

JOINT FINAL EVENT 12 & 13TH NOVEMBER 2019, SANTA OLIVA, SPAIN



Gasoline combustion modelling using detailed,
reduced and tabulated chemistry

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Prediction of gasoline combustion

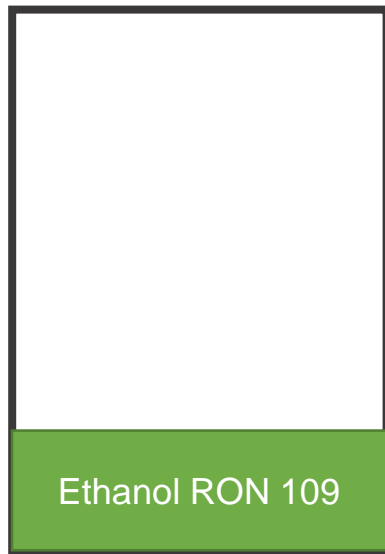
- ▶▶ Description of different gasolines using a 4 component surrogate
- ▶▶ Accurate description of
 - ▶▶ Auto-ignition & Flame Speed
 - ▶▶ Fuel oxidation
 - ▶▶ Soot formation including particle size distribution
 - ▶▶ NOx formation and NOx fuel interaction
 - ▶▶ Formation of unburned hydrocarbons
- ▶▶ Fast models (Short CPU times)

1. Represent gasoline with a 4 component surrogate
 - This allows to accurately capture ethanol content, aromatic content (soot tendency), RON, MON and heating value
2. Develop a detailed gas phase reaction mechanism for the 4 pure components and mixture of those in gas phase
 - Prediction of oxidation, auto-ignition, flame speed, NO_x , soot precursor
3. Reduced the detailed mechanism by removing unnecessary path ways
 - Speed-up of factor 10
4. For even short CPU times the combustion can be tabulated in advance. Since not everything can be tabulated, a few more informations are lost.

Gasoline Surrogate Formulation

1st free component:
Ethanol fraction

→ Surrogate = Gasoline



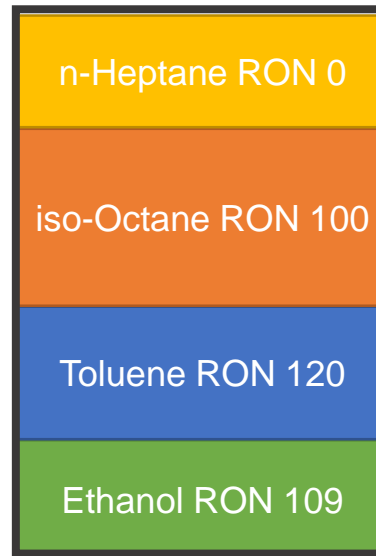
2nd free component
Toluene fraction

→ Represents Aromatic Content of Gasoline



3rd free component
RON of the Gasoline

→ Calculate n-Heptane and iso-Octane fraction



Calculate physical properties:

LHV, MON, H:C:O ratio, Density

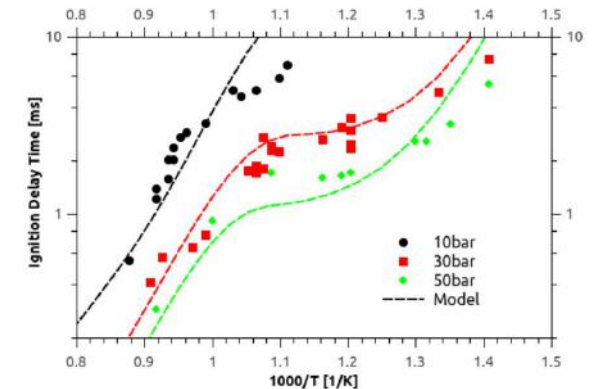


Correlation from Morgan et al. 2010 used to calculate TRF mixture <-> Octane rating
Linear molar based blending rule for ethanol / TRF mixture <-> Octane rating (Anderson et al. 2010*)

