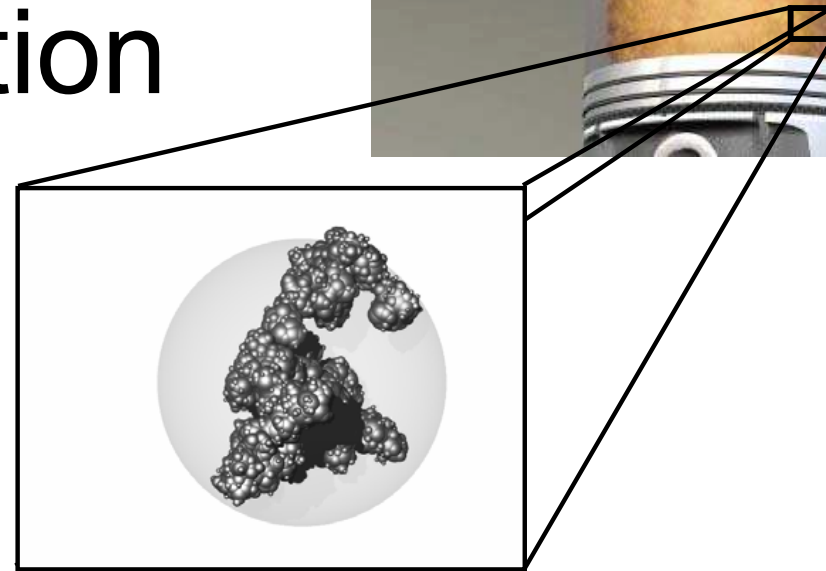
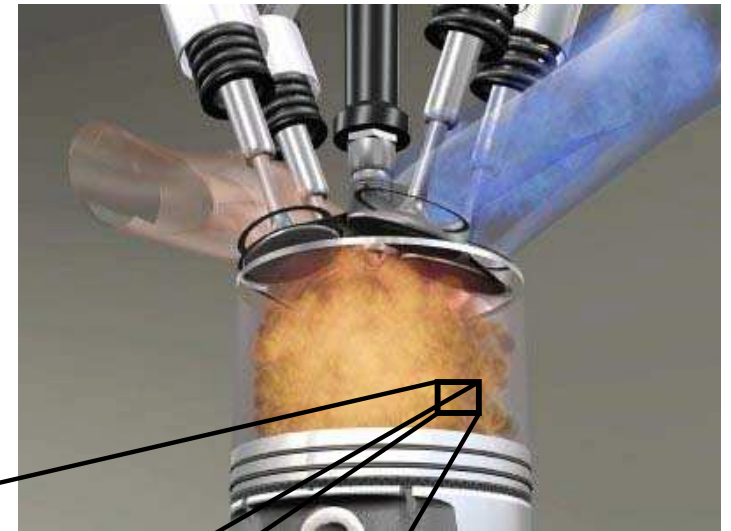


# Towards a detailed soot model for internal combustion engines



S. Mosbach, M. S. Celnik, M. Kraft,  
H. R. Zhang, S. Kubo, K.-O. Kim



**TOYOTA**

16 May 2008



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# Engine model: SRM

## Stochastic Reactor Model (SRM)

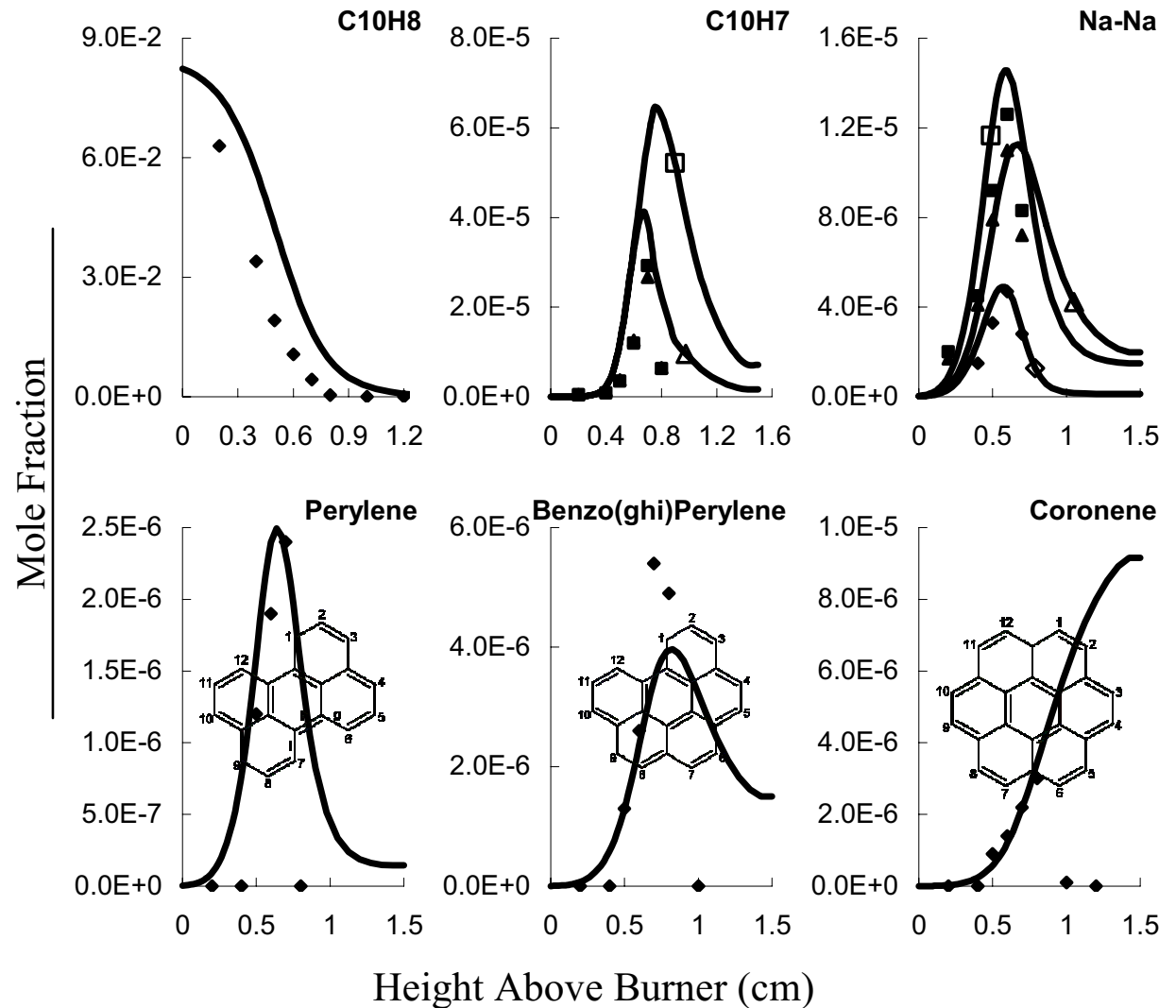
$$\begin{aligned} \frac{\partial}{\partial t} \mathcal{F}(\psi; t) = & - \underbrace{\sum_{j=1}^{S+1} \frac{\partial}{\partial \psi_j} [G_j(\psi) \mathcal{F}(\psi; t)]}_{\text{chemical reactions, volume change}} + \underbrace{\sum_{j=1}^{S+1} \frac{\partial}{\partial \psi_j} \left[ \frac{C_\phi}{2\tau} (\psi_j - \langle \psi_j \rangle) \mathcal{F}(\psi; t) \right]}_{\text{IEM mixing}} - \\ & \underbrace{- \frac{\dot{V}}{V} \mathcal{F}(\psi; t)}_{\text{piston movement}} - \underbrace{\frac{1}{h} [U(\psi_{S+1} + h) \mathcal{F}(\psi_1, \dots, \psi_S, \psi_{S+1} + h; t) - U(\psi_{S+1}) \mathcal{F}(\psi; t)]}_{\text{heat transfer}} \end{aligned}$$

- 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)



# PAHs in gas-phase chemistry

- Hongzhi R. Zhang
- Before: PRF+NO<sub>x</sub>, 157 species
- After: PRF+NO<sub>x</sub>+ variety of PAHs and highly unsaturated HCs, 208 species
- Validation against fuel-rich flame experiments

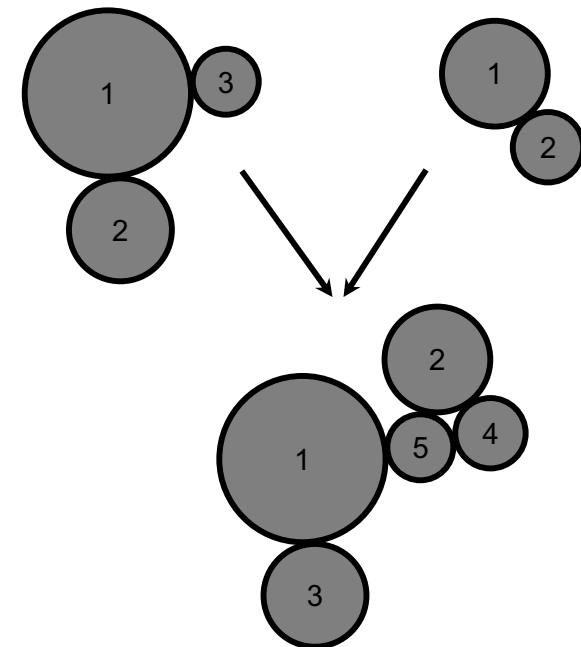
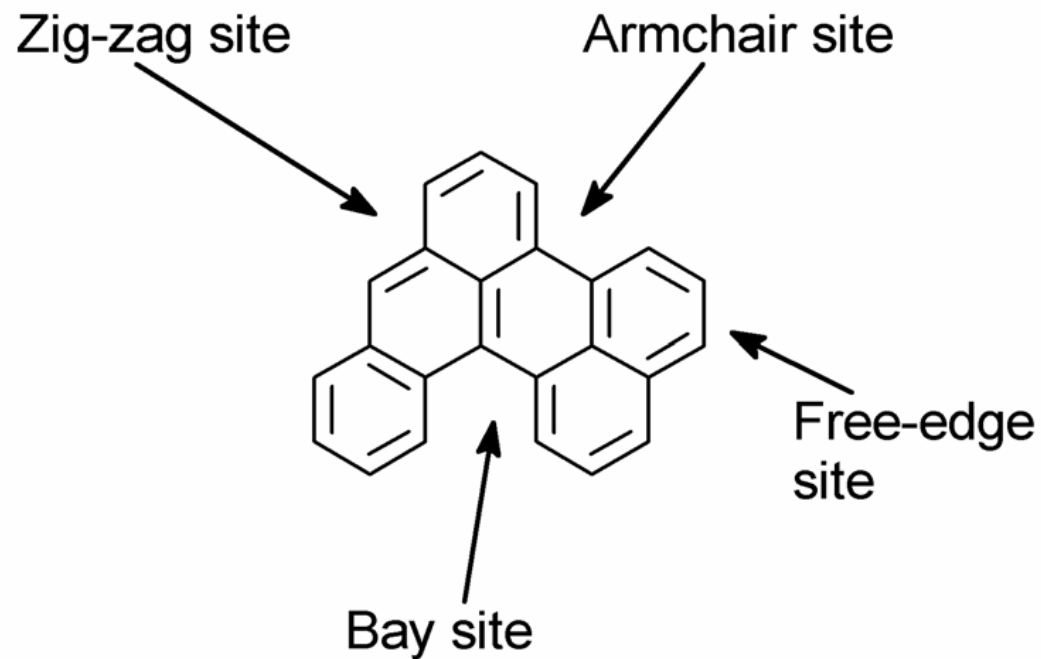


