Giornata di Studio "Giorgio Minelli" sui Motori a Combustione Interna

Modelli di combustione con cinetica tabulata per motori Diesel, RCCI e SI

POLITECNICO MILANO 1863

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Internal Combustion Engine Group
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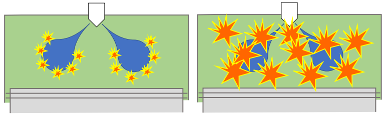
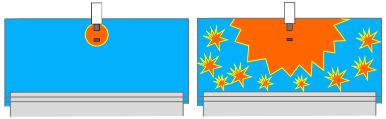
Motivation

Which approch for novel reaction controlled combustion modes?

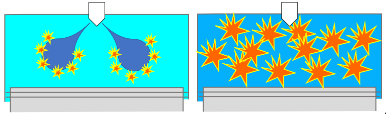
PCCI



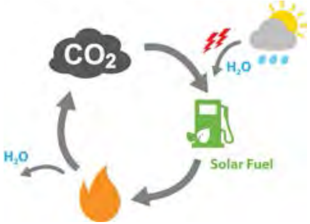
SACI



RCCI



e-fuels

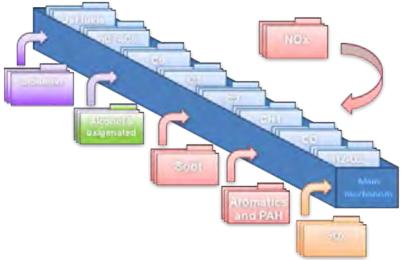


Dual-fuel combustion

Virtualization of engine design with CFD

- Prediction of engine performance and pollutant emissions
  - Computational efficiency
  - Complex flame structures and kinetic schemes

Tabulated kinetics



+

Well-mixed	CMC
RIF	Transported PDF

&

Tabulated kinetics

Tabulated kinetics

Constant-pressure homogeneous reactor tabulation

Kinetic mechanism

Conditions
p, T_u, ϕ, EGR

Homogeneous, constant-pressure reactor simulations

HR look-up table
- Composition (7 *virtual species*)
- Output species
- Progress variable reaction rate

The table generator is a PYTHON program using the CANTERA library:
- highly flexible
- fast, reliable
- fully parallel

Support for multi-component fuel

Progress variable

$$C = \sum_{i=1}^{N_S} h_{298,i} \cdot \left(Y_i(t) - Y_i(0)\right)$$

NO_x progress variable

$$C_{NO_x} = Y_{NO} + Y_{NO_2} + Y_{N_2O} + Y_{N_2O_2}$$

Tabulated kinetics

Governing equations

Mixture fraction

$$\frac{\partial \rho Z}{\partial t} + \nabla(\rho \mathbf{U} Z) - \nabla\left(\frac{\mu_t}{Sc_t} \cdot \nabla Z\right) = \dot{S}$$

Mixture fraction variance

$$\frac{\partial \rho \widetilde{Z''^2}}{\partial t} + \nabla(\rho \mathbf{U} \widetilde{Z''^2}) - \nabla\left(\frac{\mu_t}{Sc_t} \cdot \nabla \widetilde{Z''^2}\right) = 2\frac{\mu_t}{Sc} - \rho\chi$$

Progress variable

$$\frac{\partial \rho C}{\partial t} + \nabla(\rho \mathbf{U} C) - \nabla\left(\frac{\mu_t}{Sc_t} \cdot \nabla C\right) = \dot{\omega}_c$$

Unburned gas enthalpy

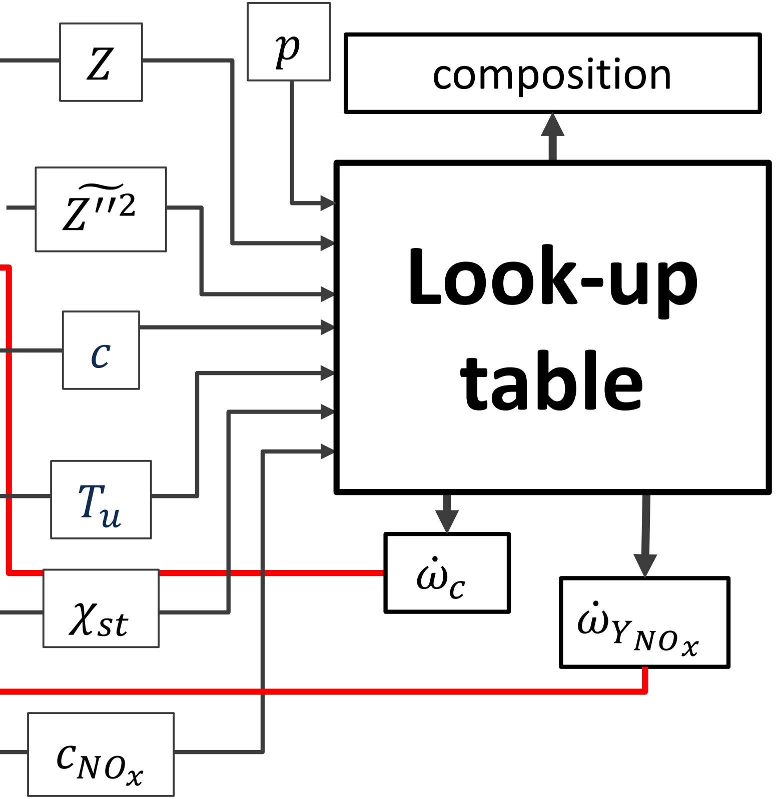
$$\frac{\partial \rho h_u}{\partial t} + \nabla(\rho \mathbf{U} h_u) - \nabla\left(\frac{\mu_t}{Pr_t} \cdot \nabla h_u\right) = \dot{Q}_s + \frac{\rho}{\rho_u}\frac{Dp}{Dt}$$

Stoichiometric scalar dissipation rate

$$\chi = C_\chi \frac{\varepsilon}{k} \widetilde{Z''^2} \qquad \chi_{st} = \frac{\chi}{\int_0^1 \frac{f(z)}{f(Z_{st})} p(z)dz}$$

NO_x progress variable

$$\frac{\partial \rho Y_{NO_x}}{\partial t} + \nabla(\rho \mathbf{U} Y_{NO_x}) - \nabla\left(\frac{\mu_t}{Sc_t} \cdot \nabla Y_{NO_x}\right) = \dot{\omega}_{Y_{NO_x}}$$

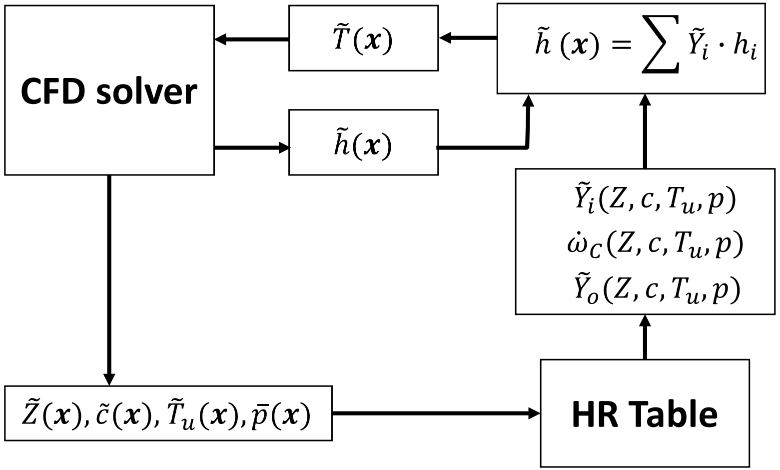


Tabulated kinetics

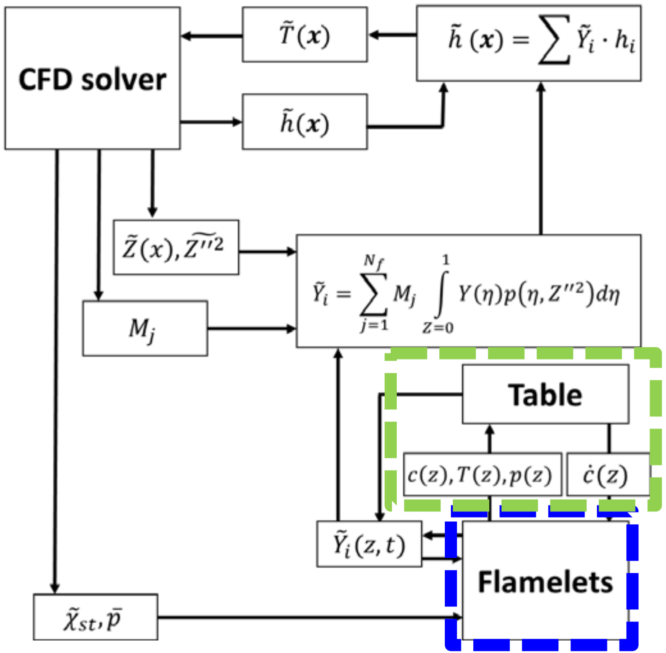
Combustion models

TWM: tabulated well-mixed

No turbulence-chemistry interaction



TRIF: Tabulated Representative Interactive Flamelet



Flamelet equations with tabulated kinetics

$$\frac{\partial C}{\partial t} = \frac{\chi_Z}{2} \frac{\partial^2 C}{\partial Z^2} + \dot{C}$$

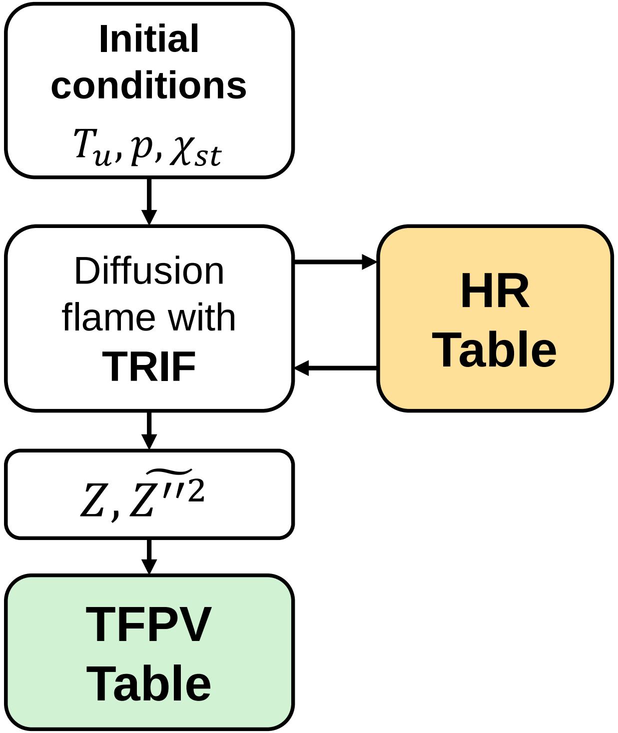
$$\frac{\partial h}{\partial t} = \frac{\chi_Z}{2} \frac{\partial^2 h}{\partial Z^2} + \frac{1}{\rho} \frac{dp}{dt}$$

Tabulated kinetics

Combustion models

TFPV: Tabulated Flamelet Progress Variable

- Approach similar to ADF (Approximated Diffusion Flames)
- Turbulence/chemistry interaction, sub-grid mixing and premixed flame propagation.
- Progress variable reaction rate function also of the stoichiometric scalar dissipation rate χ_{st}
- Correct estimation of
  - extinction in the near nozzle region;
  - re-ignition;
  - flame stabilization process;
- TFPV table generated using TRIF and a variable time-step strategy to reduce the required computational time.