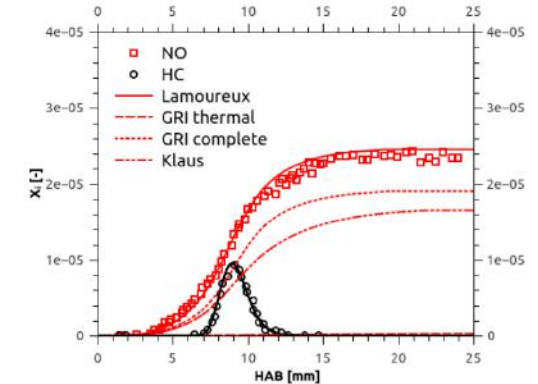
Variable Mechanism Concept

- ▶ Composed from various sources (see poster for more details)
- ▶ ETRF mechanism including emission is composed of 476 species
- ▶ Reduced mechanism 10x faster / 2.5 times smaller
- ▶ Validated against:
 - ▶ Flame speeds
 - ▶ Auto ignition delay times
 - ▶ Species formation

Auto Ignition:



NOx Model:



►► Phenomena modelled are:

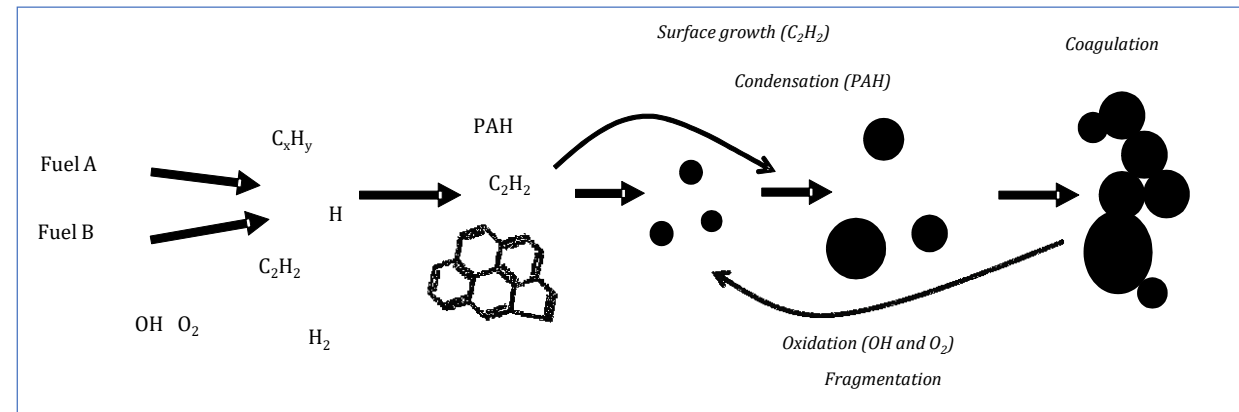
- Particle inception
- Condensation
- Coagulation and agglomeration
- Surface growth
- Fragmentation
- Oxidation

