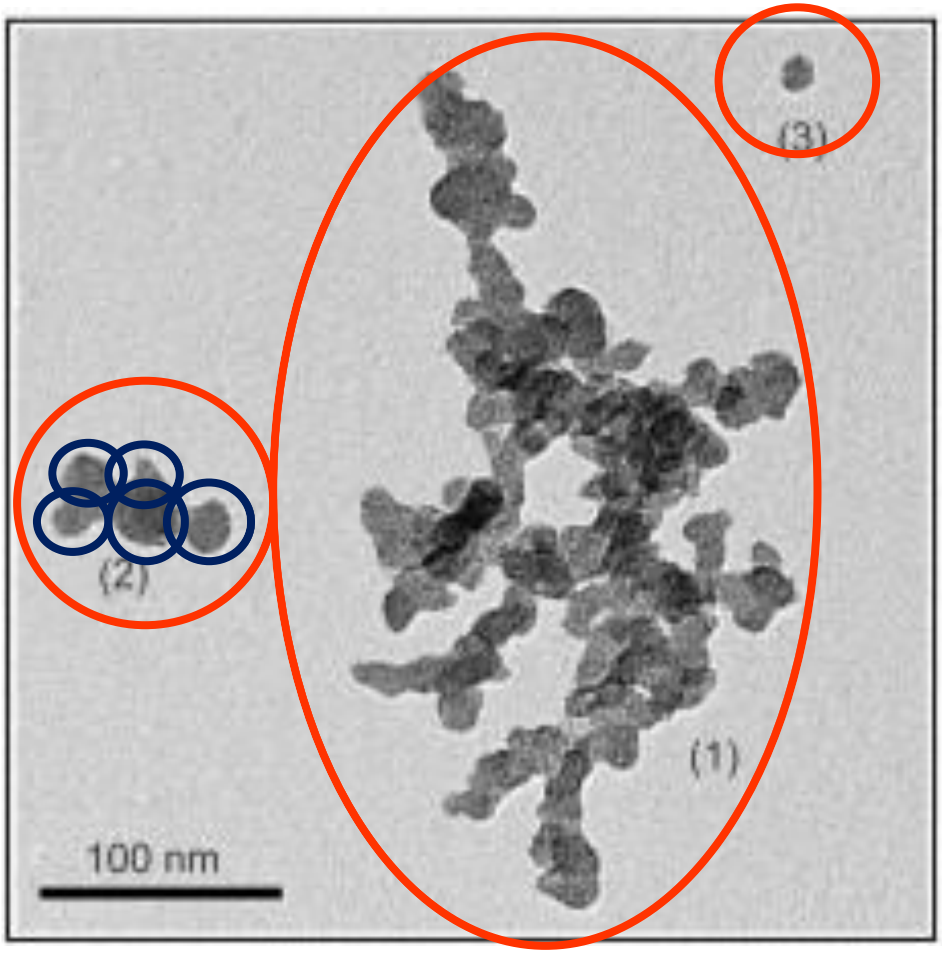
Image Post-Processing



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Simulation Methodology

CoFlame Code → Gas-phase profile → Detailed particle model

- CoFlame Code with DLR mechanism (A5)
- Post-processing gas-phase profile
- Detailed particle model solved by Monte Carlo algorithms

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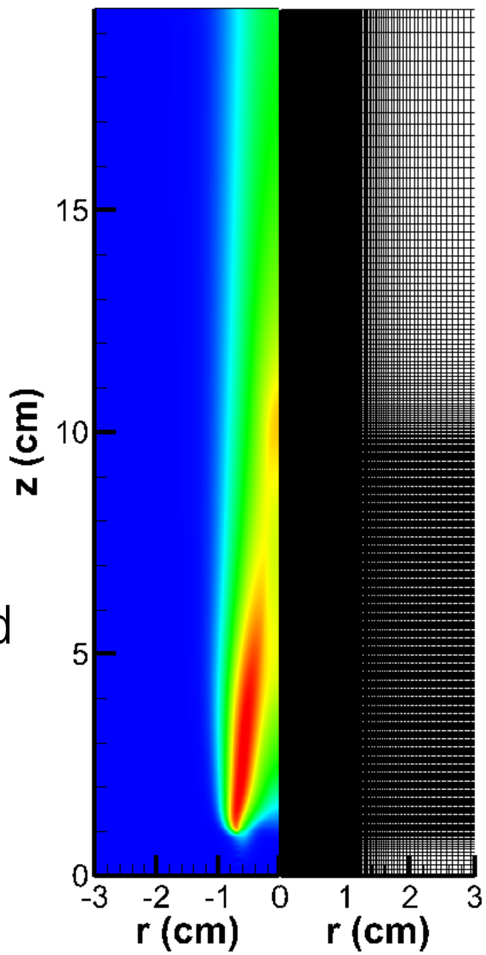
Parallel CoFlame Code

- 2D CFD code for steady coflow diffusion flames
- DOM radiation
- Strip-domain parallelization
- Conjugate heat transfer
- Fully coupled particle model solved via sectional method