Tabulated kinetics

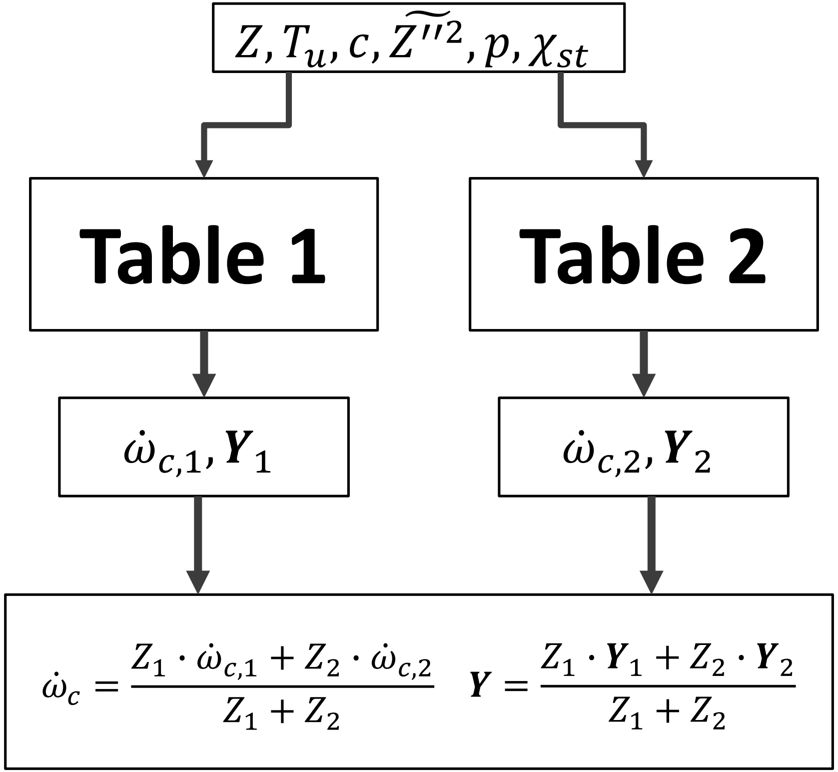
Dual fuel combustion

Assumptions

- One progress variable in any cell and infinitely fast mixing
  - "single fuel mixture fraction" is equal to the global mixture fraction
- Ignition governed by progress variable diffusion and local thermodynamic conditions
  - One table for any fuel

Model

- Transport equations for the two fuel mixture fractions (Z_1 and Z_2)
- Progress variable reaction rate is computed as the weighted average of the corresponding values for the two fuels.



Validation

Light Duty Diesel Engine

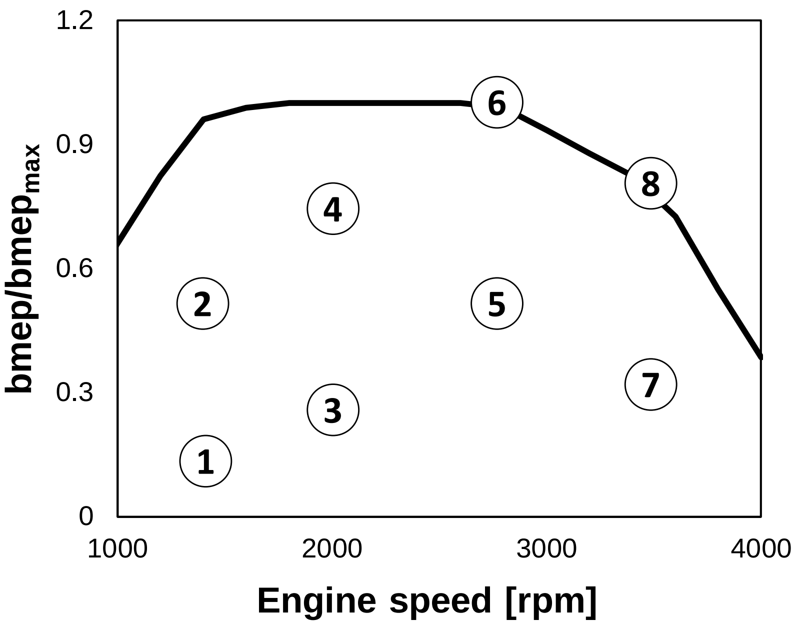
Validation: FPT F1C Engine

Conventional Diesel

Bore	96 mm
Stroke	104 mm
Compression ratio	18
IVC	-145 deg
EVO	110 deg

Swirl ratio	1.3
# holes	8
Nozzle hole diameter	140 μm
Homologation	**EU6**

Selected operating points



	Name	[rpm]	load	λ	EGR	#inj
1	**HEGR**	1400	12%	2.7	40%	3
2	**1400x50**	1400	50%	1.4	15%	3
3	**A25**	2000	25%	2.1	20%	3
4	**A75**	2000	75%	1.3	15%	3
5	**B50**	2750	50%	1.4	15%	3
6	**B100**	2750	100%	1.3	5%	2
7	**C40**	3500	40%	2.3	10%	3
8	**C100**	3500	100%	1.5	0%	1

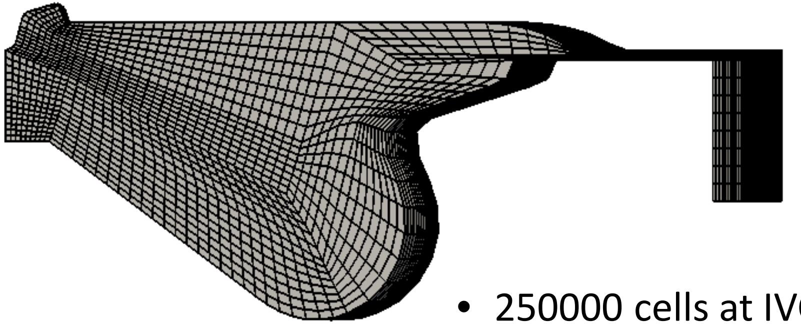
Validation: FPT F1C Engine

Conventional Diesel

Simulation setup

Mesh

- 1/8 of the combustion chamber, spray-oriented, automatically generated with the Python Polimi pre-processor



- 250000 cells at IVC
- 40000 cells at TDC

Tabulation

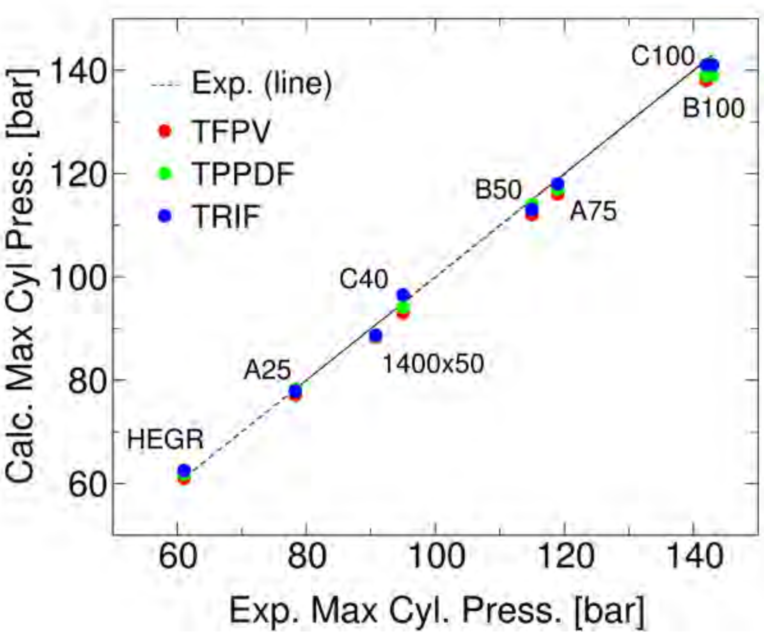
- **Fuel: n-$C_{12}H_{26}$**
- **Mechanism: Frassoldati et al (96 species)**

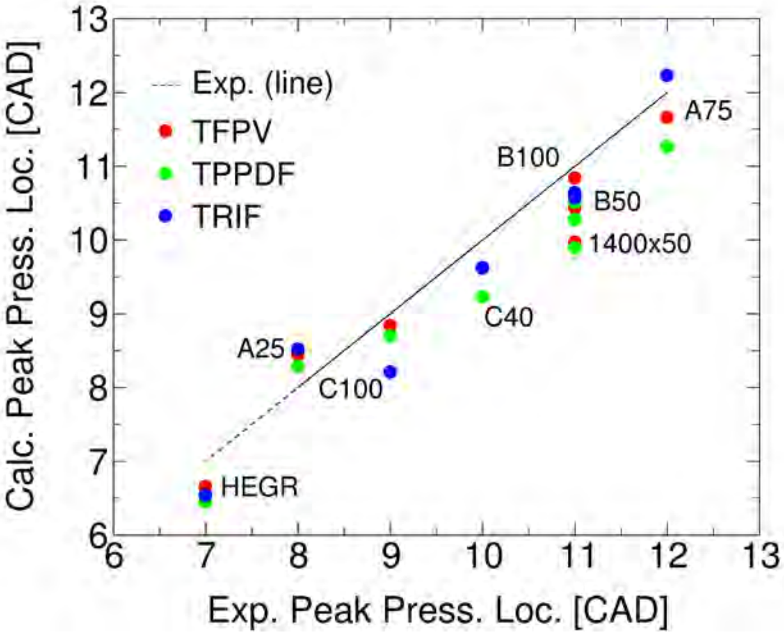
Temperature [K]	600 - 1300 K (step 50 K)
Pressure [bar]	20-200 (step 40)
Equivalence ratio	0-3 (finer resolution close to $\phi = 1$)
Mixture fraction segregation	0.0, 0.001, 0.0025, 0.01, 0.025, 0.1 1.0
Scalar dissipation rate χ_{st} [1/s]	0, 1, 3, 7, 20, 55