# Soot model: site-counting

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

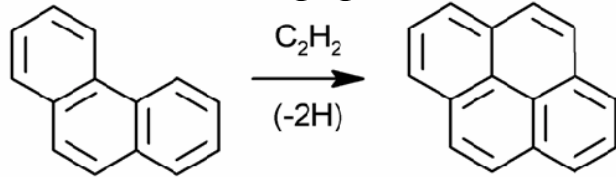
$$E = (C, H, S_{\alpha}, N_{ed}, N_{zz}, N_{ac}, N_{bay}, N_{R5}, N_{PAH}, PP_{(1-N)})$$

$PP$  = primary particle list

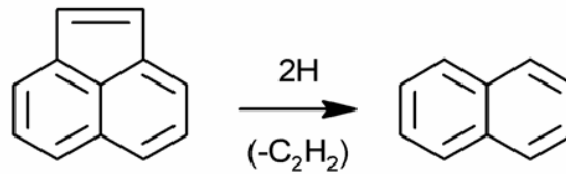


# PAH reaction steps

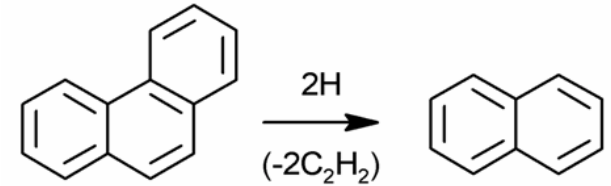
Armchair ring growth



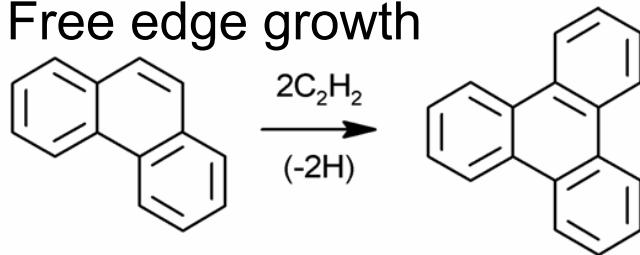
5-member ring desorption



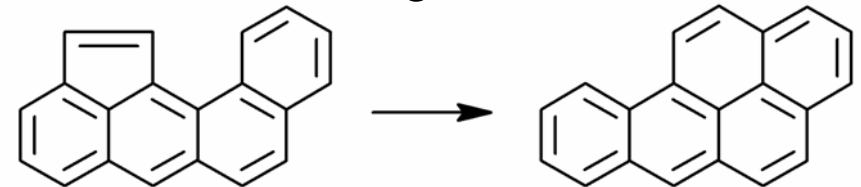
6-member ring desorption



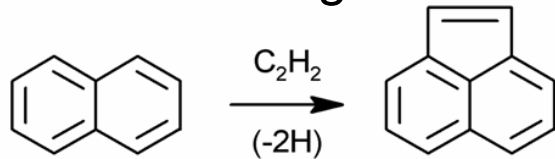
Free edge growth



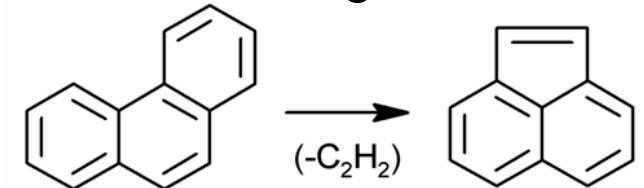
5-member ring conversion at AC



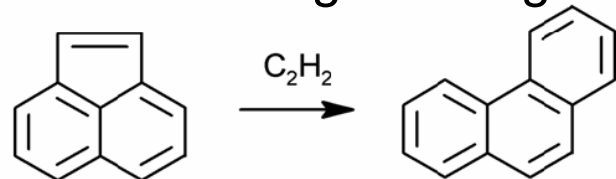
5-member ring addition



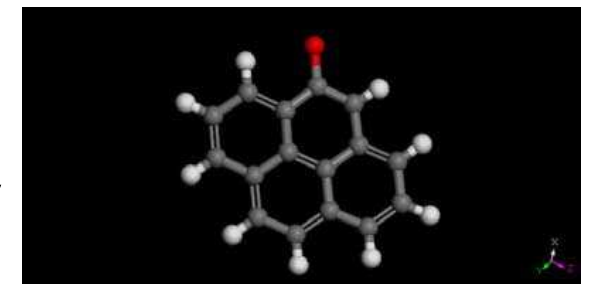
6- to 5-member ring conversion



5-member ring free edge desorption



Oxidation steps:  
rates from  
quantum chemistry



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



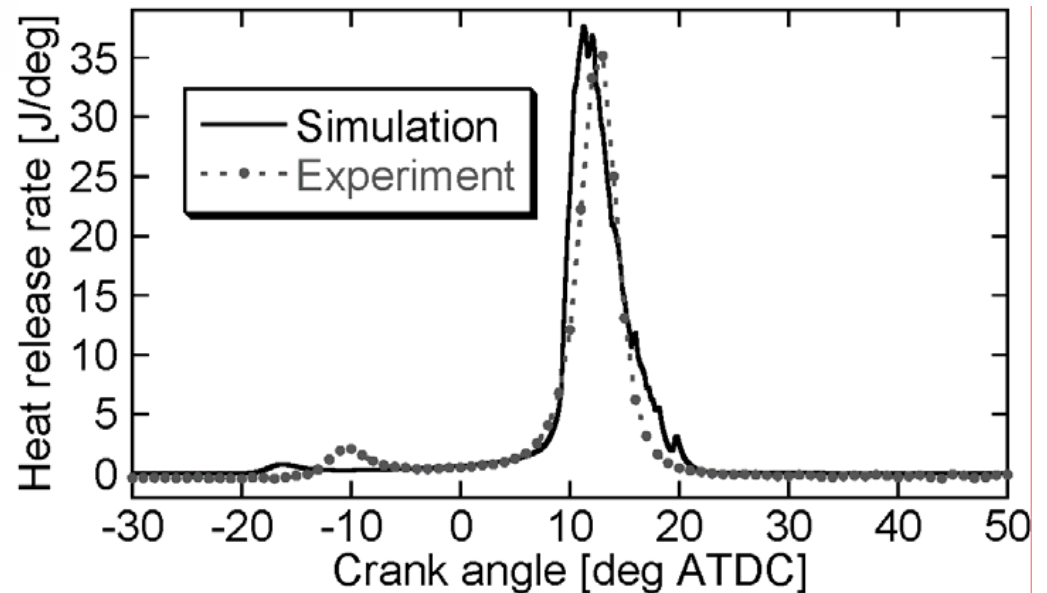
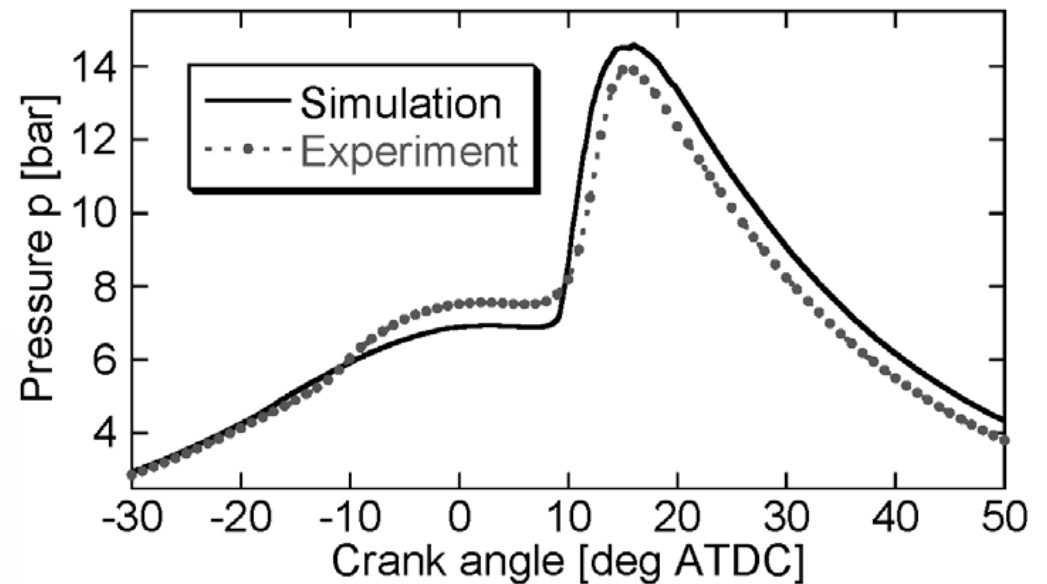
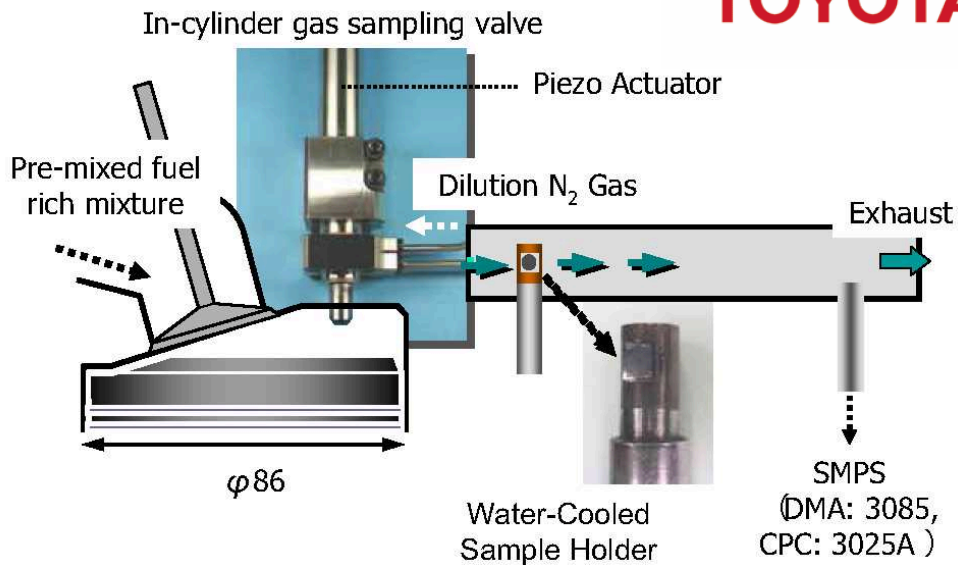
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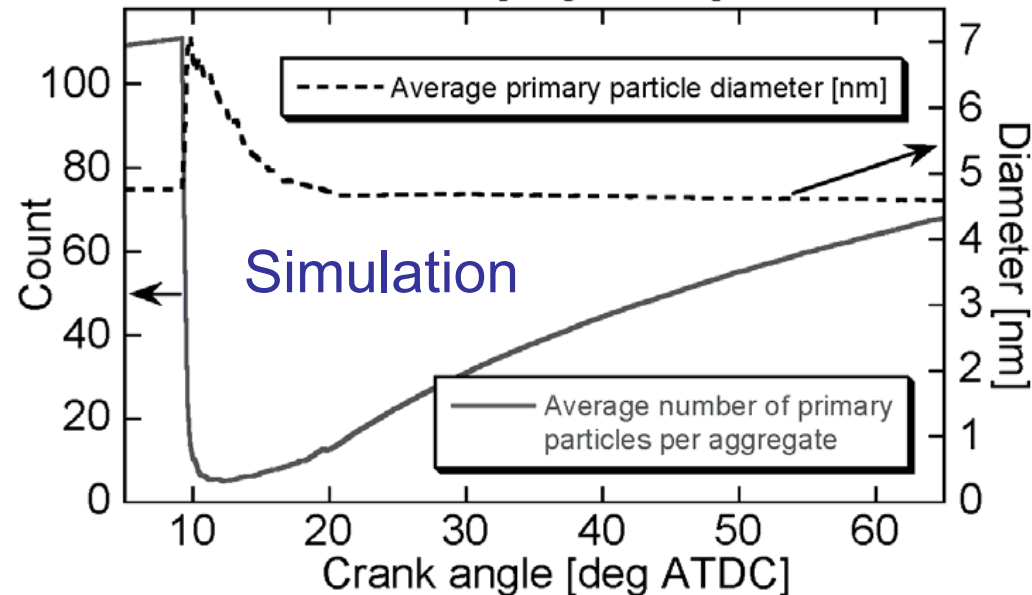
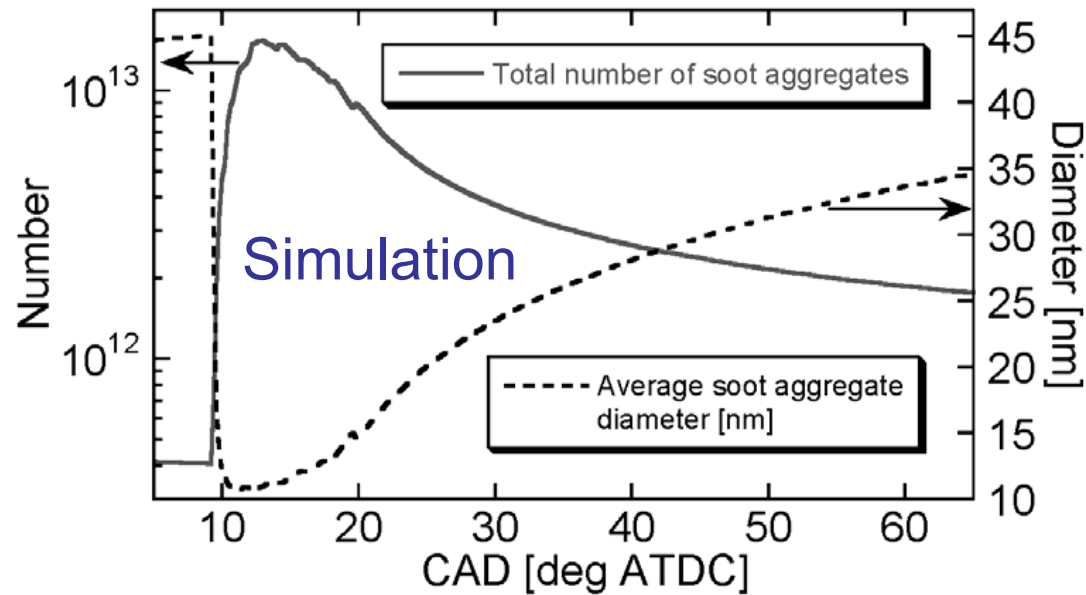