    N. Eaves et. al., CoFlame: A refined and validated numerical algorithm for modeling sooting laminar coflow diffusion flames, Computer Physics Communications, 207:464-477, 2016

    http://combustion.mie.utoronto.ca - > software



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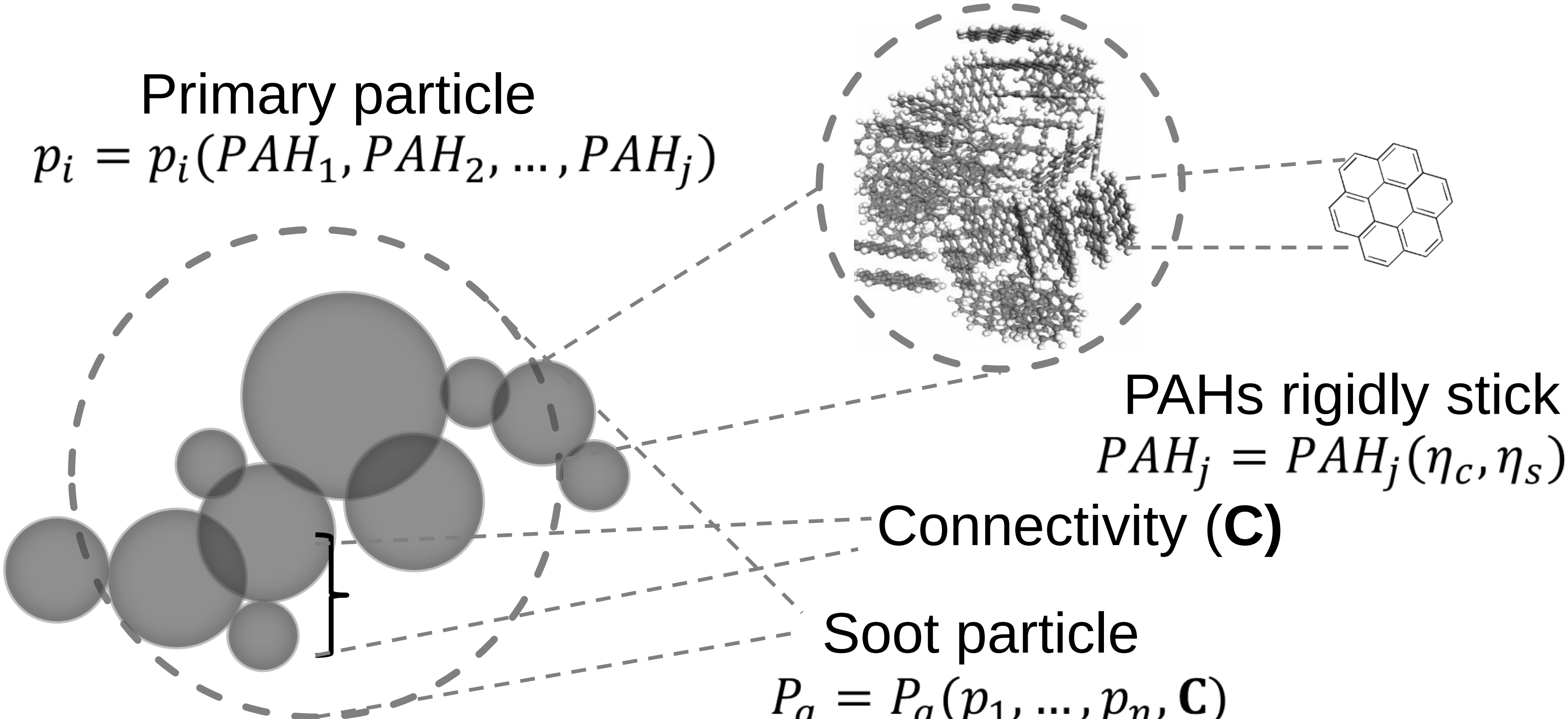
Particle Representation



Raj A. et al, Combust. Flame, 156, 896-913, 2009
Raj A. et al, Combust. Flame, 157, 523-534, 2010
Lavvas P. et al, The Astrophysical Journal, 80, 1-11, 2011

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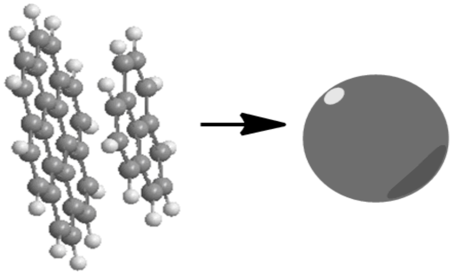
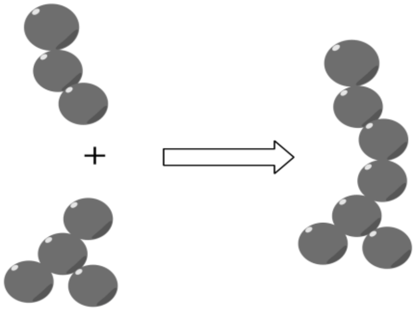
Particle Transformations

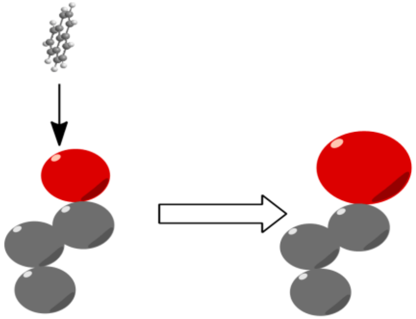
Inception:



Coagulation:



Condensation:



Yapp et al, Comb. Flame, 167, 320-334, 2016
Chen et al, Proc. Comb. Inst., 34, 1827-1835, 2013

