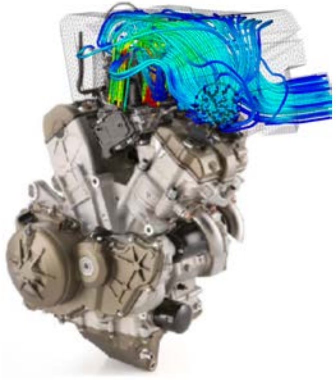
CFD modeling of IC engines:
Research work at Politecnico di Milano



Internal Combustion Engine Group

Department of Energy, Politecnico di Milano

The Internal Combustion Engine Group

Staff

Angelo Onorati, Full Professor
Gianluca D’Errico, Full Professor
Gianluca Montenegro, Associate Professor
Tommaso Lucchini, Associate Professor
Augusto Della Torre, Assistant professor
Tarcisio Cerri, Assistant professor

Post-doc/MSc researchers

Lorenzo Sforza, post-doc researcher
Giorgio D’Antonio, MSc researcher
Filippo Pavirani, MSc researcher
Andrea Marinoni, MSc researcher

PhD students

Davide Paredi
Giovanni Gianetti
Matteo Tamborski
Antonello Nappi
Qiyan Zhou

MSc thesis

20-25 per year

Visiting PhD

Aalto, Sidney, KTH, Chalmers, Freiberg, Valencia, etc.,

CFD for IC Engines: why OpenFOAM?

Requirements

Implementation of new models

- Research on fundamental topics
- Extensive validation using different type of data (engine, vessels)

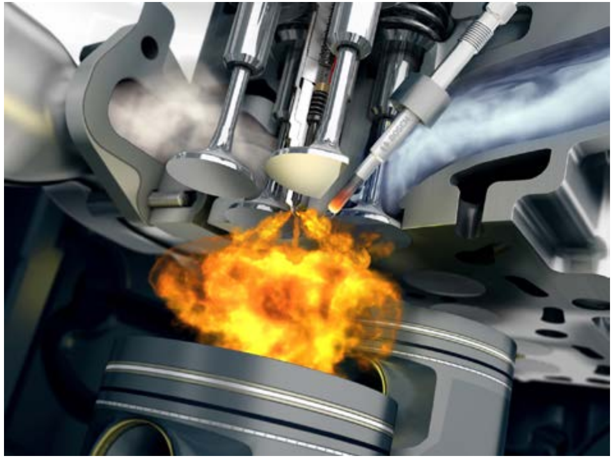
Fully integrated methodologies

Massive application in research and industrial projects

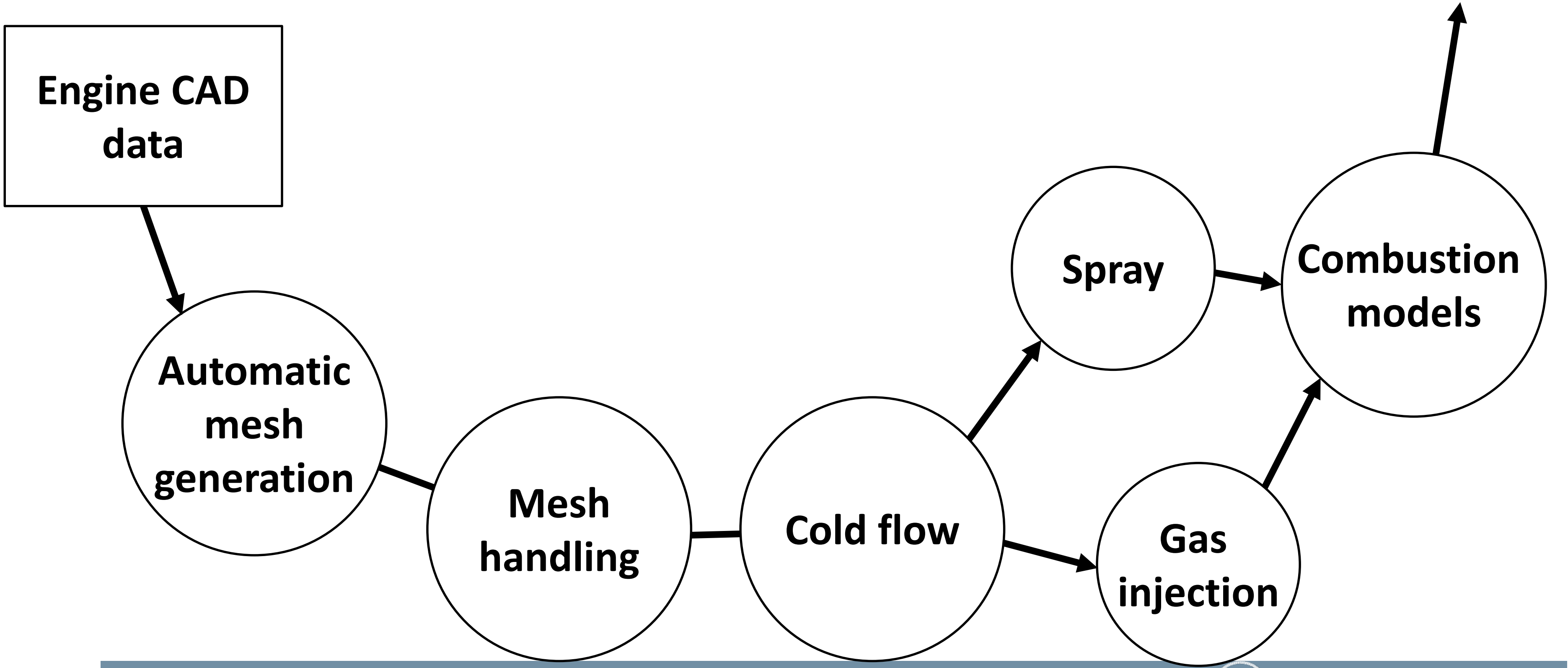
OpenFOAM is the solution

- Free and opensource
- Many pre-implemented capabilities: meshing, numerics, models
- Different available versions but very compatible
- Perfect basis to develop own libraries and solvers for complex problems