- **TPPDF, TRIF, TFPV models**

Validation: FPT F1C Engine

Conventional Diesel

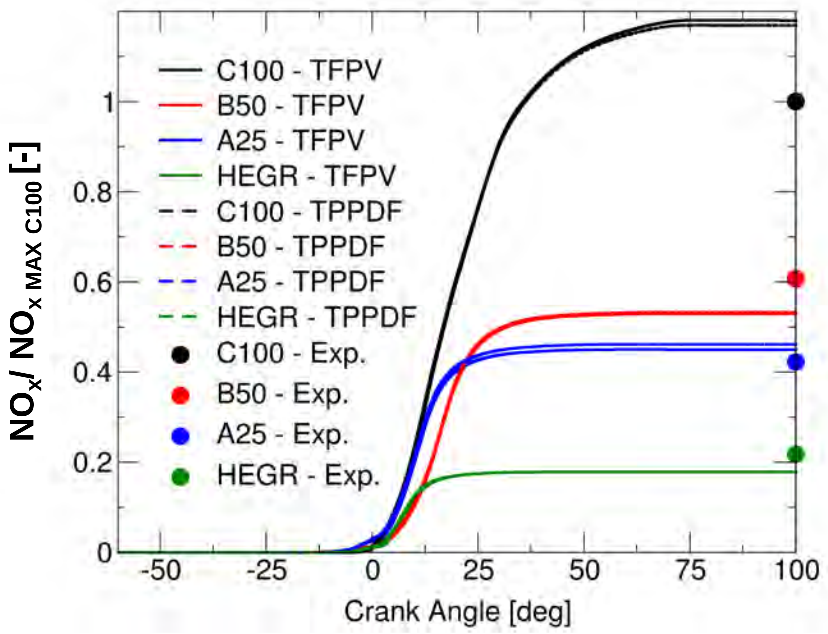


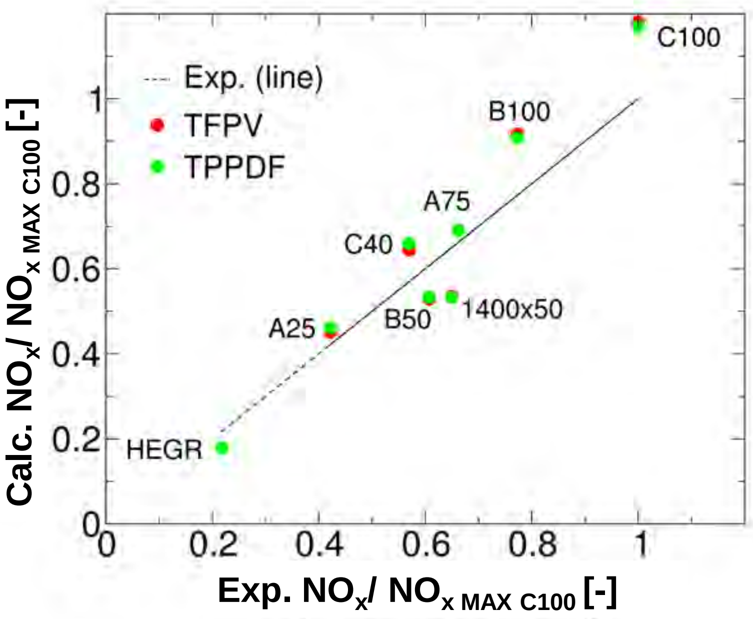


- All the models are able to capture in-cylinder pressure peak and its location
- CPU time: 15 hours on a 8 core machine for a power-cycle (dual-core, eight processor Intel Xeon E5-2630 v3 2.40GHz)

Validation: FPT F1C Engine

Conventional Diesel



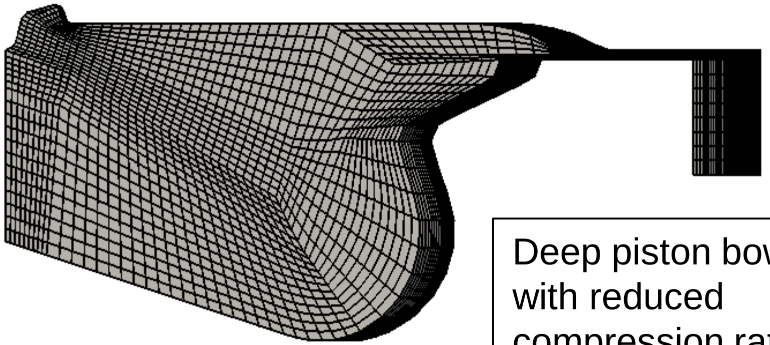


- NO_x grow during combustion process and they are frozen when cylinder temperature decreases.
- All predictions fall in the ±20% range compared to experimental data.

Validation: FPT F1C Engine

PCCI combustion

Combustion chamber



Deep piston bowl with reduced compression ratio

Operating conditions

	Name	Speed [rpm]	bmep [bar]	λ	EGR
1	PCCI1	2000	5	~1.2	~40%
2	PCCI2	2000	7.5	~1.2	~40%
3	PCCI3	3000	5	~1.2	~40%

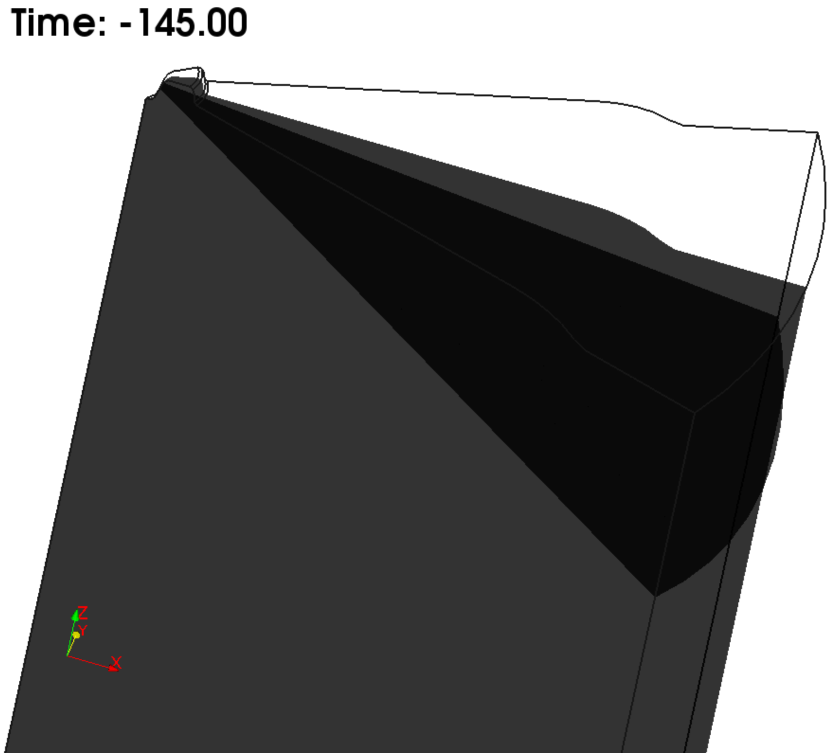
- Combustion model: TWM (TCI effects can be reasonably neglected)
- Fuel is n-heptane (n-C_7H_{16}) having similar CN as Diesel
- Tabulated mechanism: 159 species from LLNL

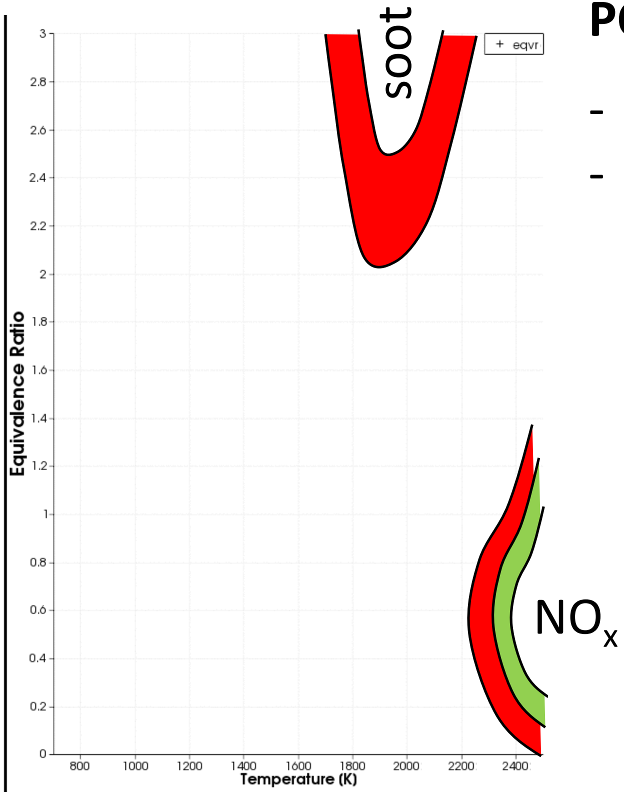
Table discretization

Temperature [K]	600-800 (step 25 K) 800 - 1000 (step 12.5 K) 1000 - 1100 (step 25 K) 1100 - 1200 (step 50 K)
Pressure [bar]	20-200 (step 20 bar)

