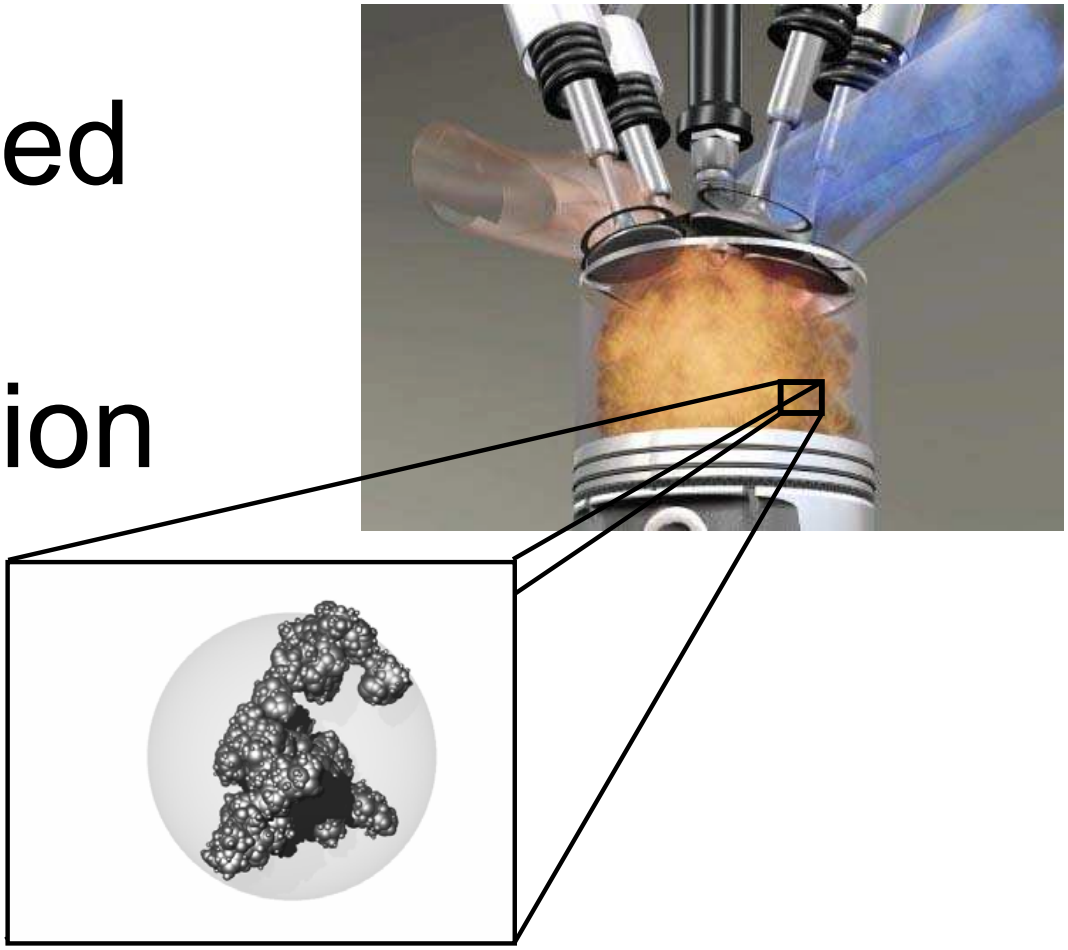
Towards a detailed soot model for internal combustion engines



S. Mosbach, M. S. Celnik, M. Kraft,

H. R. Zhang, S. Kubo, K.-O. Kim

16 May 2008

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Engine model: SRM

Stochastic Reactor Model (SRM)

$$\frac{\partial}{\partial t}\mathcal{F}(\psi;t) = \underbrace{-\sum_{j=1}^{S+1}\frac{\partial}{\partial \psi_j}\left[G_j(\psi)\mathcal{F}(\psi;t)\right]}_{\text{chemical reactions, volume change}} + \underbrace{\sum_{j=1}^{S+1}\frac{\partial}{\partial \psi_j}\left[\frac{C_\phi}{2\tau}(\psi_j - \langle\psi_j\rangle)\mathcal{F}(\psi;t)\right]}_{\text{IEM mixing}} -$$

$$\underbrace{-\frac{\dot{V}}{V}\mathcal{F}(\psi;t)}_{\text{piston movement}} \underbrace{-\frac{1}{h}\left[U(\psi_{S+1}+h)\mathcal{F}(\psi_1,\ldots,\psi_S,\psi_{S+1}+h;t) - U(\psi_{S+1})\mathcal{F}(\psi;t)\right]}_{\text{heat transfer}}$$

- Detailed chemical kinetics → Chemical mechanism: PRF + small aromatics (extended by H. R. Zhang) 208 species, 1002 reactions
- Turbulent mixing
- Convective heat transfer
- Computationally cheap (1-2 CPU-hrs/cycle)

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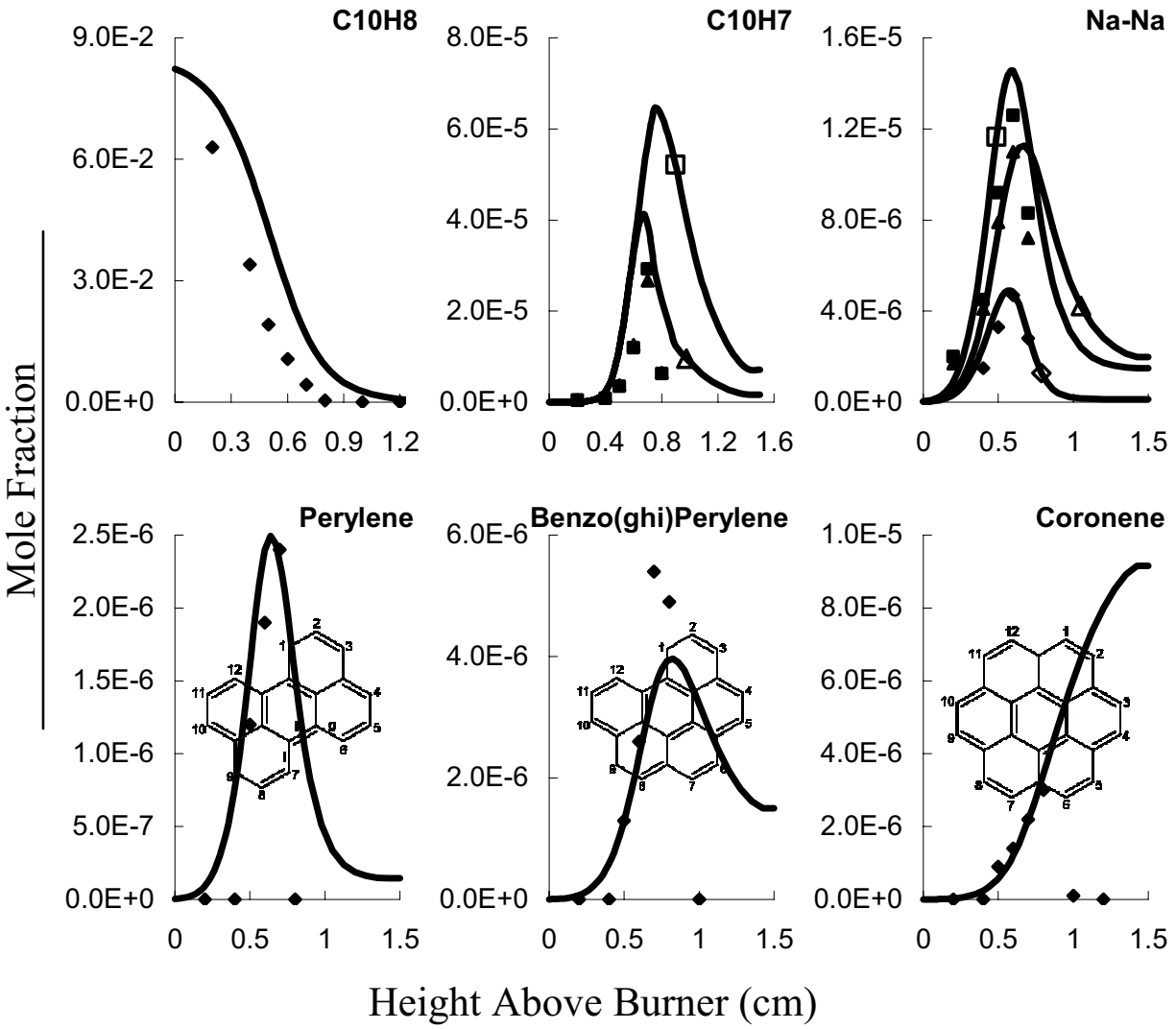
PAHs in gas-phase chemistry

- Hongzhi R. Zhang
- Before: PRF+NOx, 157 species
- After: PRF+NOx+ variety of PAHs and highly unsaturated HCs, 208 species
- Validation against fuel-rich flame experiments



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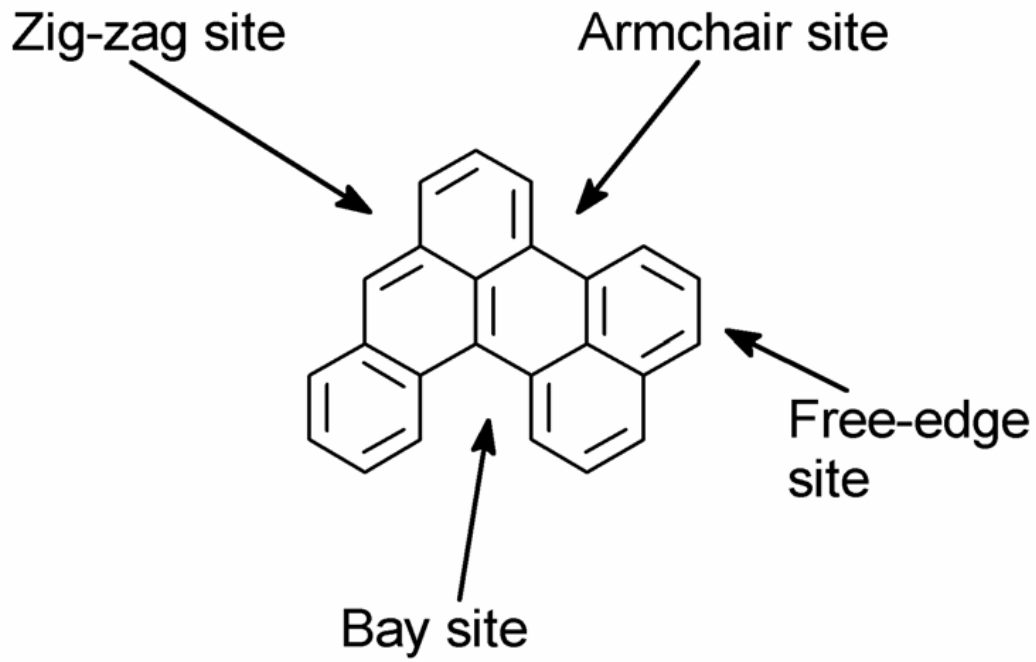
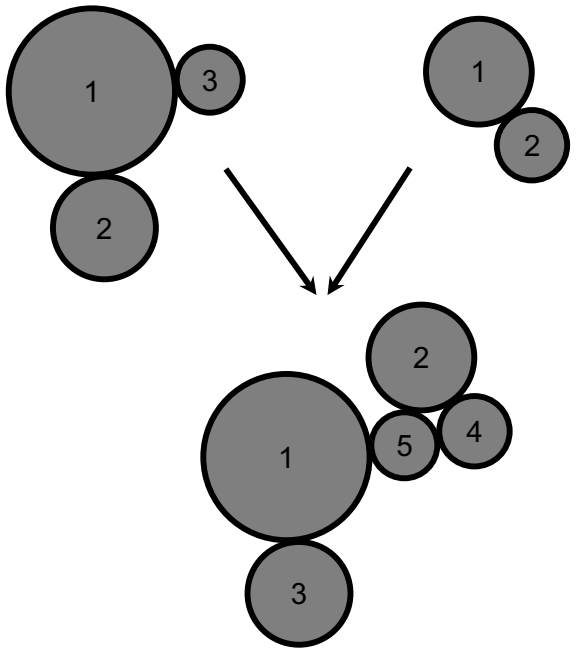
Soot model: site-counting

