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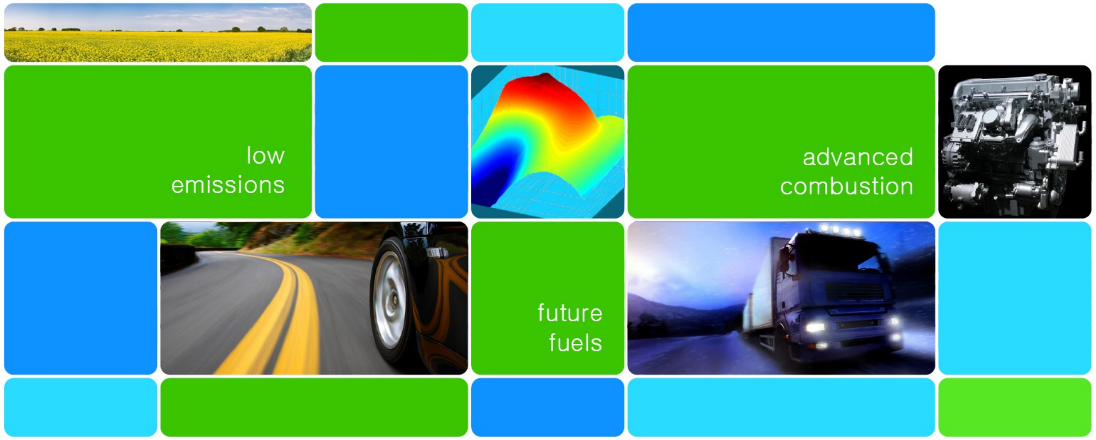


# Evolution of Particle Size Distribution within the Engine Exhaust and Aftertreatment System


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## content

What do we need to simulate PM emissions from diesel engines?

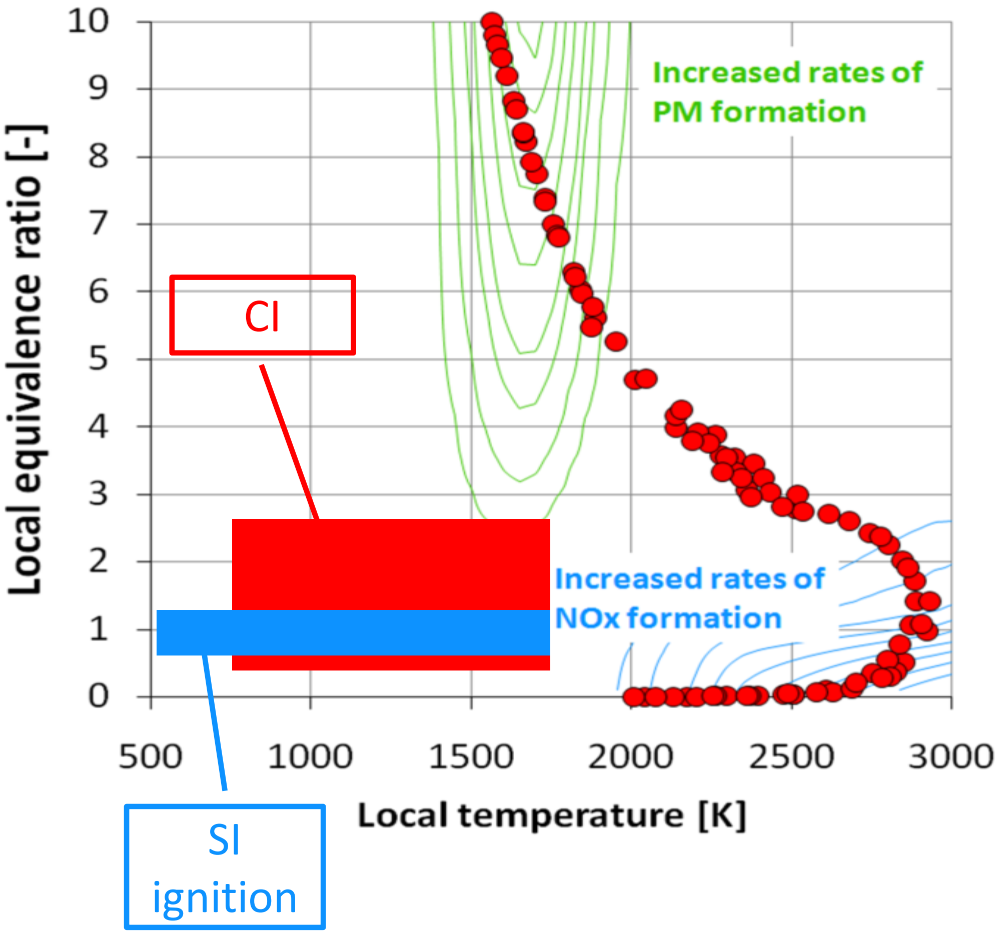
Techniques to mitigate in-cylinder PM formation

- injection timing
- split ratios
- fuel
- EGR

Exhaust and aftertreatment simulations

- model
- Exhaust duct
- DOC
- Parametric investigations
- next steps

# PM from IC engines




Thermodynamics

- compression/ expansion
- heat transfer

Mixture preparation

- injection events
- evaporation
- turbulent mixing

Combustion chemistry

- Ignition (delay)
- Flame propagation
- Local extinction
- (gas phase) emissions

Advanced particle model

- Soot formation & oxidation
- Coagulation

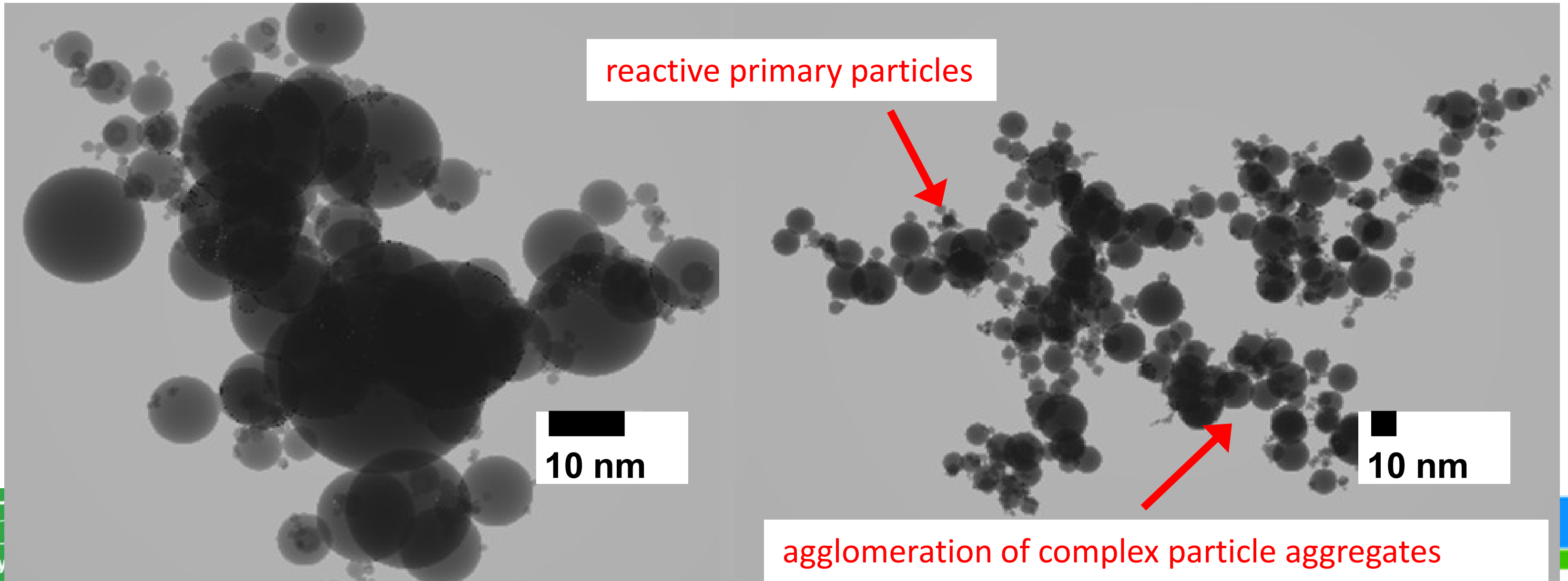
# principles of the model

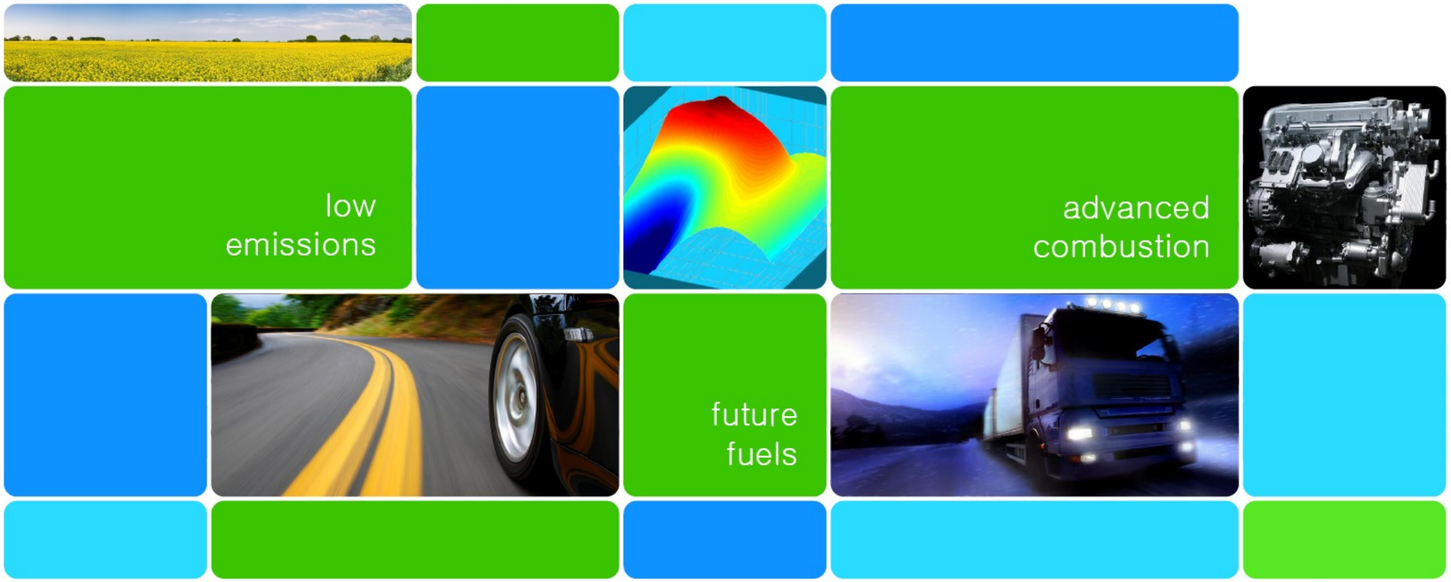
Stochastic Reactor Model

- Represent in-cylinder composition as 100 representative particles (fuel-air parcels)
- Heat transfer with walls
- Mixing
- Solution of detailed chemical kinetics (~200 species 1000 reactions)
- Injection