# Soot in engines!

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

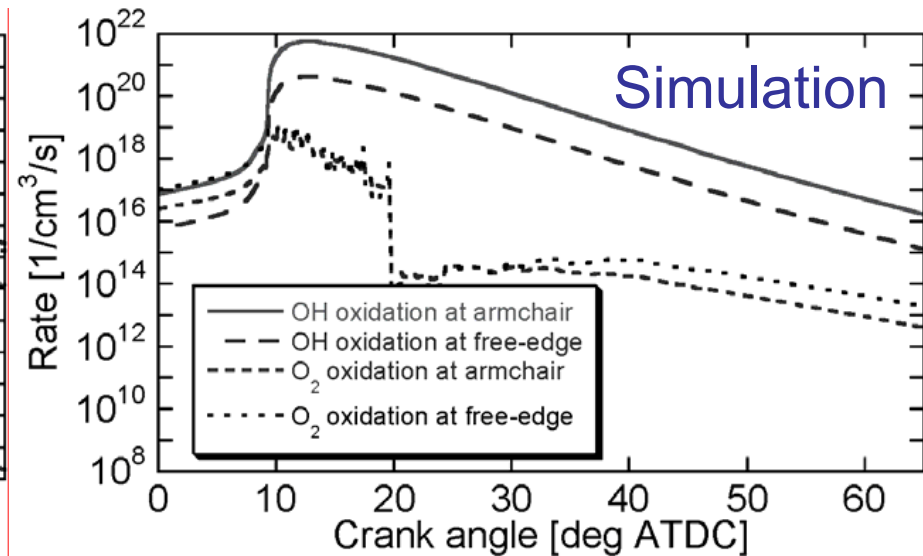
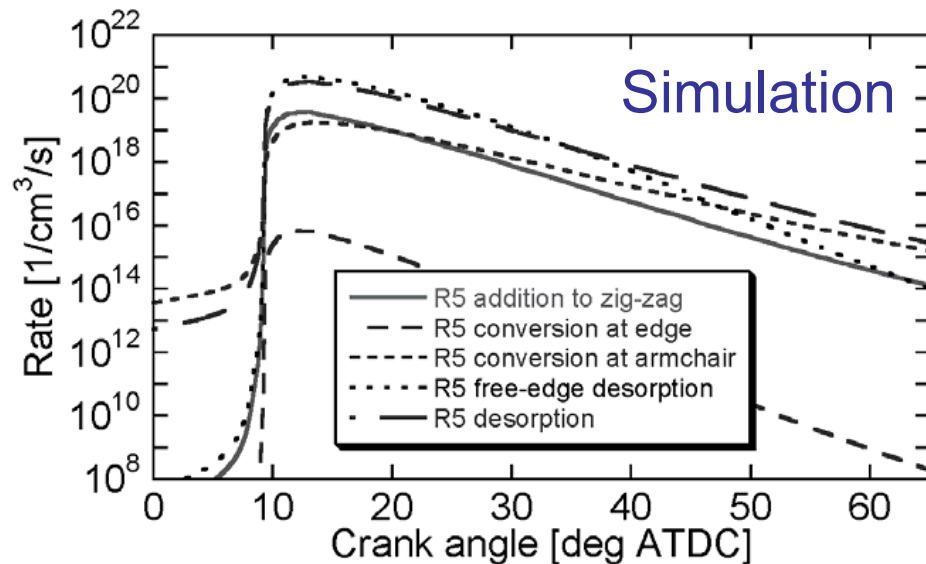
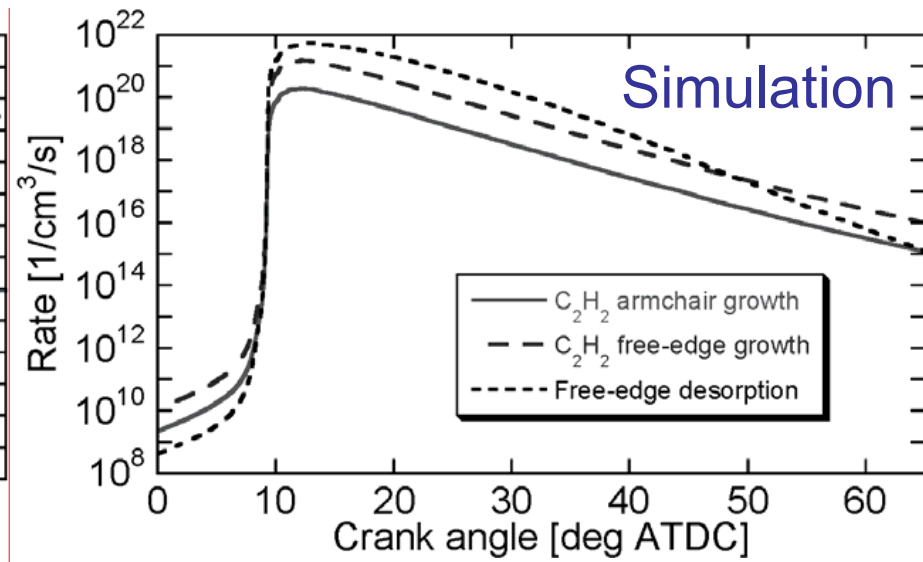
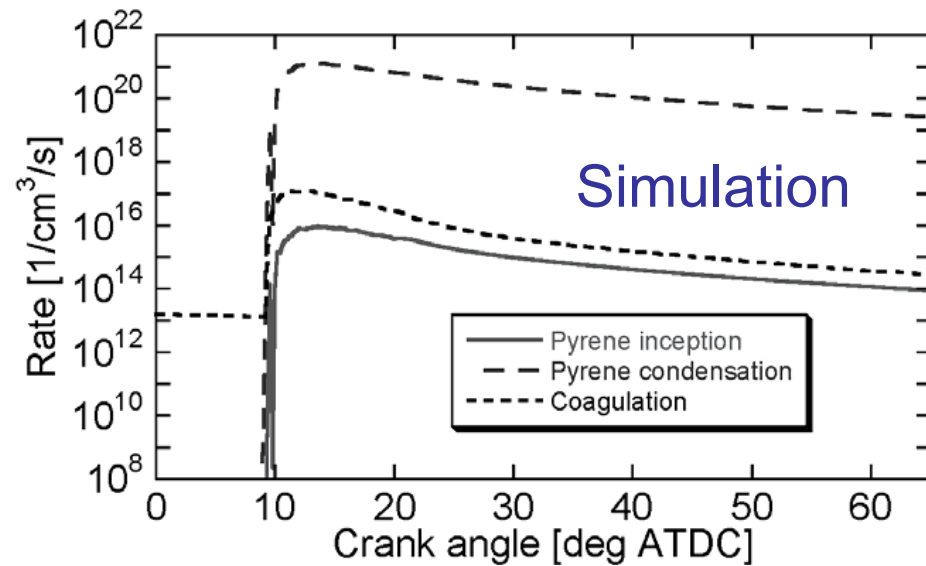