►► Moment based method

- Describes quantities of the function such as total mass, total number density

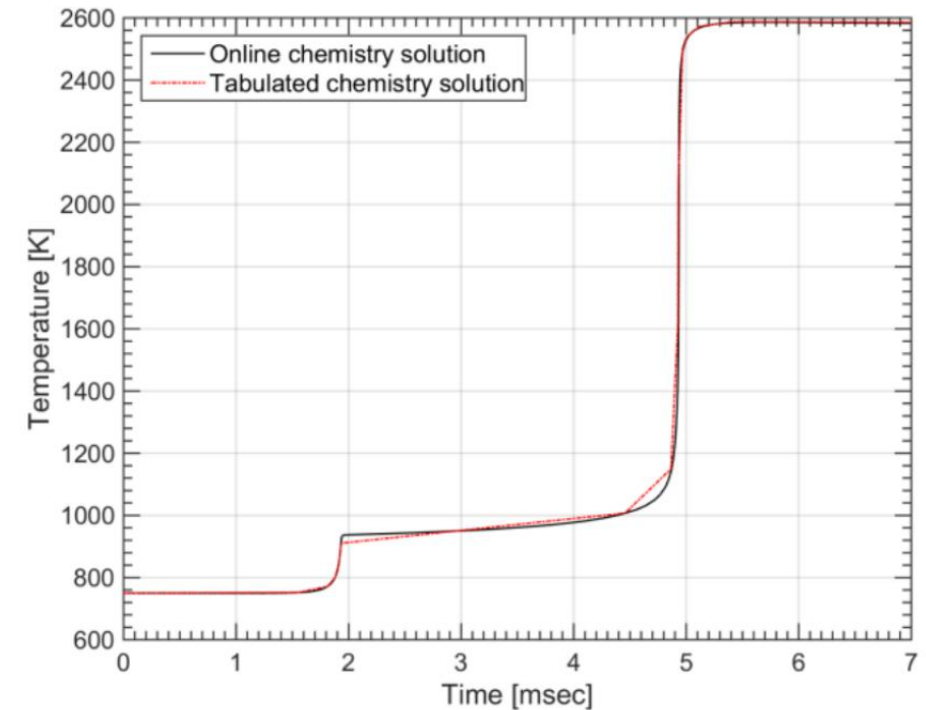
Section based method

- Deals directly with the particle site distribution



Tabulated Chemistry

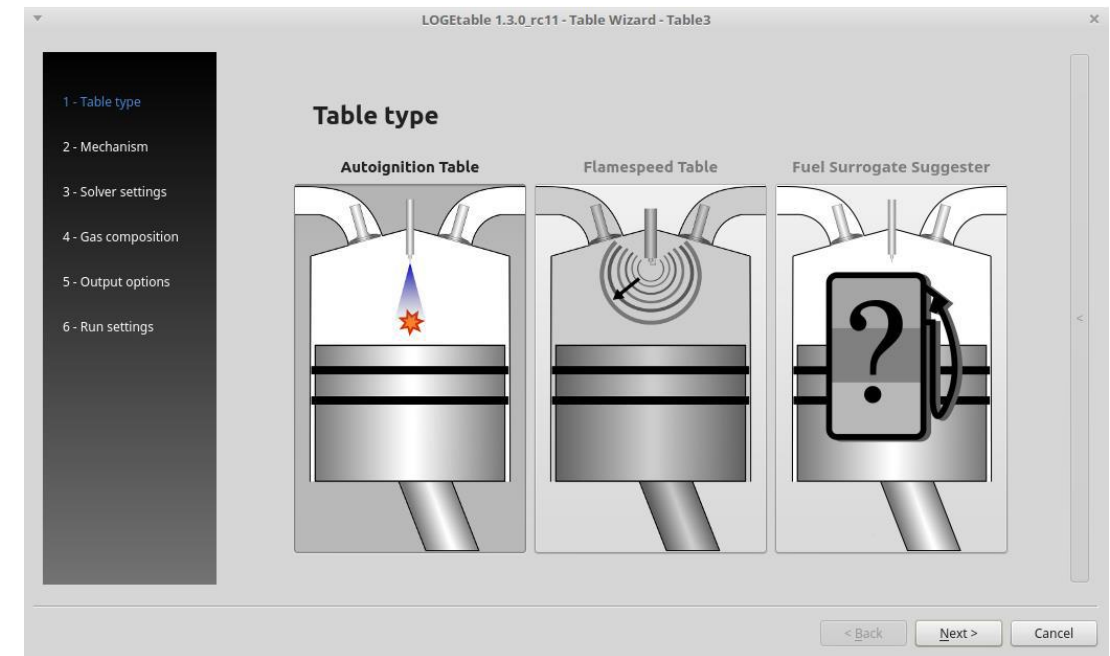
- ▶ Run a wide range of simple 0D reactors for all possible conditions
- ▶ Map combustion / species to a progress variable and tabulate them
- ▶ Use the table when running simulation
- ▶ Typical Speed ups are between factor 10 and several hundred
 - ▶ This enables large parameter studies
- ▶ Easy to use software solution to compile tables (LOGEtable)