Particle Model

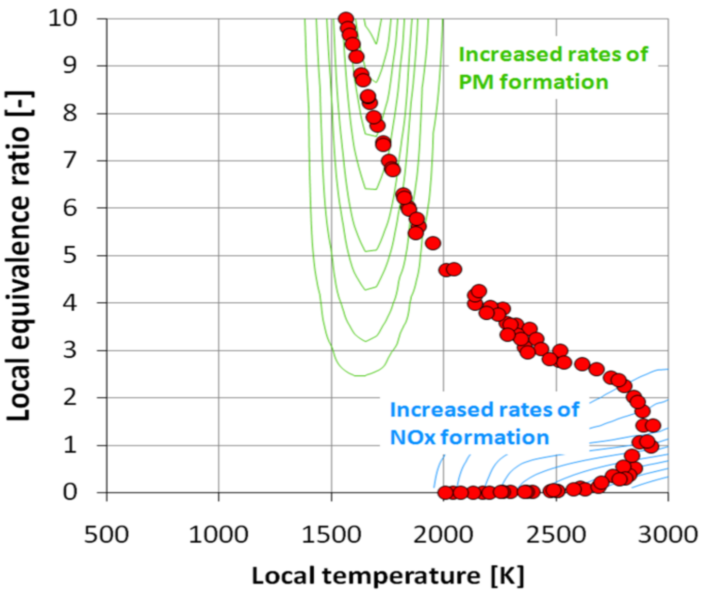
- soot chemistry includes a variety of unsaturated HCs and PAHs
- interaction of soot chemistry with the gas phase chemistry
- validation carried out in fuel-rich flame and engine experiments
- CPU time 6-90 mins/engine cycle






# In-cylinder events, mixture preparation, fuel oxidation and emission formation

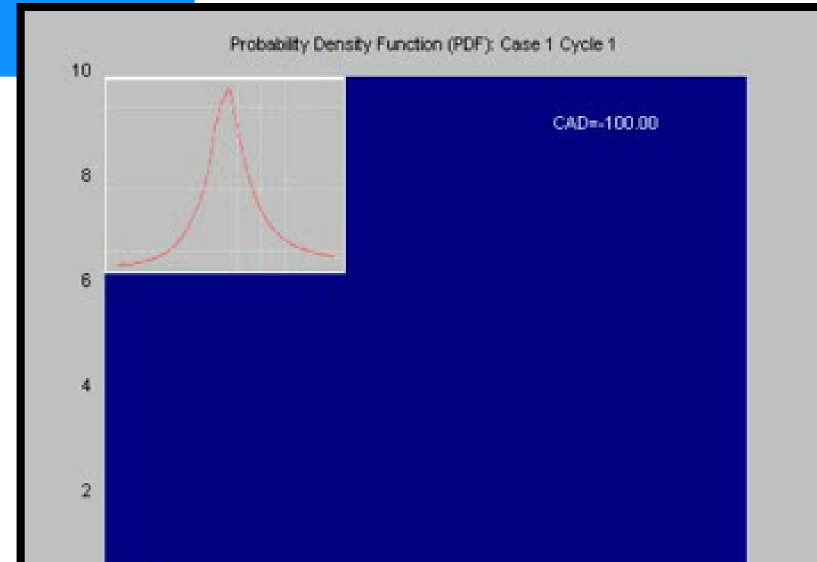
# conventional modes of com tion




| Mode | DISI | CIDI |
|---|---|---|
| SOI [aTDC] | -100 | -2 |
| EOI [aTDC] | -90 | 25 |
| C.R. | 11 | 15.0 |
| PIVC [bar] | 0.75 | 1.2 |
| TIVC [K] | 450 | 550 |
| Fuel | gasoline | diesel |
| Fuel [mg] | 10.0 | 10.0 |

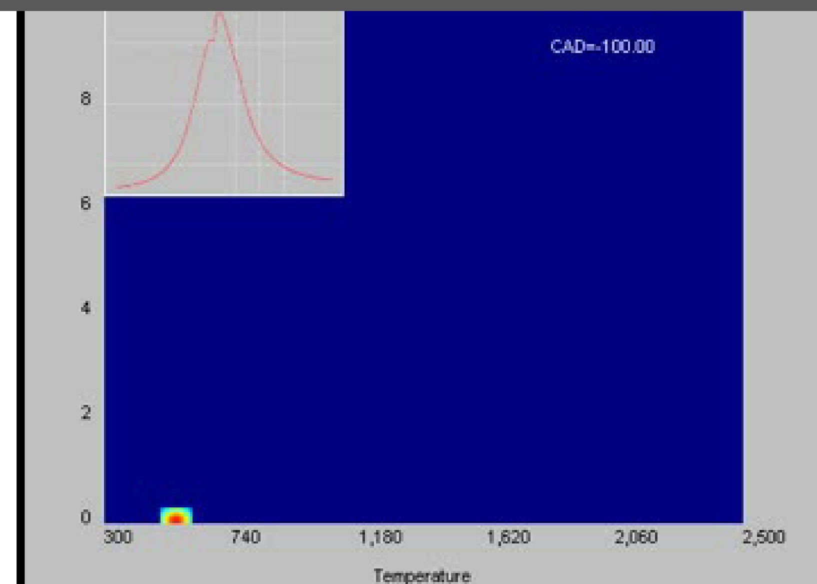
1500 RPM
2.62 BMEP
30% EGR

DISI

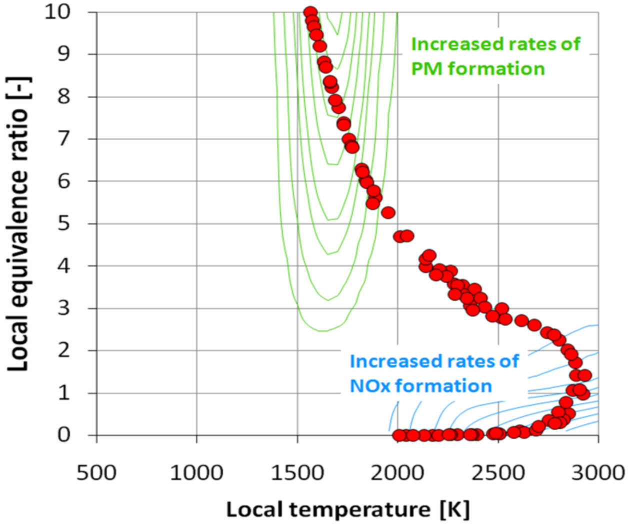



Animations available at http://www.cmclinnovations.com/products/srmsuite/phi-t-movies.html

CIDI

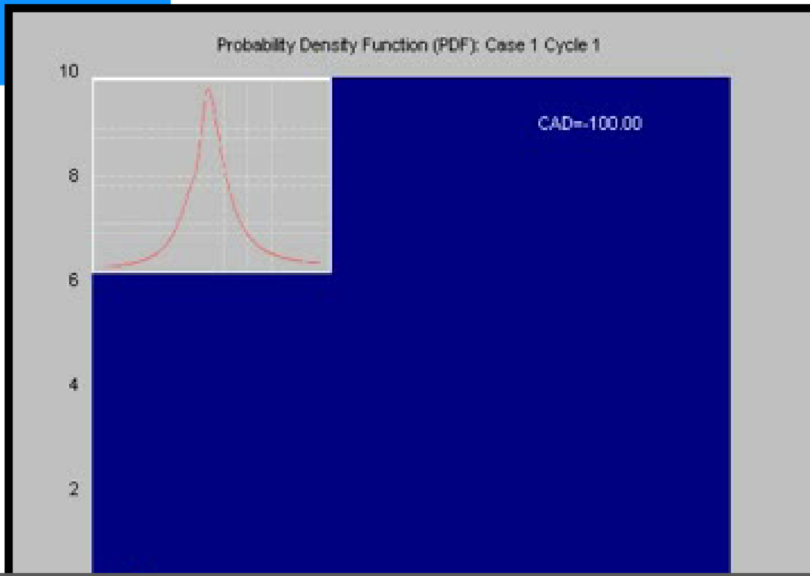


# more premixed combustion




| Mode | advanced | CIDI |
|---|---|---|
| SOI [aTDC] | -100 | -2 |
| EOI [aTDC] | -90 | 25 |
| C.R. | 15.0 | 15.0 |
| PIVC [bar] | 1.2 | 1.2 |
| TIVC [K] | 450 | 550 |
| Fuel | diesel | diesel |
| Fuel [mg] | 10.0 | 10.0 |