Describe soot particles by $9+N$ dimensional state space (ARS-SC-PP model):

$$E = (C,\ H,\ S_a,\ N_{ed},\ N_{zz},\ N_{ac},\ N_{bay},\ N_{R5},\ N_{PAH},\ PP_{(1\text{-}N)})$$

PP = primary particle list





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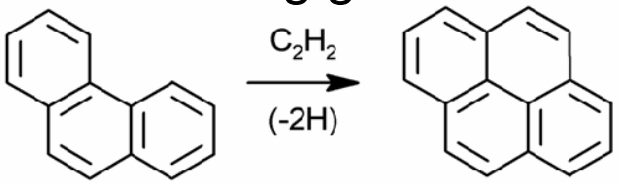
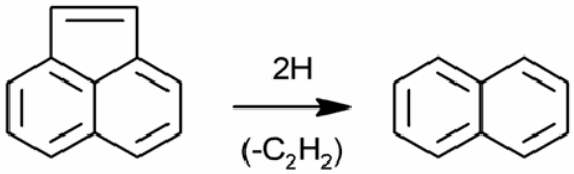
PAH reaction steps

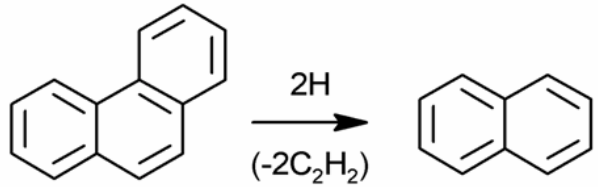
Armchair ring growth



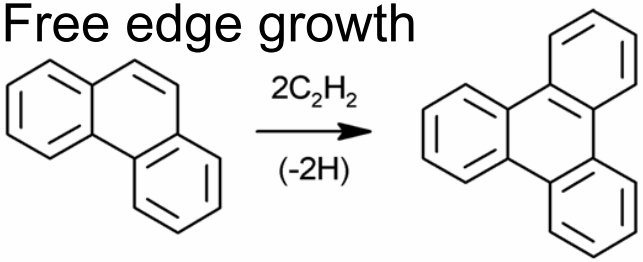
5-member ring desorption



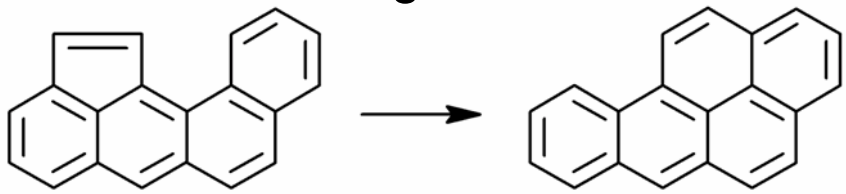
6-member ring desorption



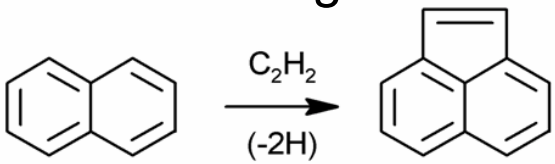
Free edge growth



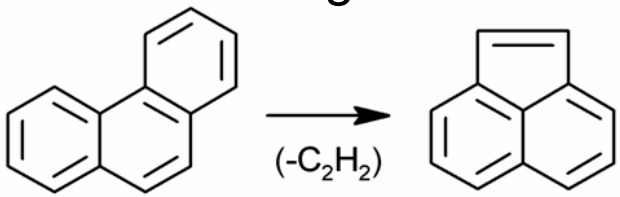
5-member ring conversion at AC



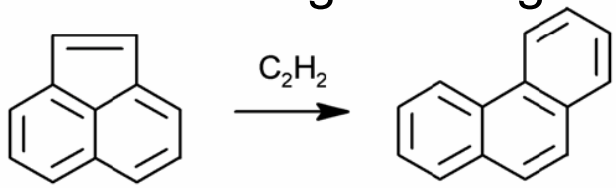
5-member ring addition



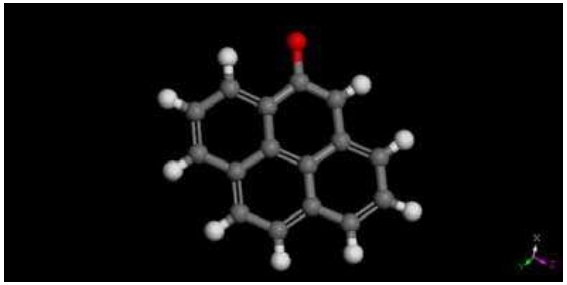
6- to 5-member ring conversion



5-member ring free edge desorption



Oxidation steps:
rates from
quantum chemistry



Frenklach, Schuetz, Ping. *Proc. Combust. Inst.* 30, 2005

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Soot in engines!

- HCCI, n-heptane
- Compression ratio 12
- Equivalence ratio 1.93
- Throttled, 20% EGR

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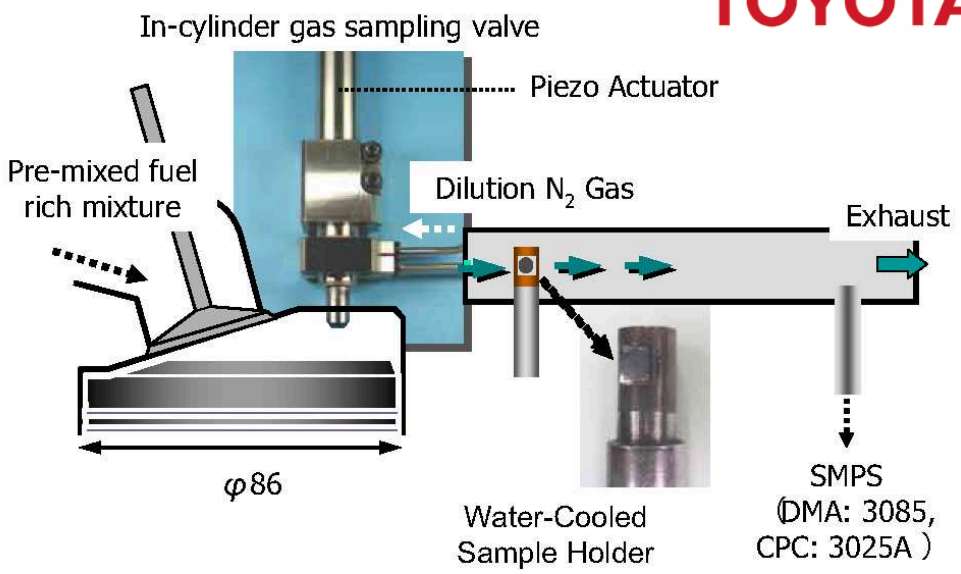