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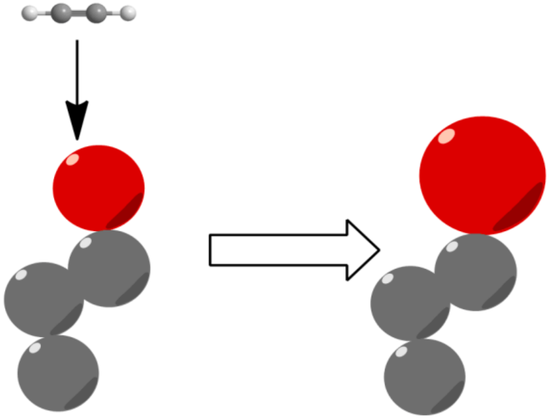
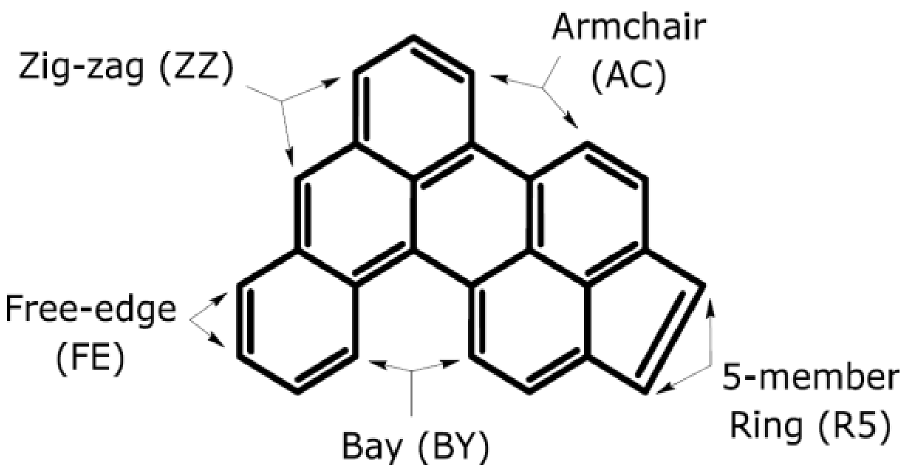
Particle Transformations

Heterogeneous reactions:



- Evolution of PAHs described by 20 jump processes
- Rates are specific to each site type
- Applies to PAHs in both the gas and particle phase (Growth factor)



Raj A. et al, Carbon, 48, 319-332, 2010

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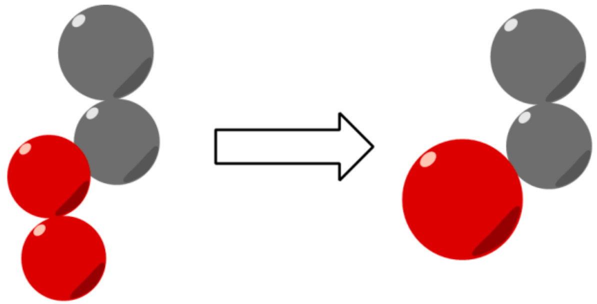
Particle Transformations

Particle rounding:



Two mechanisms for particle rounding:

- Mass addition: condensation and heterogeneous reactions
- Sintering: Rearrangement of molecules in adjacent primary particles.

Yapp et al, Comb. Flame, 167, 320-334, 2016
Chen et al, Proc. Comb. Inst., 34, 1827-1835, 2013