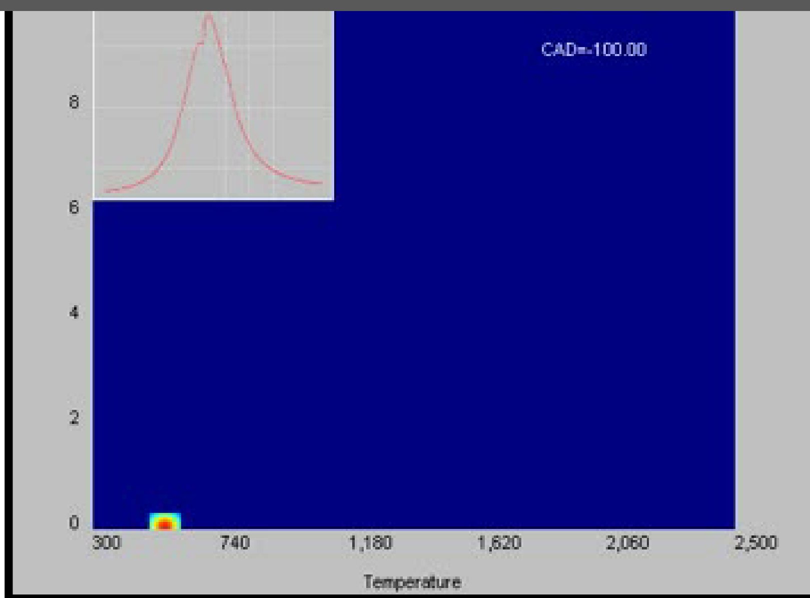
PPCI




1500 RPM
2.62 BMEP
30% EGR

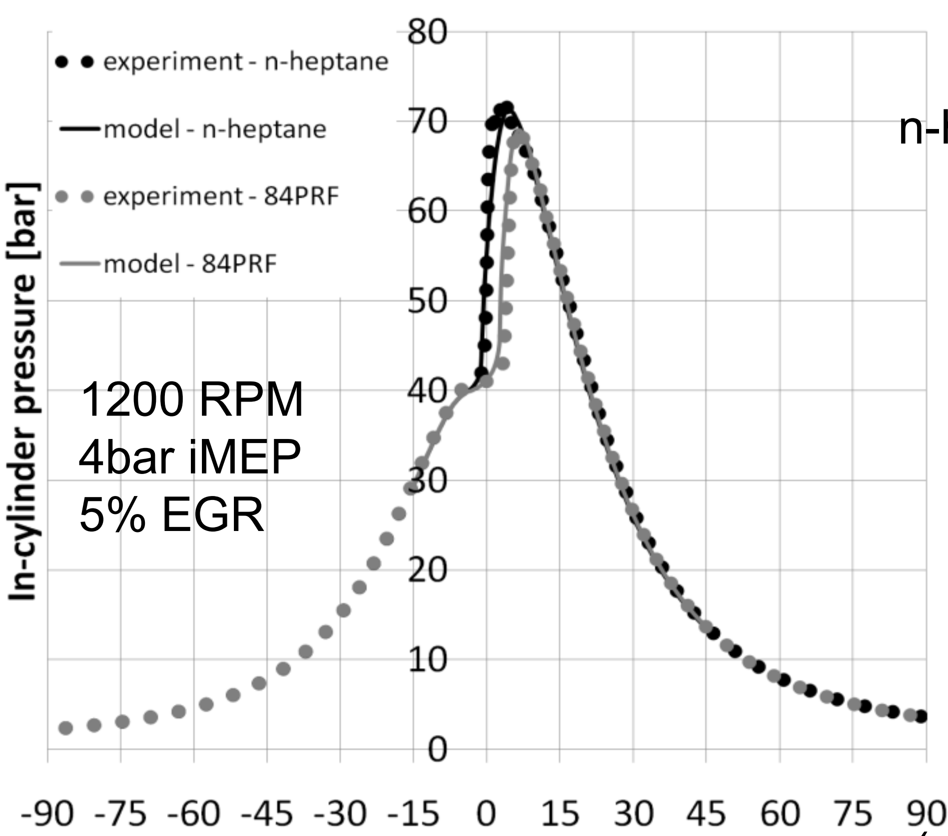
[Animations available at http://www.cmclinnovations.com/products/srmsuite/phi-t-movies.html](http://www.cmclinnovations.com/products/srmsuite/phi-t-movies.html)

CIDI



# impact of fuel: ignition resis ce

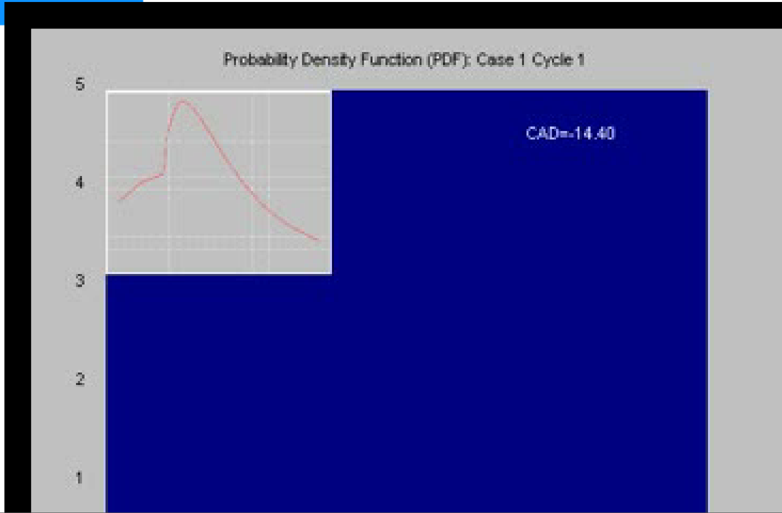
Results from SAE 2011-01-1184



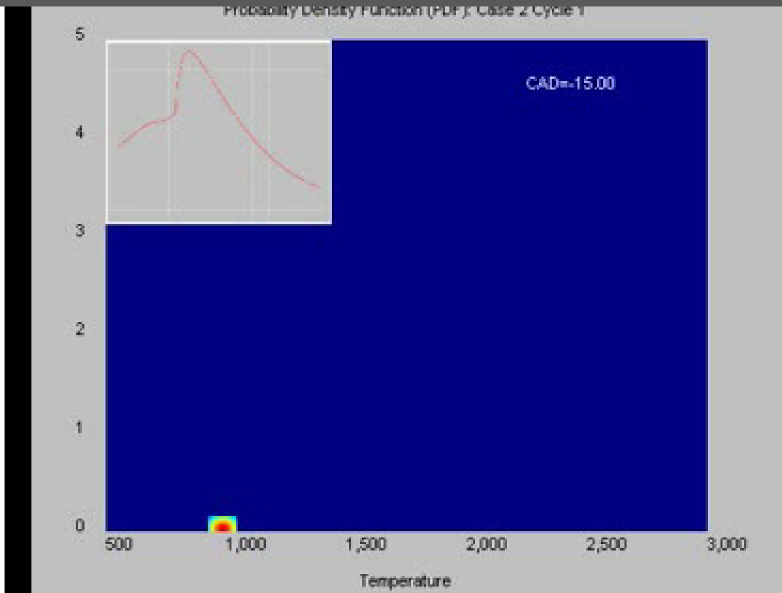

n-heptane (diesel)

84 PRF (gasoline)

| Fuel | Gasoline | Diesel |
|---|---|---|
| SOI [aTDC] | -8 | -8 |
| EOI [aTDC] | -4 | -4 |

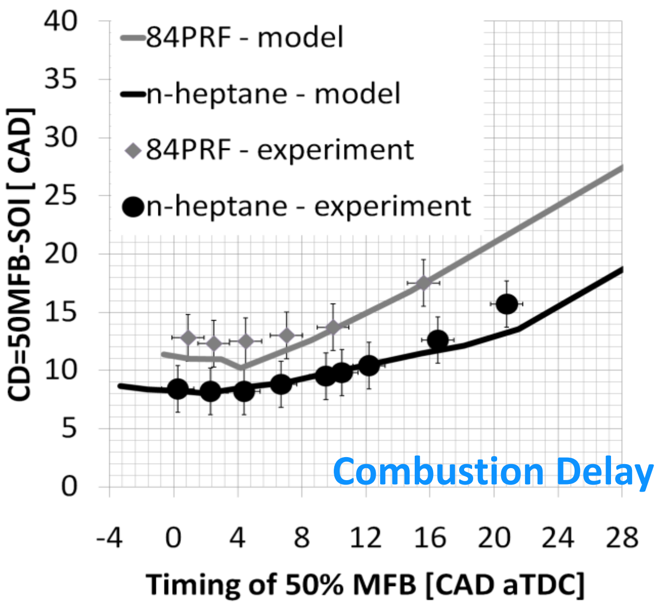


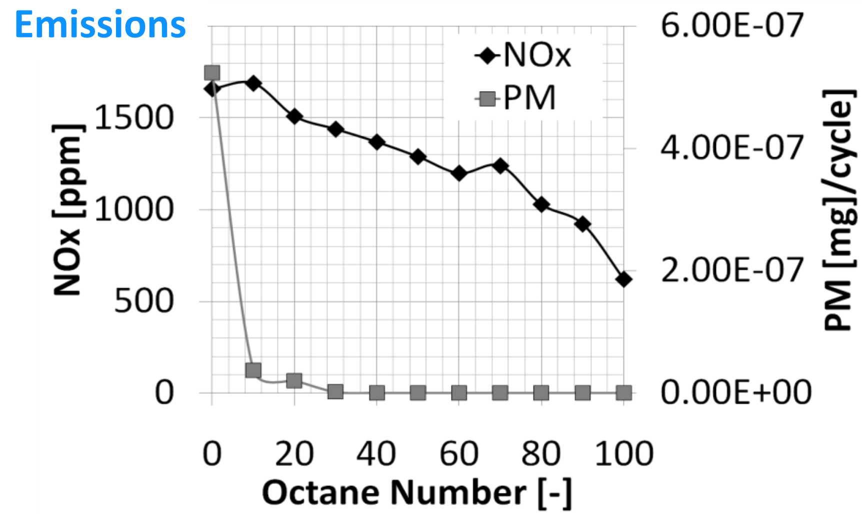

Animations available at http://www.cmclinnovations.com/products/srmsuite/phi-t-movies.html