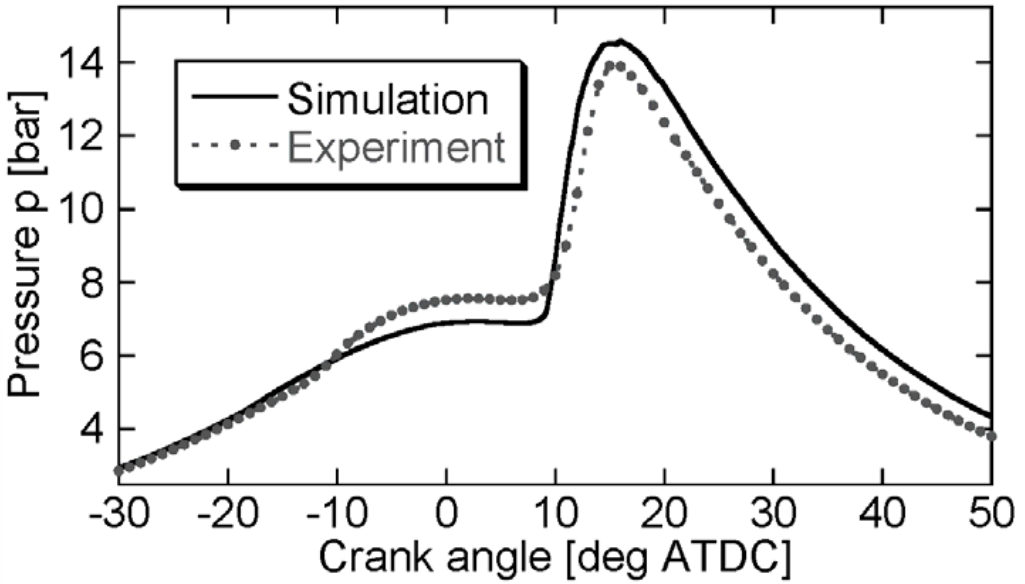

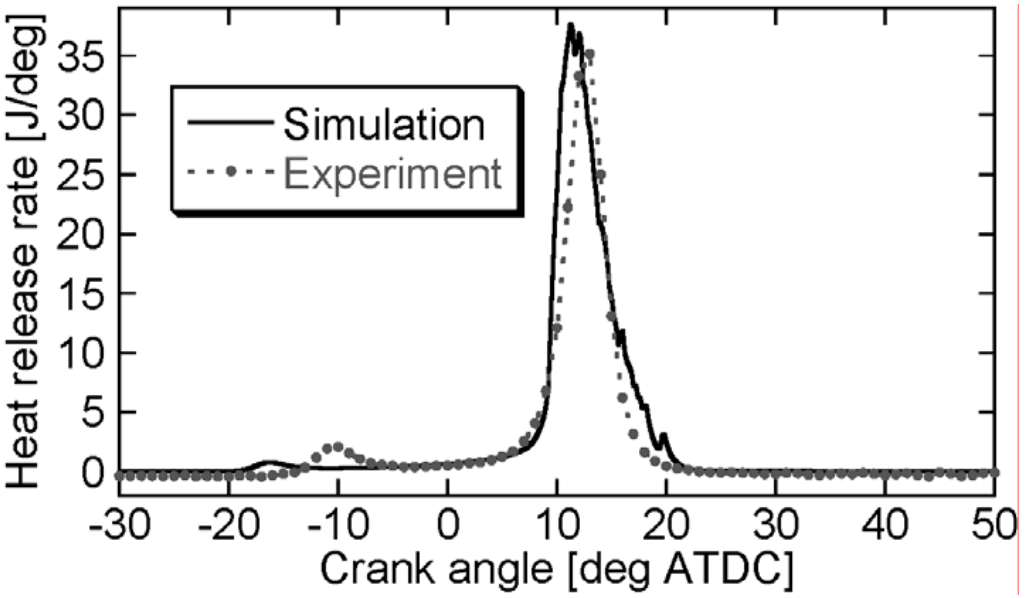

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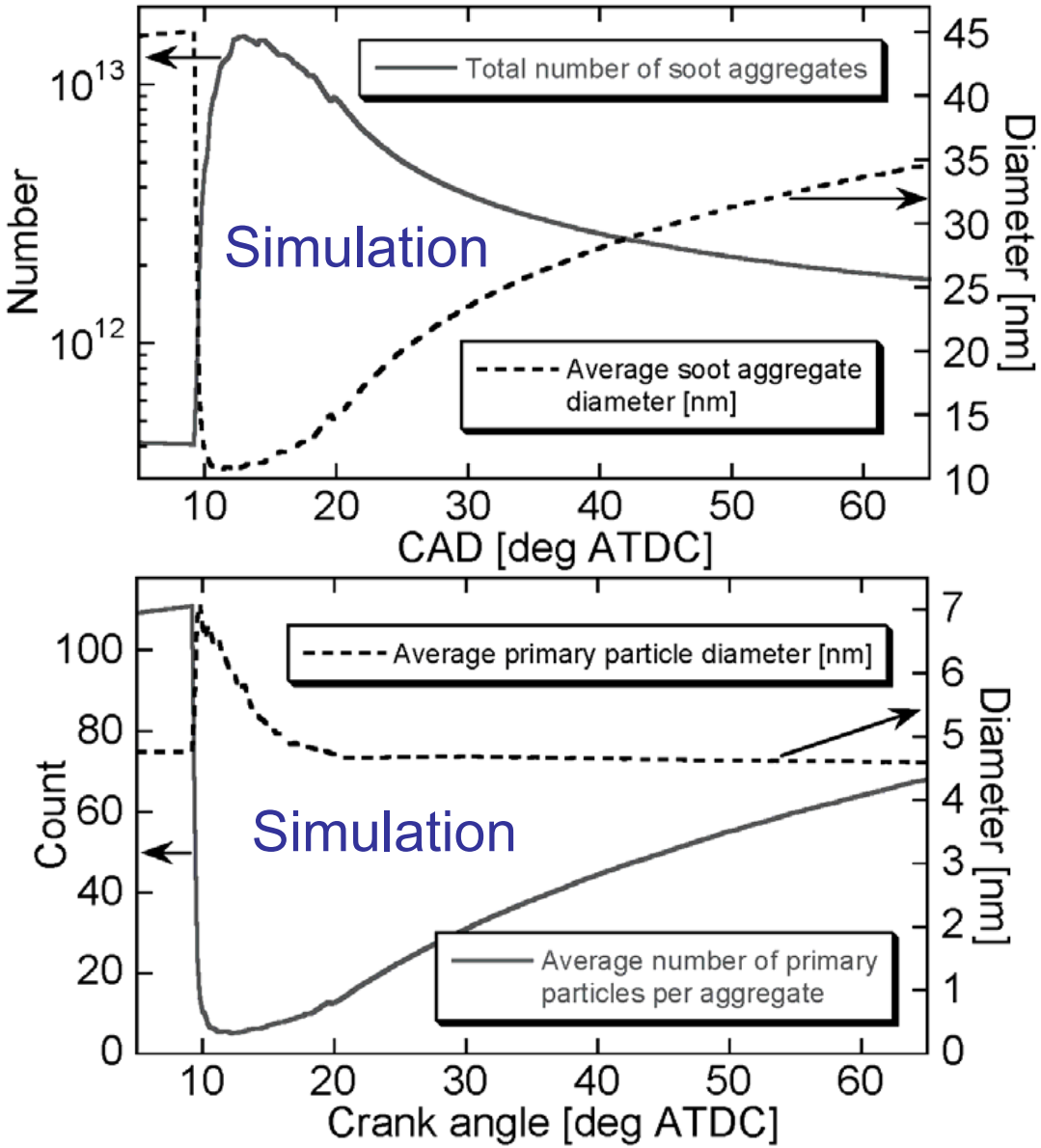
Averaged soot quantities



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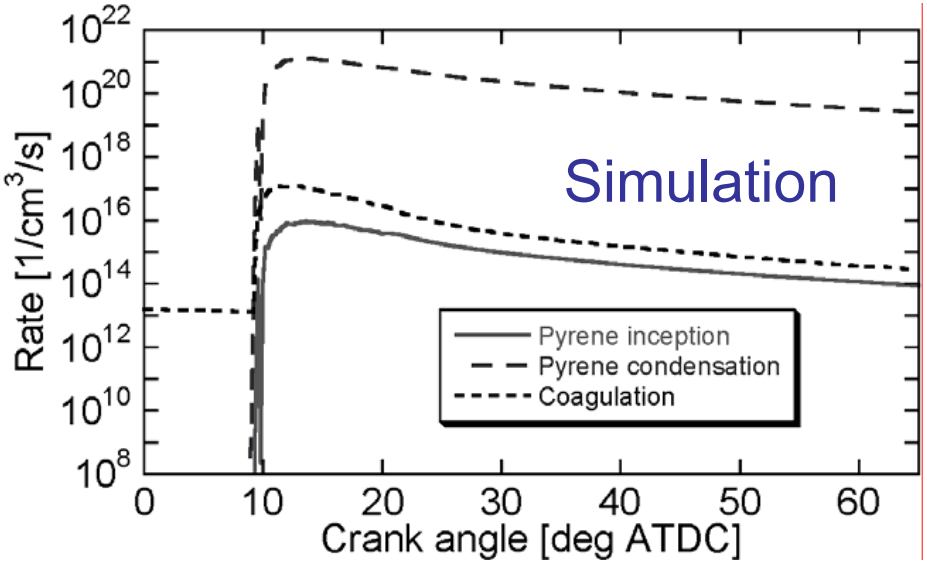
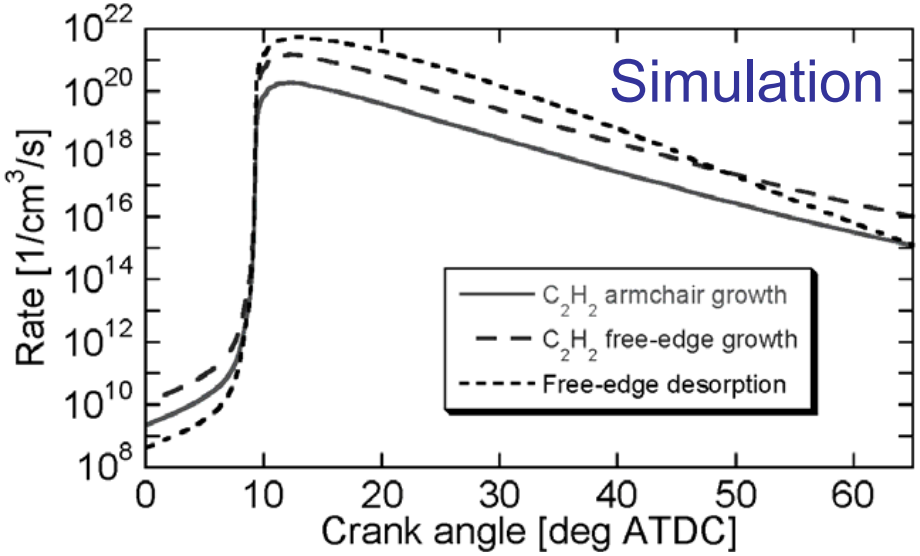
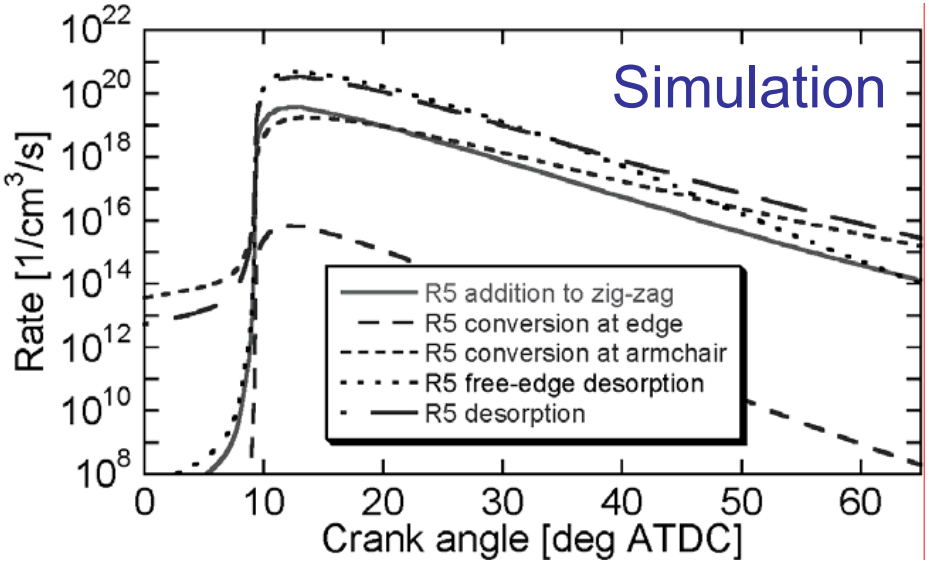
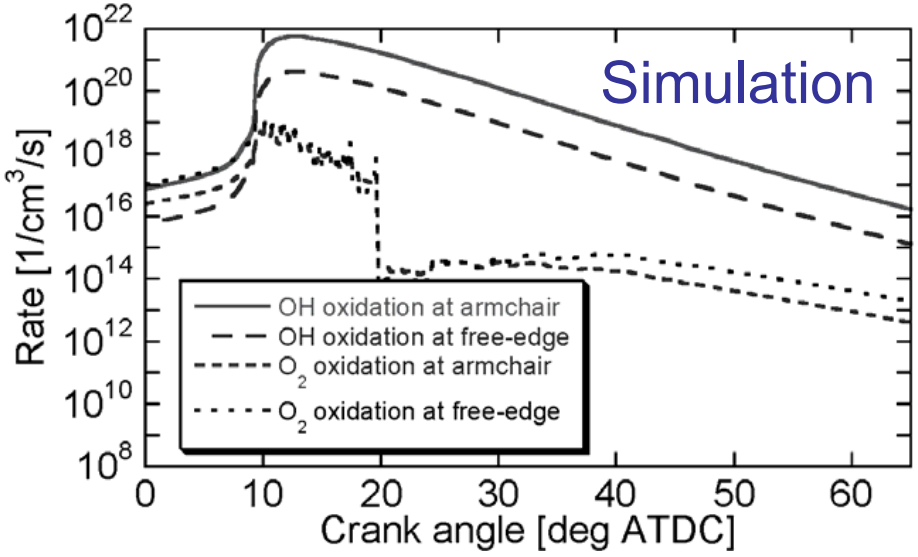
Rates of soot processes