In-cylinder flows



In-cylinder simulations workflow



Engine CAD data

Automatic mesh generation

Mesh handling

Cold flow

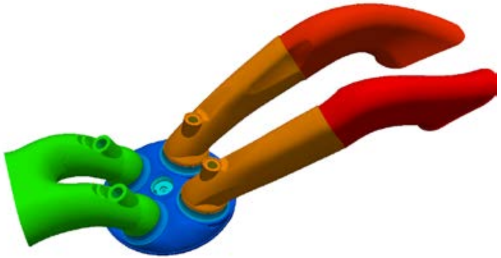
Spray

Gas injection

Combustion models

Spark-ignition engines: mesh generation and handling

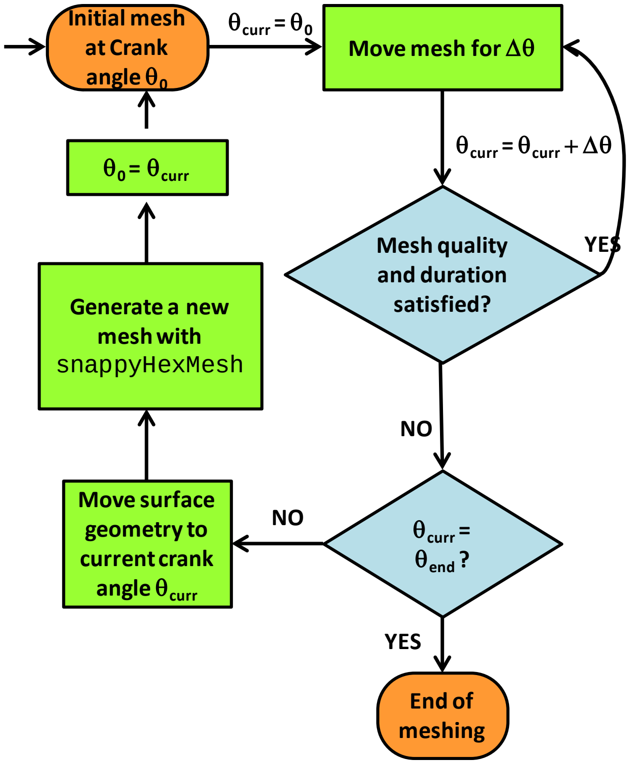
Input data



Input engine geometry data:

- STL geometry
- stroke, bore, connecting rod length
- valve lift curves
- rounds per minute

Automatic meshing



Initial mesh at Crank angle θ_0

$\theta_{curr} = \theta_0$

Move mesh for $\Delta\theta$

$\theta_{curr} = \theta_{curr} + \Delta\theta$

Mesh quality and duration satisfied?

YES

NO

$\theta_{curr} = \theta_{end}$?