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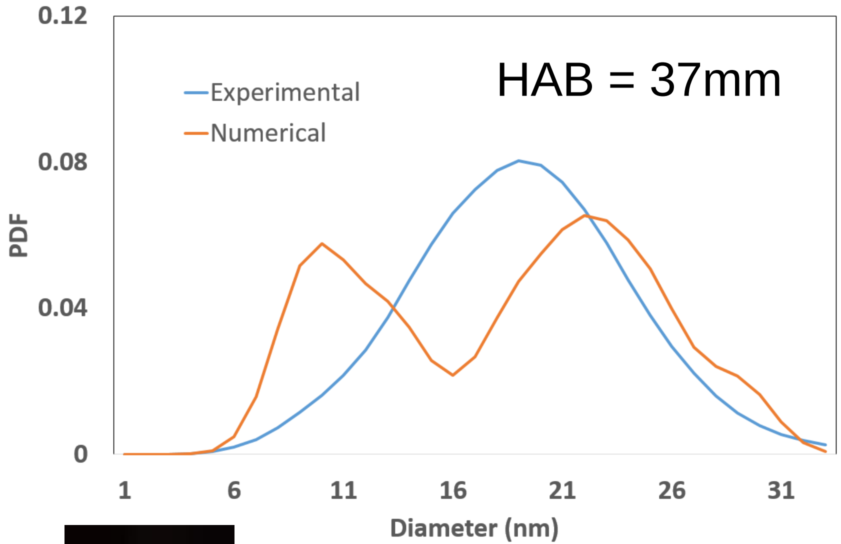
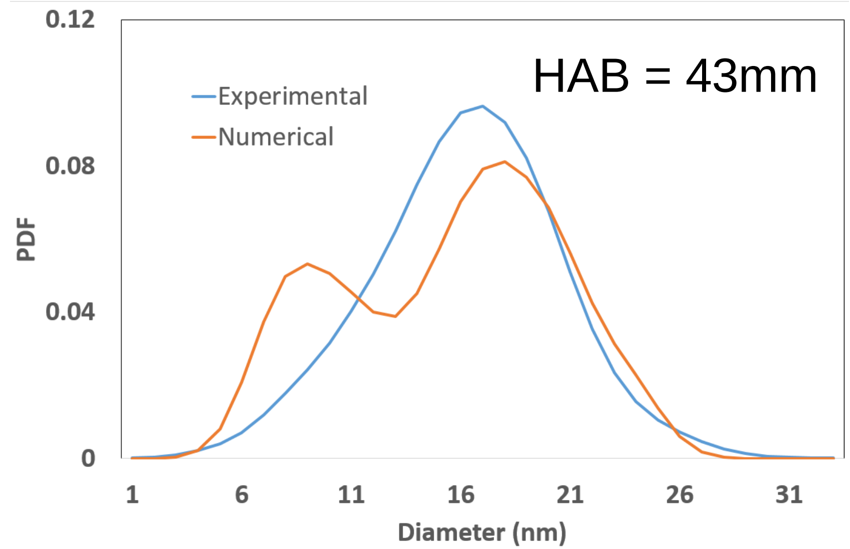
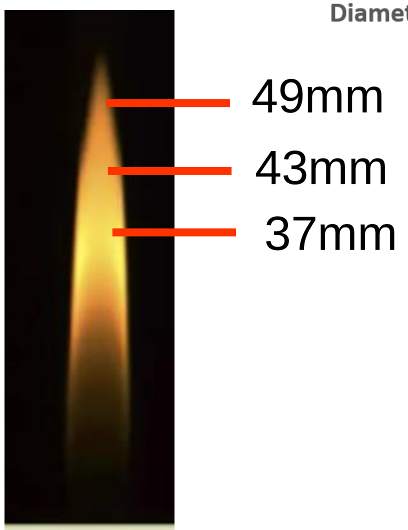
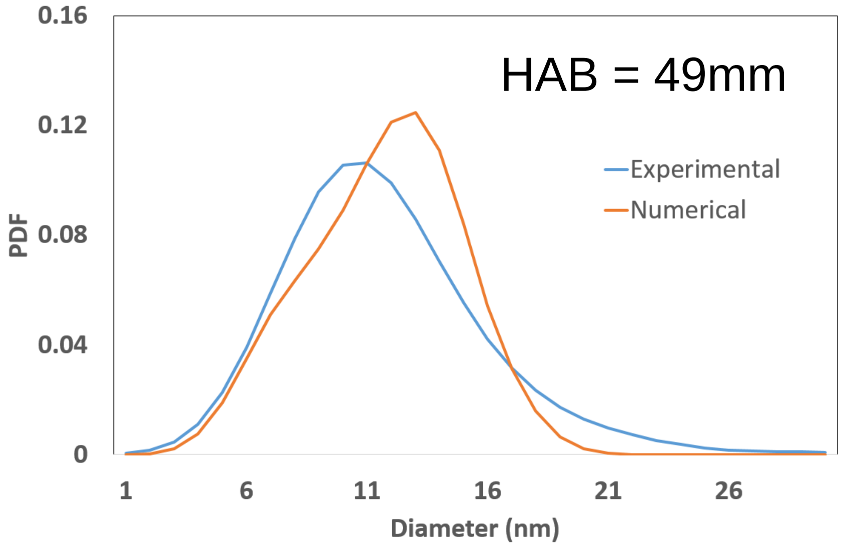
Results: PPSDs