Validation: FPT F1C Engine

PCCI combustion





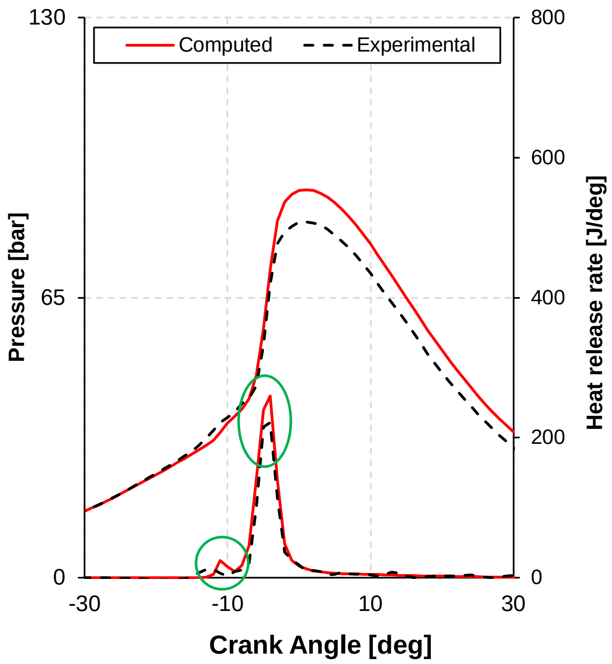
PCCI1 condition

- combustion
- T-ϕ maps

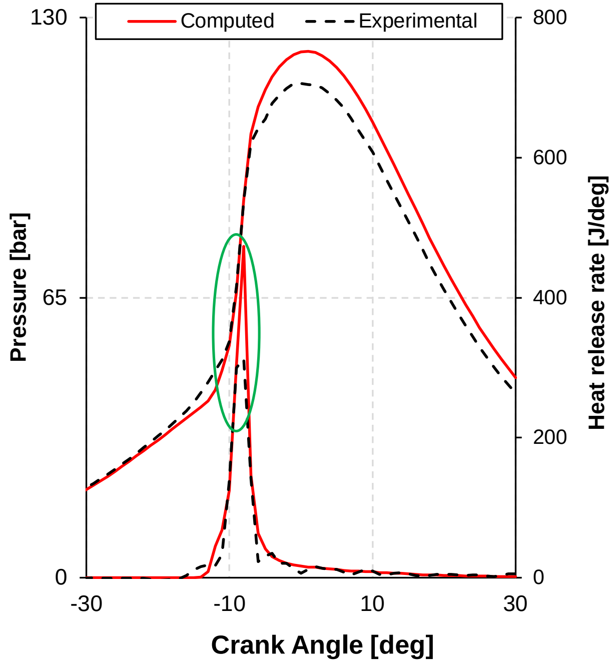
Validation: FPT F1C Engine

PCCI combustion: cylinder pressure

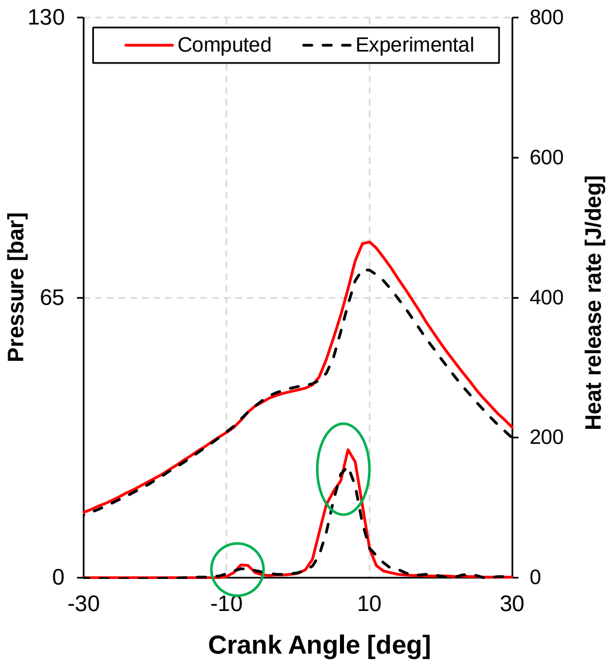
PCCI1: 2000 rpm x 5bar



PCCI2: 2000 rpm x 7.5 bar

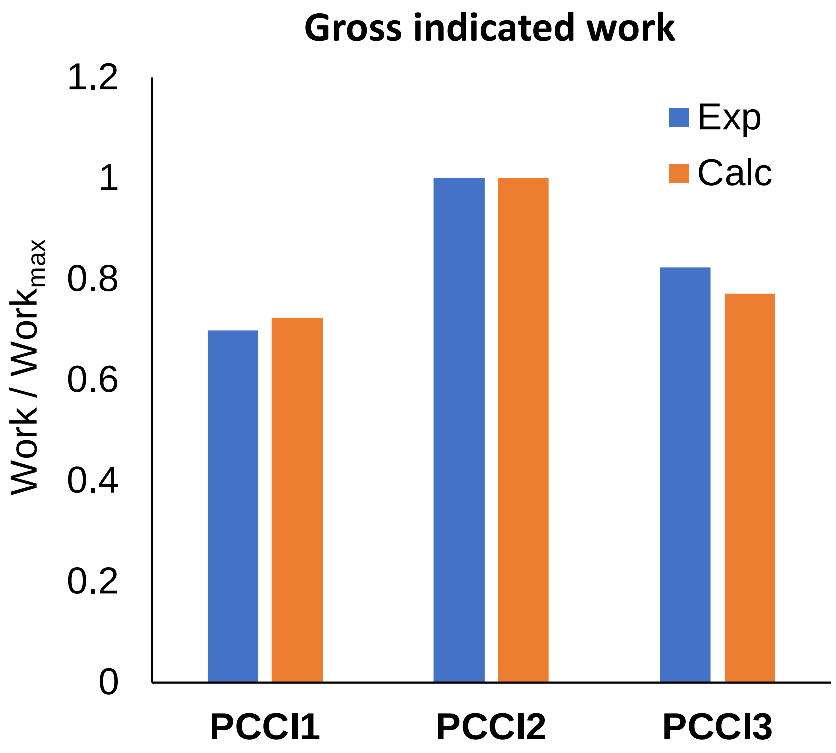


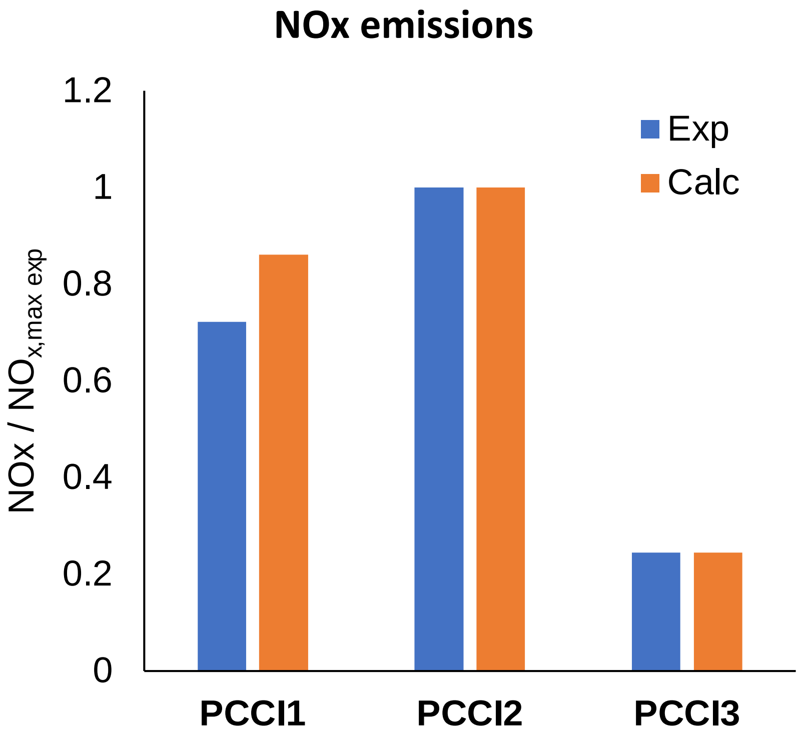
PCCI3: 3000 rpm x 5 bar



Validation: FPT F1C Engine

PCCI combustion: consistency





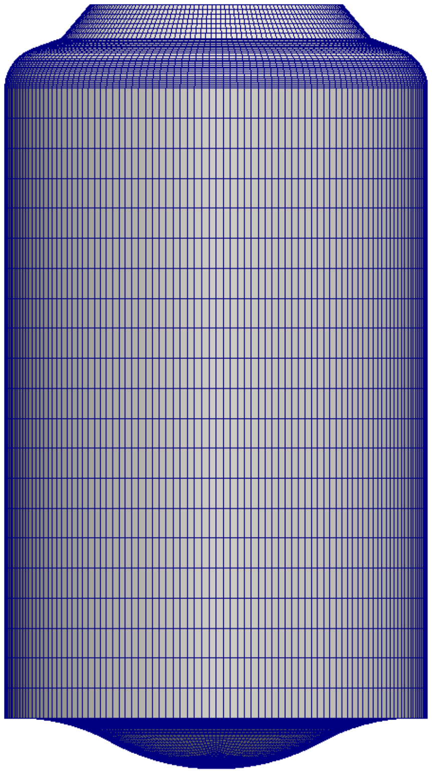
Validation

Large Bore Diesel Engine

Validation: Large Bore Diesel Engine

Conventional Diesel: simulation setup

	"Low" Load	"High" Load
Speed [rpm]	~80	~100
SOI [CAD BTDC]	2	-2
$m_{inj}/m_{inj,full}$	0.85	1
Mesh	deforming, 650000 cells	
Fuel type	$n\text{-}C_7H_{16}$ (gas phase) IDEA (liquid properties)	
Tabulated mechanism	$n\text{-}C_7H_{16}$ from LLNL (159 species)	
Tabulation	ϕ=0.2-3; T=500-1250 K; p=2-20 MPa	