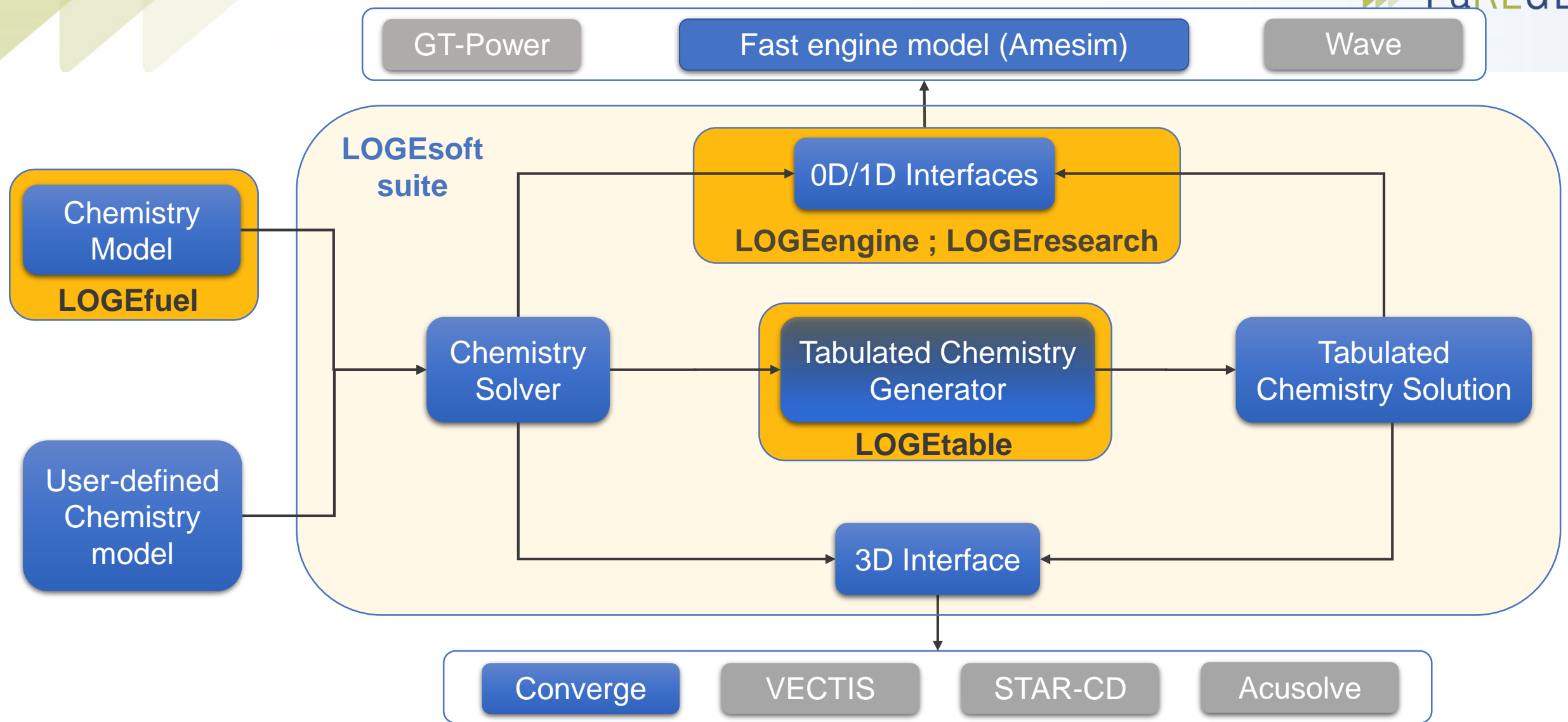


Constant pressure reactor calculation at 10 bar and 750 K for n-heptane/air mixture at stoichiometry.