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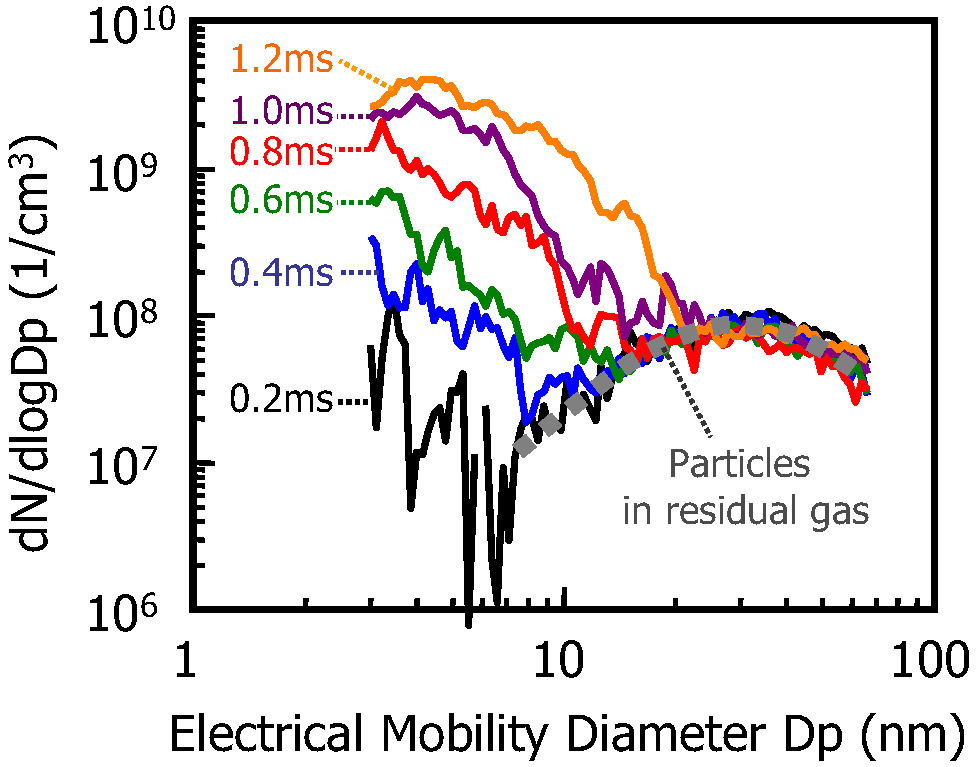
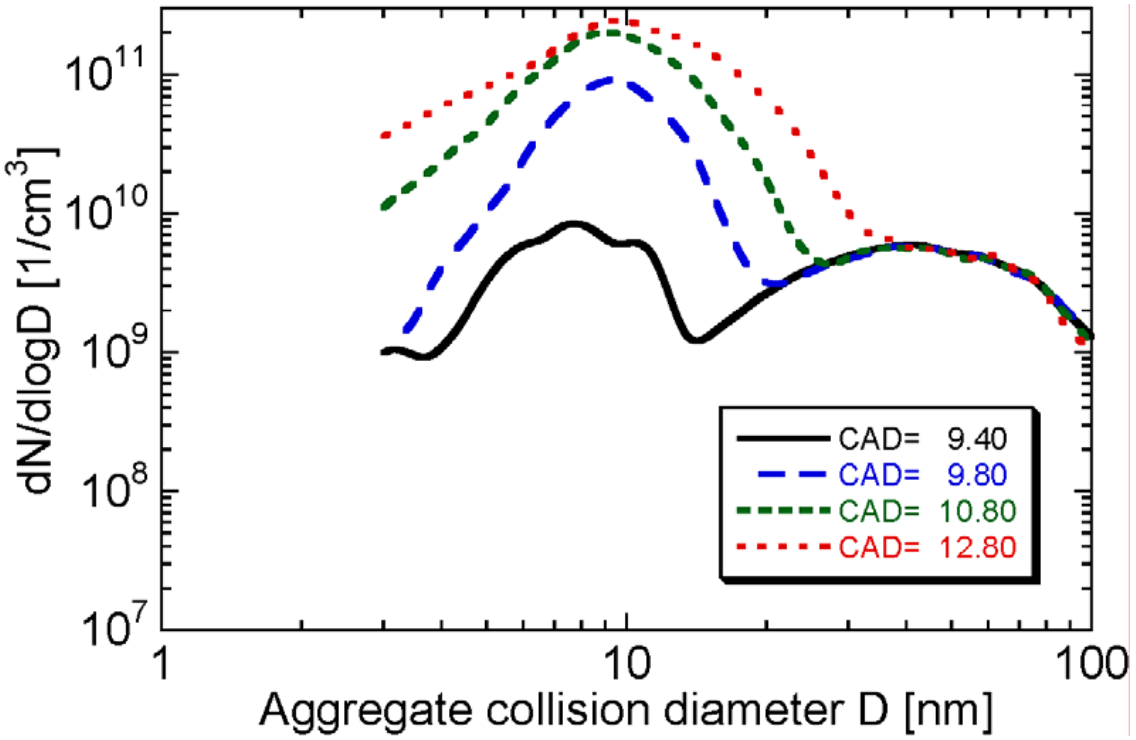
Aggregate size distributions (I)

Experiment



Simulation



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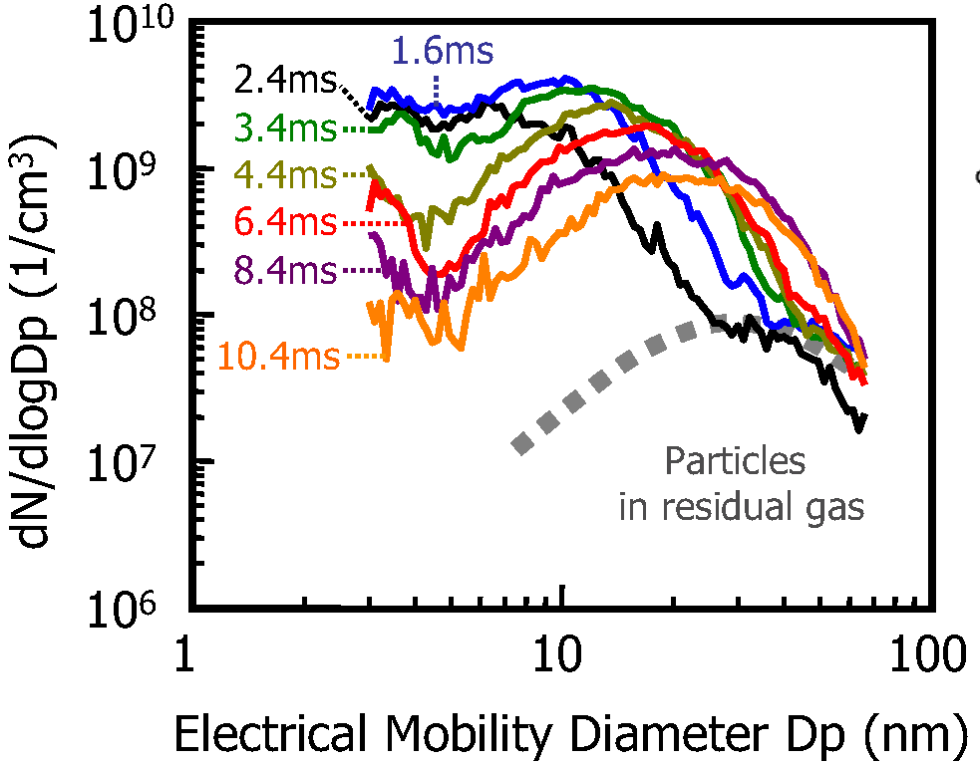
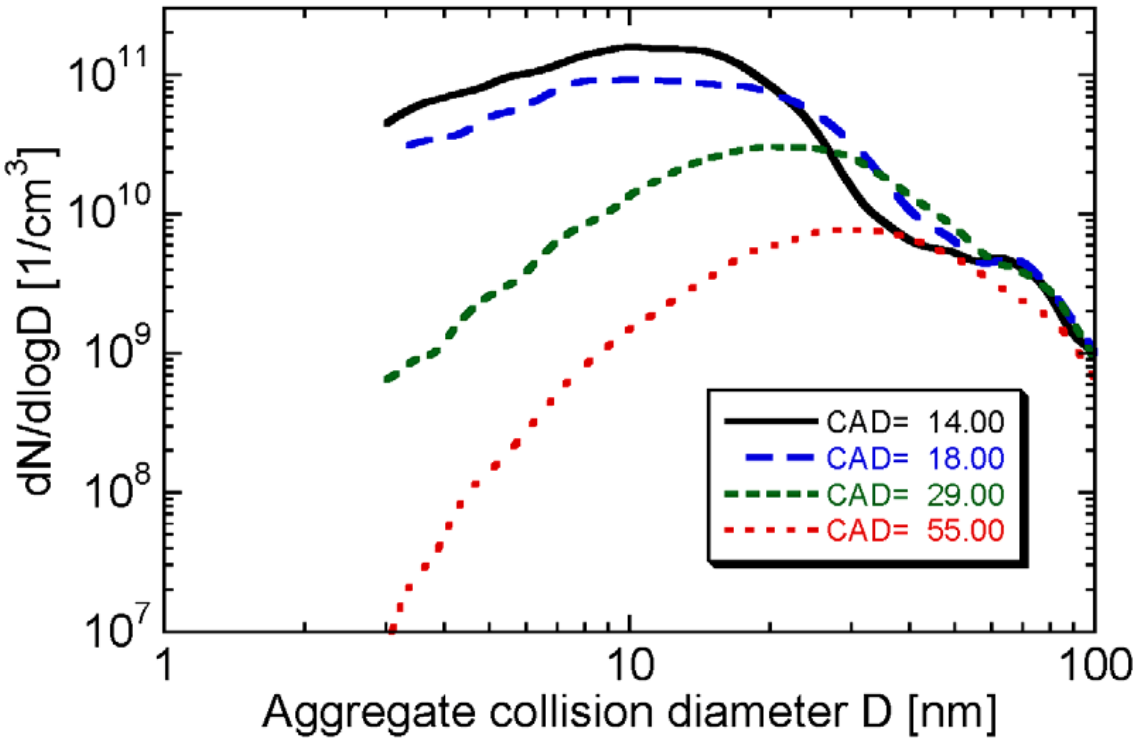
Aggregate size distributions (II)