# Averaged soot quantities





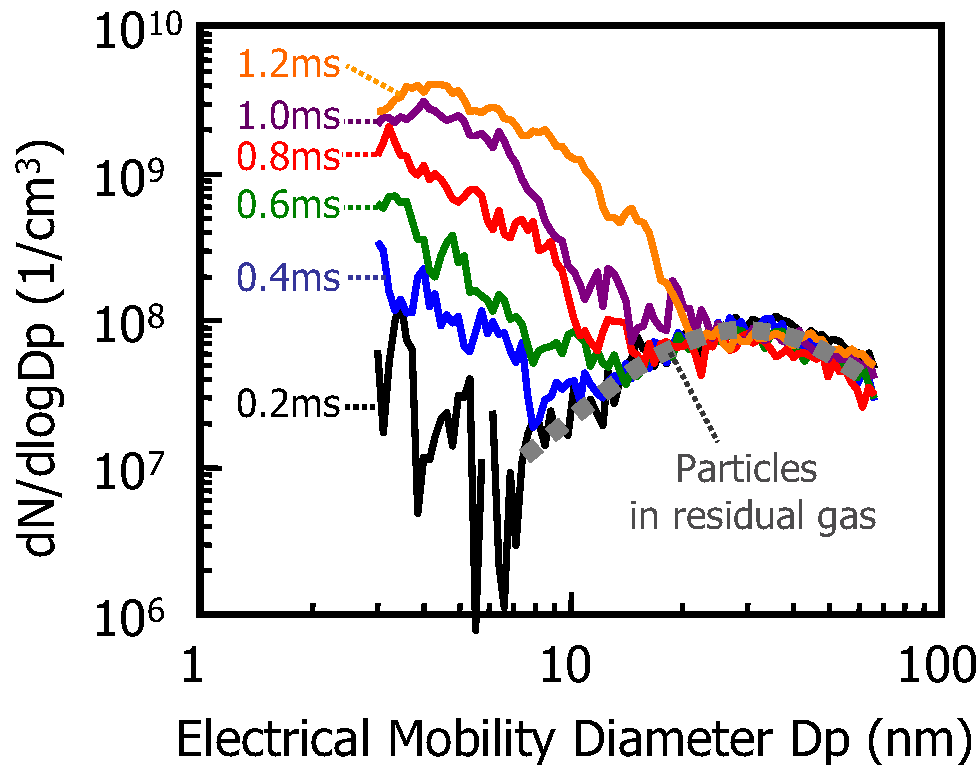
# Rates of soot processes



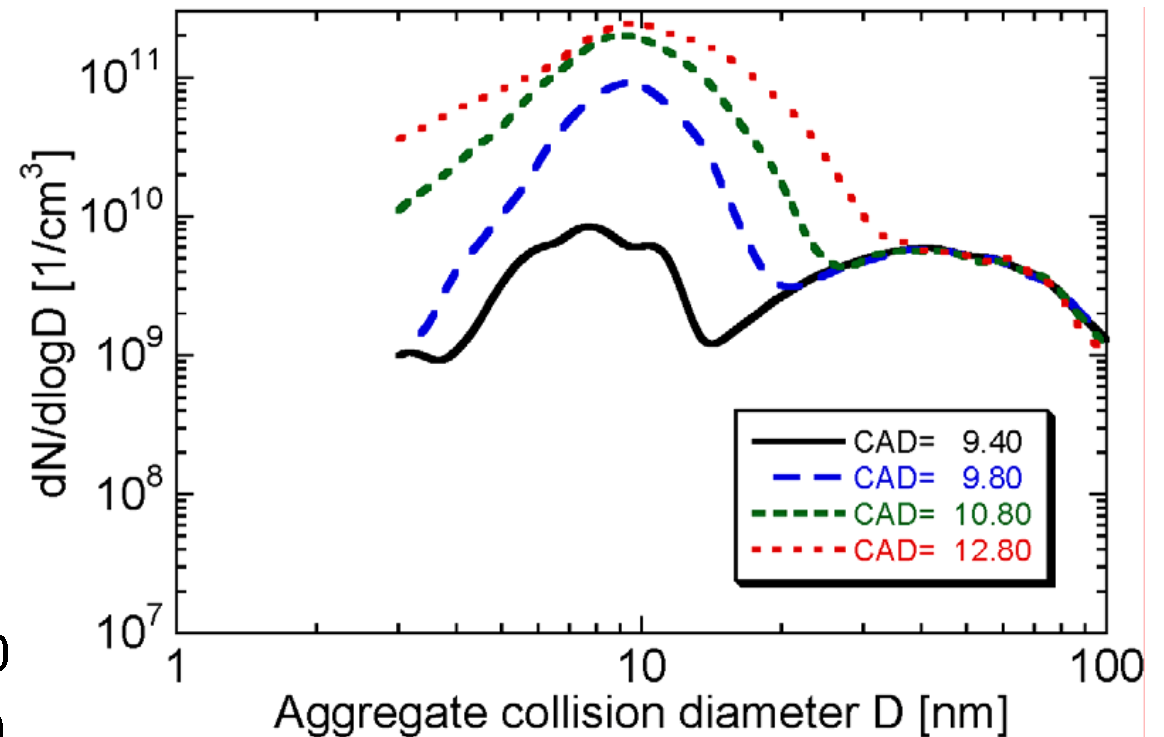


# Aggregate size distributions (I)

## Experiment

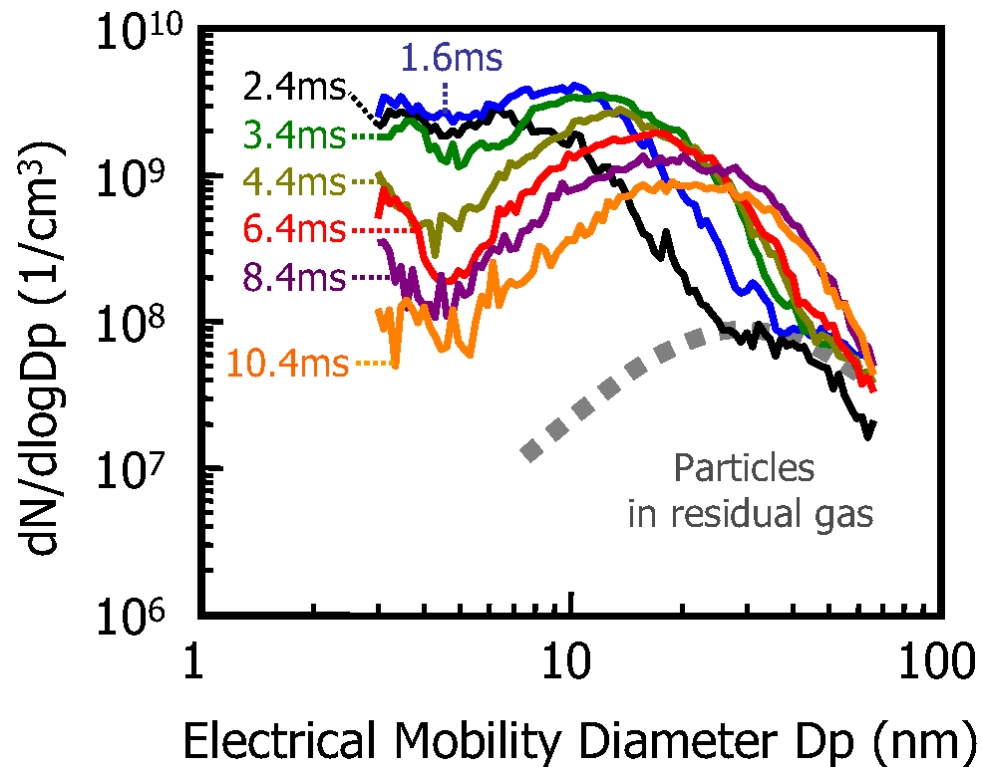


## Simulation

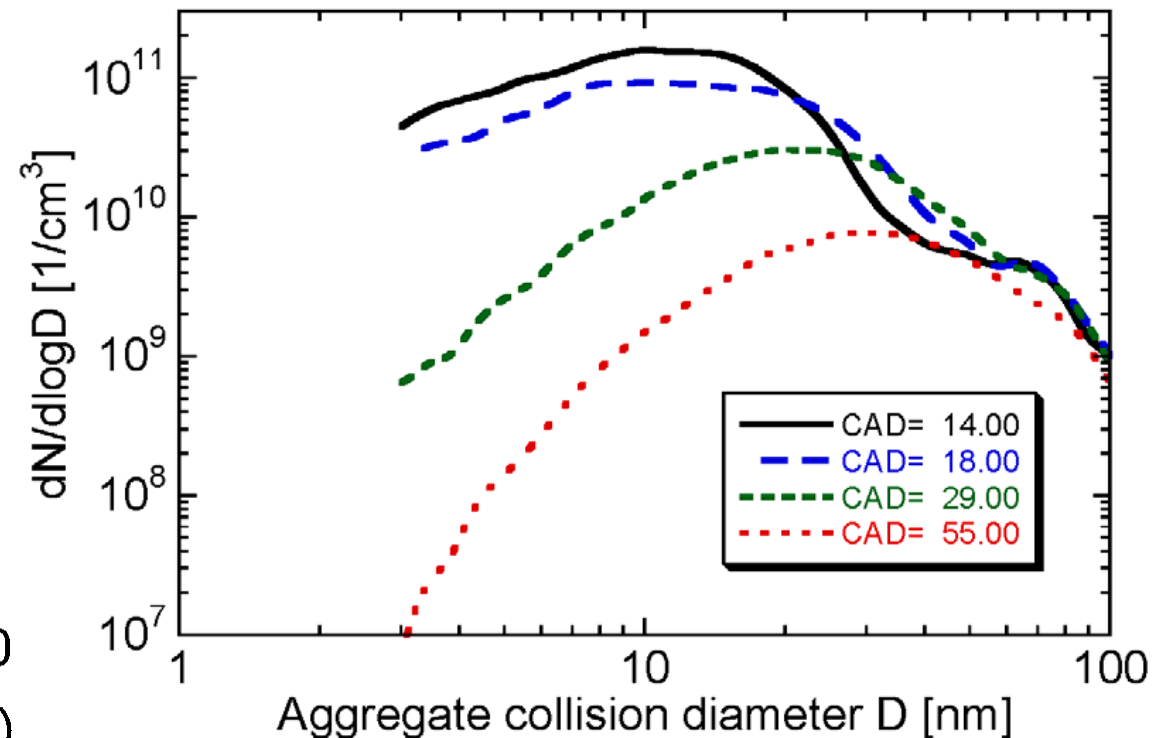


# Aggregate size distributions (II)

## Experiment

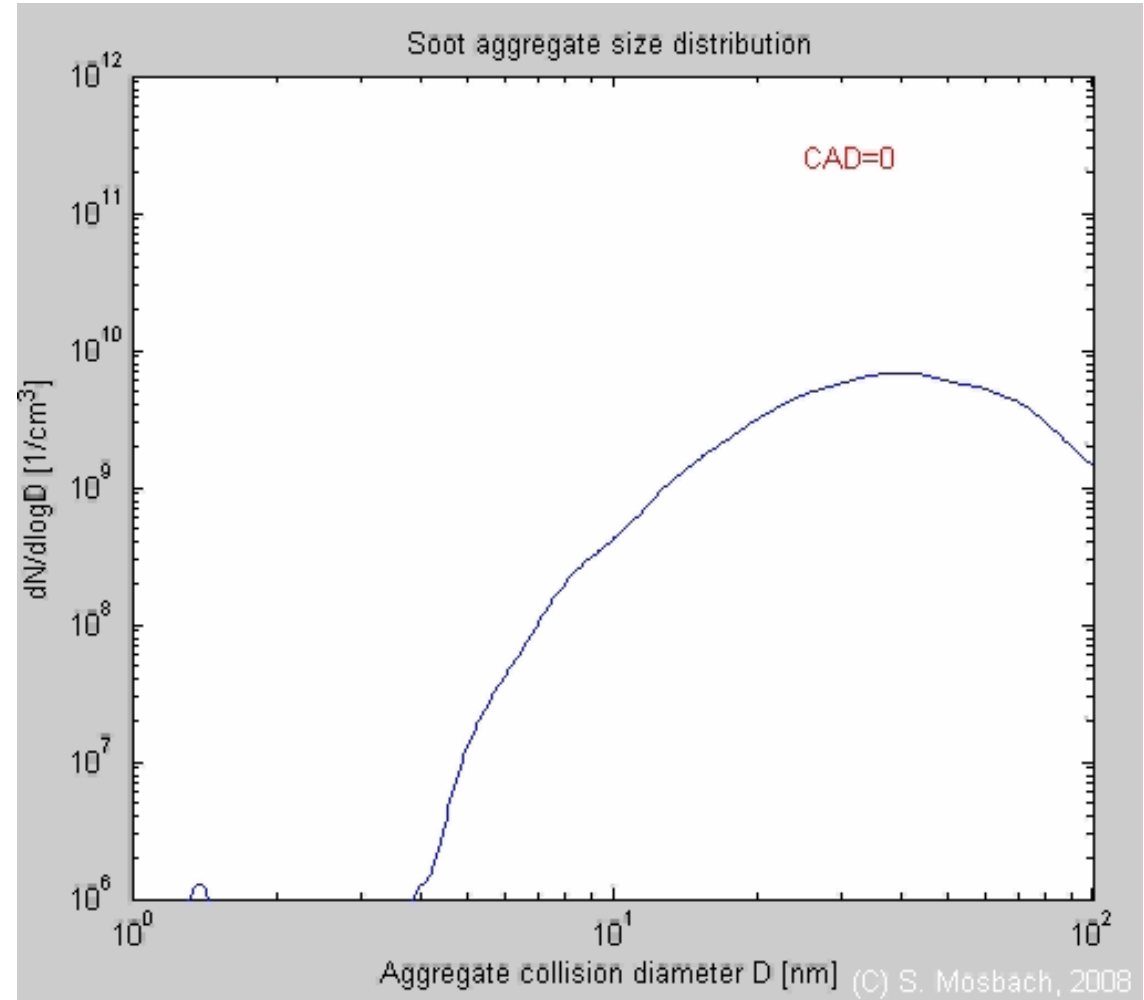
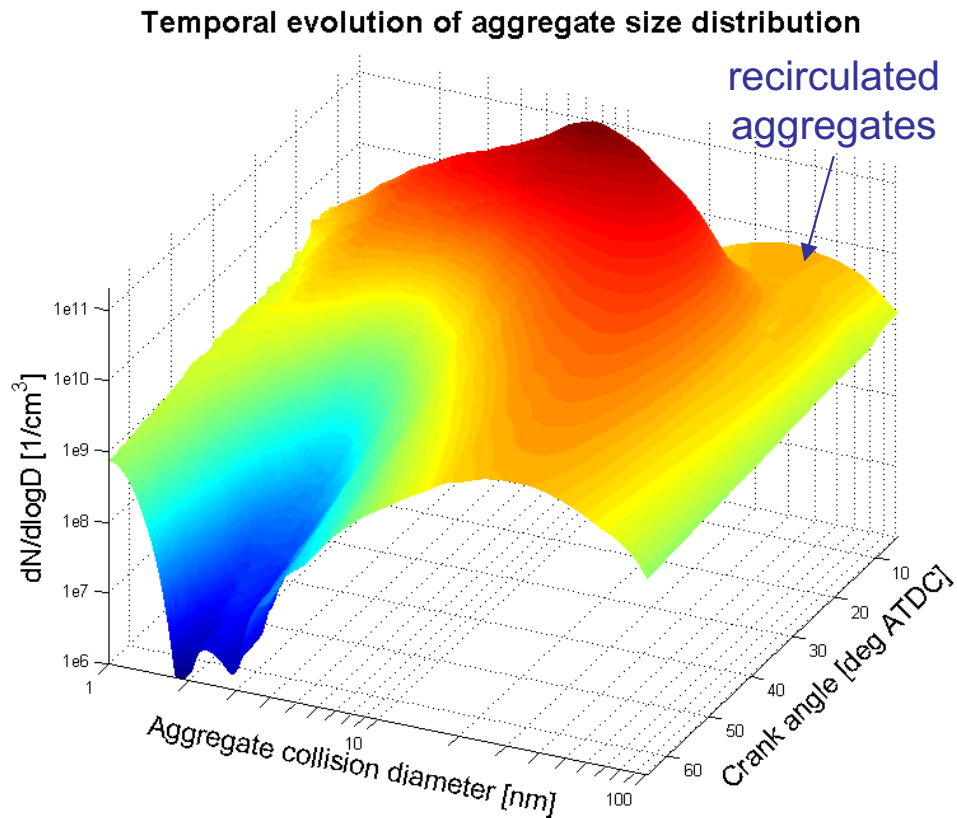