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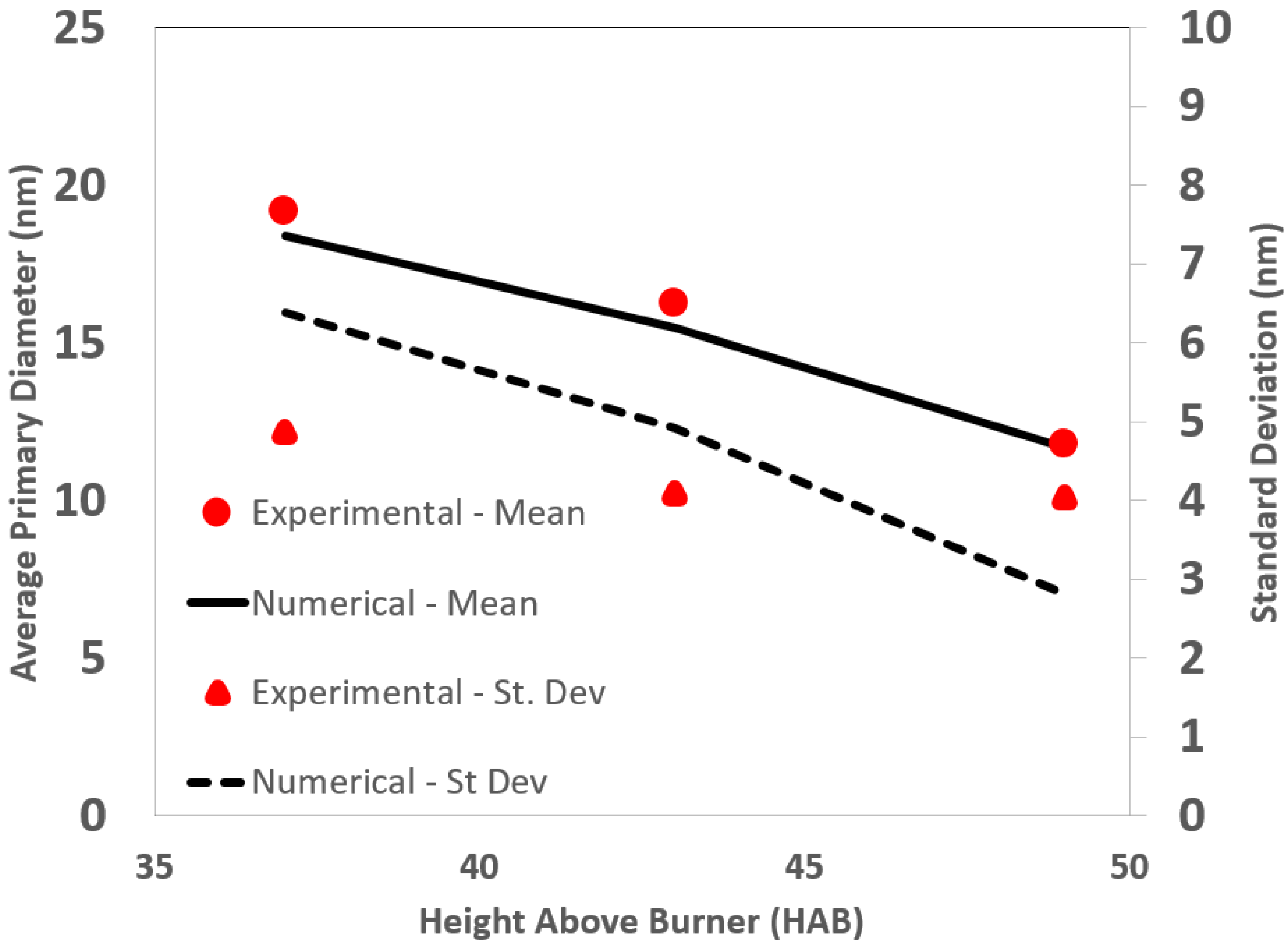
Results: PPSD Trend



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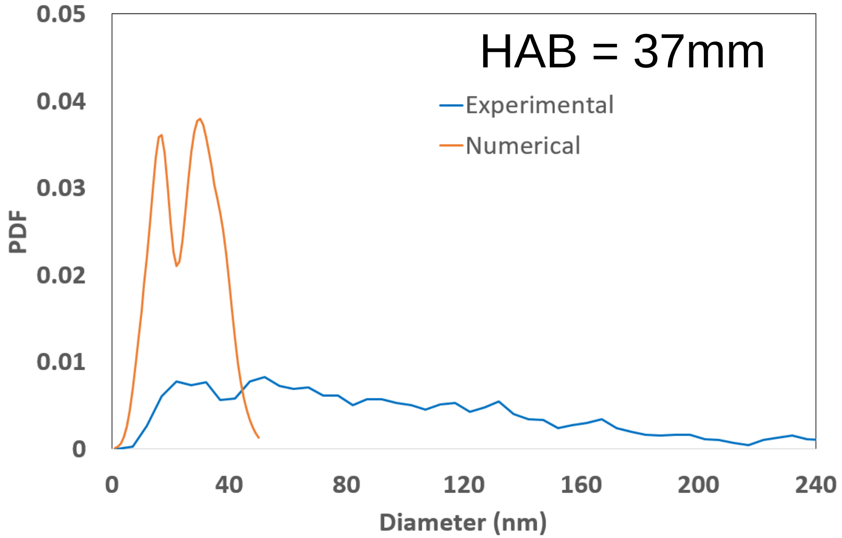
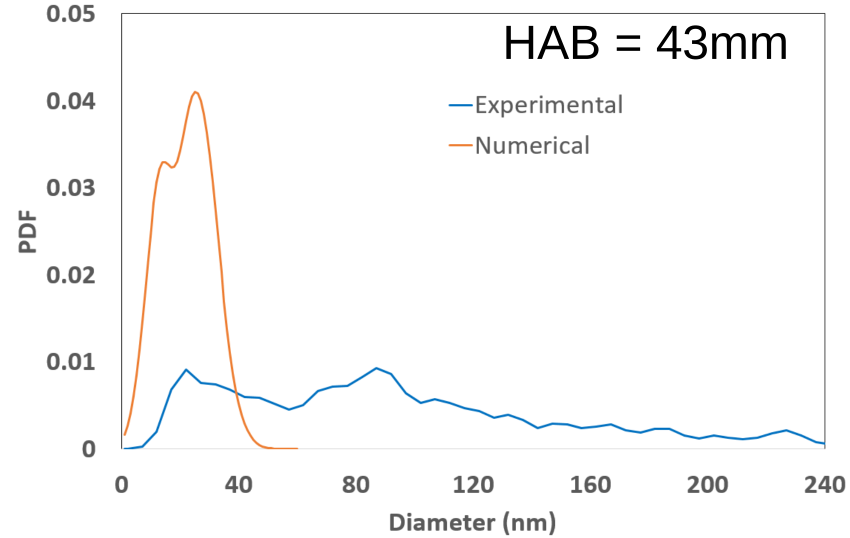
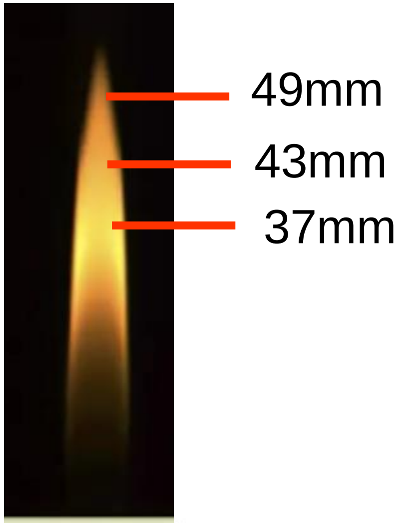
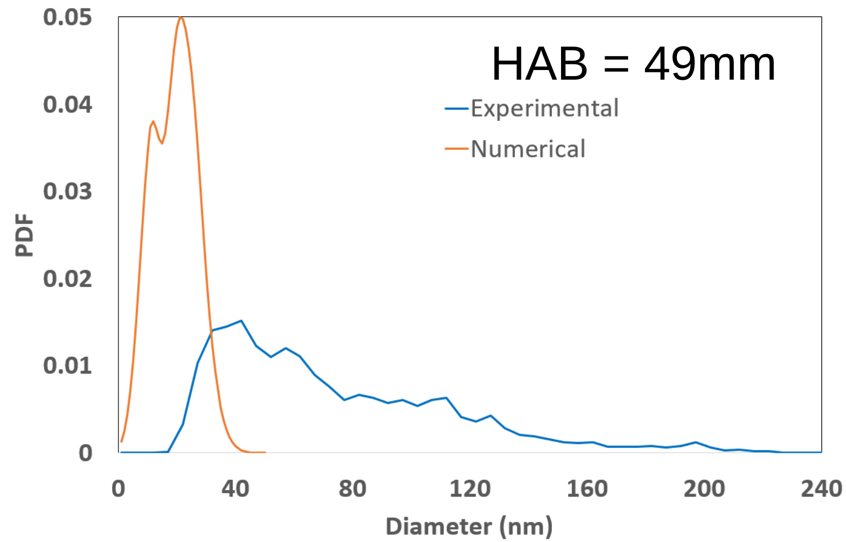
Results: ASDs