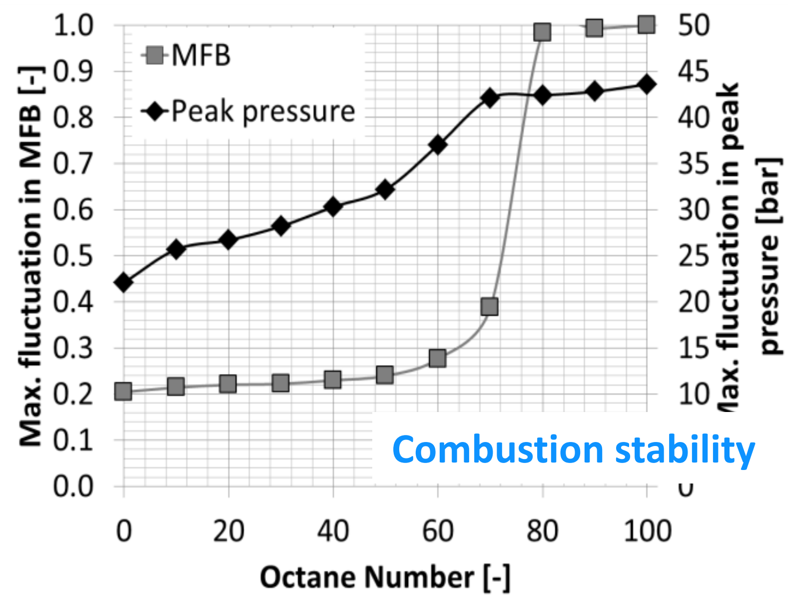


# ignition resistance

Results from SAE 2011-01-1184



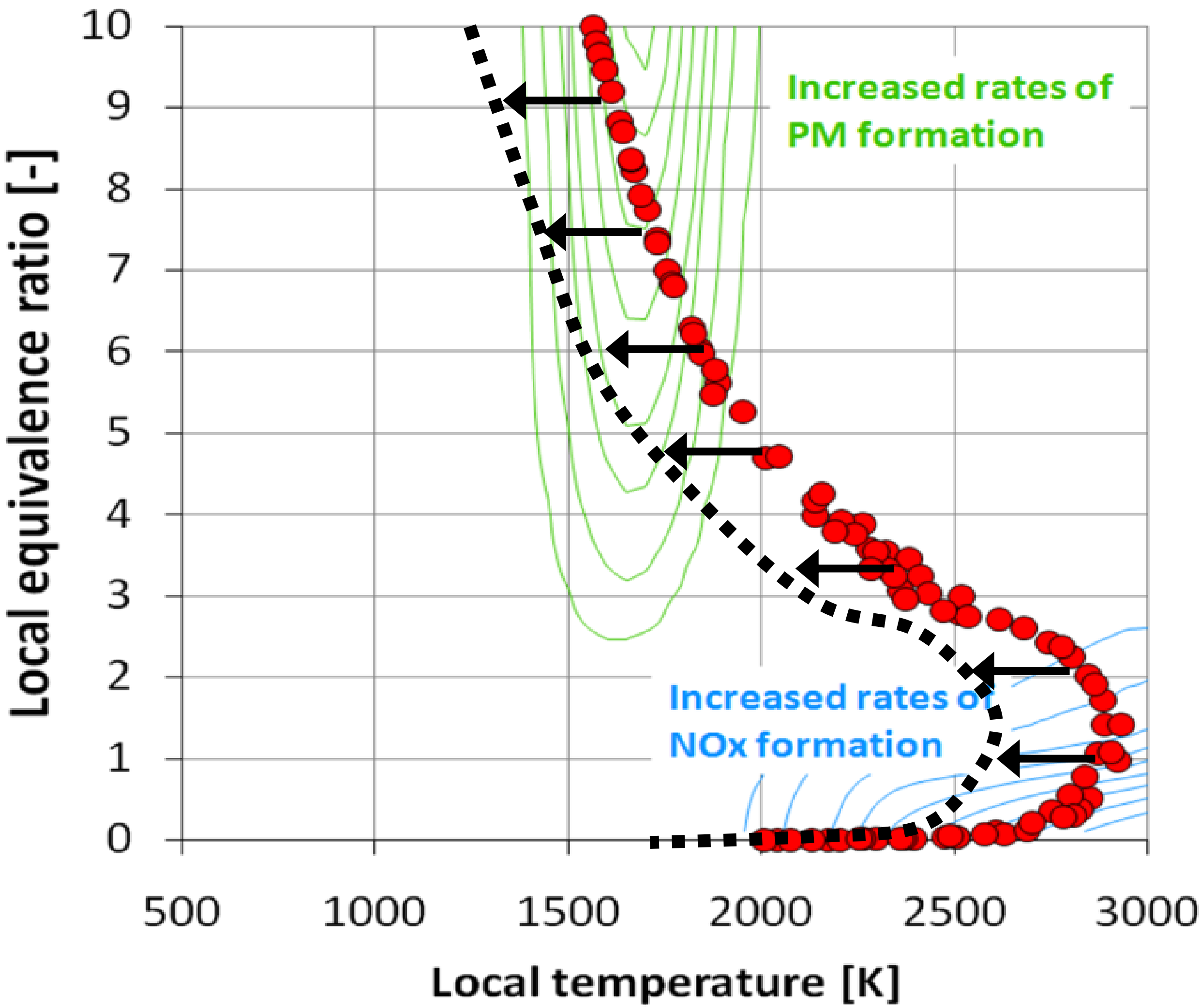




- For each fuel, injection timing optimised to achieve 50%MFB at 5CADaTDC

- Emissions
- Cycle-to-cycle variations

- **New fuel/engine optima**

# Impact of EGR



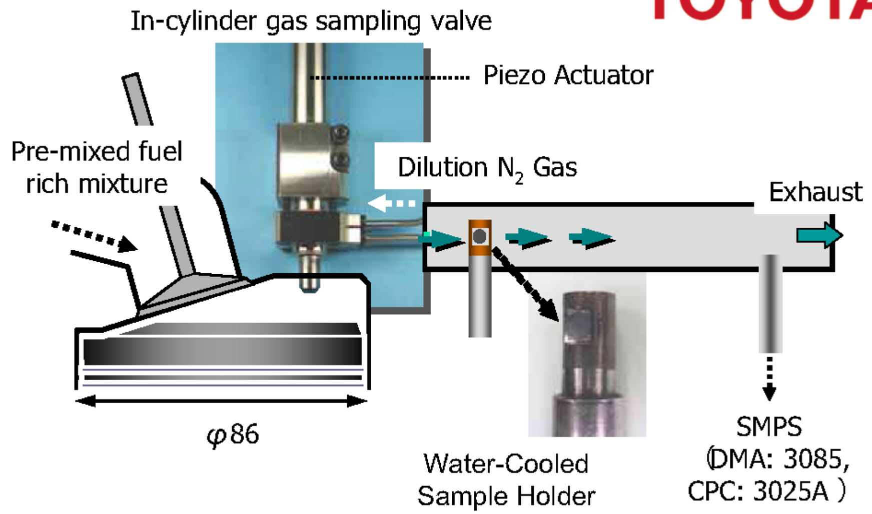

Lower combustion temperatures

…proved more interesting when considering PM formation

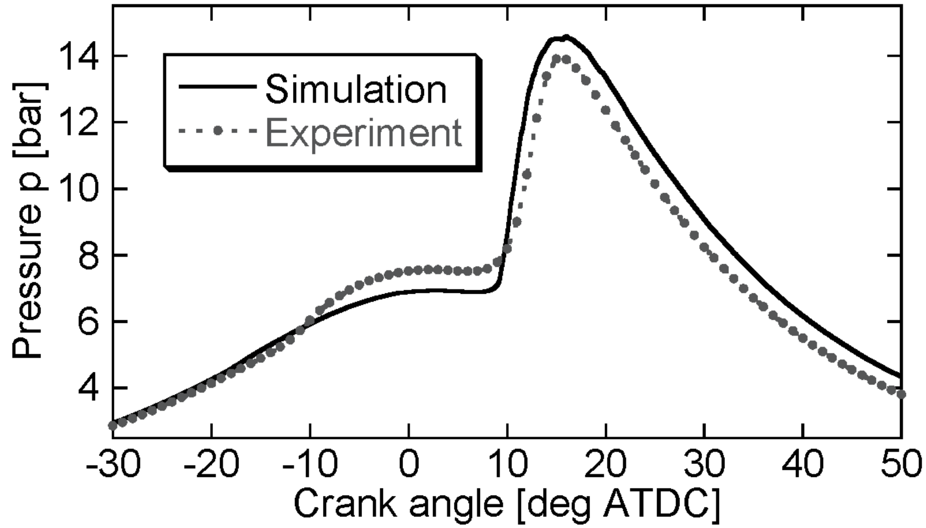
# Impact of EGR

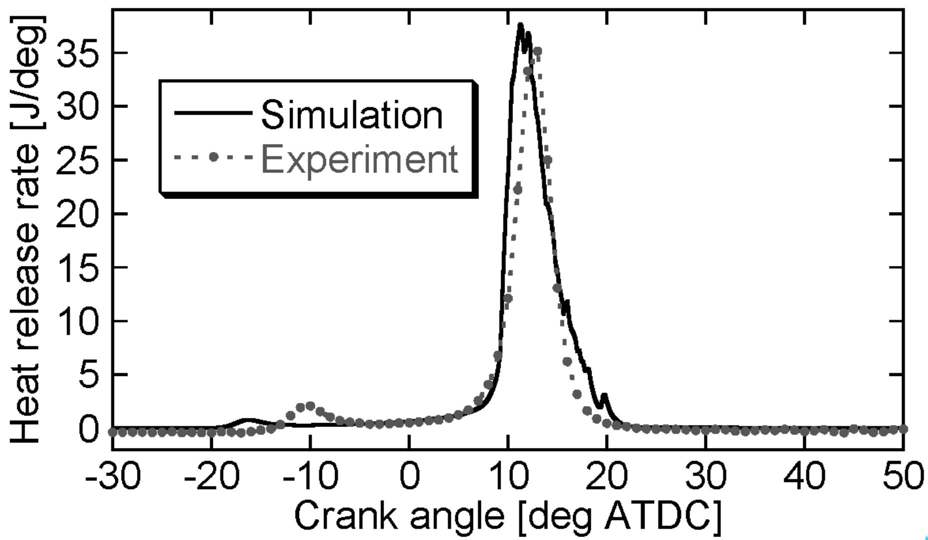
- HCCI, n-heptane
- Compression ratio 12
- Equivalence ratio 1.93
- Throttled, 20% EGR