## Simulation



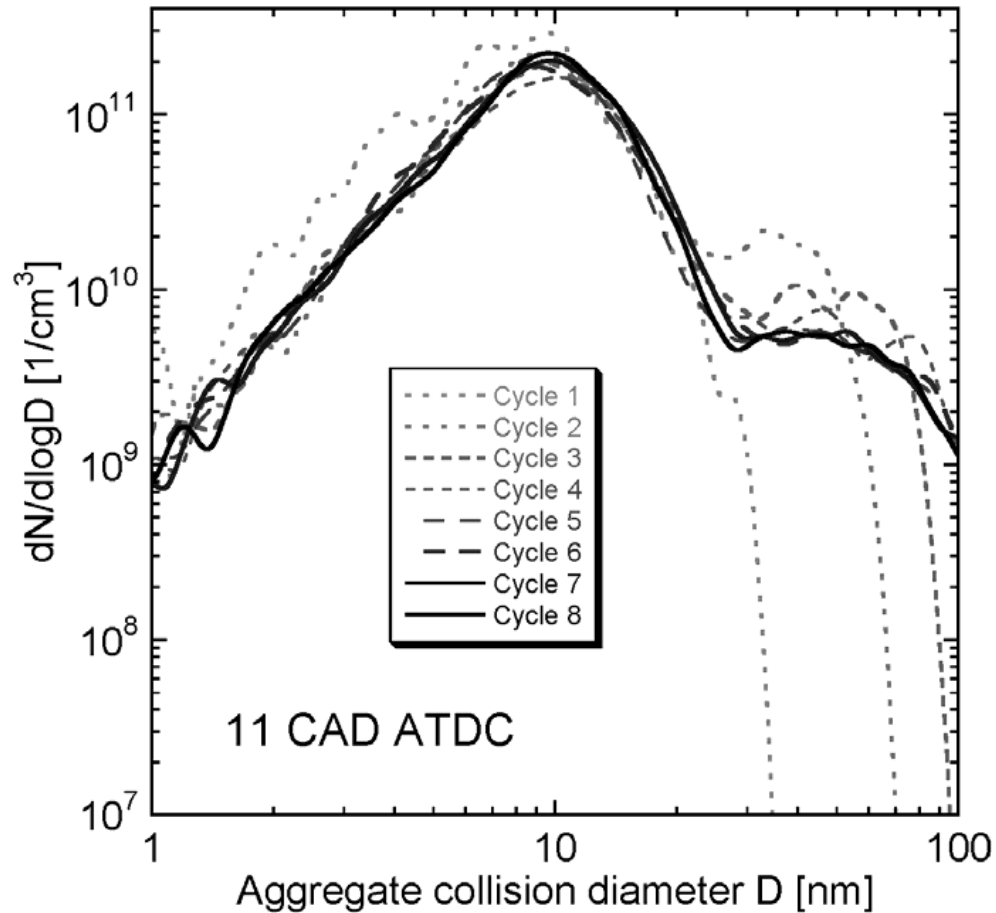
# Aggregate size distributions (III)