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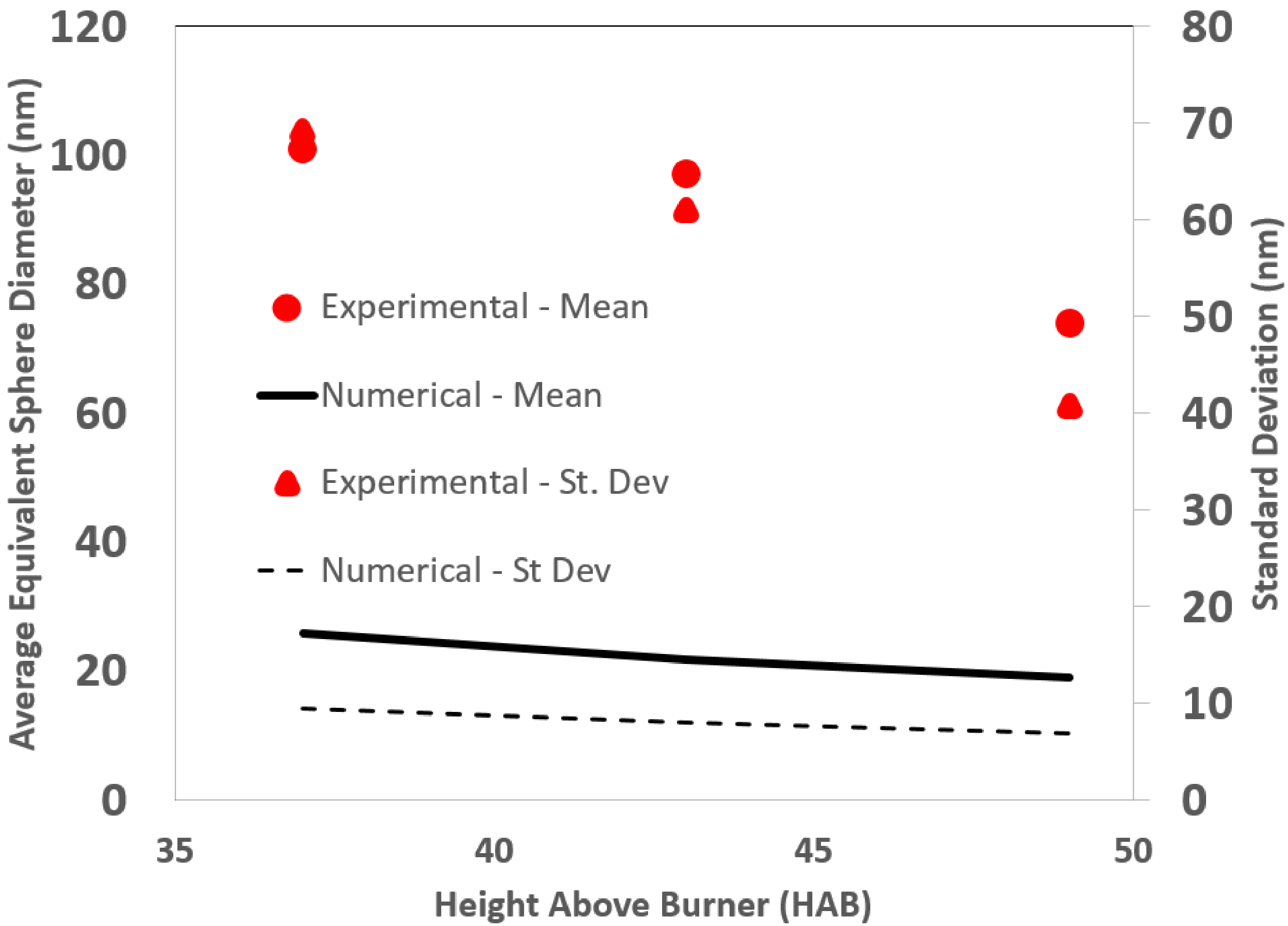
Results: ASD Trend