TOYOTA




**Towards a detailed soot model for internal combustion engines**
***Combustion and Flame***, 156 (6), 1156-1165, 2009

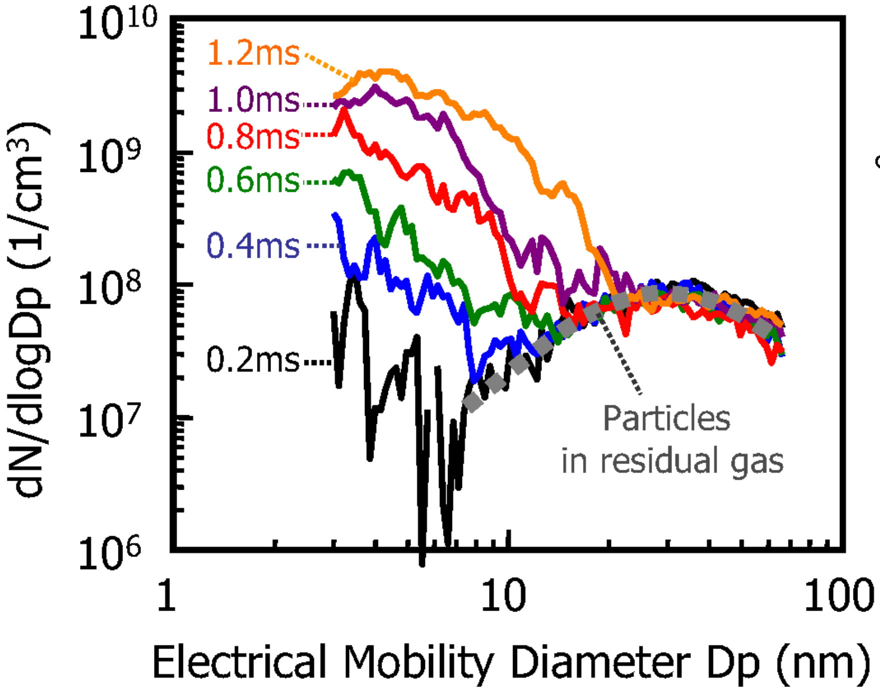


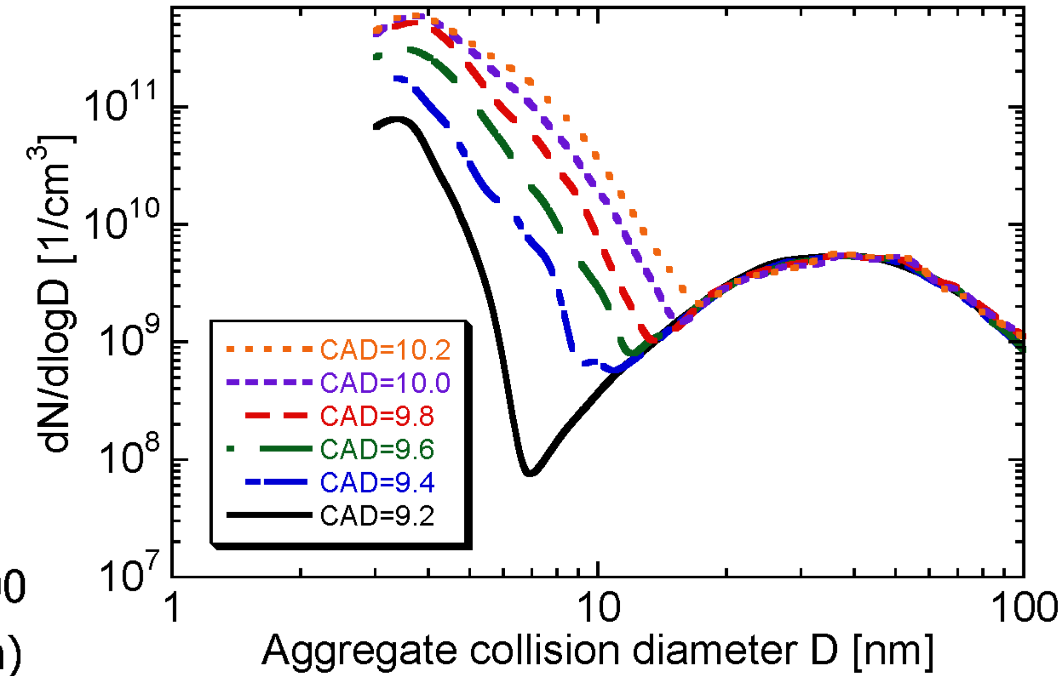
# aggregate size distribution e ution

**Towards a detailed soot model for internal combustion engines**
***Combustion and Flame***, 156 (6), 1156-1165, 2009

Experiment




Simulation



# Impact of EGR

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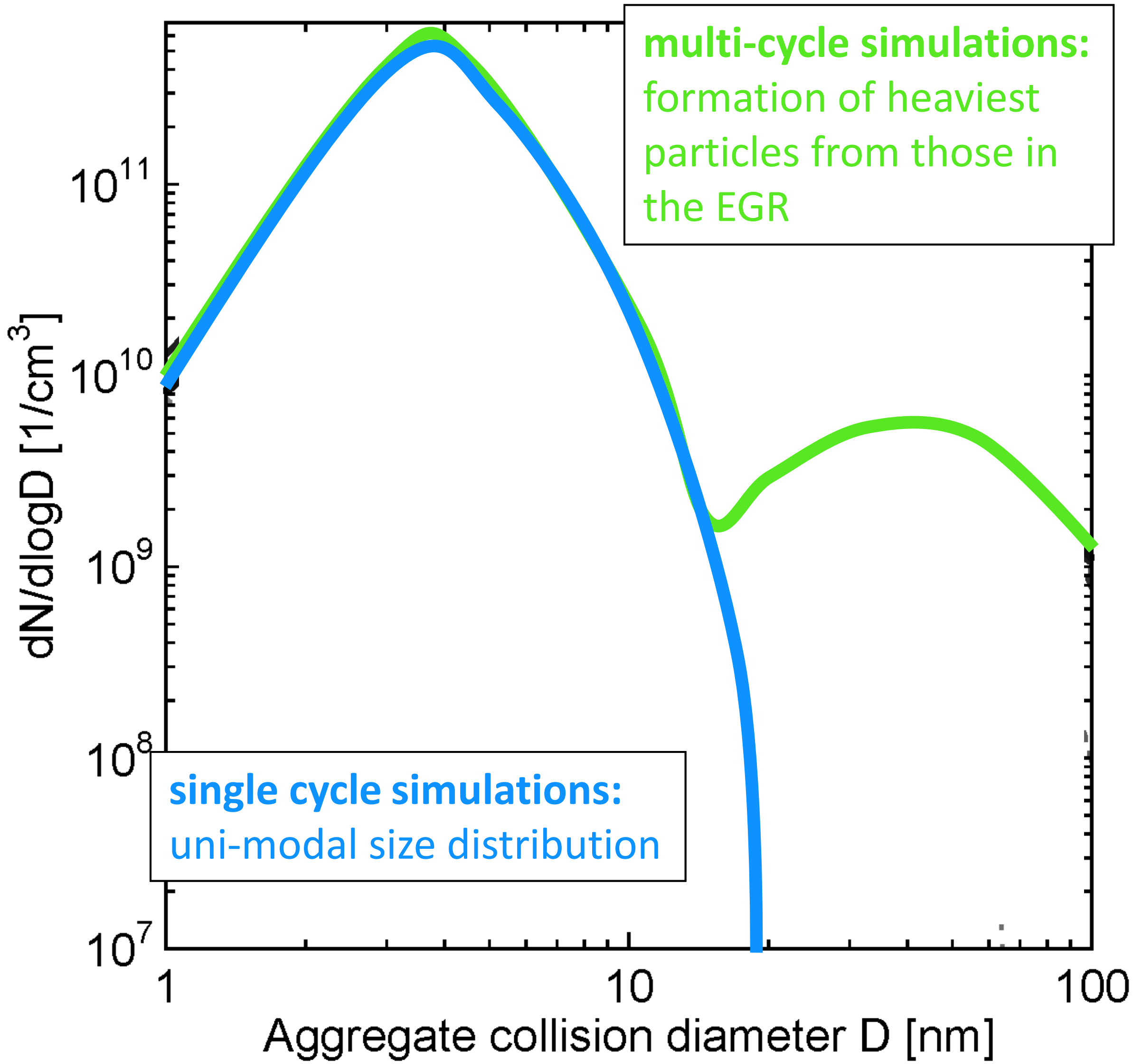
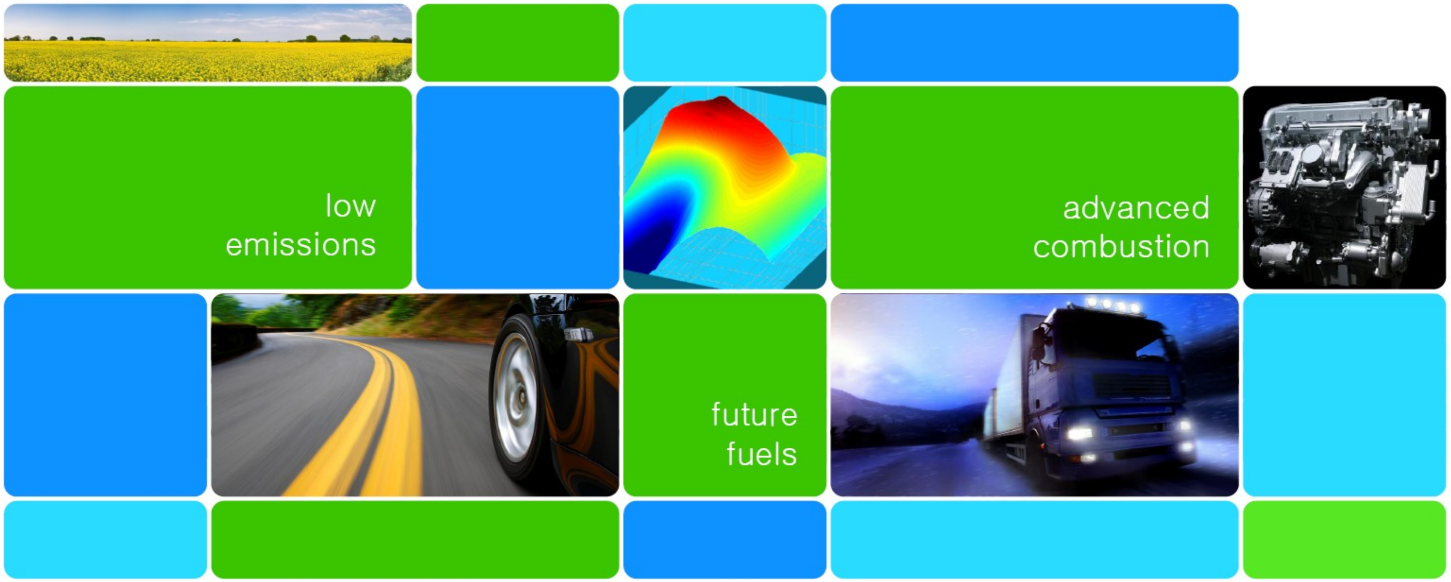
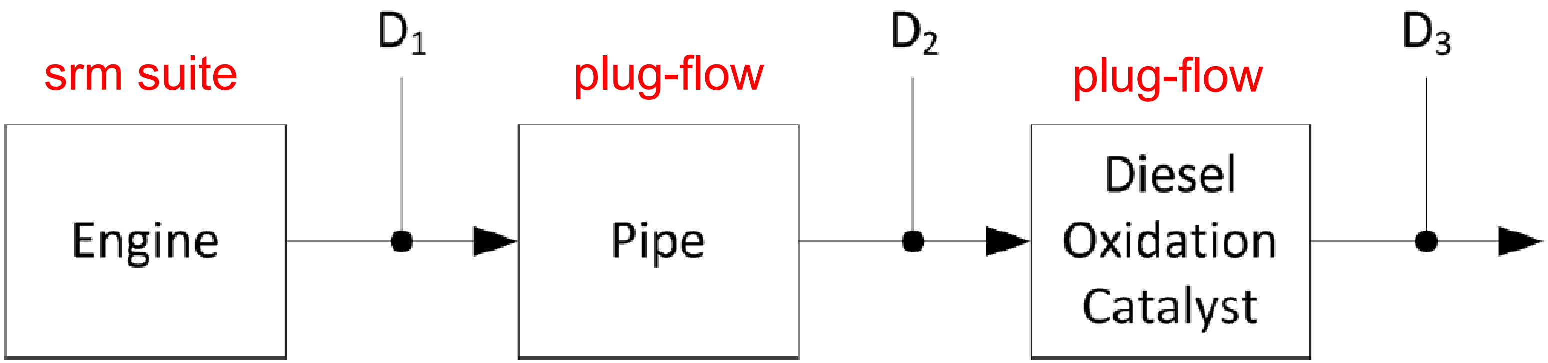