Experiment



Simulation



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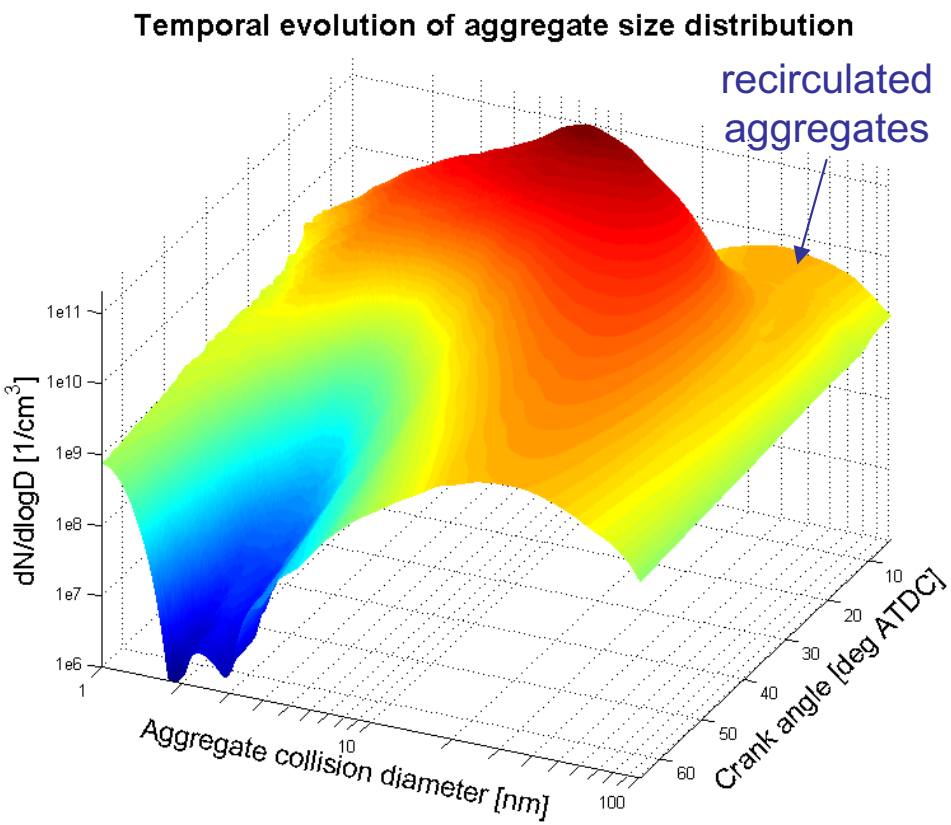
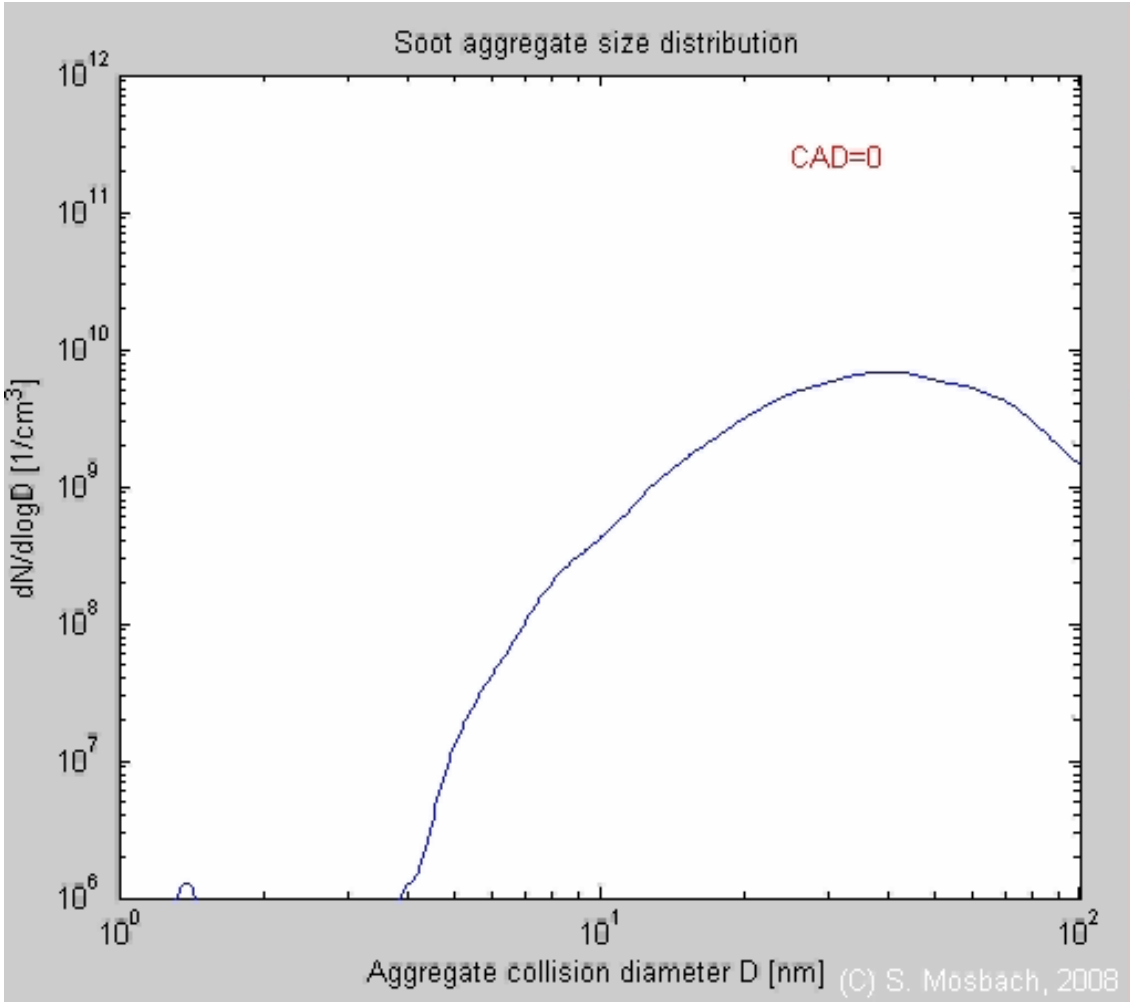
Aggregate size distributions (III)

Simulation





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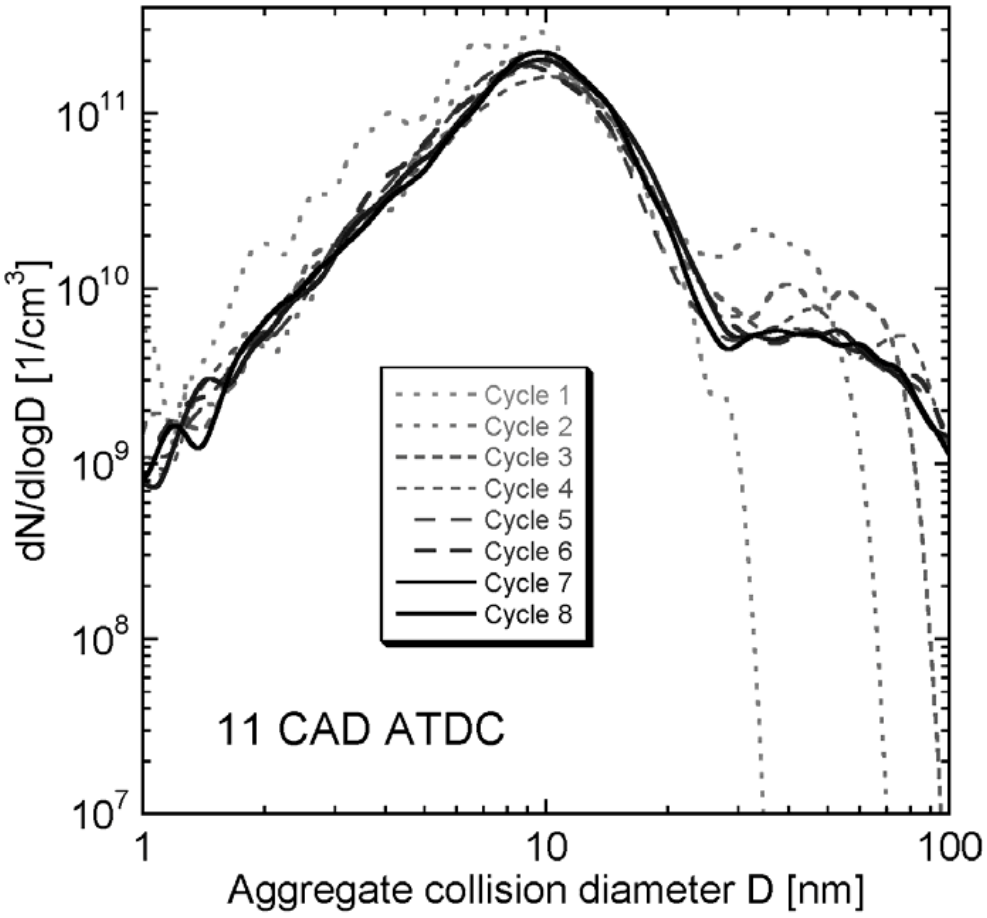
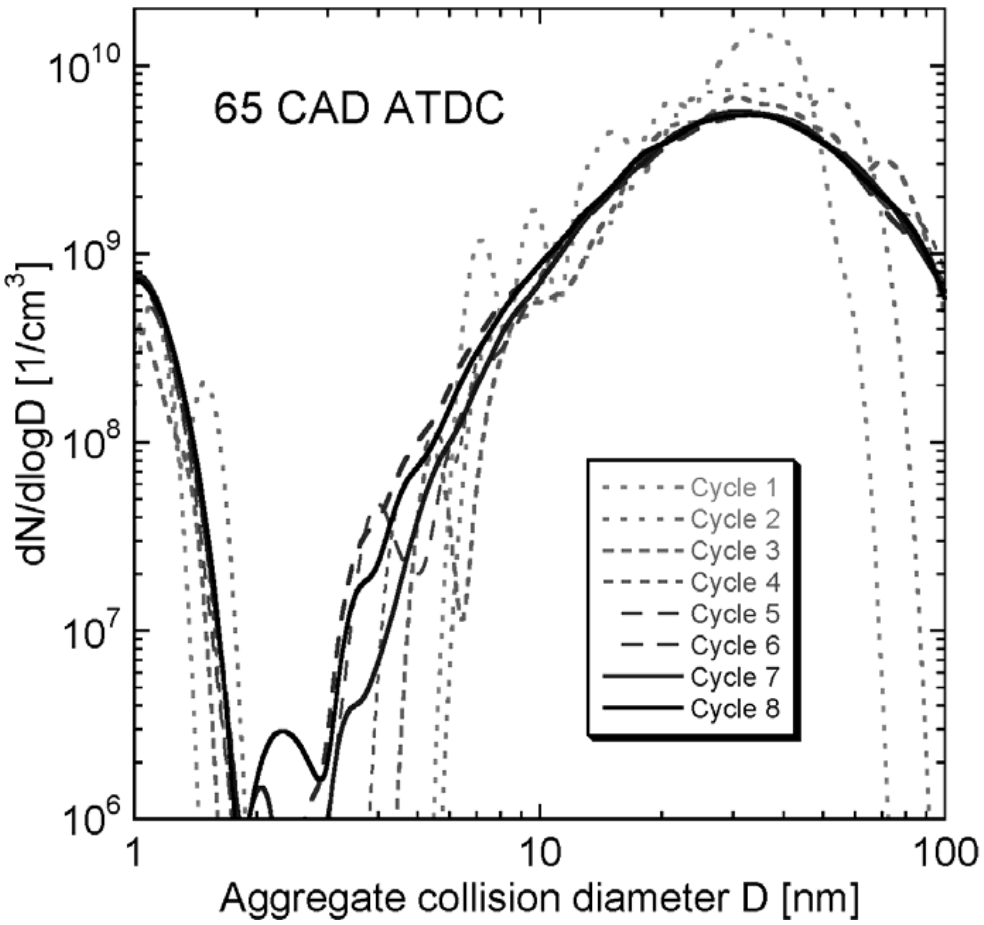
Role of EGR