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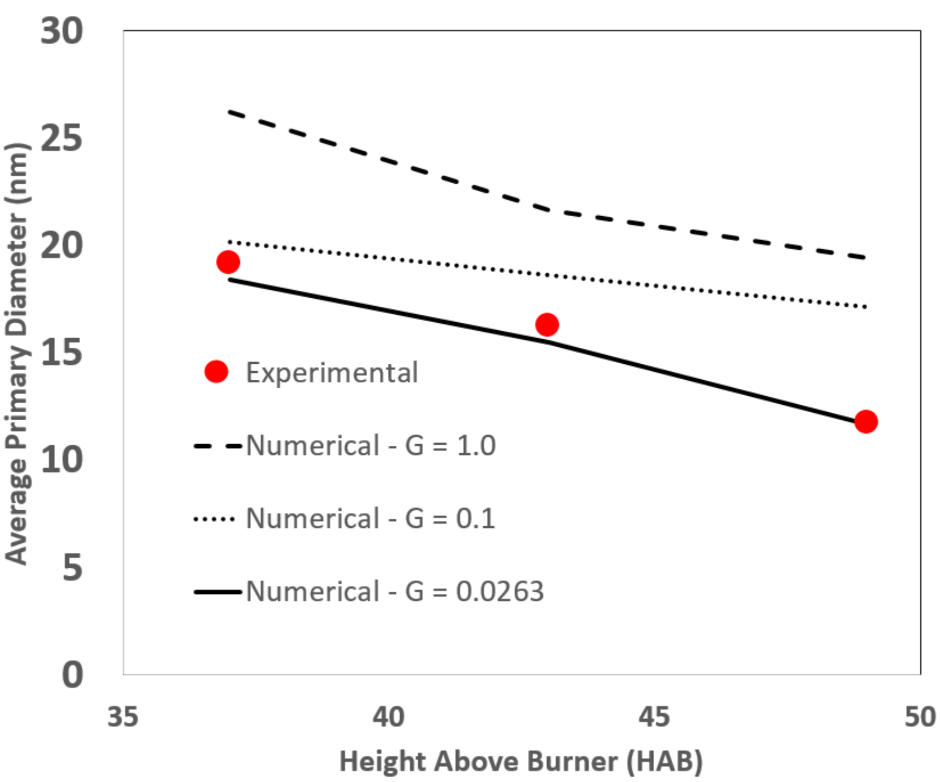
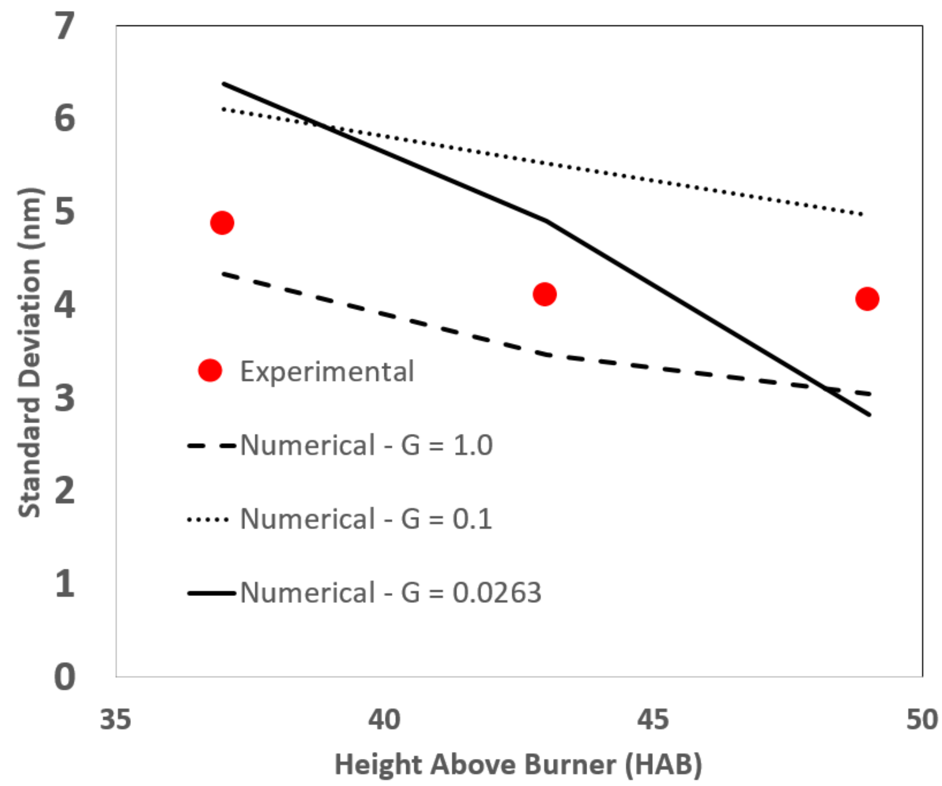
Results: PPSD Growth Factor