# Post-combustion, exhaust and aftertreatment

# model schematic




Cu-Cr-Ag-K-Ce-Zr-Al catalyst

ble 5: *Operating Parameters for the Cylindrical Connecting Pipe*

| Parameter | Value |
|---|---|
| Diameter (m) | $6 \times 10^{-2}$ |
| Length (m) | 0.5 |
| Effective Volume ($m^3$) | $1.41 \times 10^{-3}$ |
| Mean Residence Time (ms) | 32.9 |

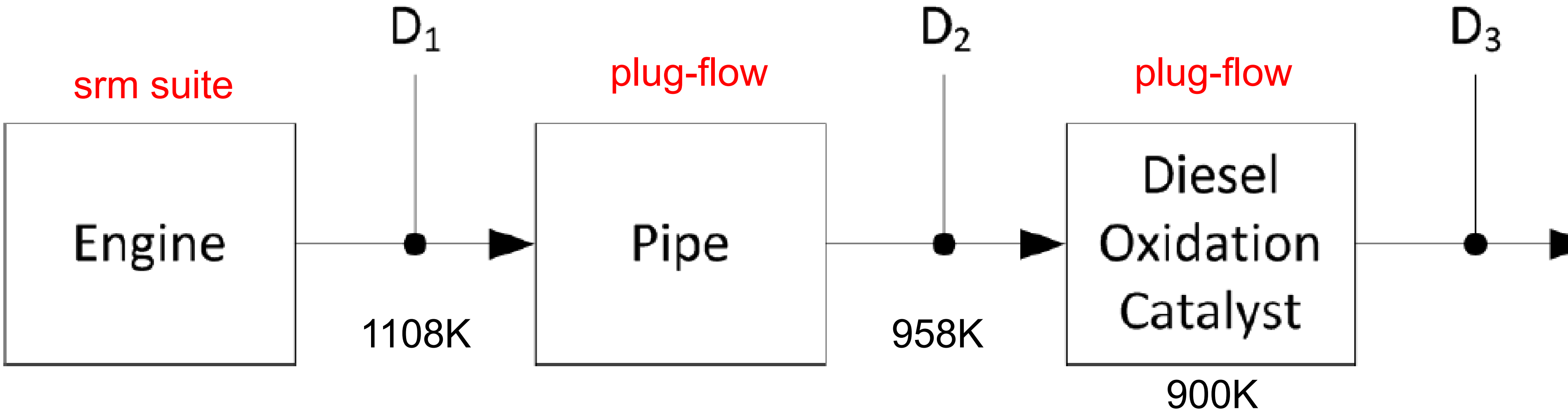
**Table 6:** *Operating Parameters for the Diesel Oxidation Catalyst*

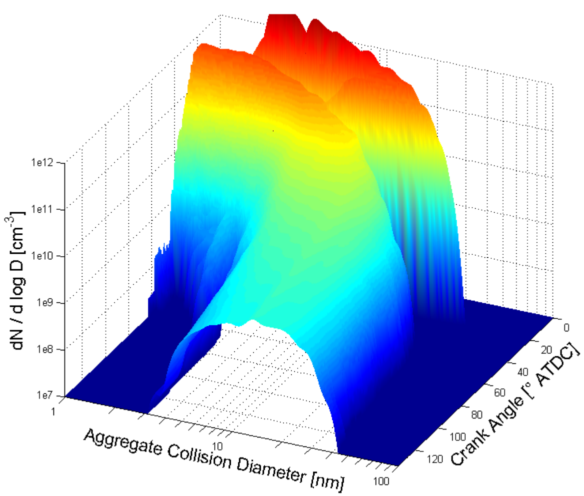
| Parameter | Value |
|---|---|
| Volume ($m^3$) | $1.7 \times 10^{-3}$ |
| Open Frontal Area | 0.706 |
| Effective Volume ($m^3$) | $1.20 \times 10^{-2}$ |
| Mean Residence Time (ms) | 280 |

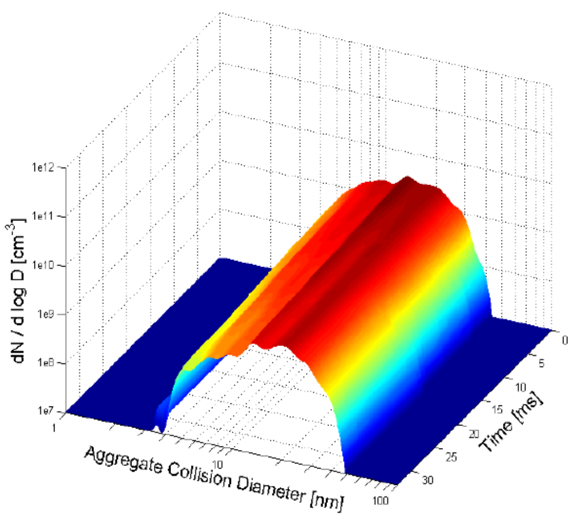
Addition of PM/catalytic reactions to chemical kinetic mechanism

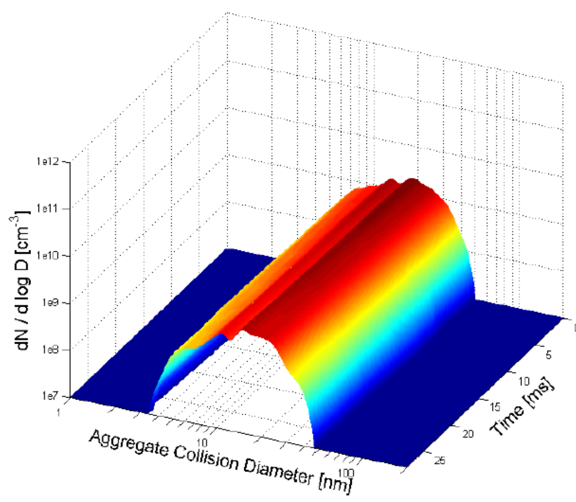
BCs: Temperatures, pressures and residence time from standard GT-Power simulations

# results

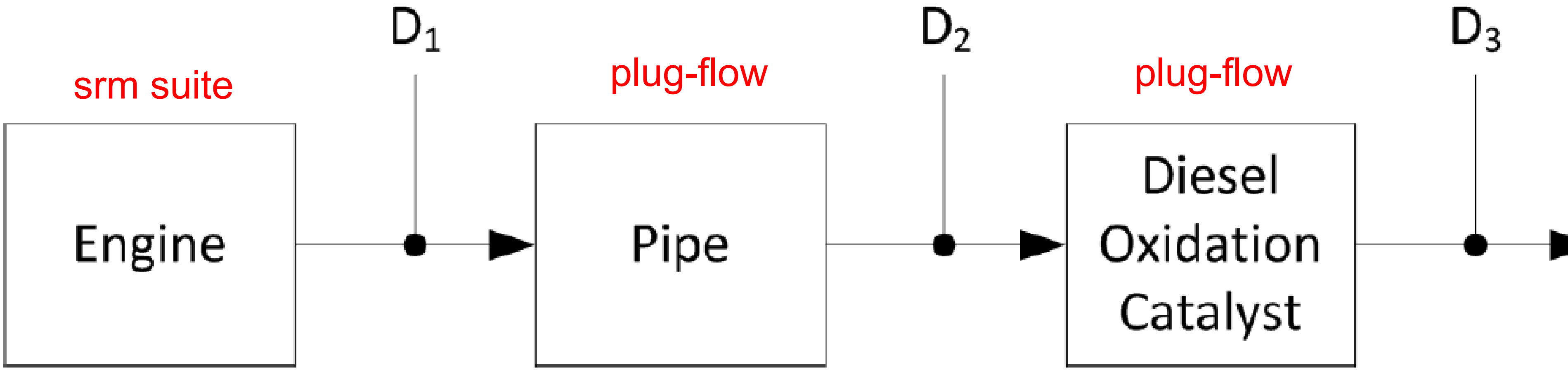

D1
D2
D3
srm suite
plug-flow
plug-flow
Engine
Pipe
Diesel Oxidation Catalyst
1108K
958K
900K


dN / d log D [cm^-3]
Aggregate Collision Diameter [nm]
Crank Angle [° ATDC]