Simulation



Simulation



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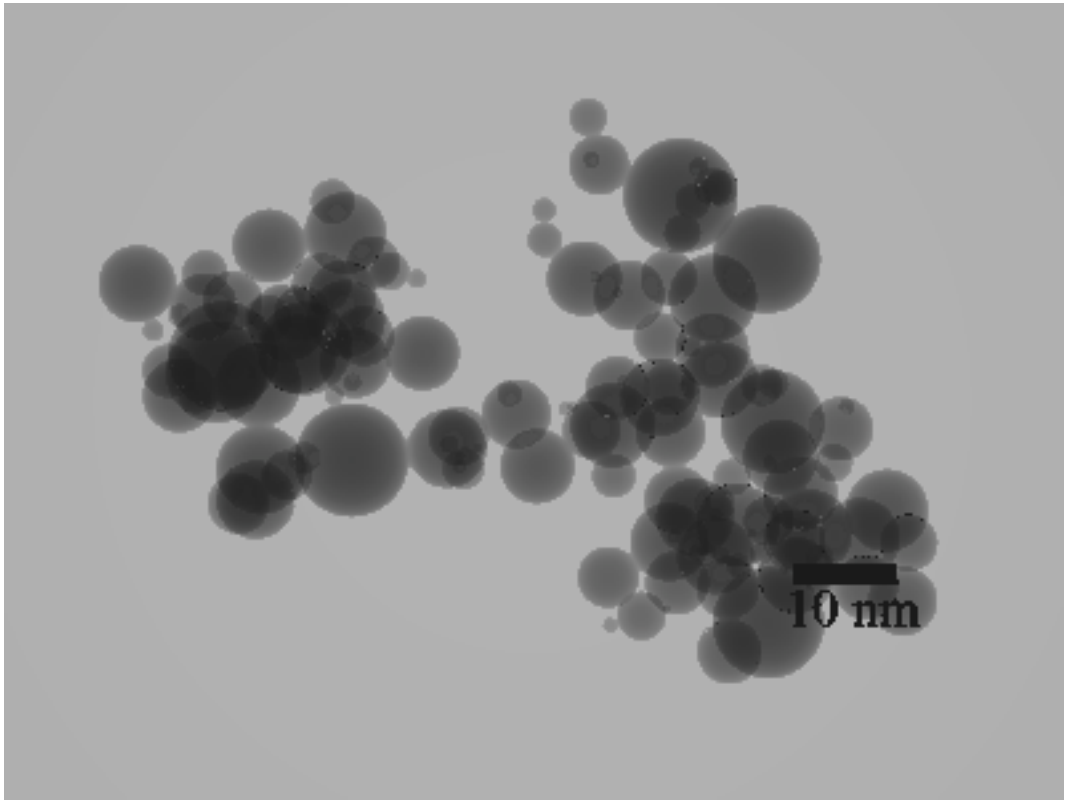
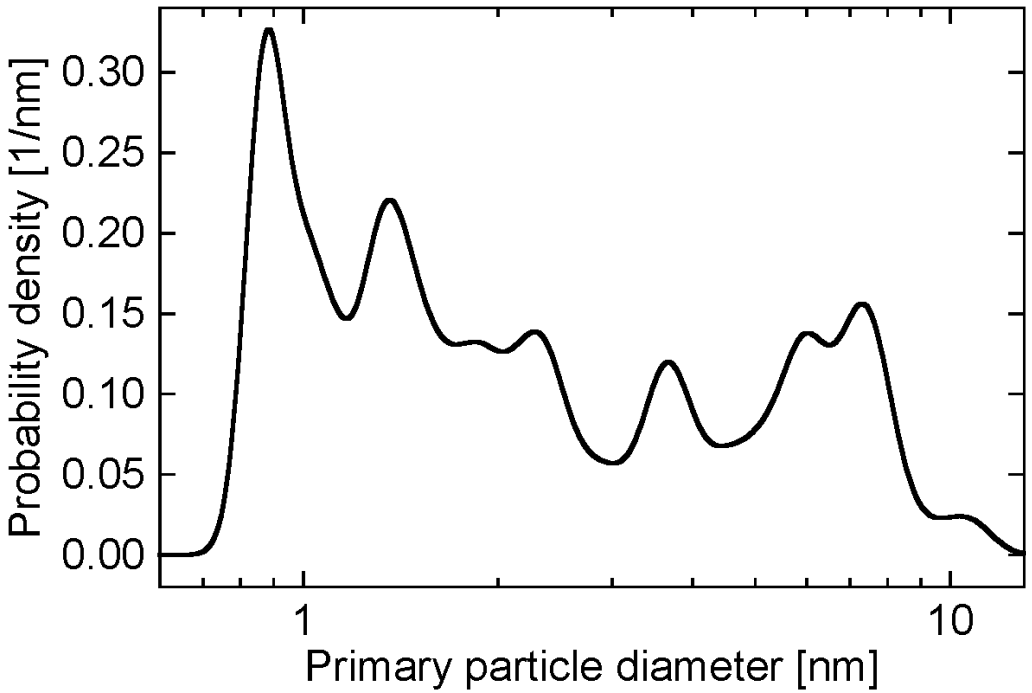
Sampled aggregates (I)

Simulation



Simulation



49.4 CAD ATDC, 129 primaries, coll. diam. 64 nm

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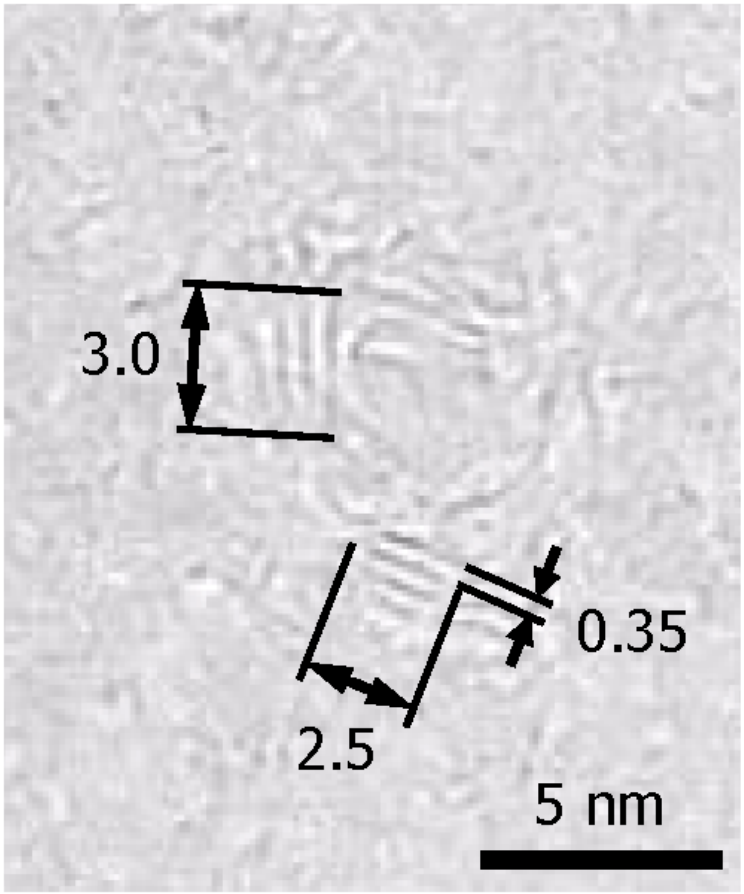
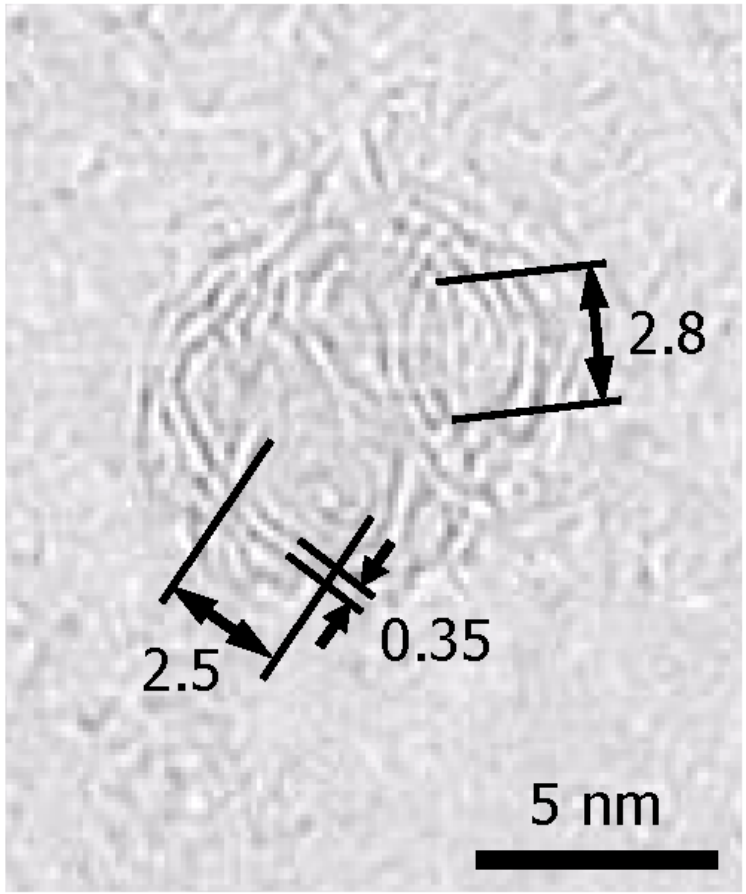
Sampled aggregates (II)

Experiment, sampled at ~16 CAD ATDC





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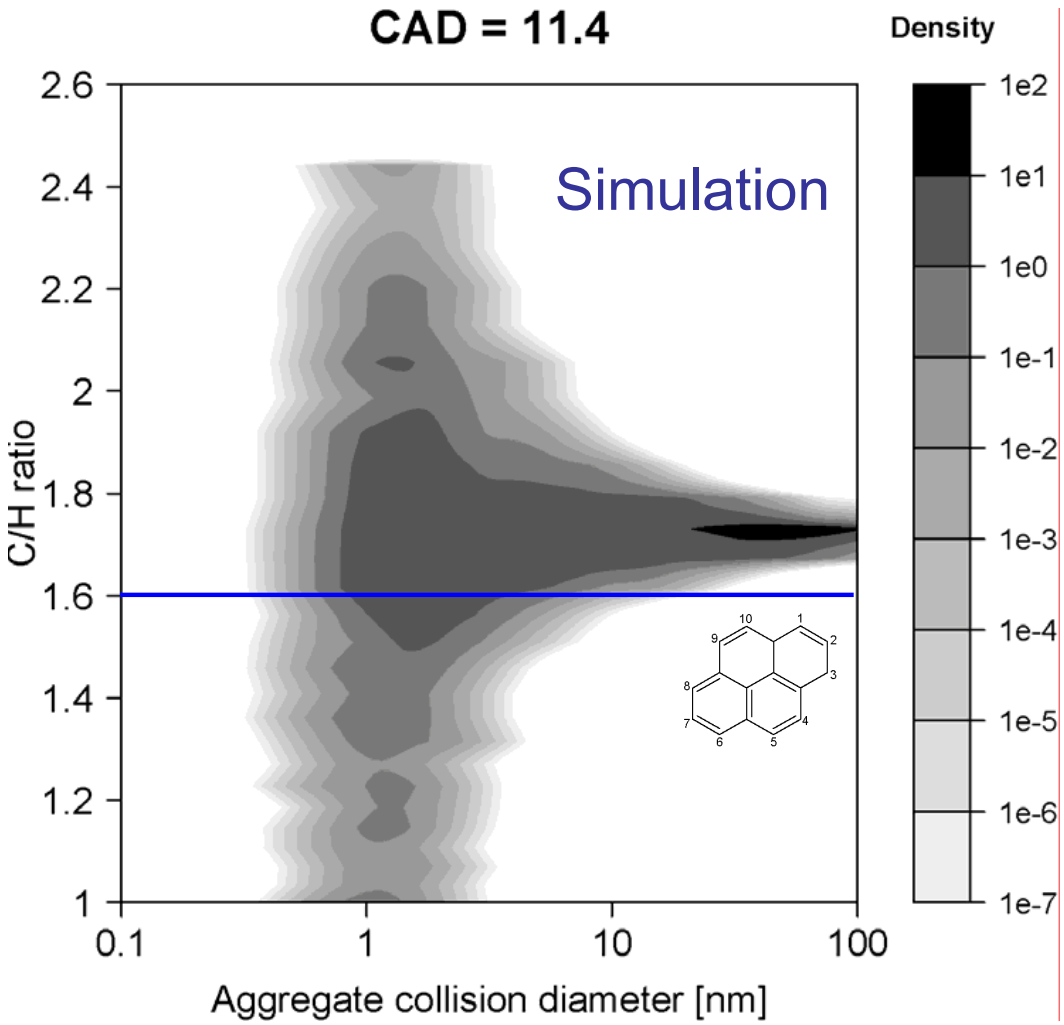
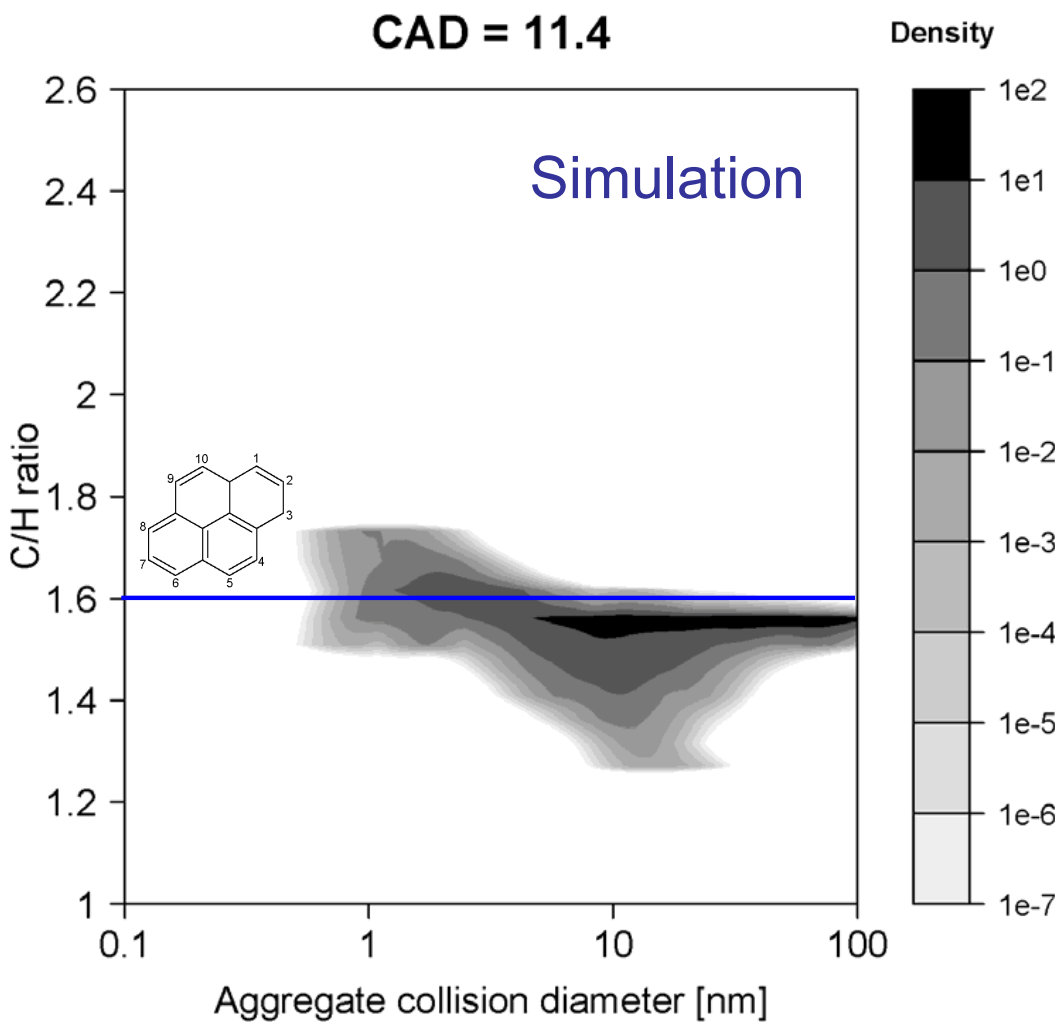
Aggregate composition pdfs (I)