## Simulation

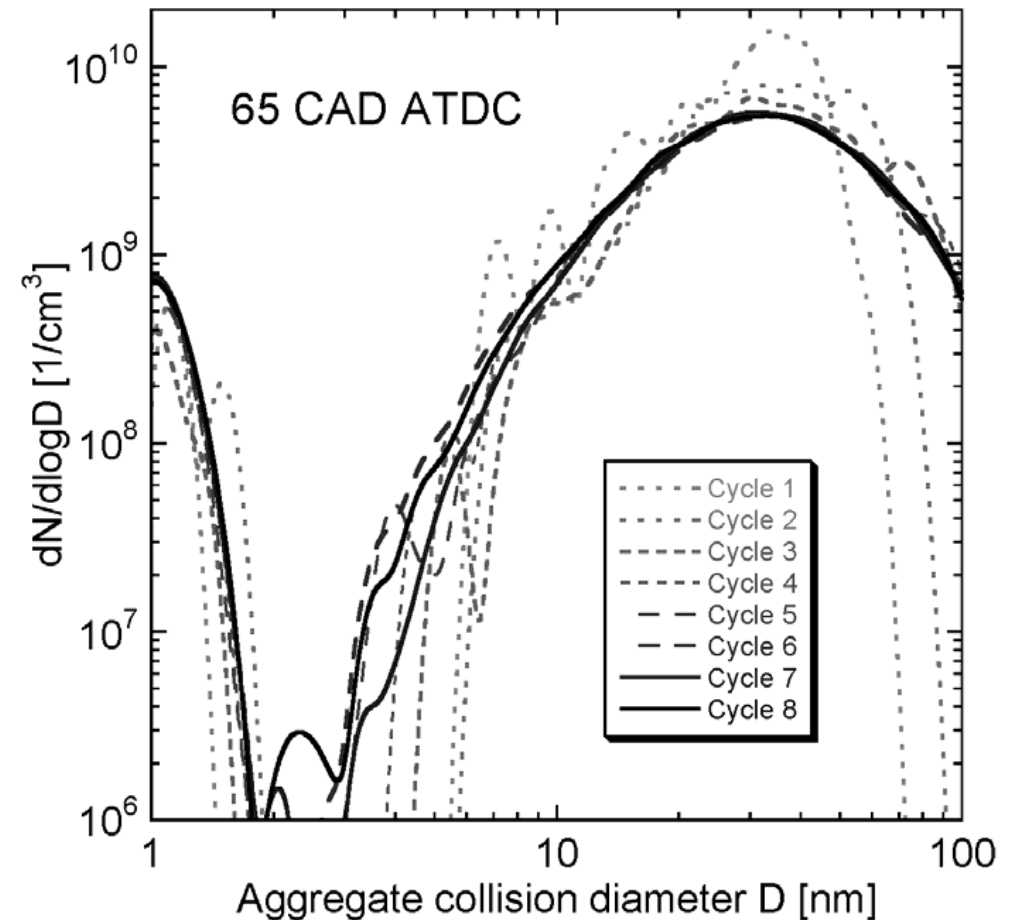


# Role of EGR

Simulation

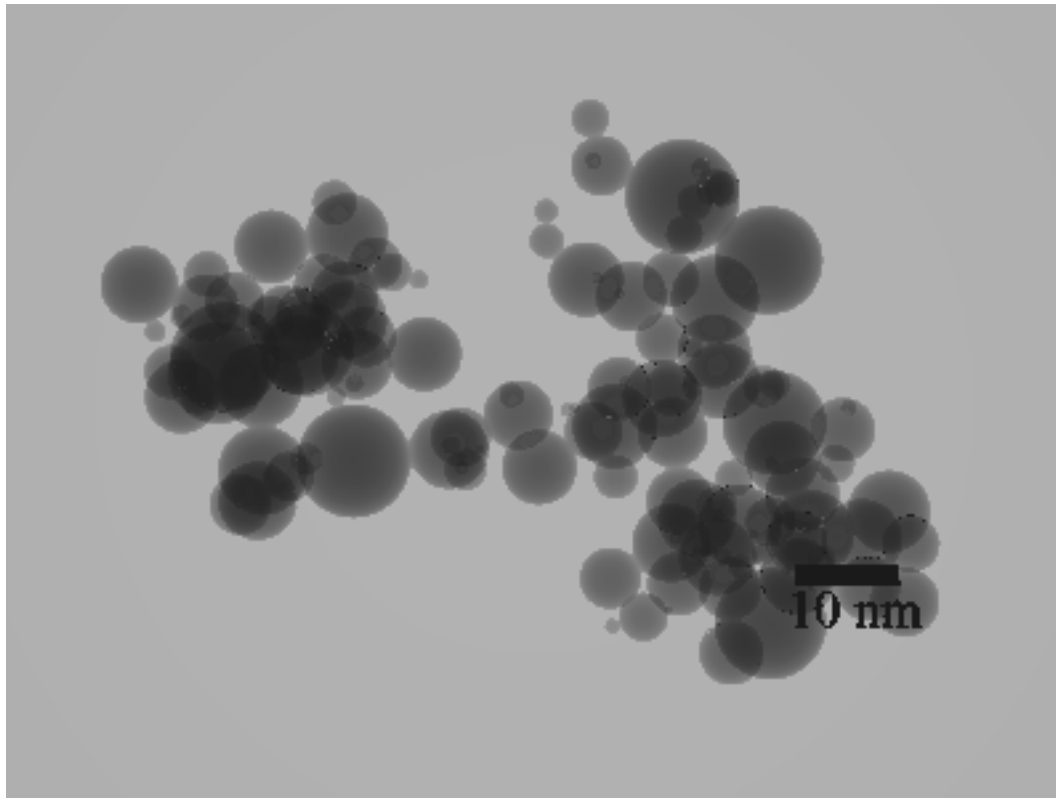


Simulation

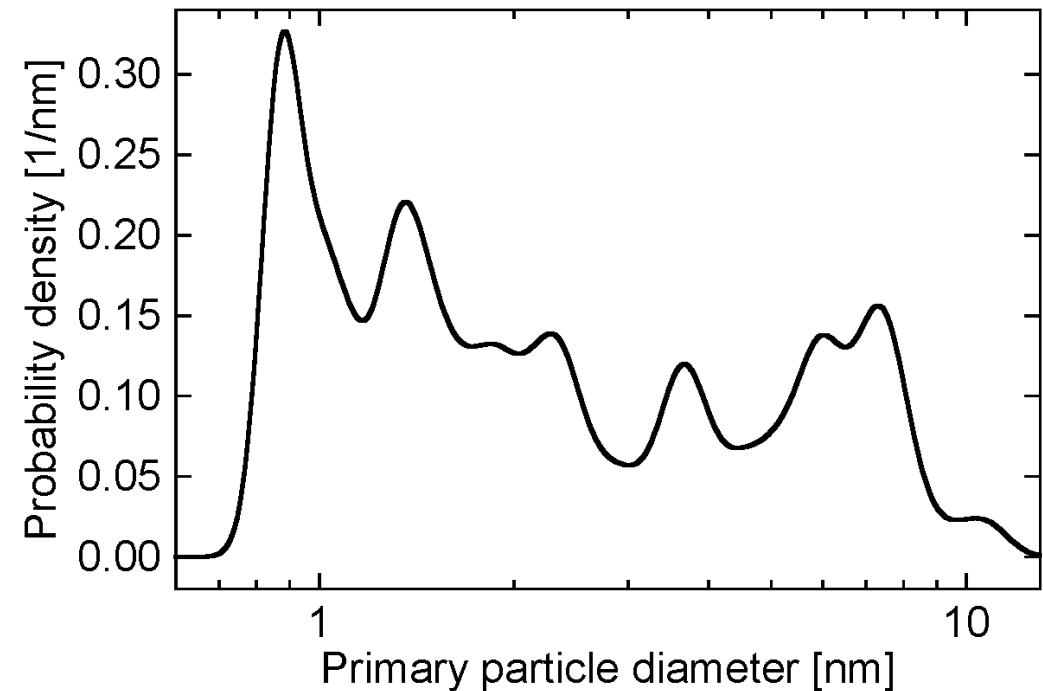


# Sampled aggregates (I)

Simulation



Simulation



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



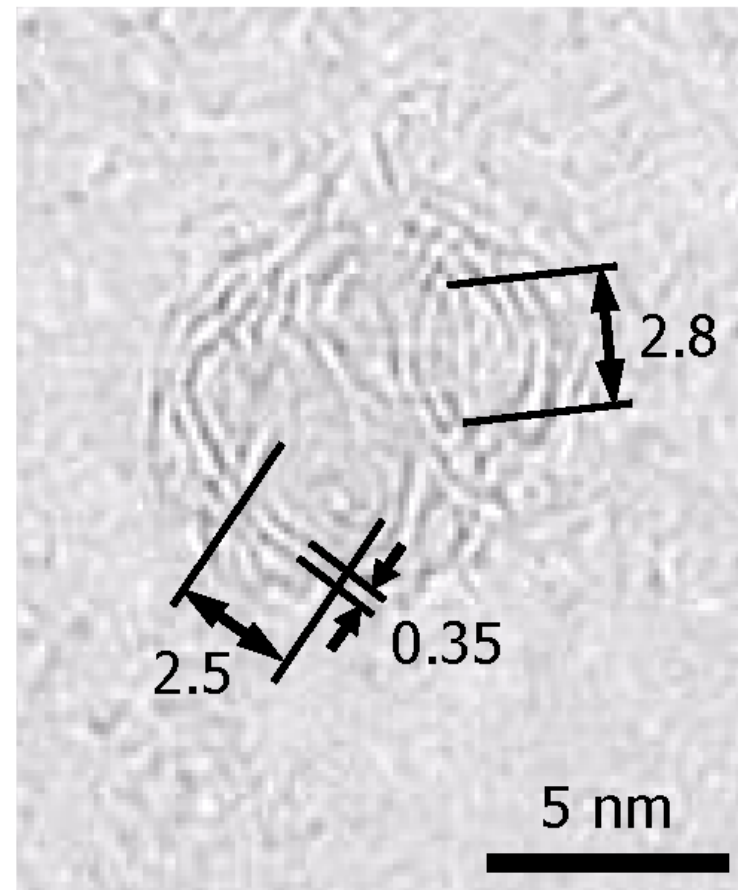
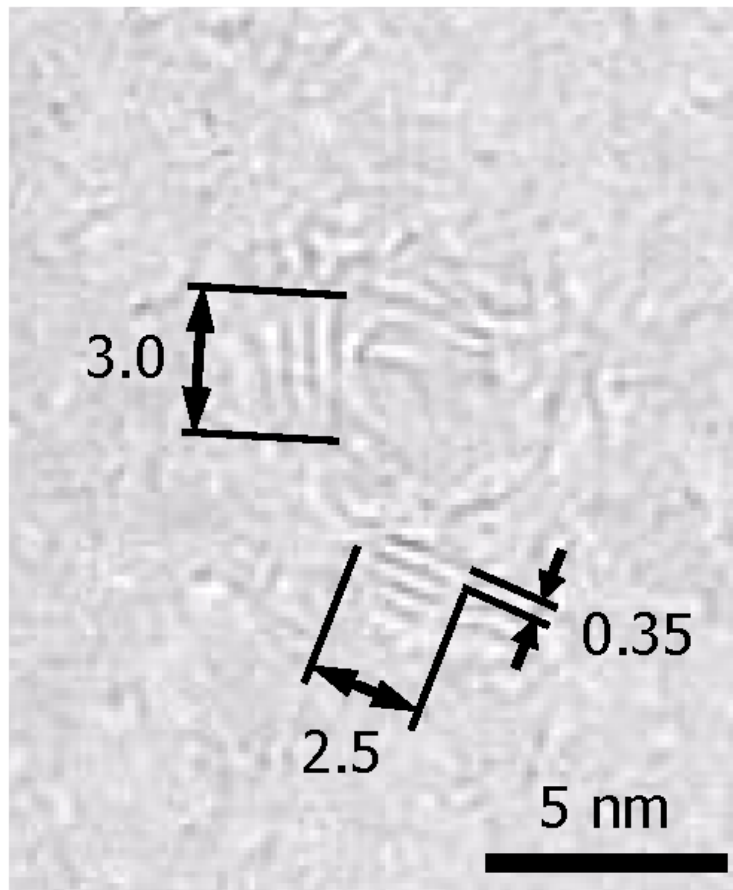
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# Sampled aggregates (II)