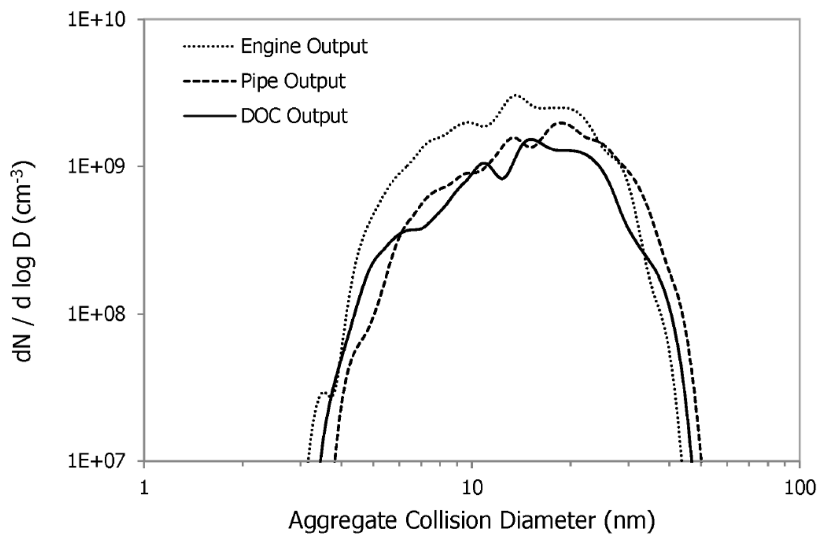

dN / d log D [cm^-3]
Aggregate Collision Diameter [nm]
Time [ms]

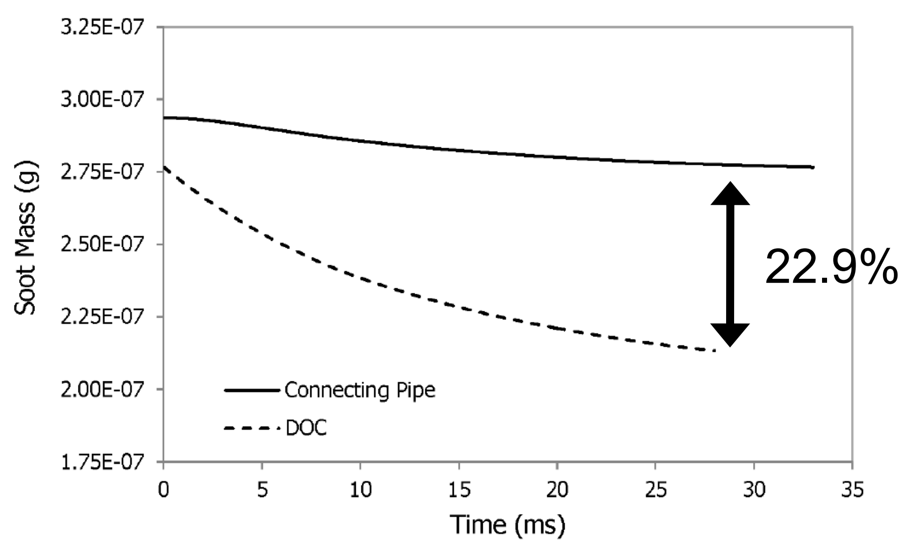

dN / d log D [cm^-3]
Aggregate Collision Diameter [nm]
Time [ms]