YES

End of meshing

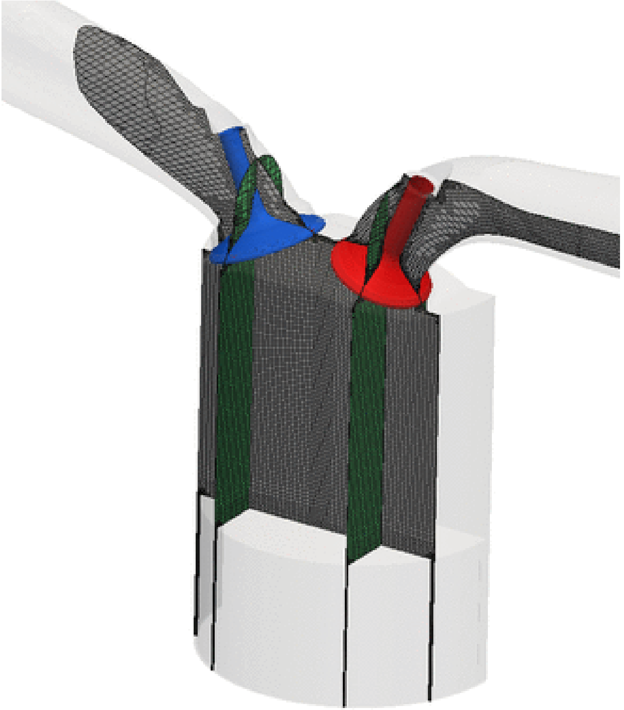
NO

Move surface geometry to current crank angle θ_{curr}

Generate a new mesh with `snappyHexMesh`

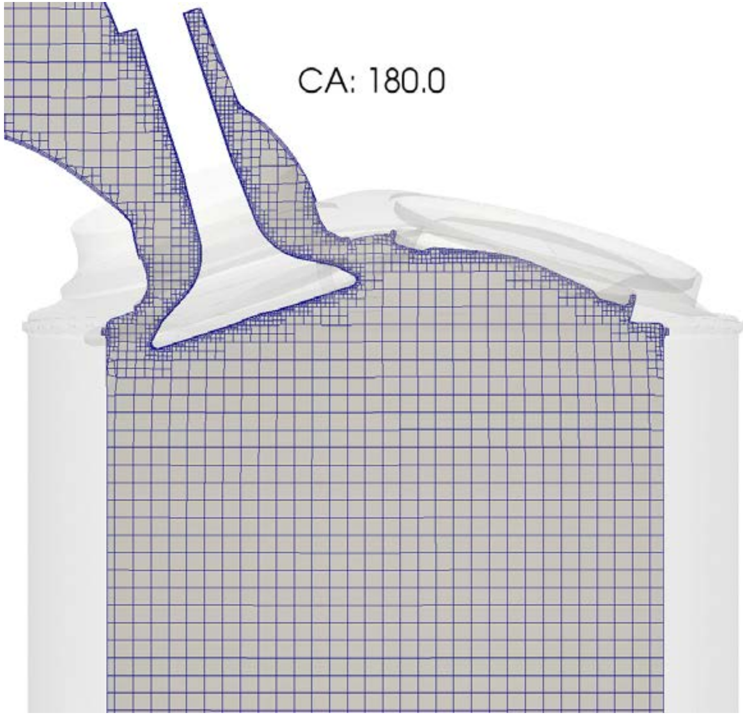
$\theta_0 = \theta_{curr}$

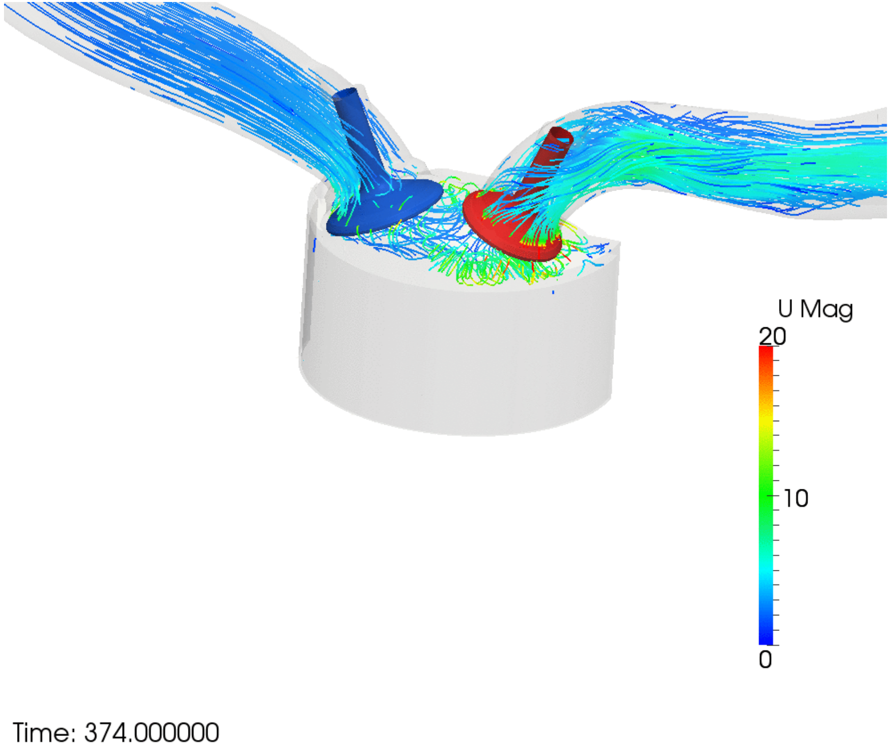
Mesh-motion



Spark-ignition engines: mesh generation and handling

Mesh motion and full-cycle simulation



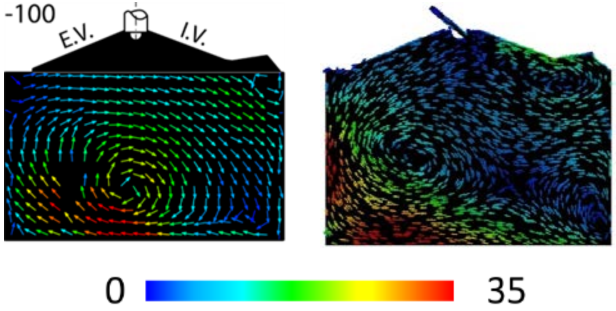


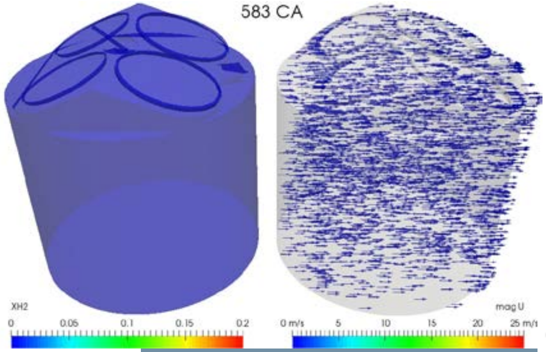
SI engines: direct-injection

Natural gas / hydrogen

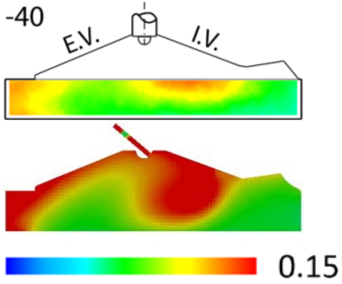
SANDIA H_2 engine

Velocity field at 100 CAD BTDC





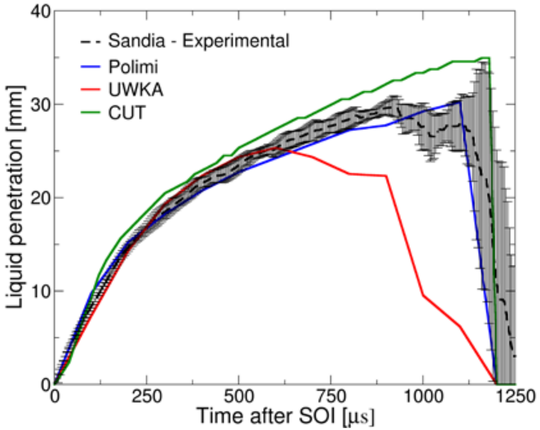
Equivalence ratio distribution



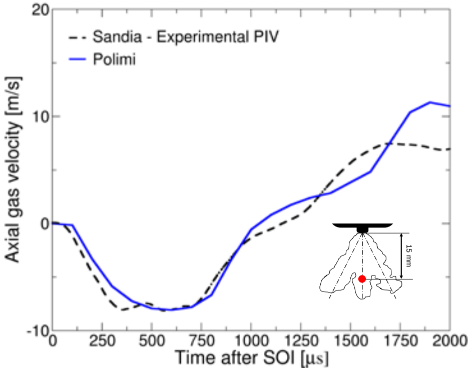
Liquid fuels

ECN spray G

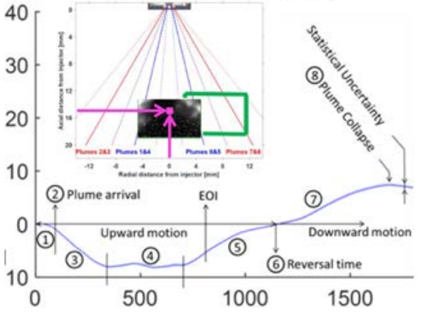