Experiment, sampled at  $\sim 16$  CAD ATDC

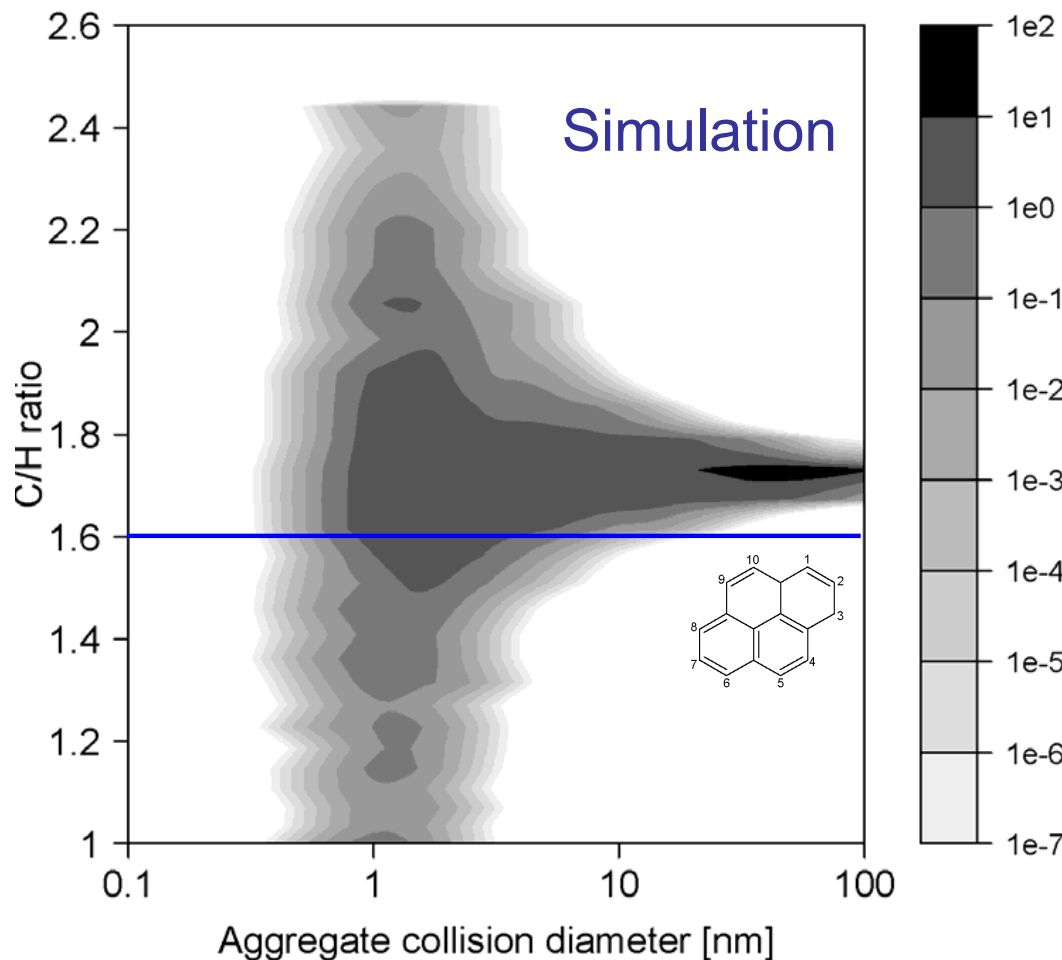




# Aggregate composition pdfs (I)

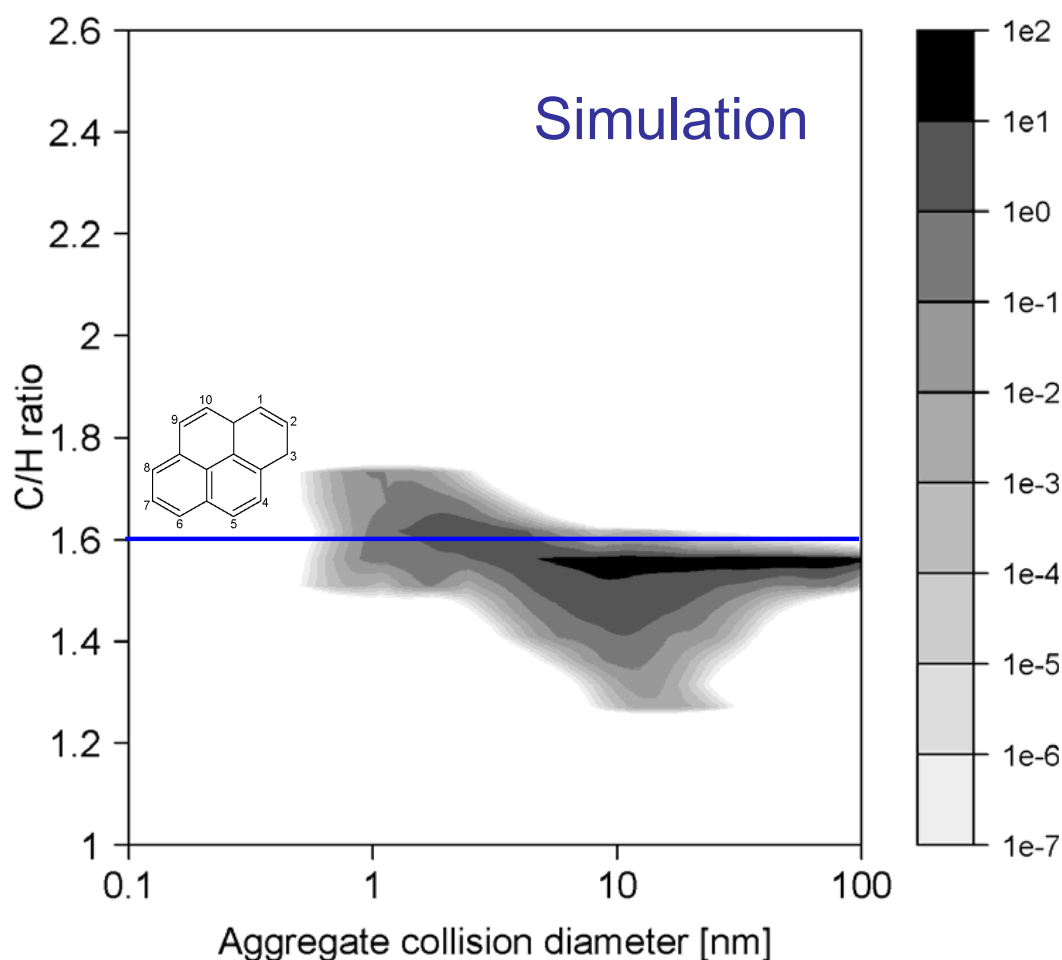
large inception rate

CAD = 11.4



large condensation rate

CAD = 11.4



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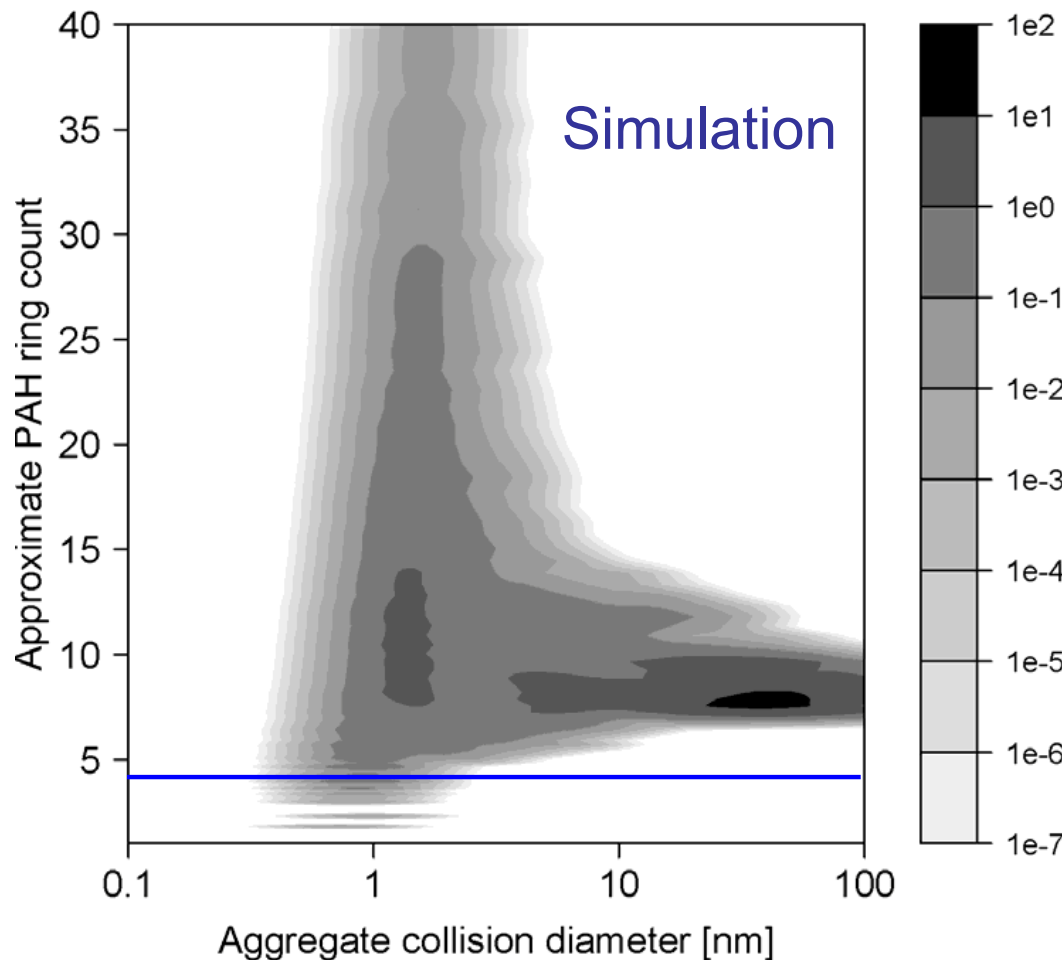
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# Aggregate composition pdfs (II)

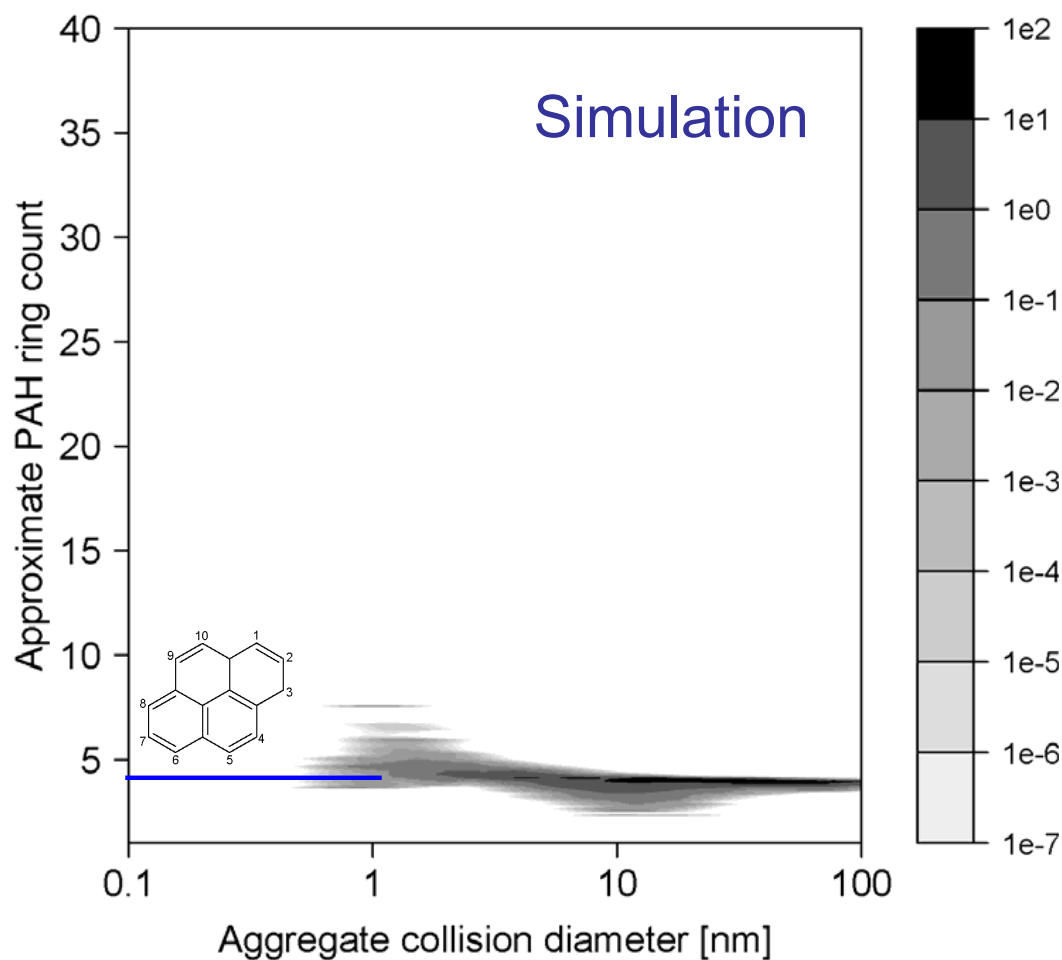
large inception rate

CAD = 11.4



large condensation rate

CAD = 11.4



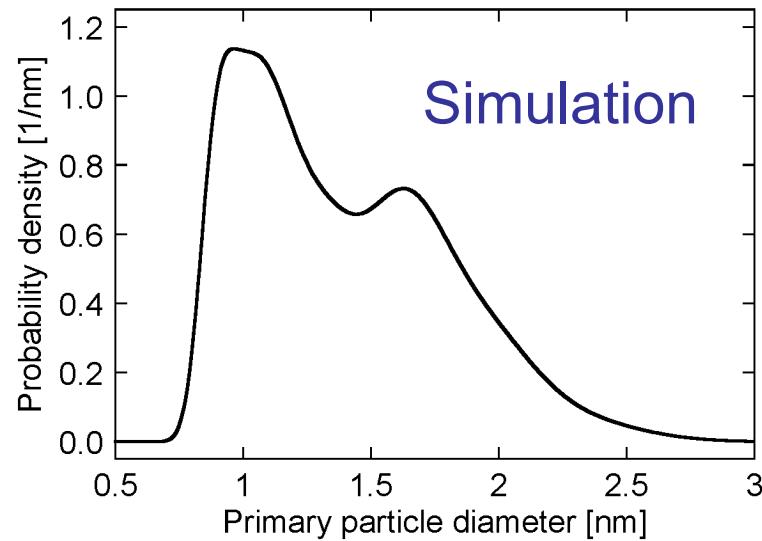
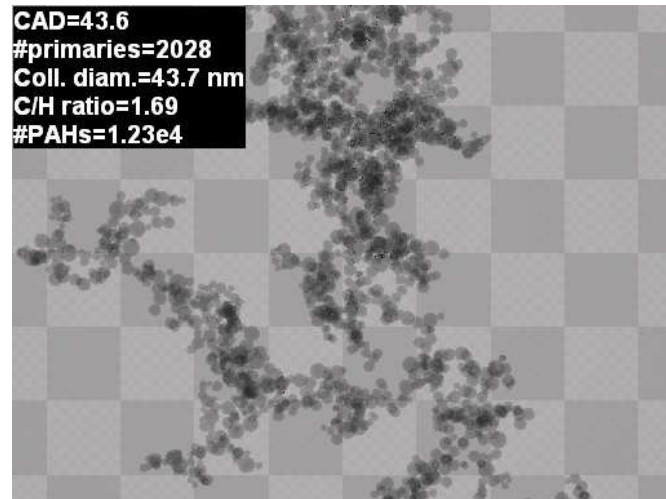
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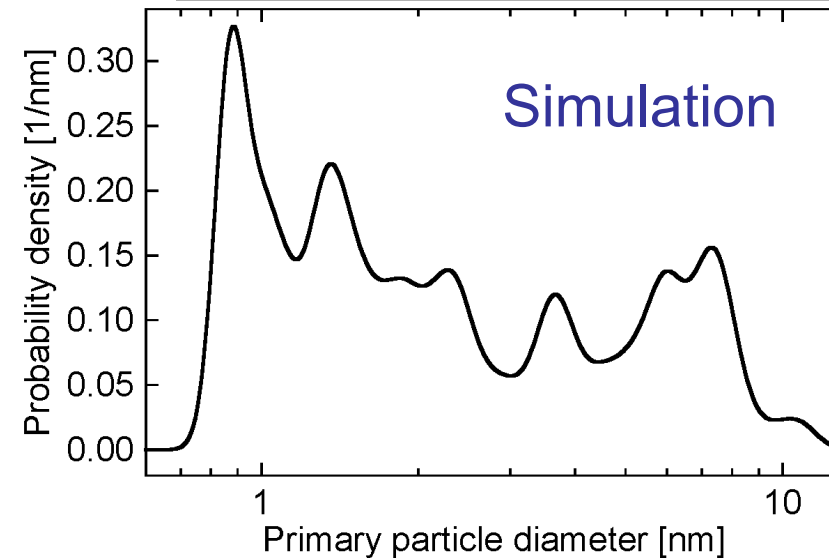
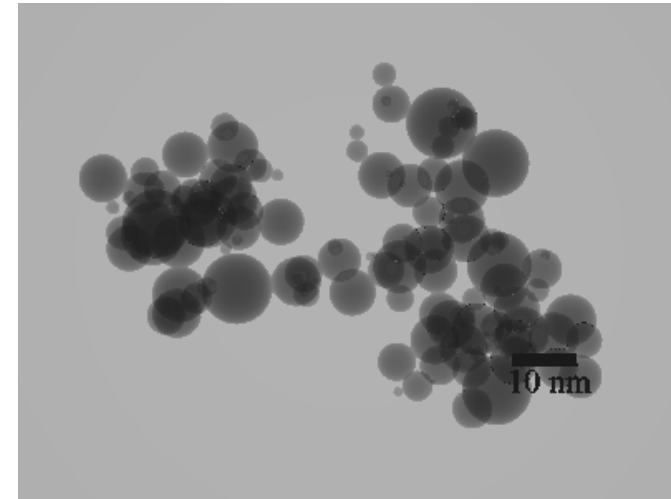