large inception rate



large condensation rate



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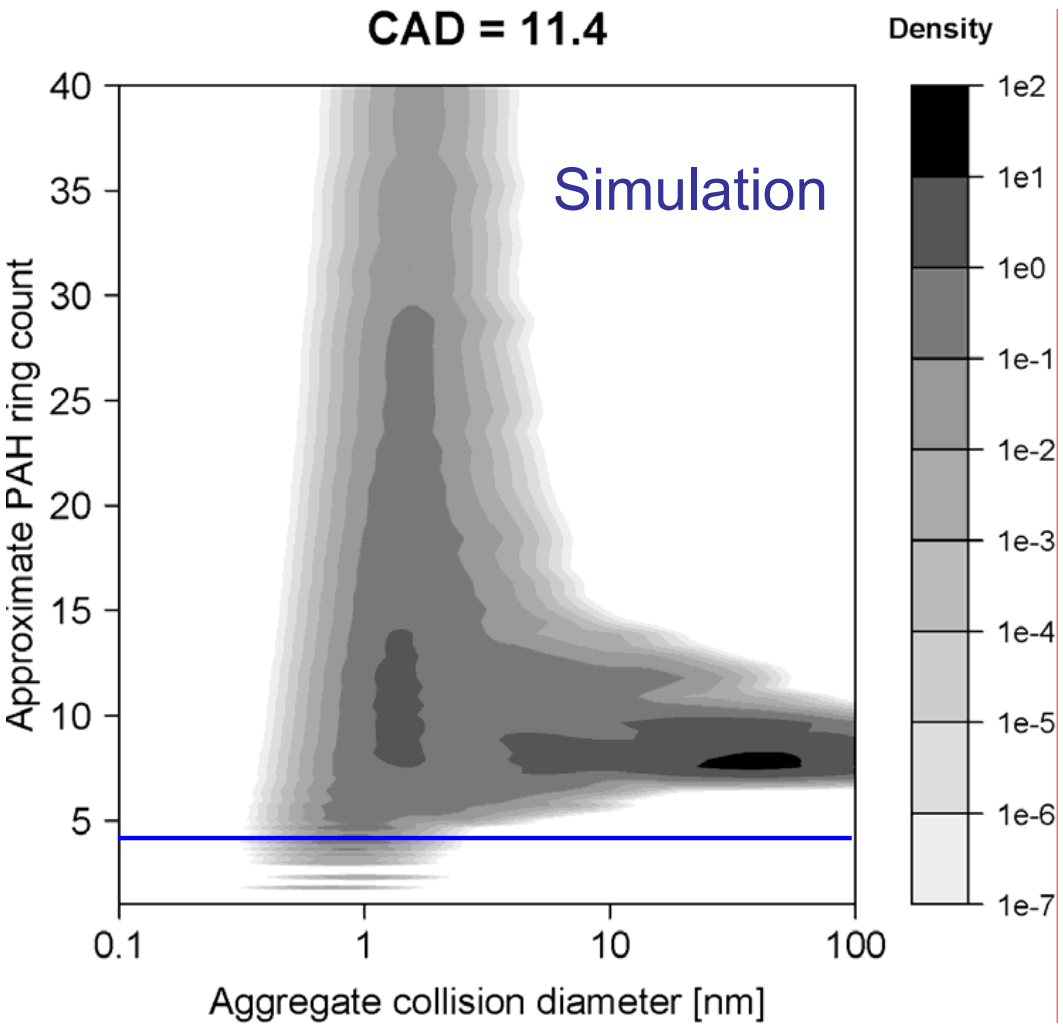
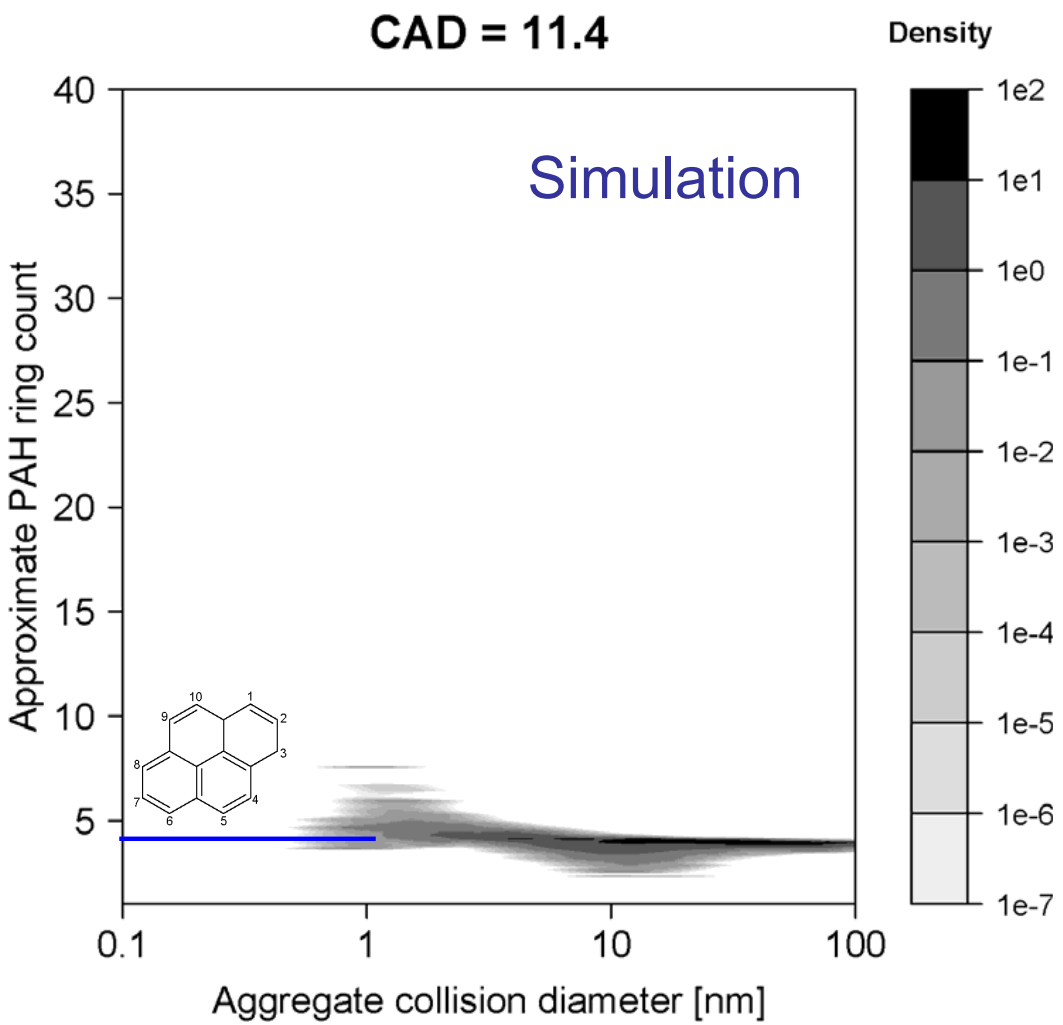
Aggregate composition pdfs (II)