Spray penetration



Validation with PIV data



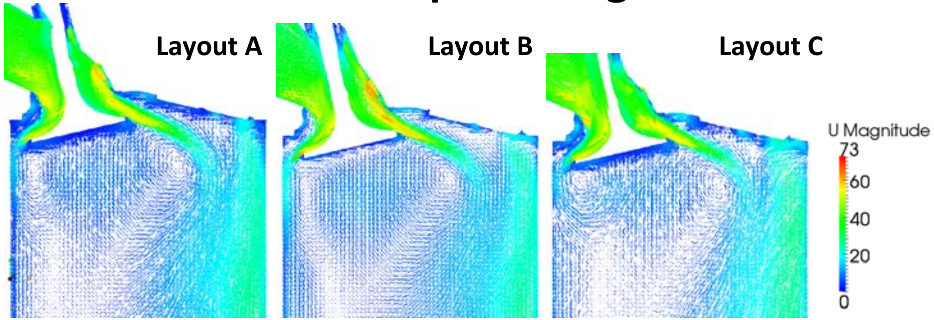
15-mm axial velocity



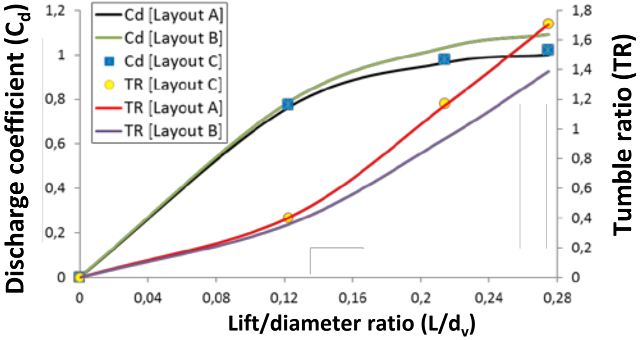
Spark-ignition engines: EU project HDGas

- Purpose: development of dedicated SI, natural gas engines for heavy duty
- OpenFOAM and LibICE used for design of combustion chamber and analysis of fuel-air mixing

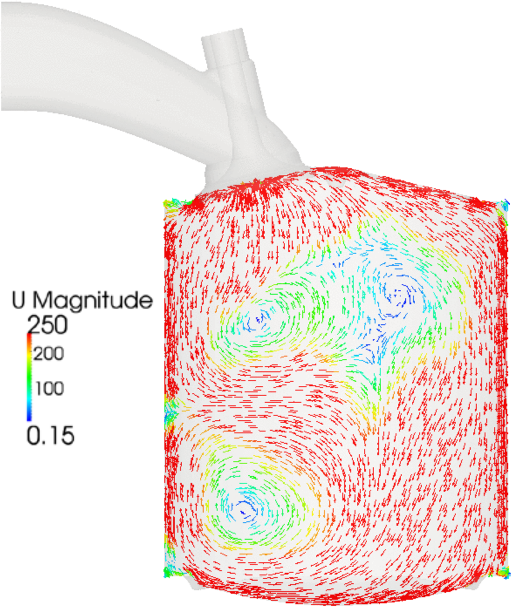
Intake port design

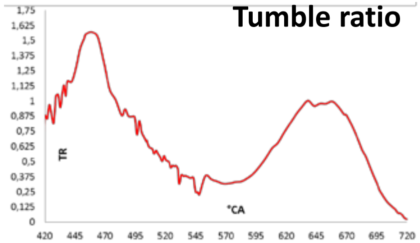


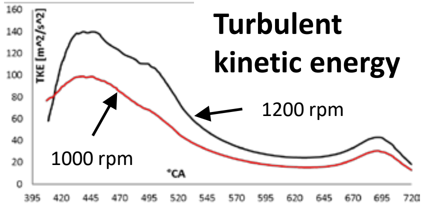
- ➢Discharge coefficient (C_d)
- ➢Tumble ratio (TR)

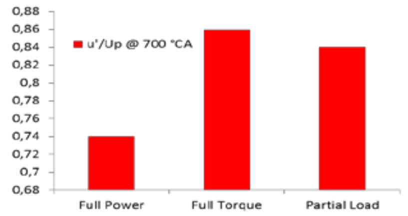


Charge motions analysis







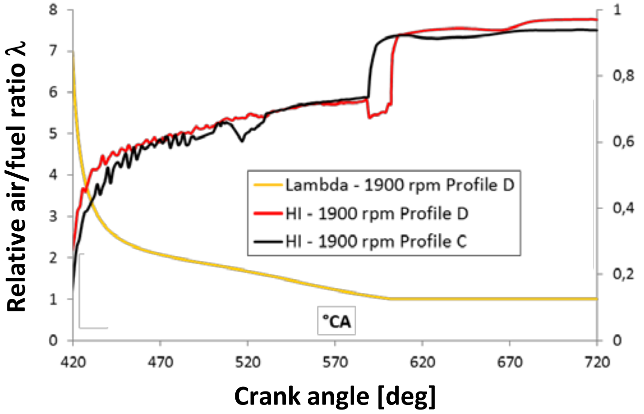


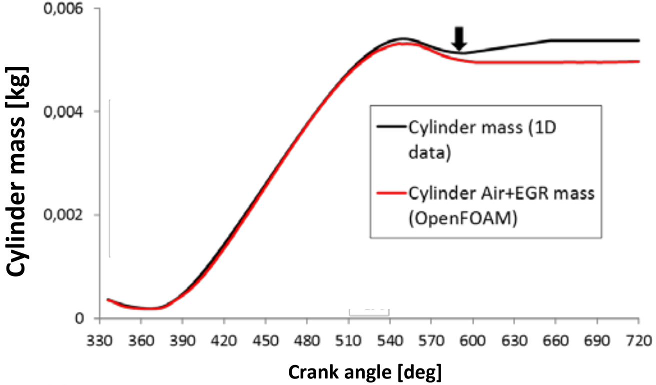
Acknowledments: S. Golini, N. Rapetto (FPT Industrial)