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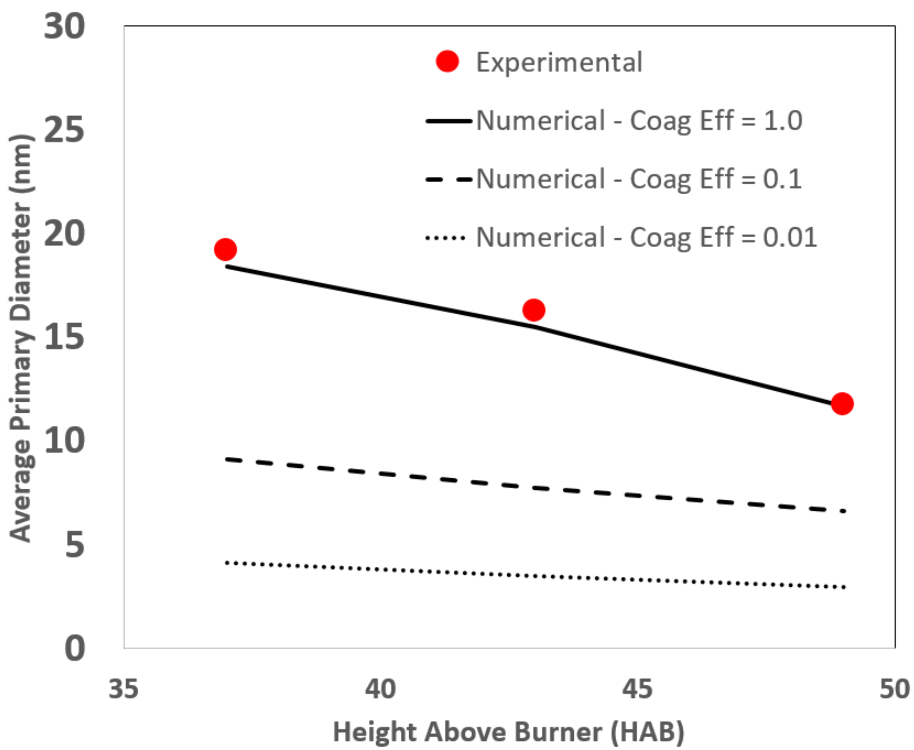
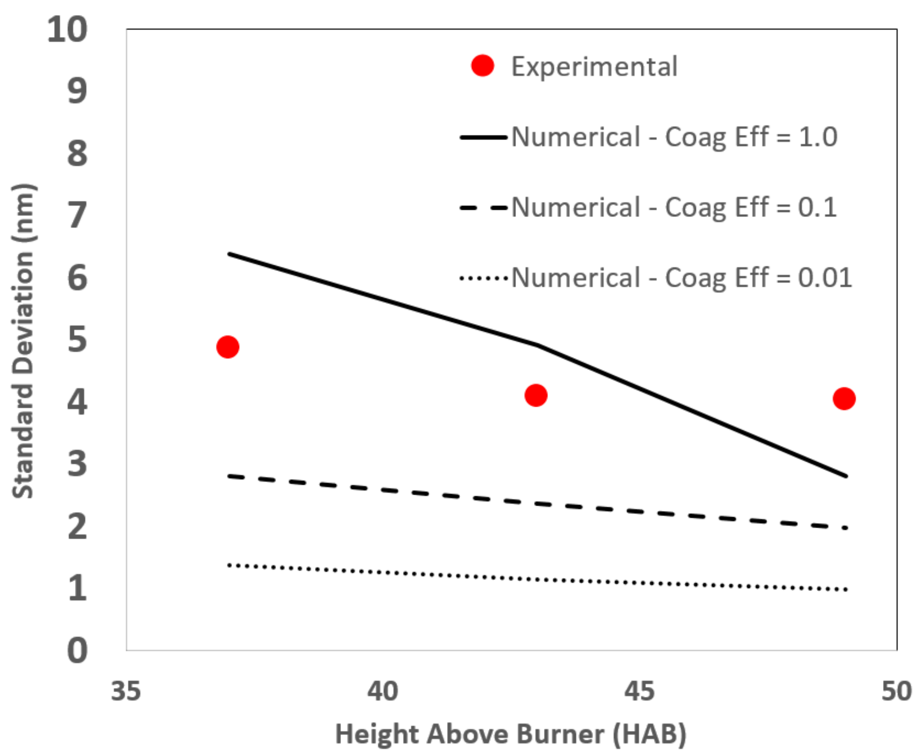
Results: PPSD Coagulation Eff.





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Conclusions

- Experimental and numerical results for PPSD and APSD
  - First in literature for PPSD
- Average size/dispersion reduce with HAB
  - Qualitative agreement
  - Aggregate size/dispersion under-predicted
- Additional 2D measurements
- Complete sensitivity analysis
- Improvement of model performance

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CAMBRIDGE CARES

CAM.CREATE C4T Cambridge Centre for Carbon Reduction in Chemical Technology

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HORIZON 2020

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