# results

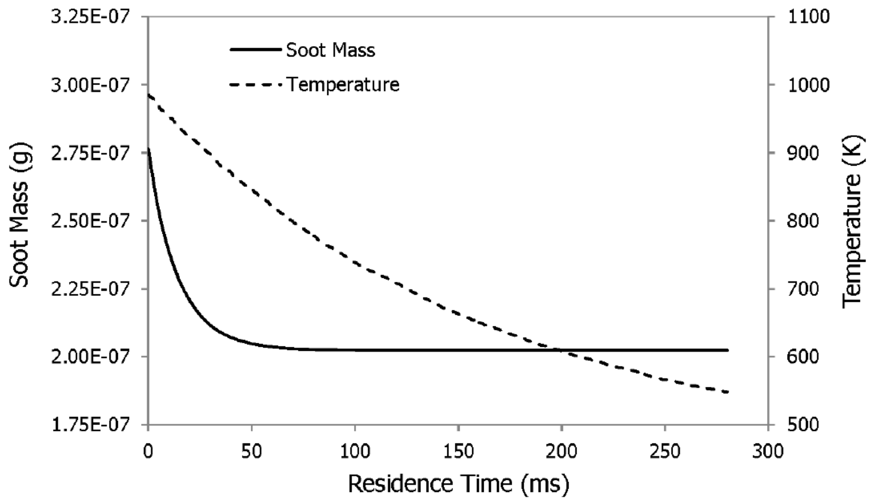



Experiment: 20% reduction of PM



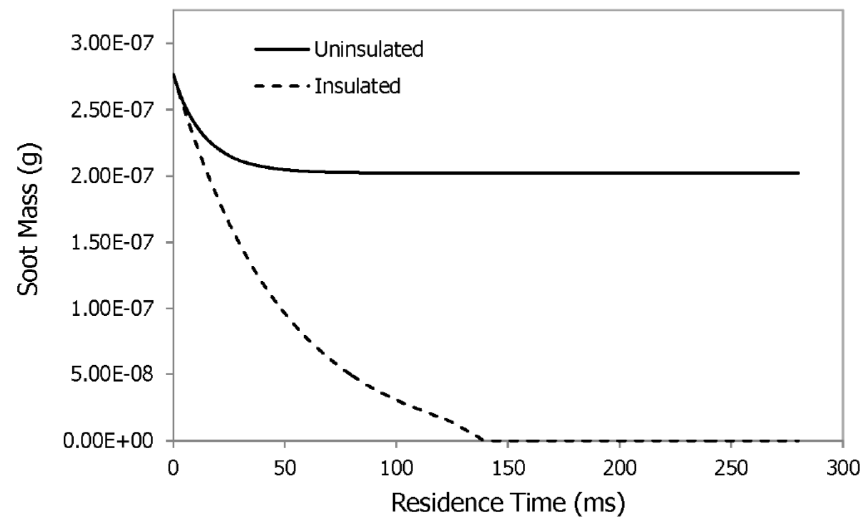



# DOC parametric study

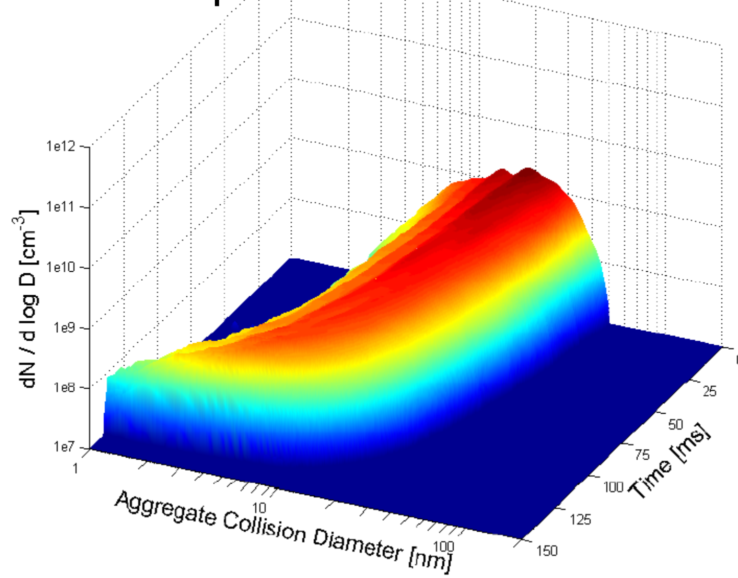



impact of residence time

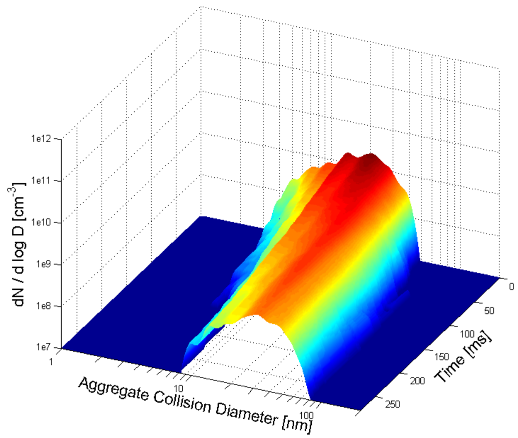
1000K initial



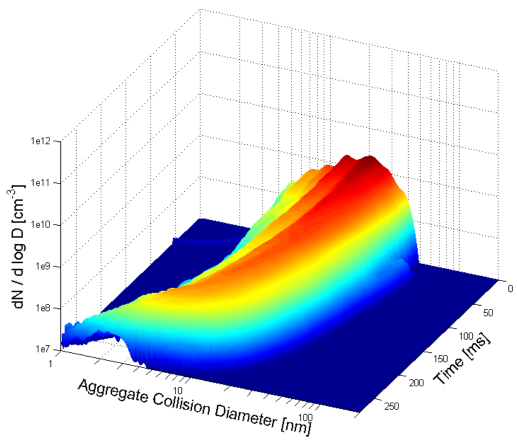

impact of insulation



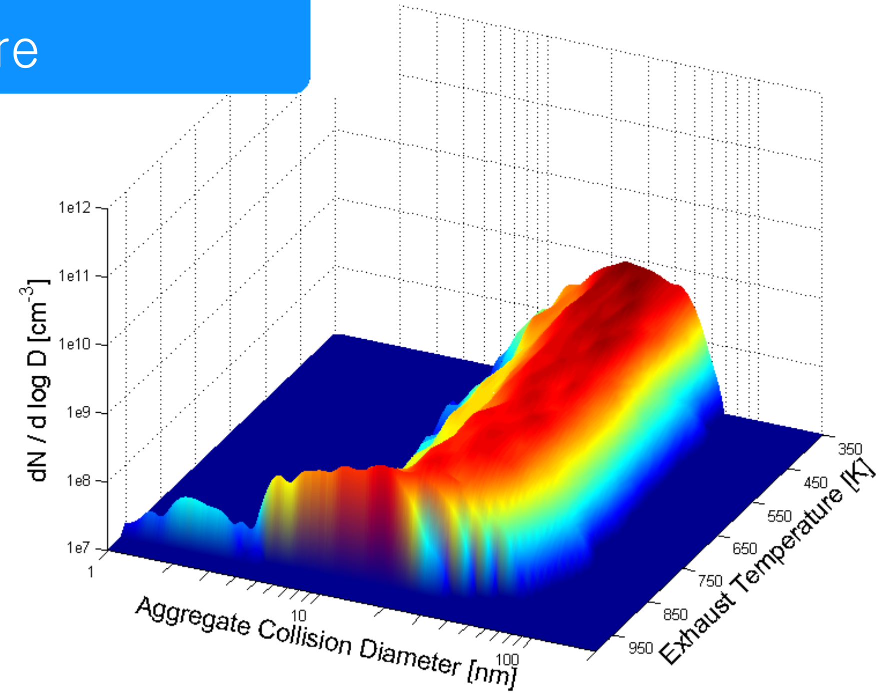
# DOC parametric study – tem rature

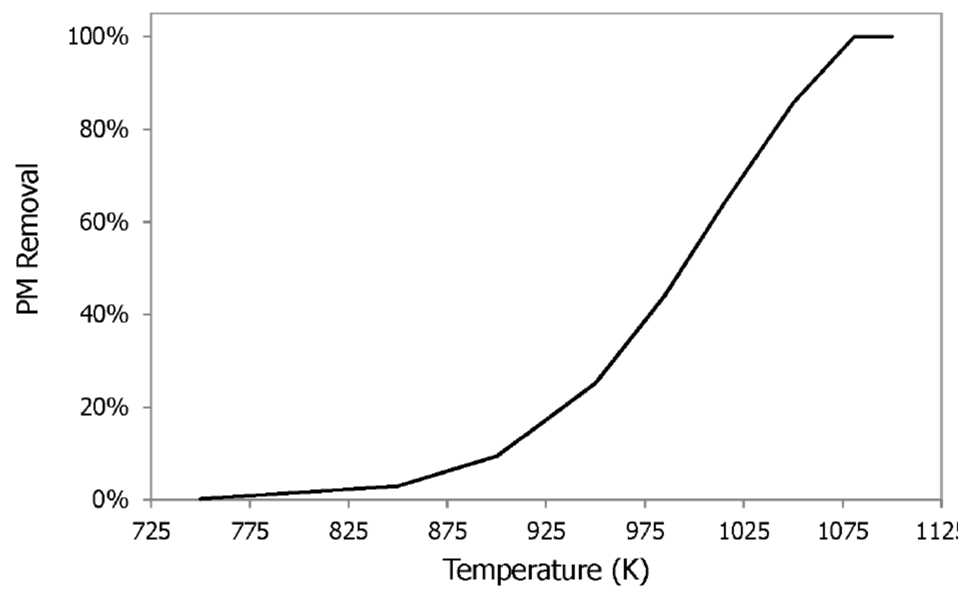



700 K



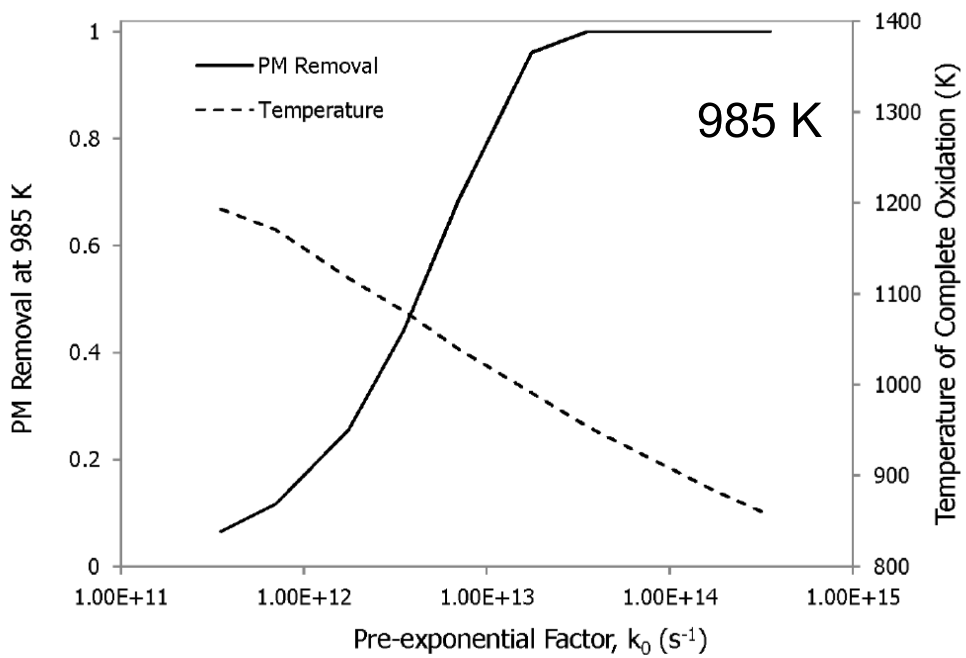

950 K

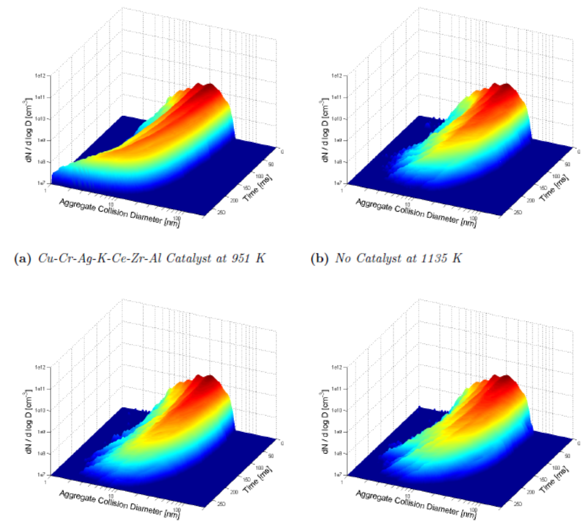


# DOC parametric study – cat t material

| Catalyst | Carbon Form | $k_0$ ($s^{-1}$) | $E_a$ (kJ $mol^{-1}$) |
|---|---|---|---|
| **Cu-Cr-Ag-K-Ce-Zr-Al** | Diesel Soot | $3.52 \times 10^{12}$ | 160 |
| **$Al_2O_3$** | Carbon Black | $4.33 \times 10^{13} \pm 20\%$ | $251 \pm 20\%$ |
| **1Ce10Al** | Carbon Black | $6.48 \times 10^{12} \pm 20\%$ | $250 \pm 20\%$ |
| **3Ce10Al** | Carbon Black | $3.28 \times 10^{5} \pm 20\%$ | $119 \pm 20\%$ |
| **10Ce10Al** | Carbon Black | $1.21 \times 10^{4} \pm 20\%$ | $90 \pm 20\%$ |
| **$CeO_2$** | Carbon Black | $2.20 \times 10^{4} \pm 20\%$ | $90 \pm 20\%$ |




(a) *Cu-Cr-Ag-K-Ce-Zr-Al Catalyst at 951 K* (b) *No Catalyst at 1135 K*

(c) ****Al2O3*** at 1129 K* (d) ****CeO2*** at 1132 K*

Light off temperature largely independent of $k_0$

# summary/next steps

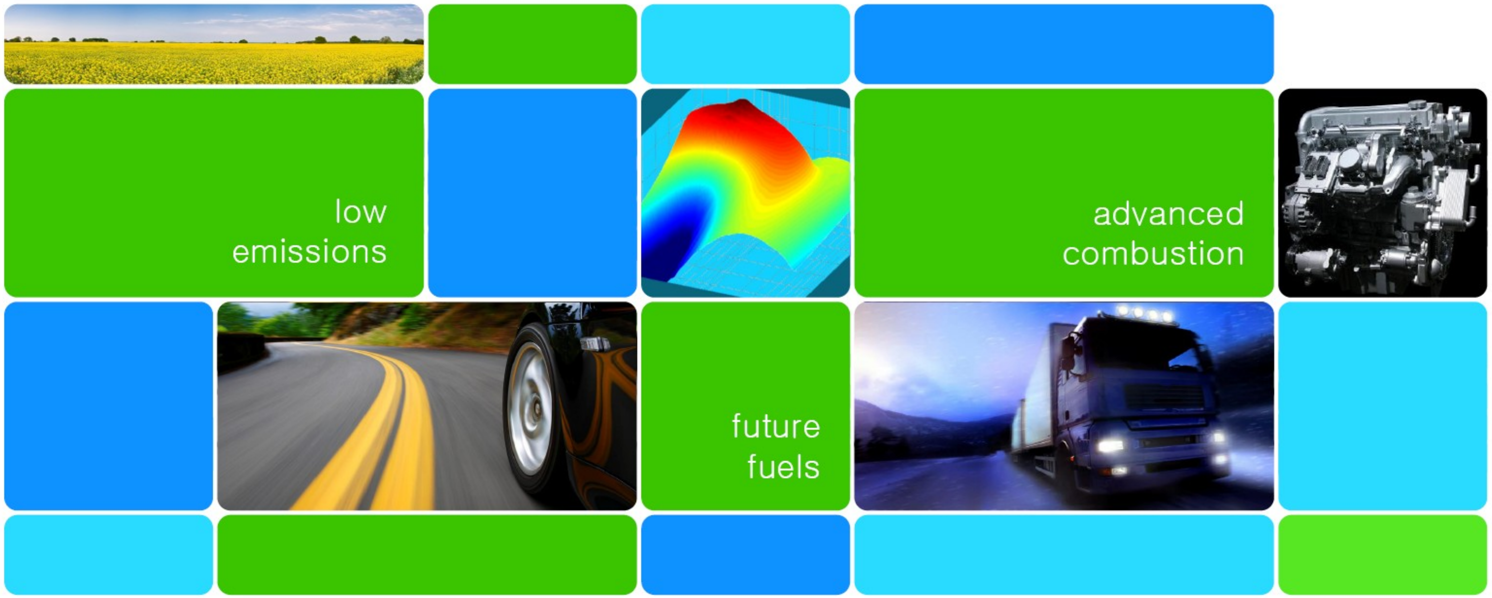
PM produced by modern IC engines can be simulated in terms of mass and size/mass distributions

Simulation can be employed to

(a) avoid PM formation
(b) facilitate its oxidation through catalytic aftertreatment

Aftertreatment solutions require further validation

- quality of experimental data
- knowledge of reaction rates




Thank you for listening...any questions?

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