Spark-ignition engines: EU project HDGas

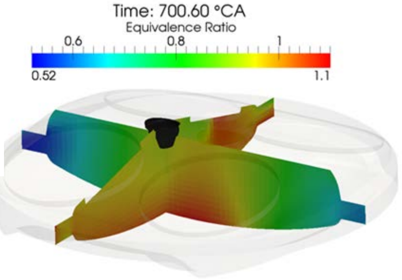
Simulation of the fuel-air mixing process

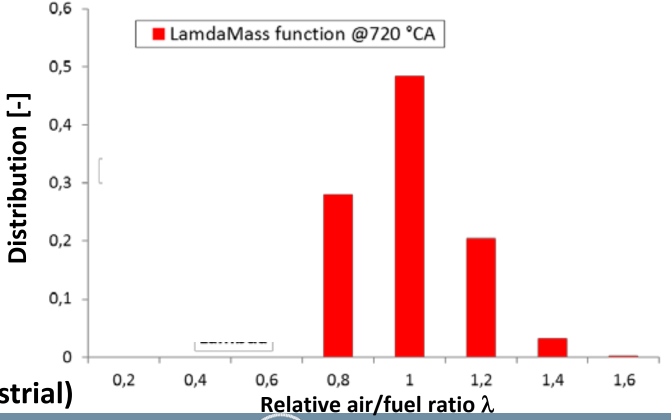
Contours of equivalence ratio





Equivalence ratio distribution at spark-timing





Acknowledments: S. Golini, N. Rapetto (FPT Industrial)

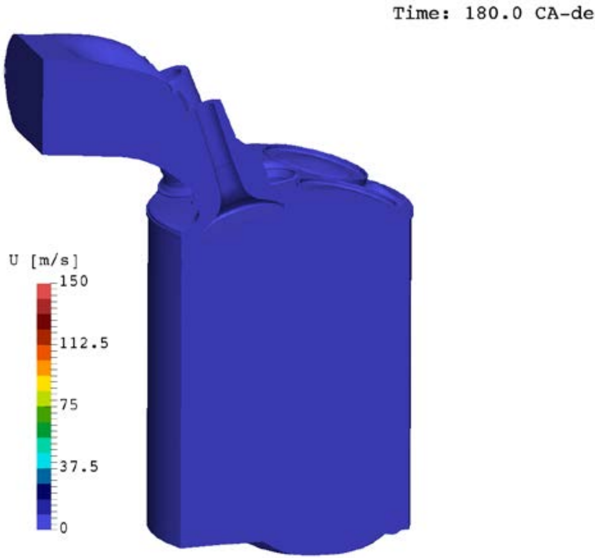
Spark-ignition engines: EU project UPGRADE

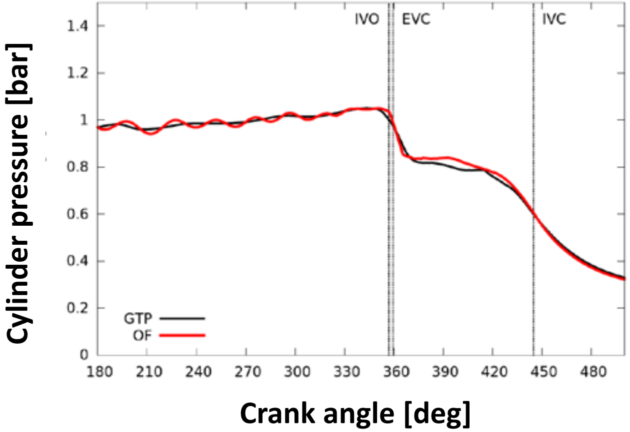
- Purpose: development of a new generation of GDI Engines with high efficiency and low-soot
- OpenFOAM and LibICE used to perform full-cycle simulations (gas exchange, fuel-air mixing and combustion) in both production and optical engines.

Turbocharged engine with Multi-air® technology

2000 rpm, bmep = 2 bar
2000 rpm, bmep = 4 bar
1500 rpm, full load
2500 rpm, bmep = 13 bar

Full-cycle simulations (gas exchange only)



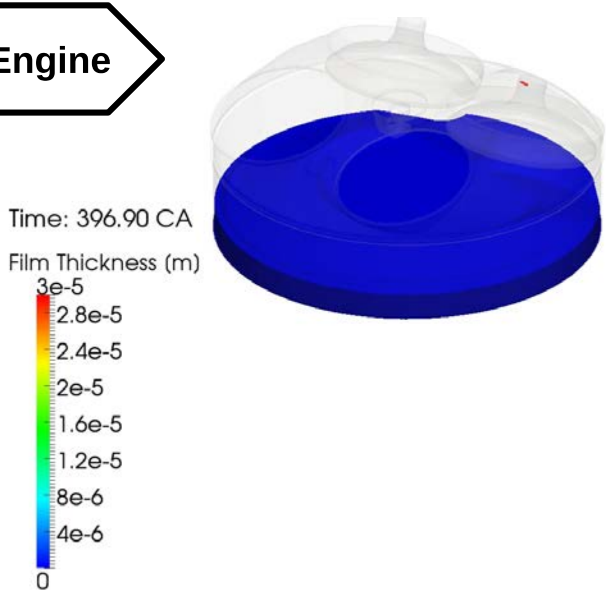


Acknowledments: A. Gerini, S. Zandiri, F. Perna (CRF)