Table generation with LOGEtable

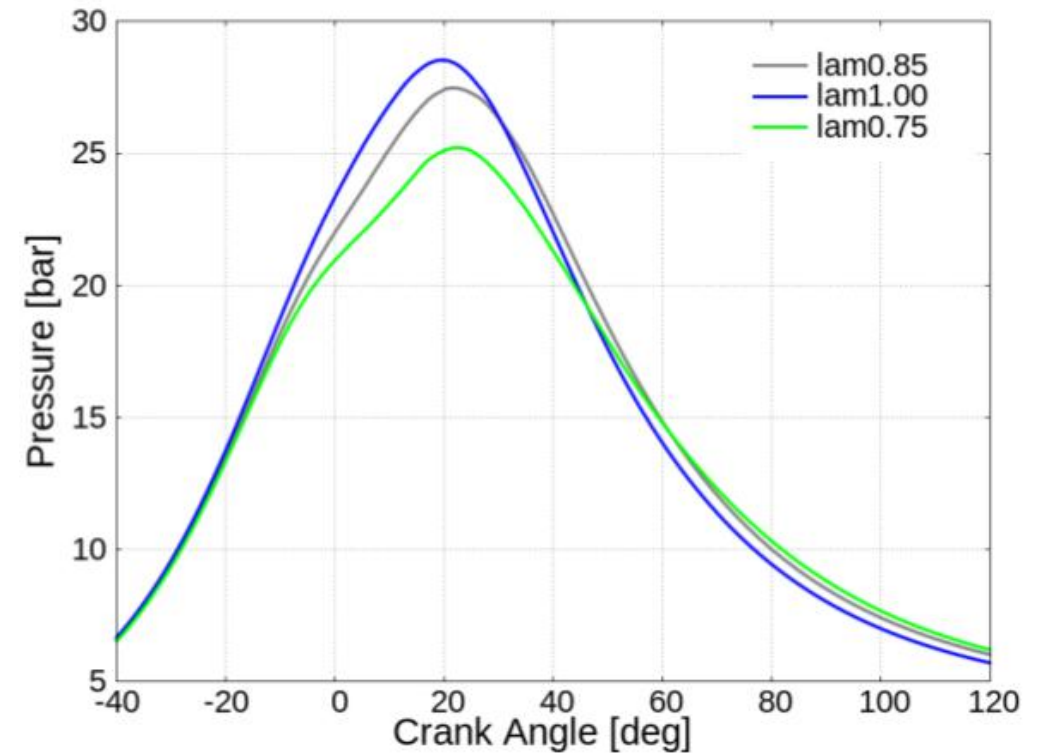
- ▶▶ Easy to use tool to pre-compile look-up tables
 - ▶▶ Windows / Linux incl. HPC
 - ▶▶ Can read any reaction mechanism in standard format
 - ▶▶ Very fast and stable solver
 - ▶▶ Can also generate laminar flame speed tables
- ▶▶ Includes surrogate formulation tool developed in this project and more than 20 fuel components