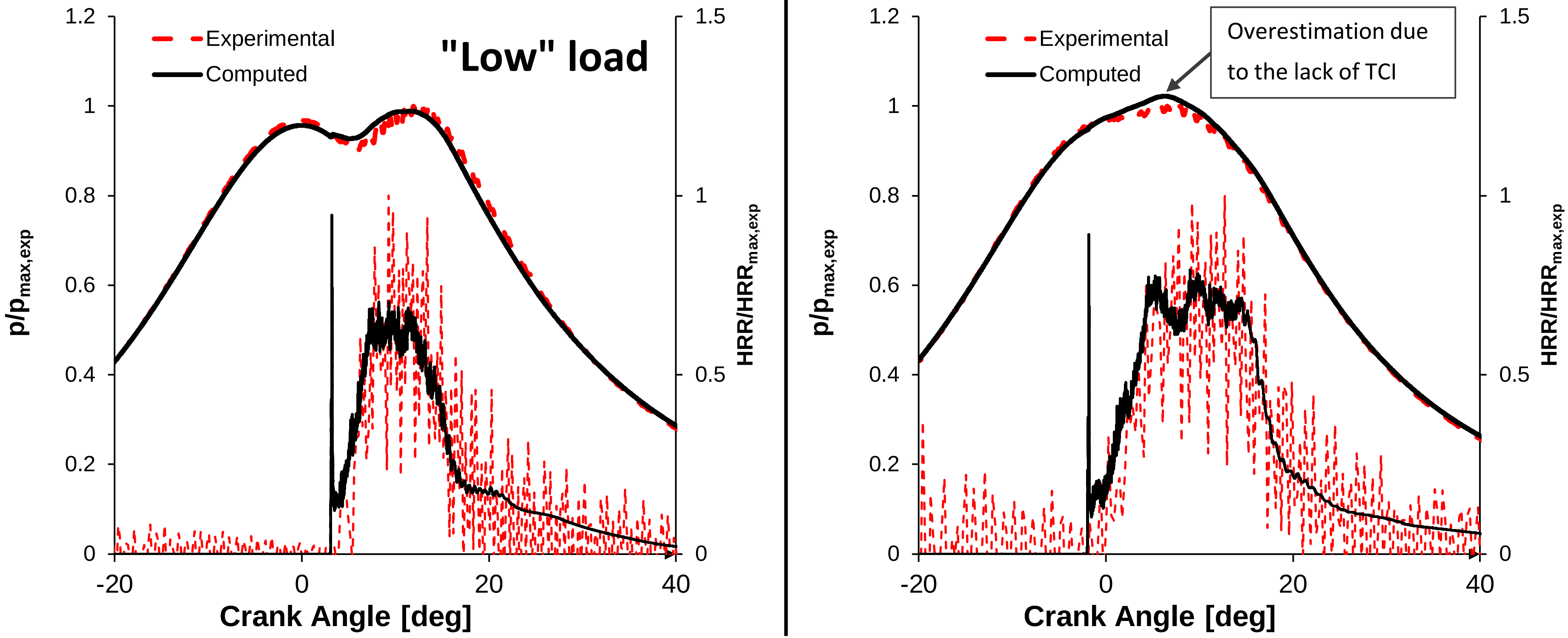
*To allow optical access, the engine runs with a single injector

*Operating conditions adjusted to enable optical experiments and not representative of the real engine operation

Validation: Large Bore Diesel Engine

Conventional Diesel: validation

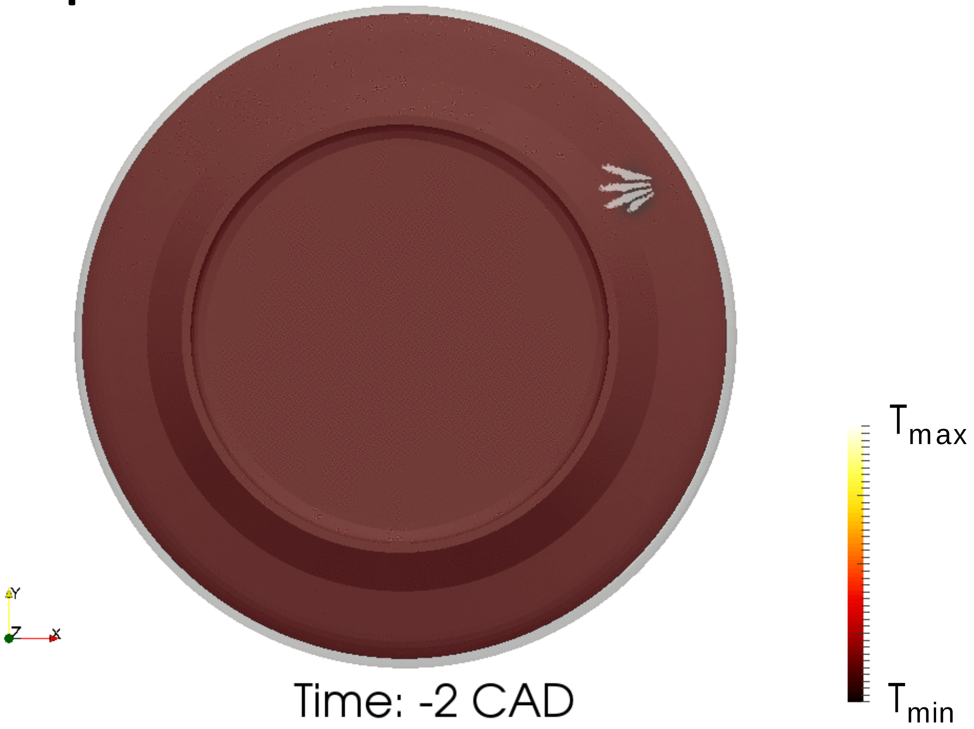
All data normalized with respect to the corresponding maximum experimental value



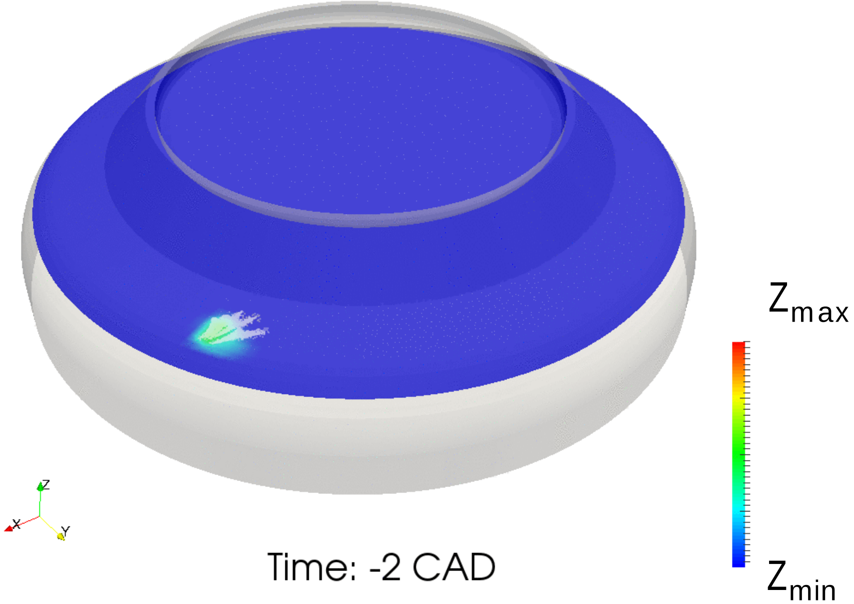
Validation: Large Bore Diesel Engine

Conventional Diesel: validation – High Load

Temperature



Mixture fraction



Validation: Large Bore Diesel Engine

Dual-fuel mode

Diesel fuel and natural gas directly injected into the cylinder with different SOI times

	"Low" Load	"High" Load
Speed [rpm]	~80	~100
SOI Diesel [CAD BTDC]	-1	-1.5
SOI CNG [CAD BTDC]	1	0

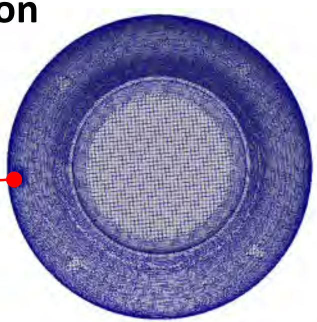
*To allow optical access, the engine runs with one diesel and one natural gas injector
*Operating conditions adjusted to enable optical experiments and not representative of the real engine operation

Validation: Large Bore Diesel Engine

Dual-fuel mode: simulation setup

Boundary conditions for gas injection

Gas injector



Spray + Mixture fraction field

- Velocity: derived from measured mass flow rate
- Temperature : fixed value
- Pressure: zero gradient
- Mixture fraction $Z = 1$
- Mixture fraction $Z_1 = 1$
- Mixture fraction $Z_2 = 0$

Tabulated kinetics

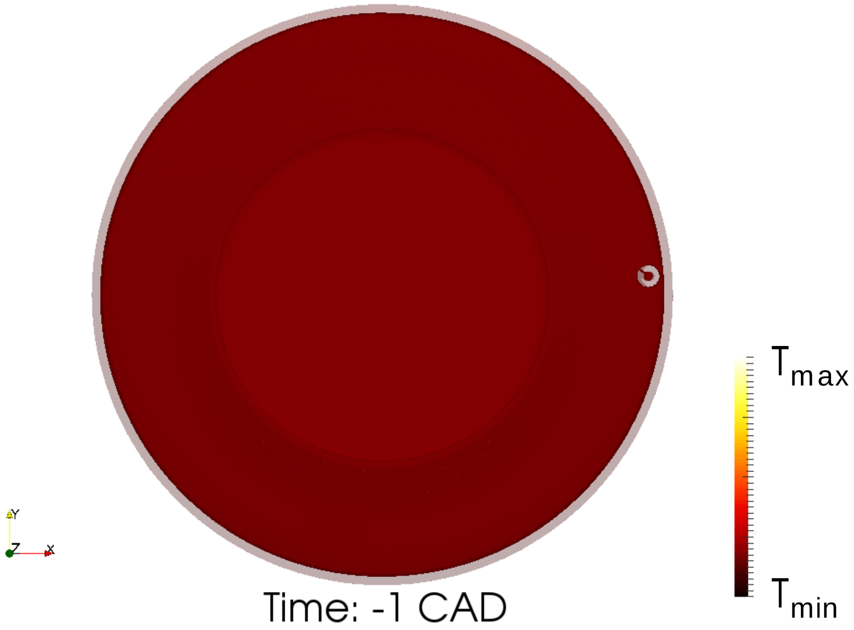
Diesel fuel type	n-C_7H_{16} (gas phase) IDEA (liquid properties)
Tabulated mechanism	n-C_7H_{16} from LLNL (159 species)
Tabulation	ϕ=0.2-3; T=500-1250 K; p = 2-20 MPa