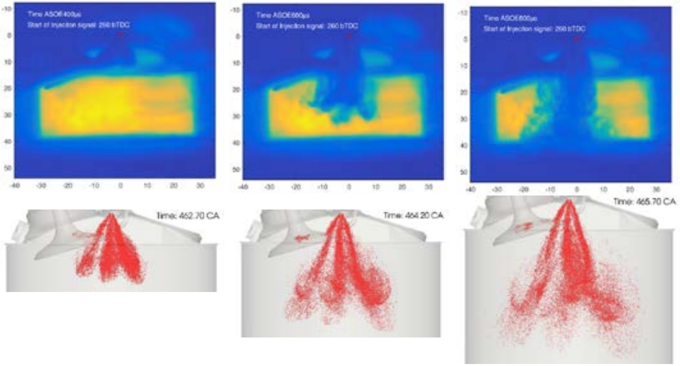
Spark-ignition engines: EU project UPGRADE

Simulation of the fuel-air mixing process with wall-film

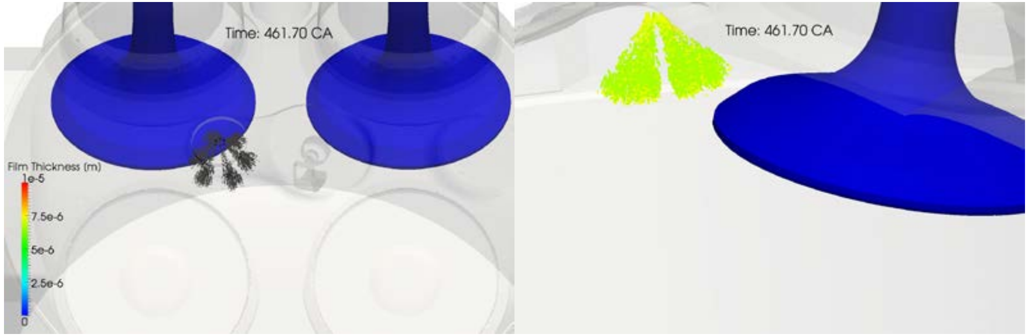
CRF Engine



IFPEN Engine



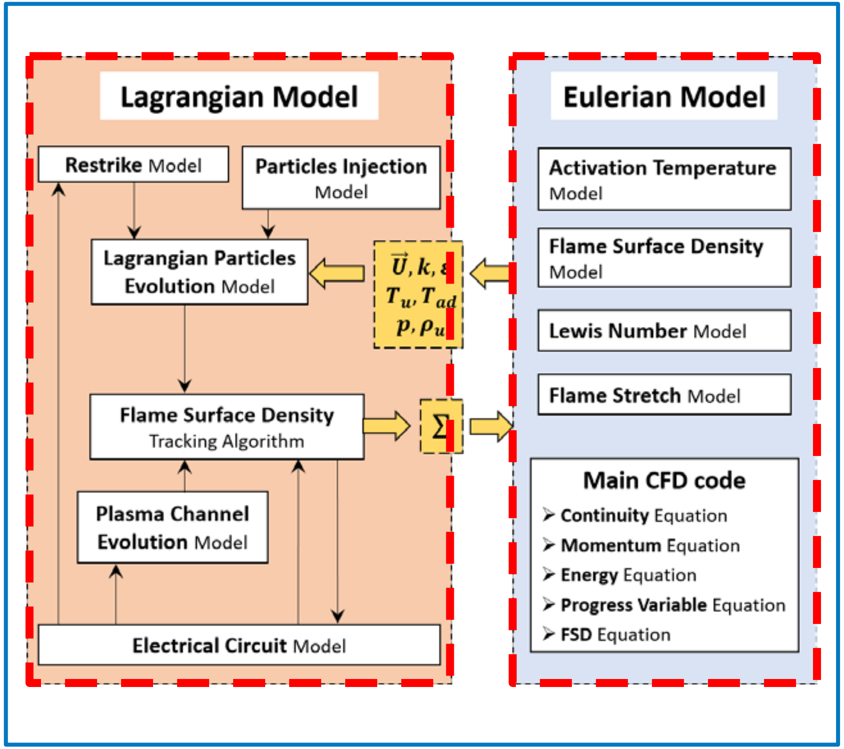
Exp. data courtesy of IFPEN (Dr. M. Bardi)



Acknowledments: A. Gerini, S. Zandiri, F. Perna (CRF)