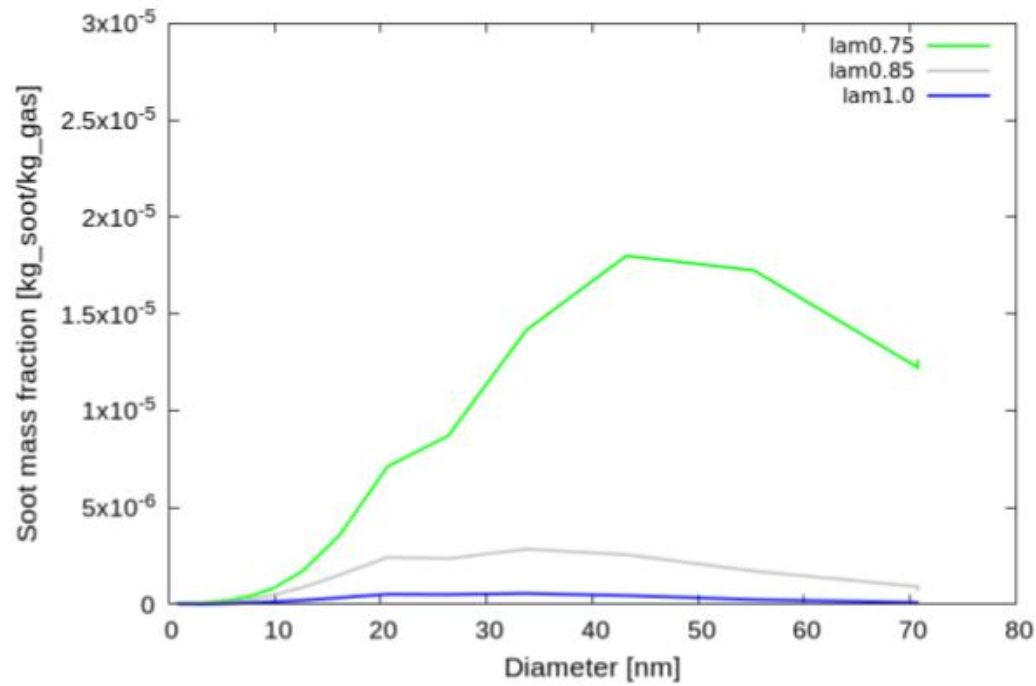


Results – Particle Formation Prediction using Tabulated Chemistry

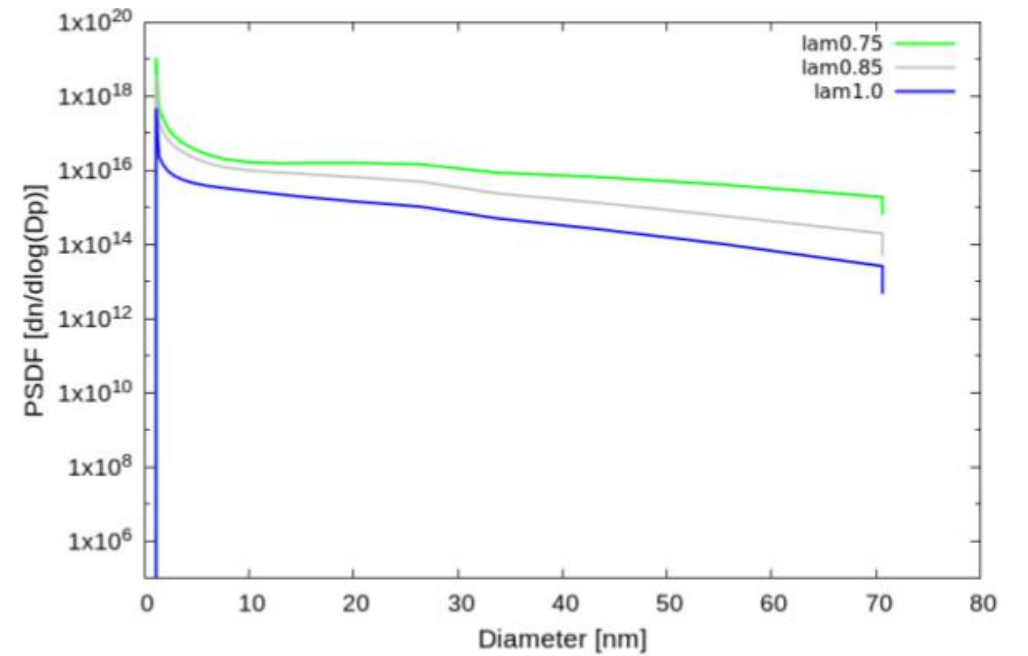
- ▶▶ Tabulated chemistry coupled with CONVERGE CFD code
- ▶▶ GDI sample cases for $\lambda=1.0, 0.85, 0.75$ by injecting more fuel
- ▶▶ Strong wall impingement
- ▶▶ Ignition timing was optimised to match similar CA 50
- ▶▶ Section based soot model
- ▶▶ 10h simulation time on modern workstation