Natural gas	CH_4 (gas phase)
Tabulated mechanism	CH_4 from GRI (53 species)
Tabulation	ϕ=0.2-3; T=500-1250 K; p = 2-20 MPa

Validation: Large Bore Diesel Engine

Dual fuel combustion

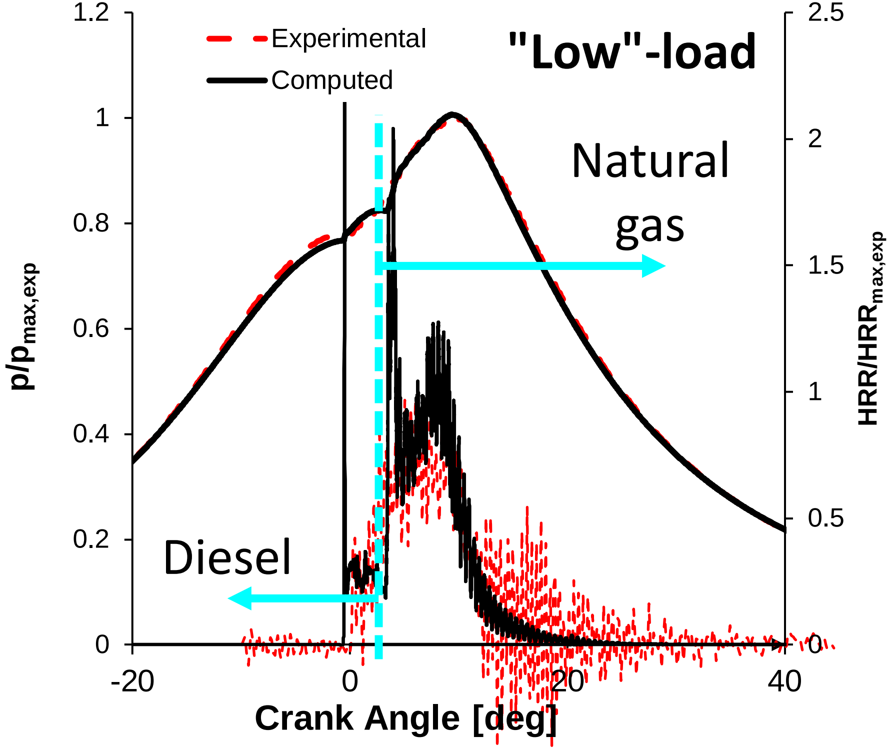
The diesel jet is first ignited, diffusion of progress variable ignites natural gas shortly after its injection

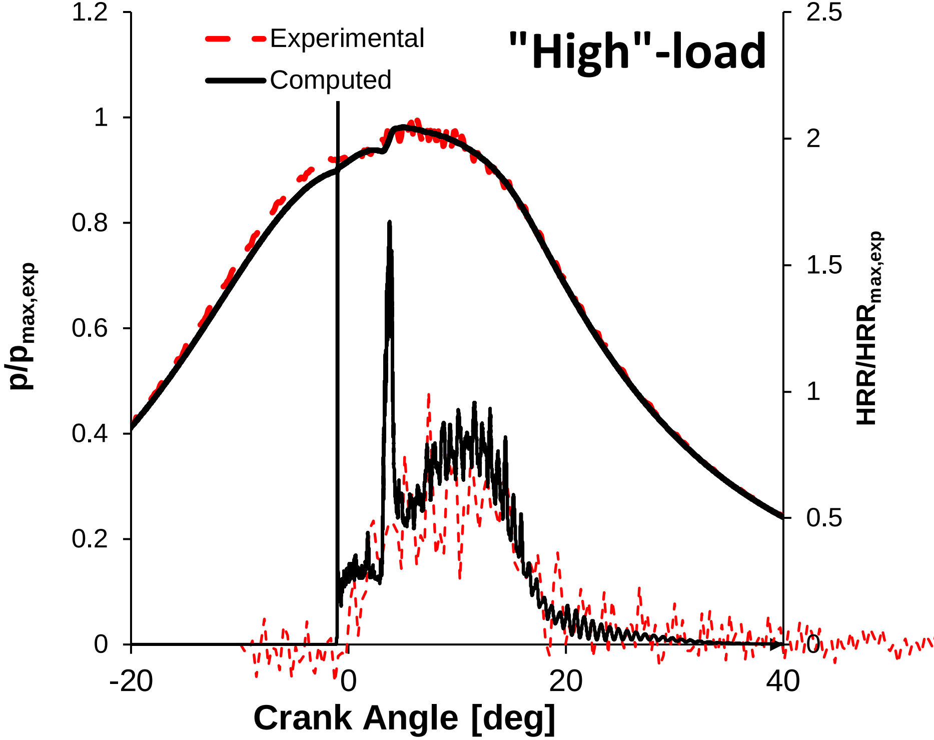


Validation: Large Bore Diesel Engine

Dual-fuel combustion: validation

All data normalized with respect to the corresponding maximum experimental value





SI engine

Challenges for SI engine modelling?

Mesh handling, DI injection, ignition, combustion, knock

OpenFOAM-x.x.x

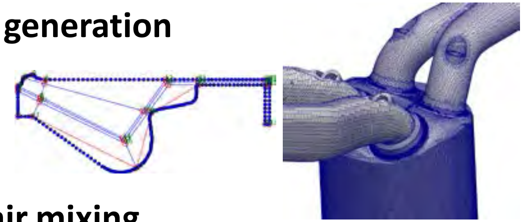
↓

Lib-ICE

- **Library**: physical models, mesh management
- **Applications**: solvers (cold flow, SI, Diesel, after-treatment), utilities

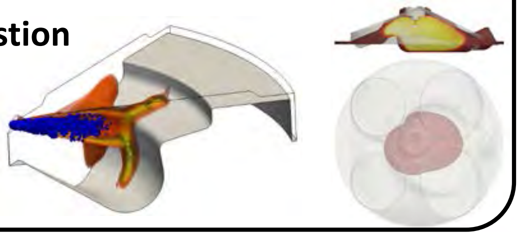
Engine simulation workflow

Mesh generation

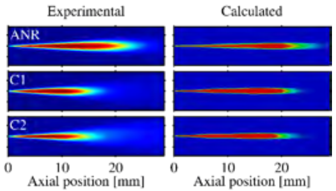


Fuel-air mixing

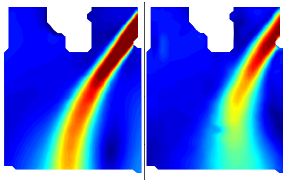
Combustion



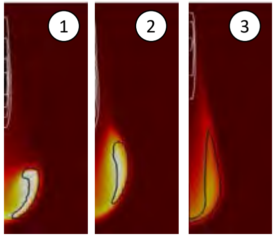
Development/validation



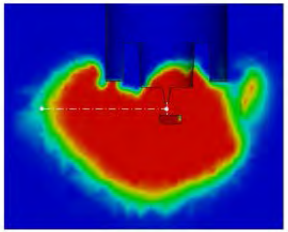
Spray modeling



Engine flows



Diesel combustion



SI combustion

SI engines: simulation workflow

Global overview

SI engines

Mesh management
- Automatic mesh generation
- Mesh motion
- Topological changes

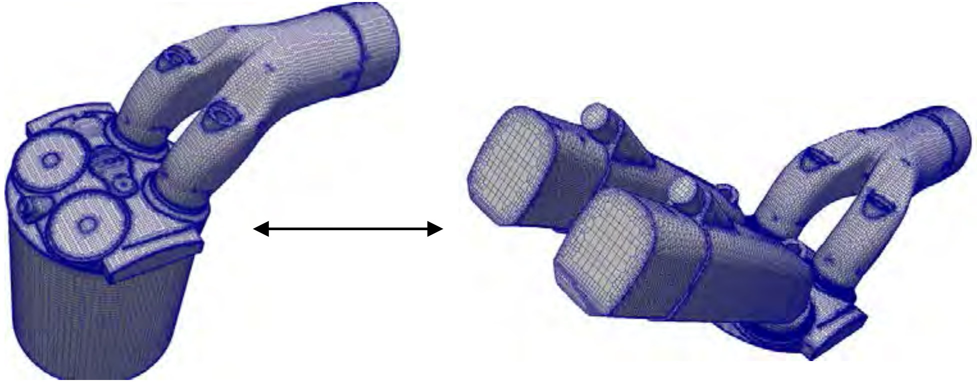
Cold flow
- Discretization
- Turbulence models
- Mesh quality

Fuel-air mixing
- Lagrangian spray
- Sub-models
- Nozzle flow

Combustion
- Simplified or detailed kinetics
- Ignition
- Pollutants

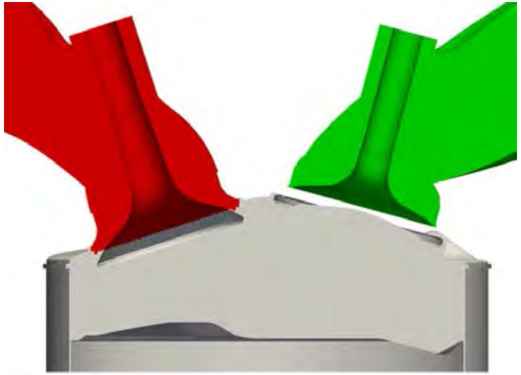
Mesh generation and management

Mesh manipulation: IFP Energies nouvelles optical engine and 1.0 liter, 3 cyl. VVA engine



IFP optical engine

- Multiple meshes
- Mesh to mesh interpolation strategy
- Ducts are removed when not used
- 1 mm internal cell size
- 0.5 mm internal cell size under the injector
- Local refinement down to 0.125 mm at the valves