Spark-ignition engines: combustion modeling

Comprehensive approach for spark-ignition combustion



Lagrangian Model

Restrike Model

Particles Injection Model

Lagrangian Particles Evolution Model

$\vec{U}, k, \varepsilon$
T_u, T_{ad}
p, ρ_u

Flame Surface Density Tracking Algorithm

Σ

Plasma Channel Evolution Model

Electrical Circuit Model

Eulerian Model

Activation Temperature Model

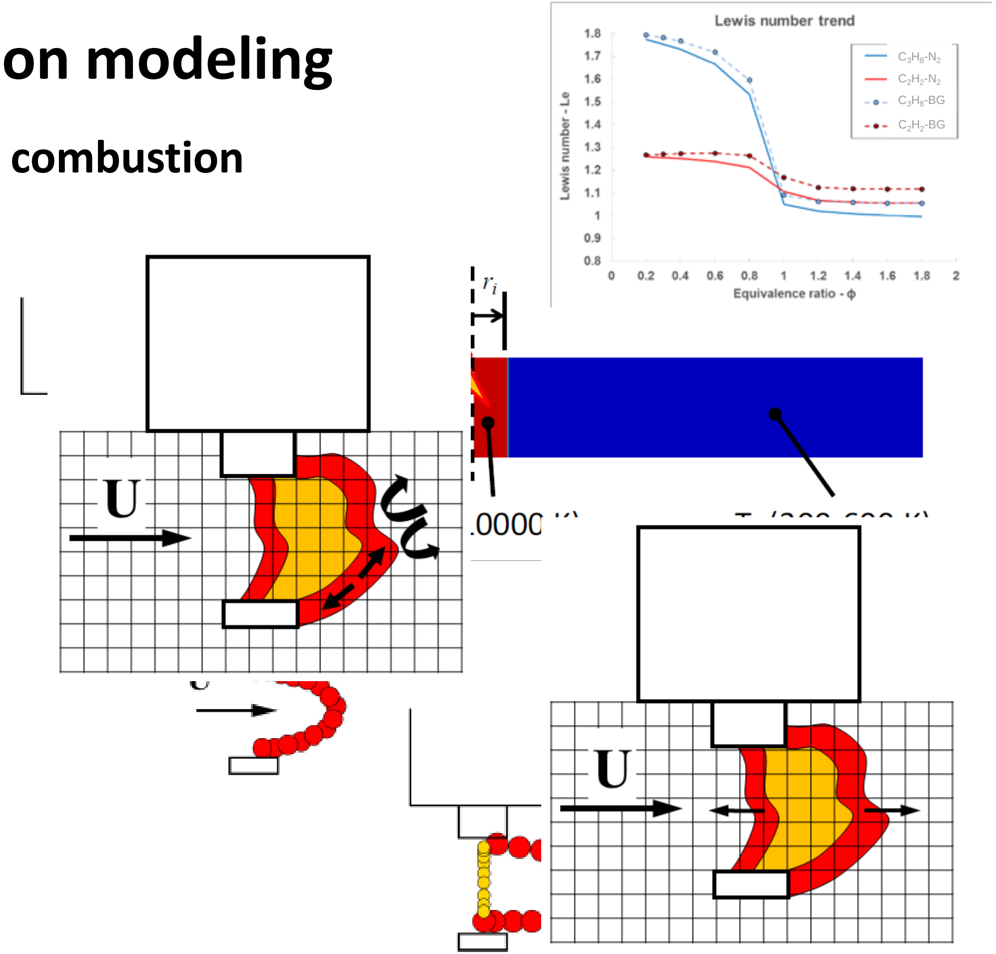
Flame Surface Density Model

Lewis Number Model

Flame Stretch Model

Main CFD code

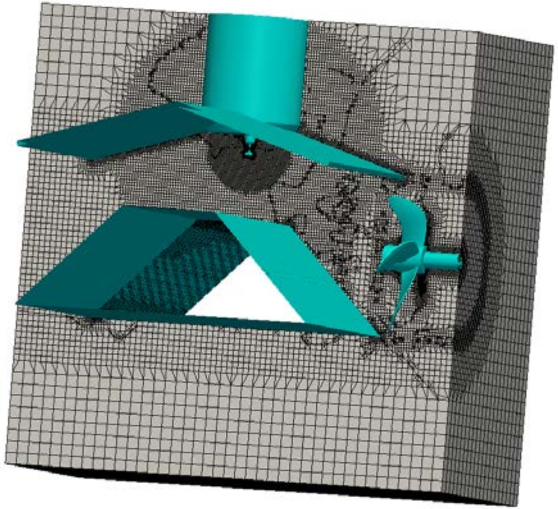
- **Continuity** Equation
- **Momentum** Equation
- **Energy** Equation
- **Progress Variable** Equation
- **FSD** Equation

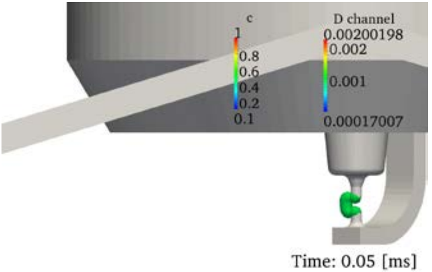


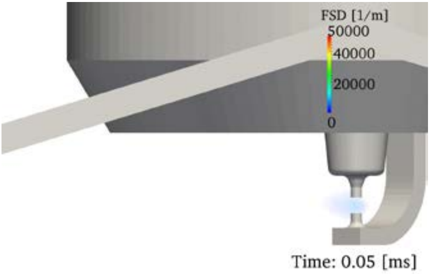
Spark-ignition engines: combustion modeling

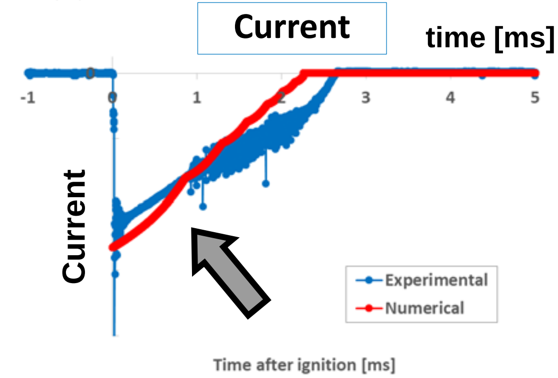
Comprehensive approach for spark-ignition combustion – CHIBA VESSEL

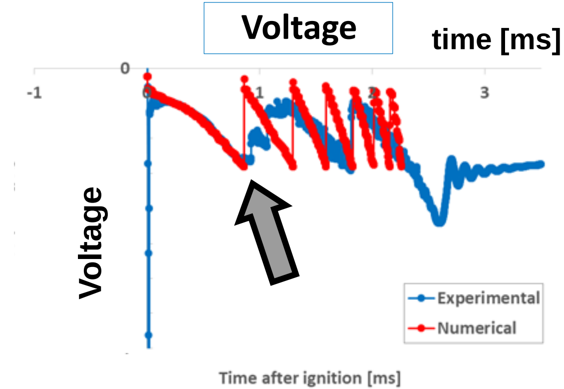
Cold-flow initialization → **Combustion simulation**











Acknowledments: T. Shiraishi, T. Hori(Nissan); prof. Moriyoshi (Chiba University)