Pressure trace

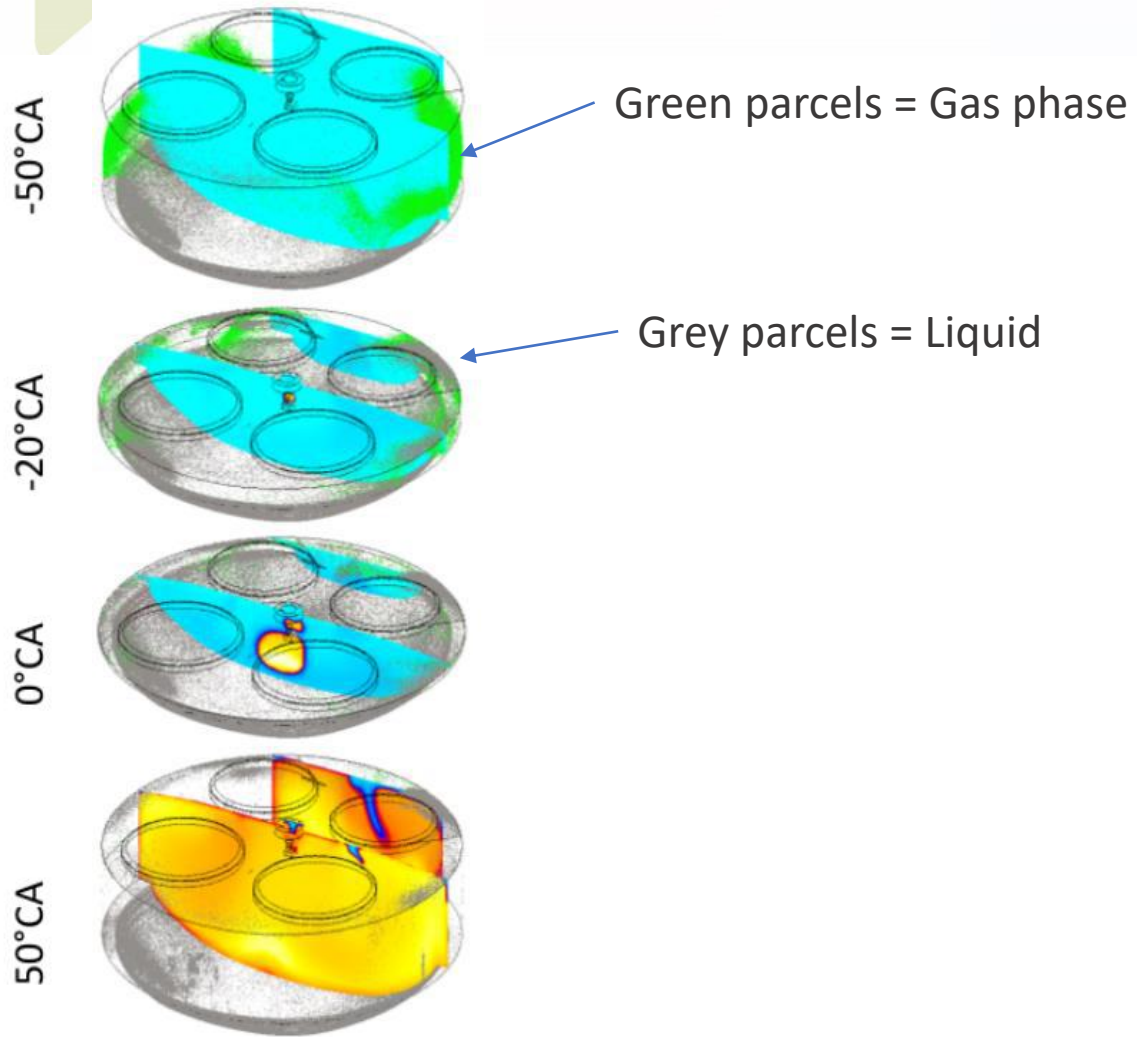


Soot mass fraction distribution at +80 CAD

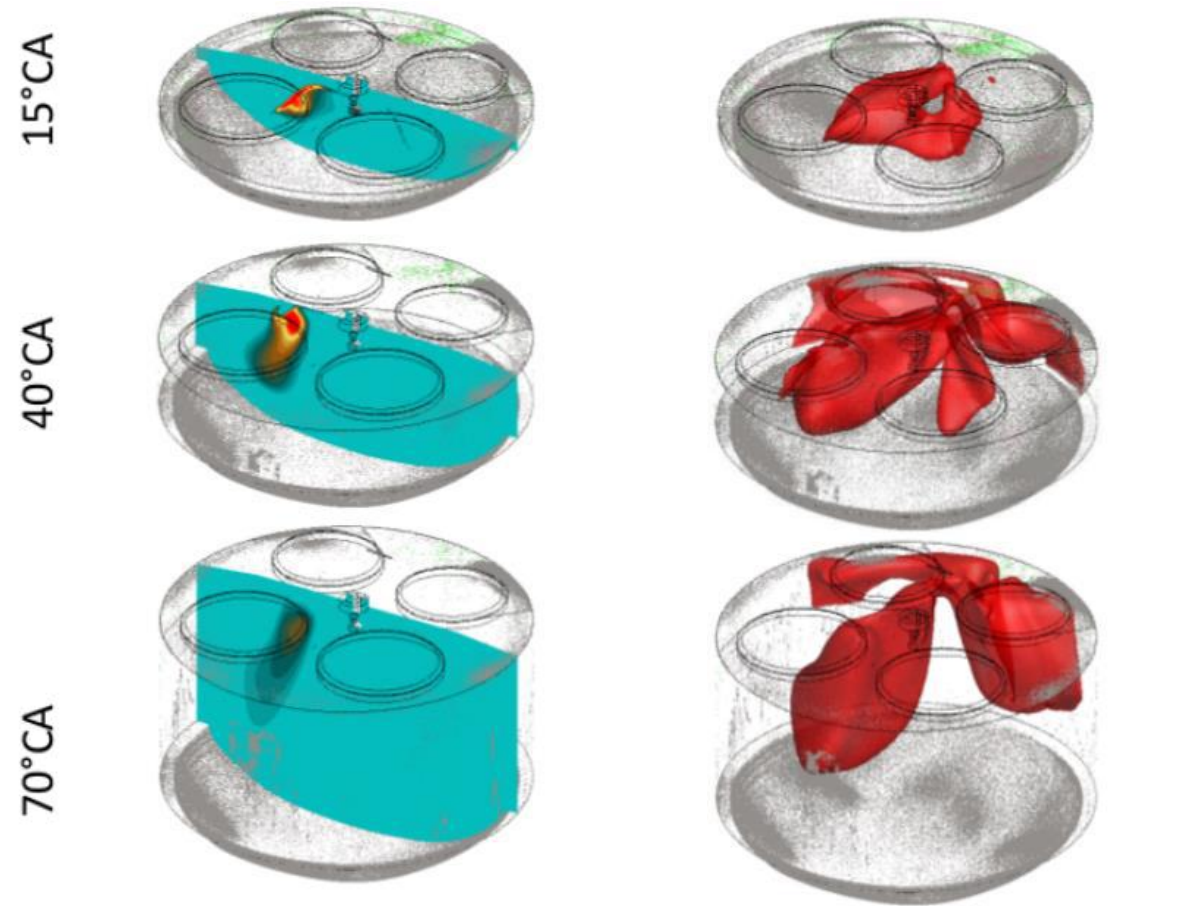


Particle size distribution at +80 CAD

Closer look at $\lambda=0.75$



Temperature



Nucleation rate
(Vertical slice)

Iso-surface of surface growth
and fragmentation rate

- ▶▶ Complete tool chain:
 - ▶▶ Surrogate formulation
 - ▶▶ Combustion prediction
 - ▶▶ Emission formation prediction
 - ▶▶ NOx
 - ▶▶ Soot incl. particle size distribution
 - ▶▶ Very fast models for engine design
 - ▶▶ Exploitable:
 - ▶▶ Improved software for combustion pre tabulation
 - ▶▶ Improved gasoline surrogates
- ▶▶ Live demo's of the software and more details at the booth!