# Inception vs. condensation

large inception rate



large condensation rate



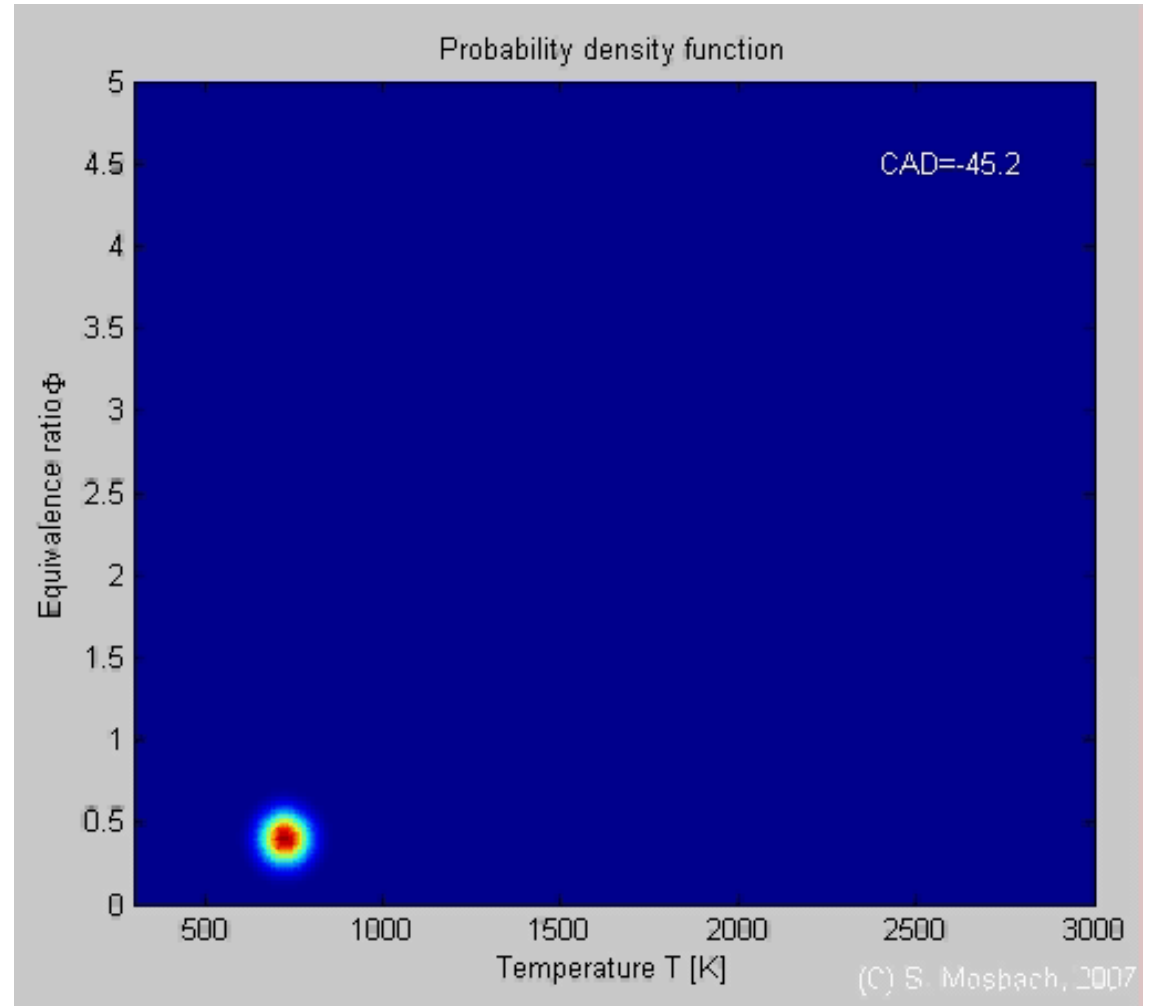
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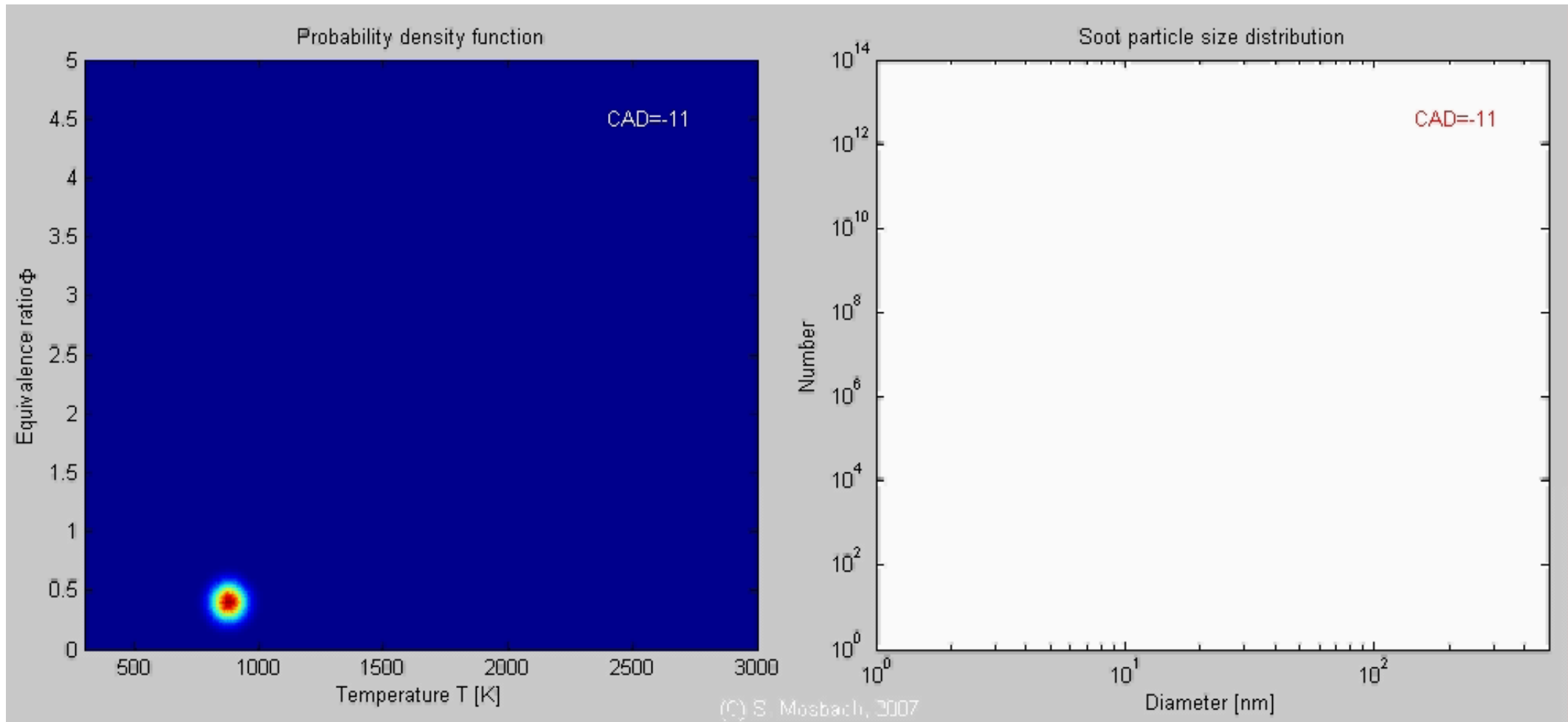
# Future engine soot models (I)

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



# Future engine soot models (II)

Soot formation in a partially stratified HCCI engine:



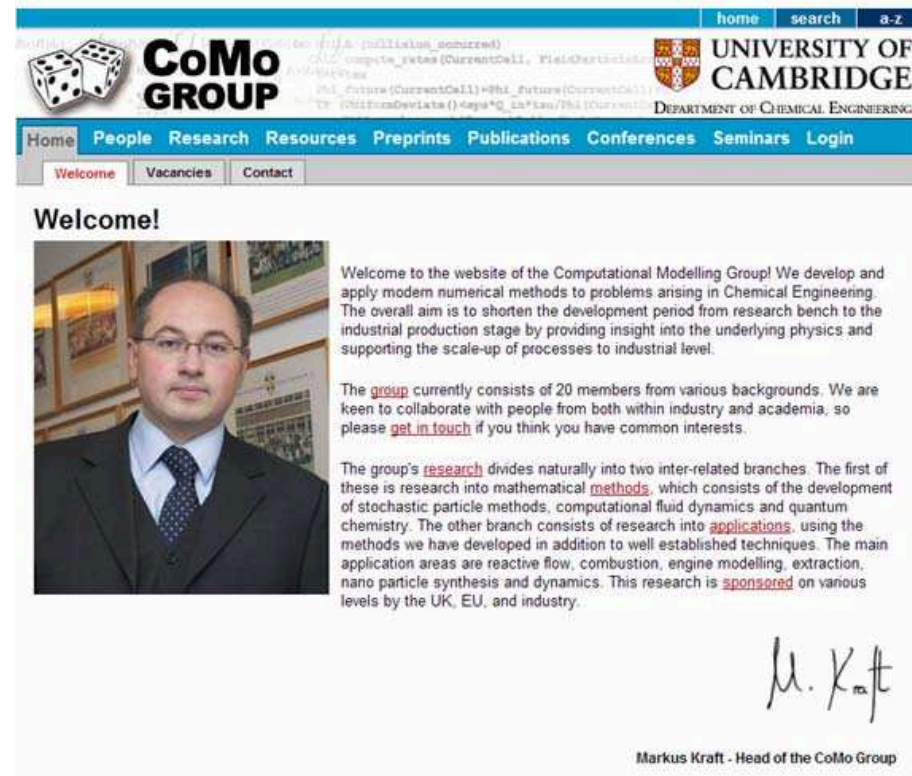
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# Thank you!

## Please visit our website:



The screenshot shows the homepage of the CoMo Group website. At the top, there is a navigation bar with links for 'home', 'search', and 'a-z'. Below this is the CoMo Group logo, which consists of two dice and the text 'CoMo GROUP'. To the right of the logo is the University of Cambridge logo and the text 'UNIVERSITY OF CAMBRIDGE' and 'DEPARTMENT OF CHEMICAL ENGINEERING'. Below the navigation bar is a menu with links for 'Home', 'People', 'Research', 'Resources', 'Preprints', 'Publications', 'Conferences', 'Seminars', and 'Login'. Below the menu is a 'Welcome' section with a photo of Markus Kraft, a man in a suit and glasses. To the right of the photo is a welcome message: 'Welcome to the website of the Computational Modelling Group! We develop and apply modern numerical methods to problems arising in Chemical Engineering. The overall aim is to shorten the development period from research bench to the industrial production stage by providing insight into the underlying physics and supporting the scale-up of processes to industrial level.' Below the welcome message is a paragraph about the group: 'The group currently consists of 20 members from various backgrounds. We are keen to collaborate with people from both within industry and academia, so please [get in touch](#) if you think you have common interests.' Below that is a paragraph about the group's research: 'The group's [research](#) divides naturally into two inter-related branches. The first of these is research into mathematical [methods](#), which consists of the development of stochastic particle methods, computational fluid dynamics and quantum chemistry. The other branch consists of research into [applications](#), using the methods we have developed in addition to well established techniques. The main application areas are reactive flow, combustion, engine modelling, extraction, nano particle synthesis and dynamics. This research is [sponsored](#) on various levels by the UK, EU, and industry.' At the bottom right of the page is a signature of Markus Kraft and the text 'Markus Kraft - Head of the CoMo Group'.

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