large inception rate



large condensation rate



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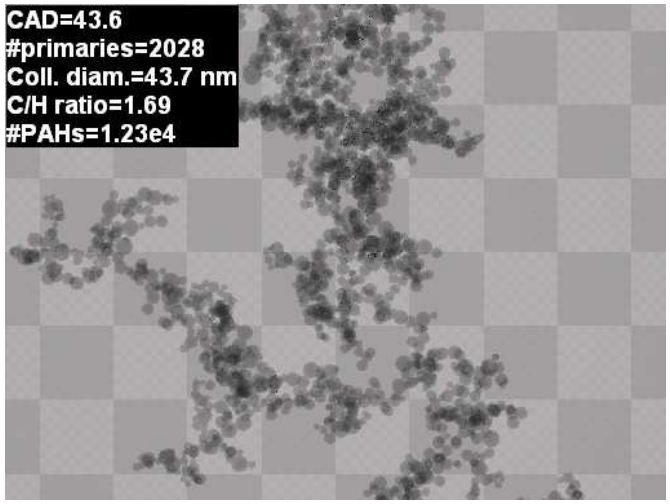
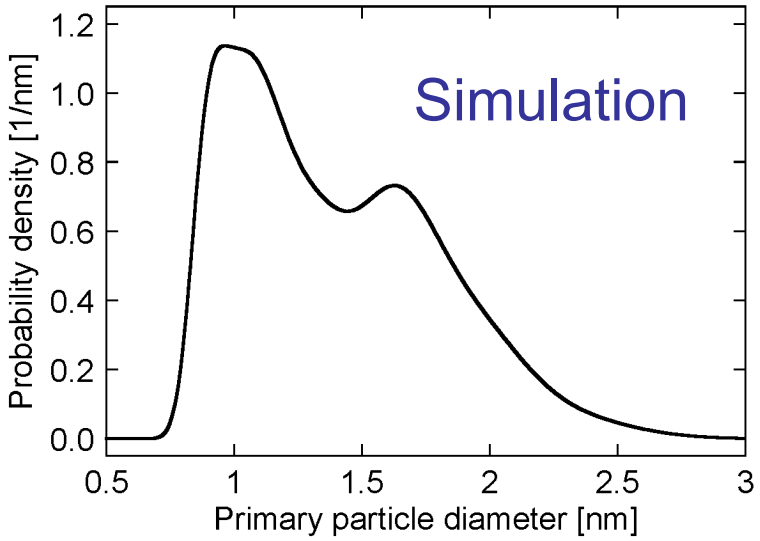
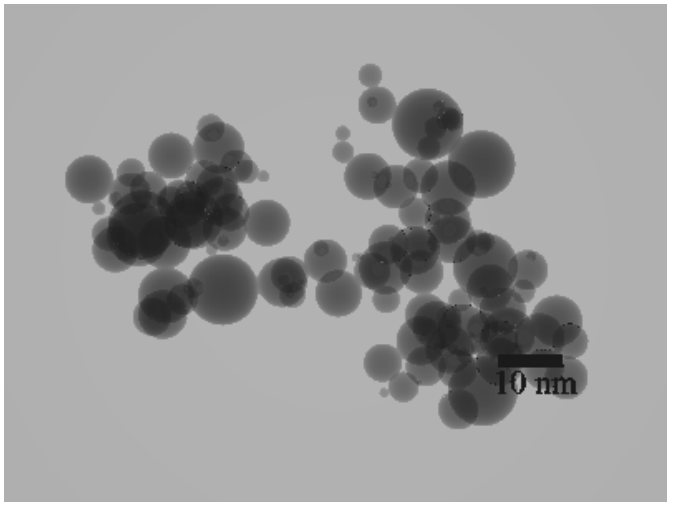
Inception vs. condensation

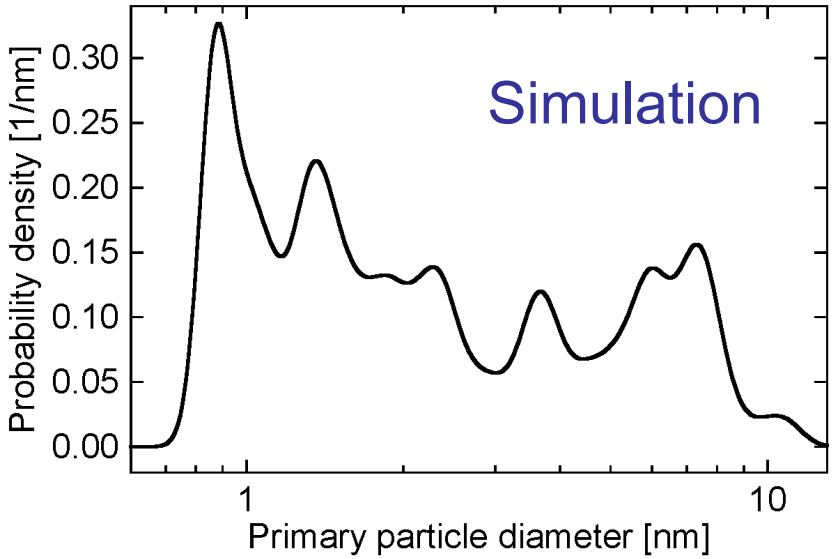
large inception rate





large condensation rate





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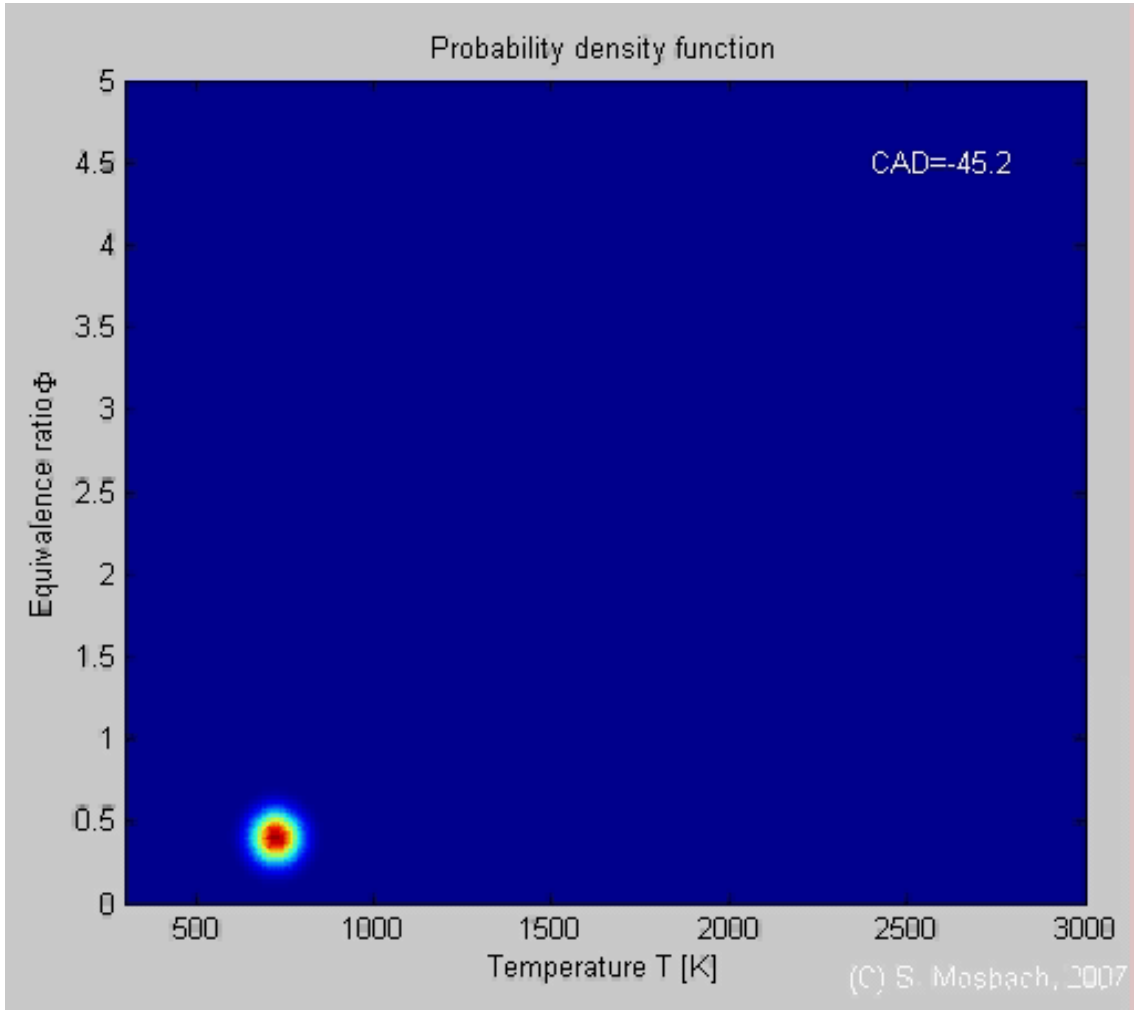
Future engine soot models (I)

- Partially stratified HCCI
- Partially premixed CIDI
- Conventional CIDI
- (Partially stratified) DISI



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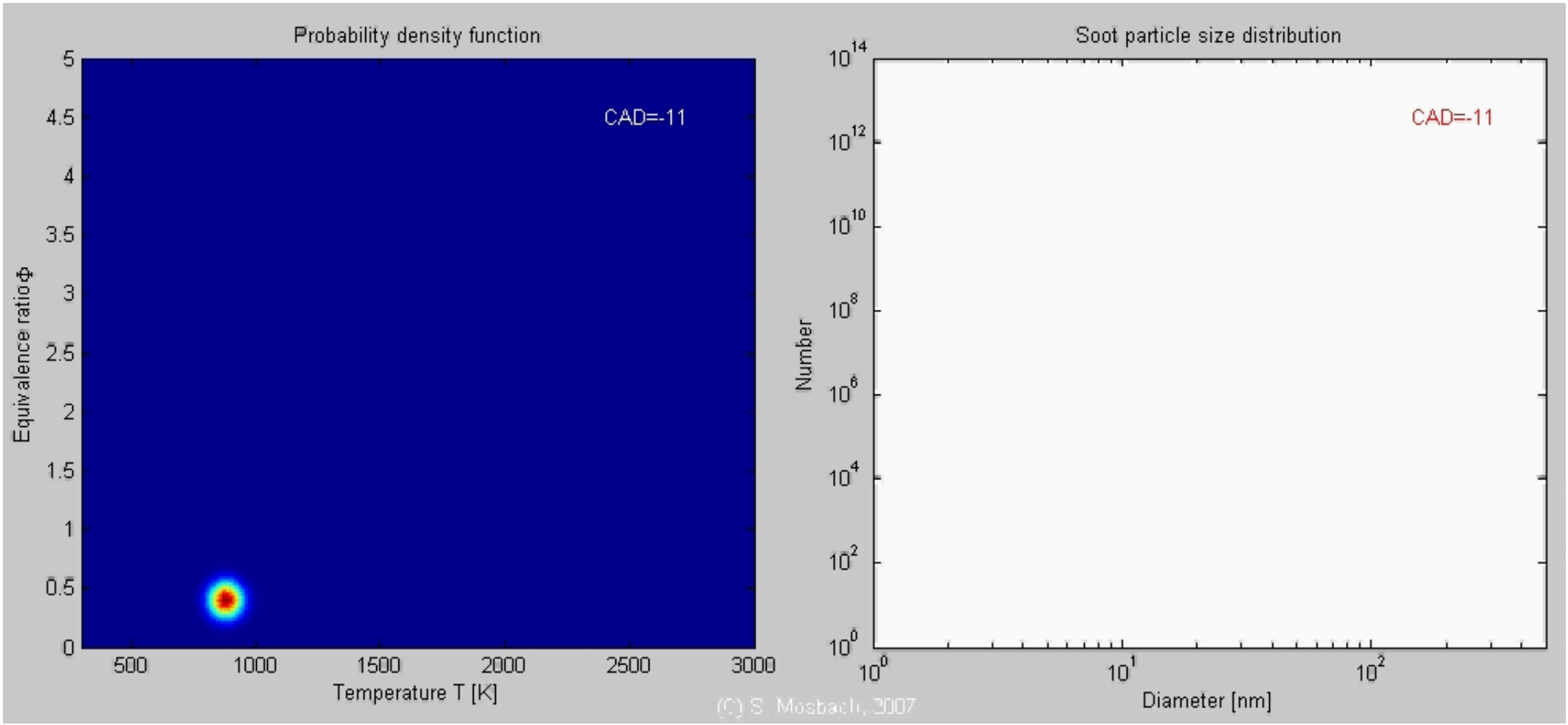
Future engine soot models (II)

Soot formation in a partially stratified HCCI engine:



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