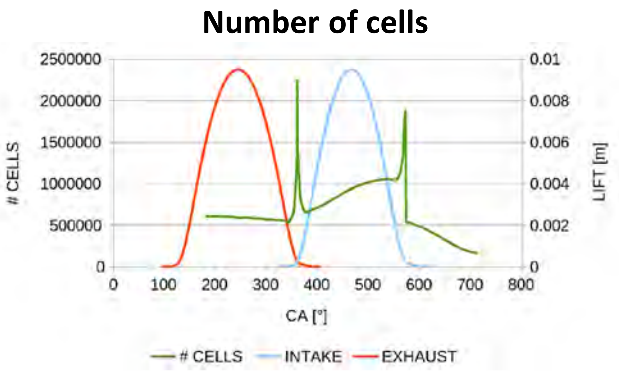


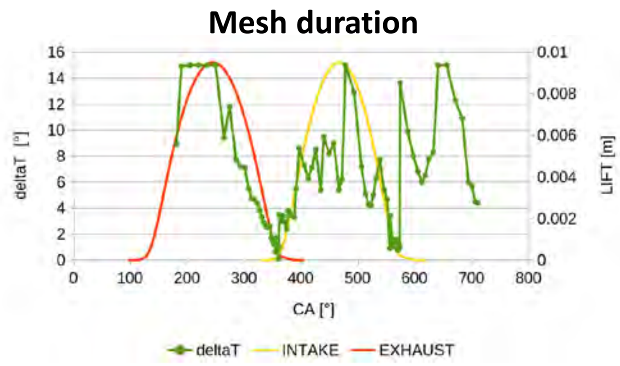
1.0 liter, 3 cyl. VVA engine

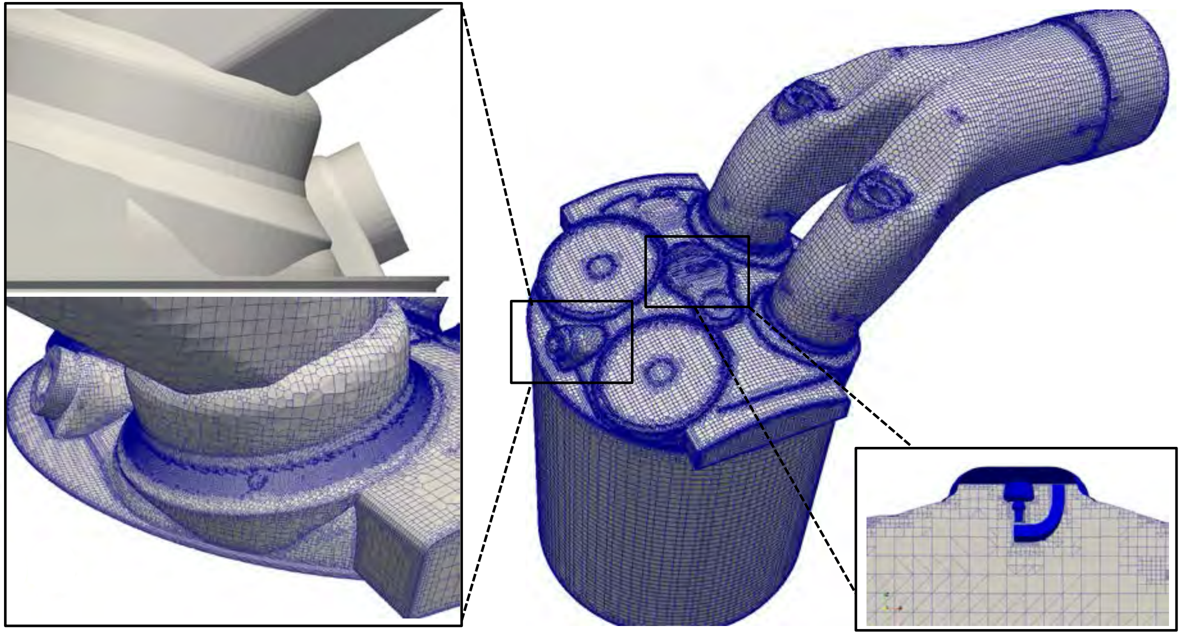
- Unsteady flow in detached ducts is simulated along with the engine
- Pressure waves helping cylinder filling are taken into account
- Fuel backflow into the intake ducts is taken into account

Mesh generation and management

Mesh generation: IFP Energies nouvelles optical engine

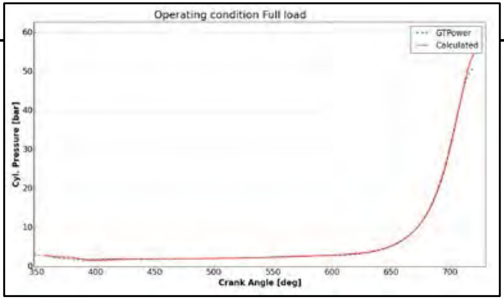


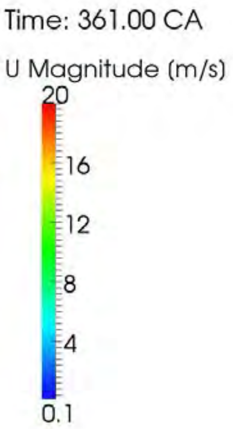


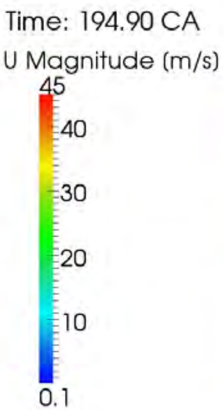


SI Engines: cold flow

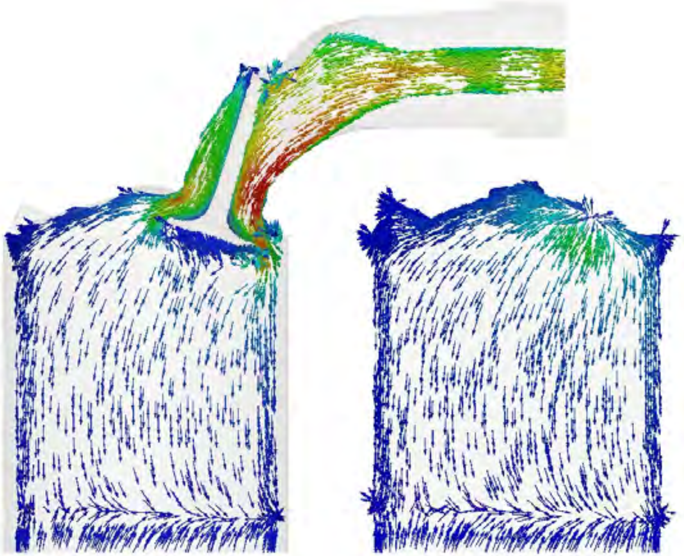
IFP optical engine: flow field post processing







Intake flow streamlines and in-cylinder velocity vectors for a plane cutting through the valves stem

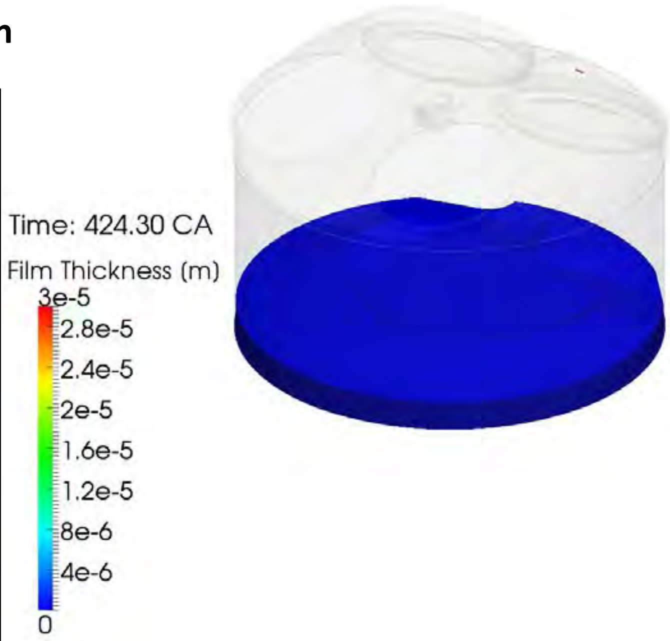


SI Engines: GDI air-fuel mixing

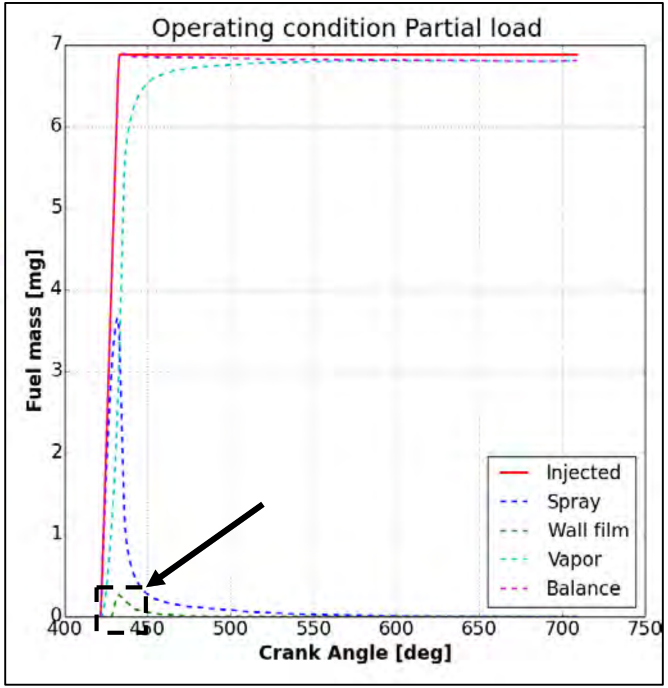
1.0 liter, 3 cyl. VVA engine – Partial load condition: fuel balance

- **Complete wall-film evaporation**

Crank Angle [deg]

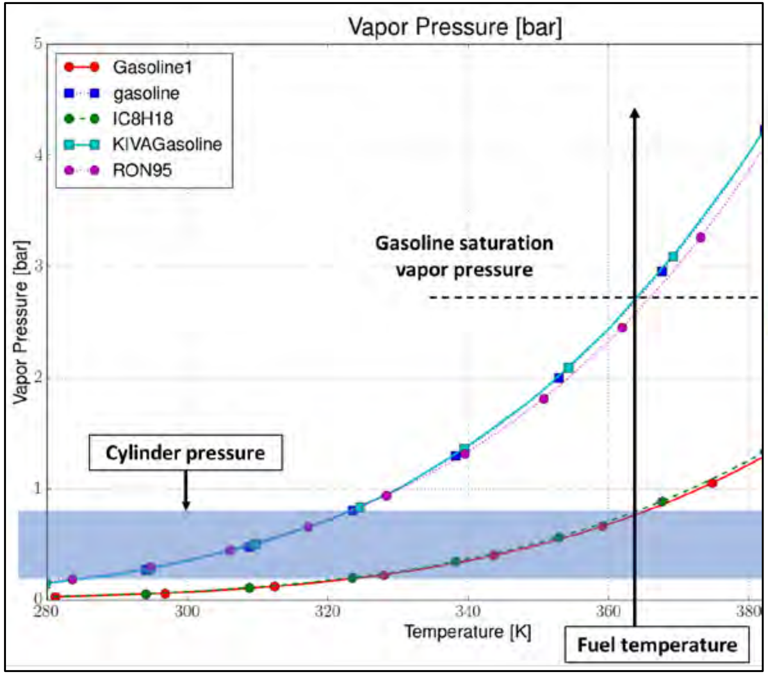


- **Accurate global fuel balance**

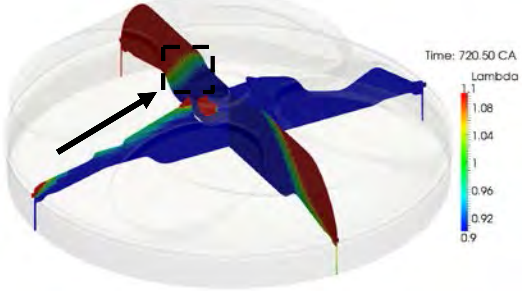


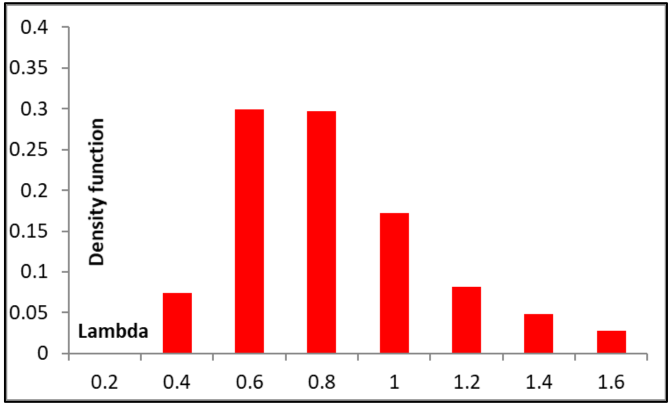
SI Engines: GDI air-fuel mixing

1.0 liter, 3 cyl. VVA engine – Partial load condition: mixture analysis



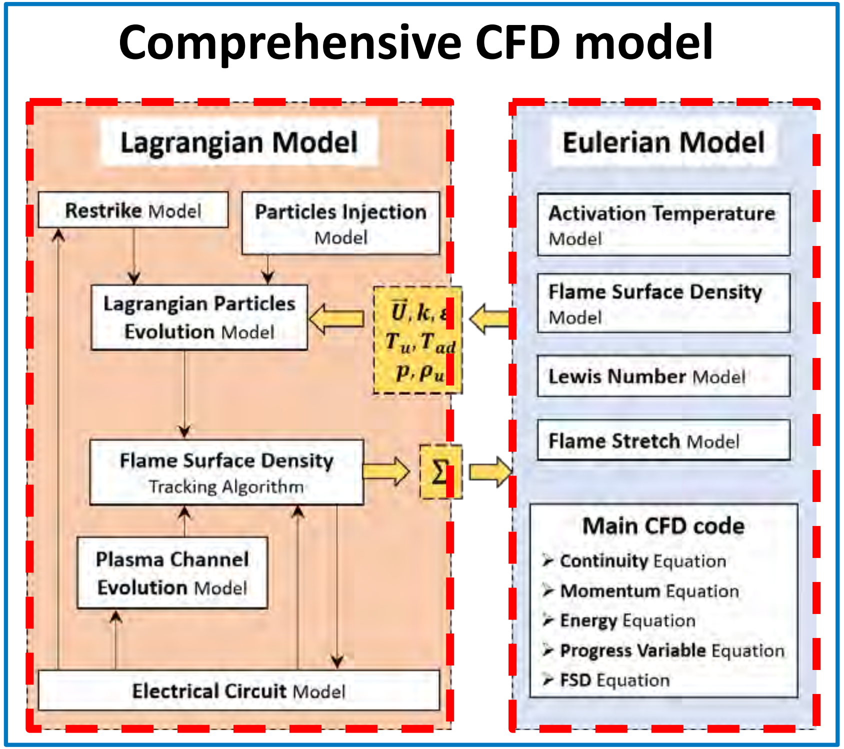
➢ **Flash boiling condition: larger spray cone**

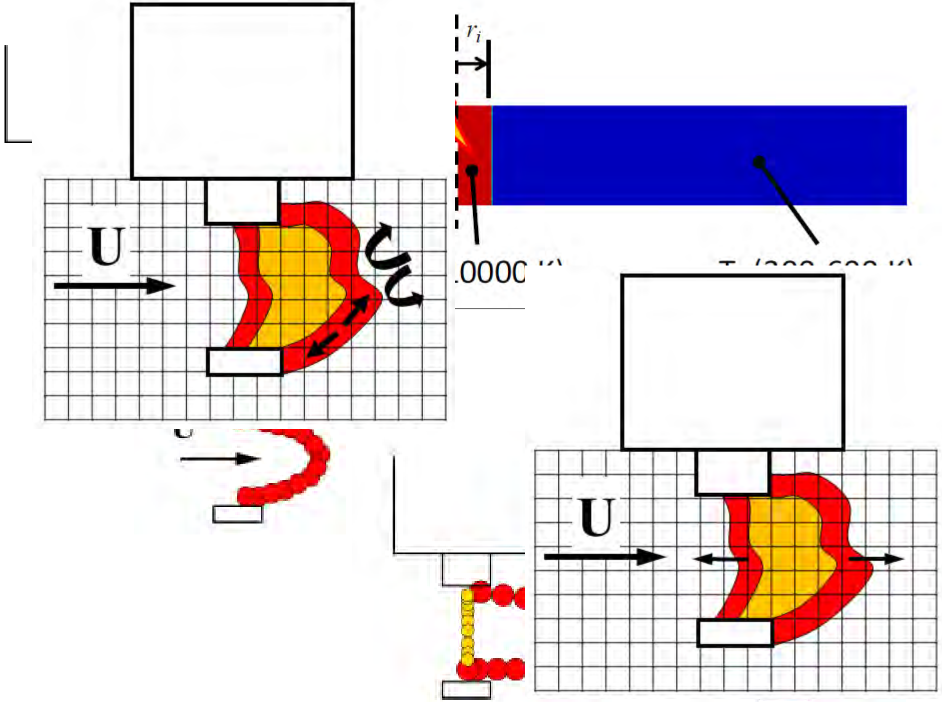




The *Lagrangian-Eulerian* model for SI combustion

SI combustion engine modeling using the Open-FOAM® technology





SI combustion simulation of diluted mixtures

SI combustion engine modeling using the Open-FOAM® technology

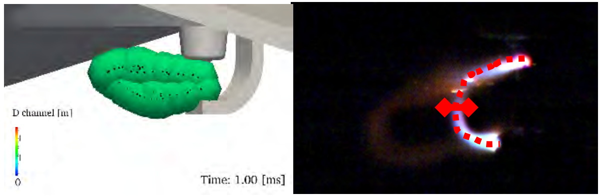
Validations

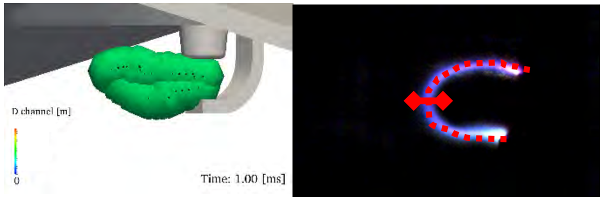
- Michigan Tech University vessel
- Chiba University vessel
- Herweg-Maly side chamber

$\uparrow l_{channel}$ and $\uparrow d_{channel}$

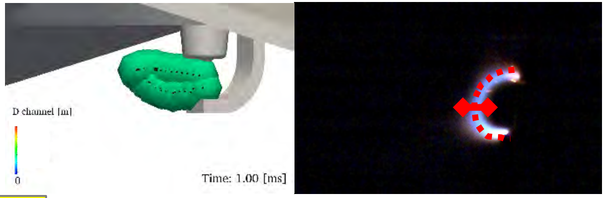
Plasma channel shape

Stoichiometric mixture with EGR





Lean mixture



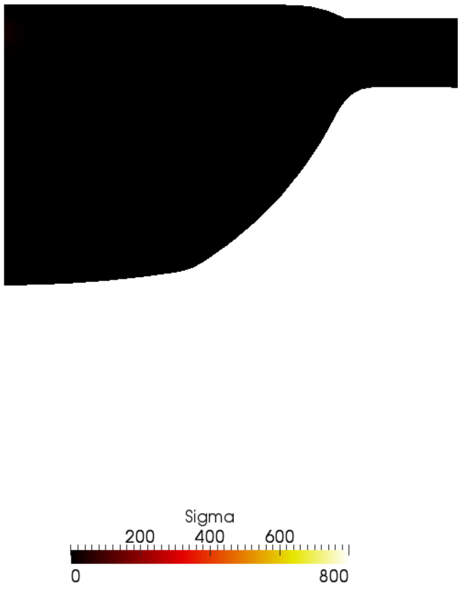
$\uparrow i_s$

SI combustion simulation

SI combustion engine modeling using the Open-FOAM® technology

Next Steps

- Use of **tabulated well-mixed (TWM)** in the unburnt mixture **to predict knock** in SI engines.
- Integration of the **Tabulated Flamelet Progress Variable (TFPV)** in the post-flame zone to determine non-equilibrium composition and soot precursor due to mixture fraction fluctuations in GDI engines.



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Thanks for your attention!!!