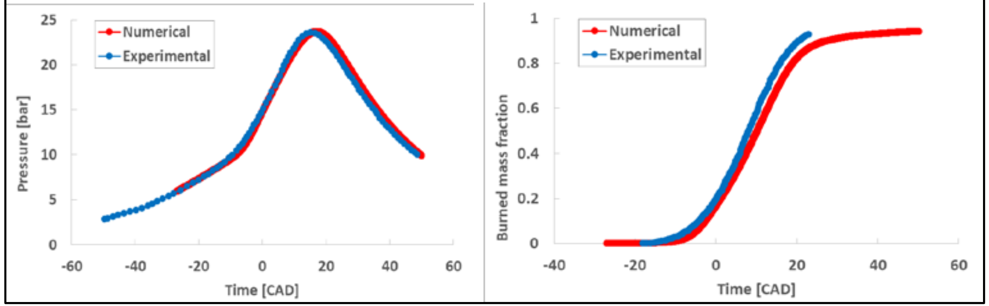
Spark-ignition engines: combustion modeling

GM pancake engine

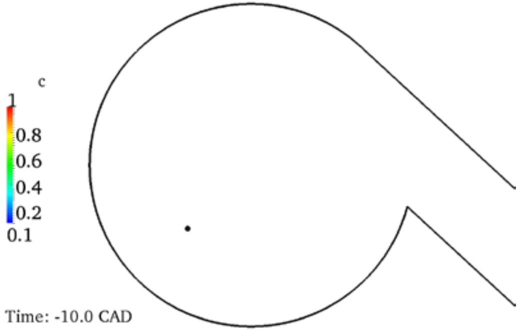
Computational mesh

flame propagation

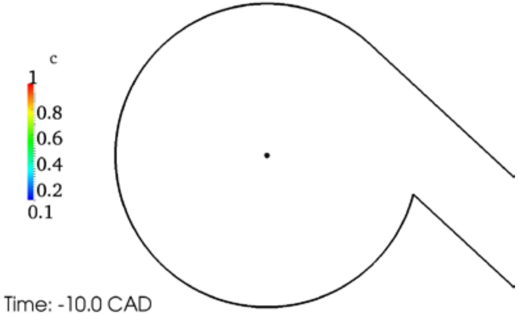
Validation (cyl. press and cumulative heat release)



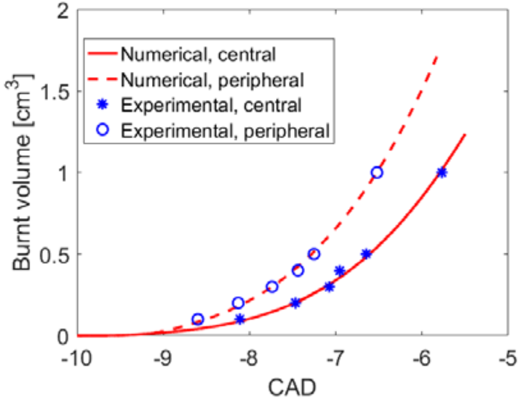
Side-chamber engine (Herweg and Maly)



Peripheral ignition

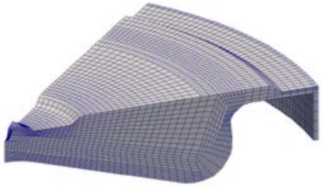


Central ignition



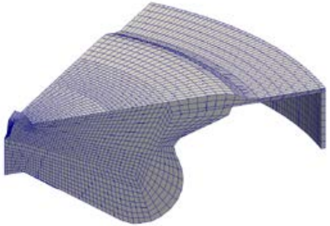
Diesel engines: mesh generation and handling

Automatic mesh generation

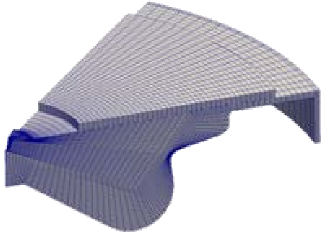


Bowl #1

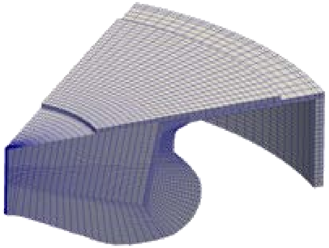
Bowl #2



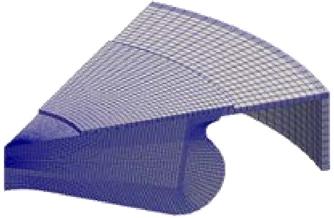
Bowl #3



Bowl #4



Bowl #5

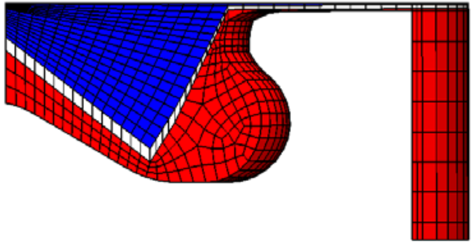


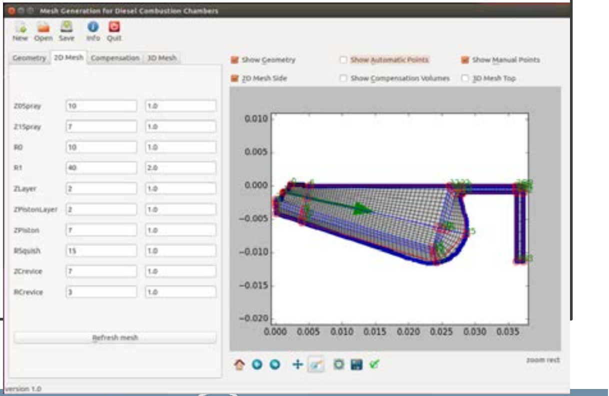
Bowl #6

From CAD to SIMULATION: 10 minutes

Mesh handling

Dynamic layering





Mesh Generation for Diesel Combustion Chambers

☑ Show Geometry
☐ Show Automatic Points
☑ Show Manual Points
☑ 2D Mesh Side
☐ Show Compensation Volumes
☐ 3D Mesh Top

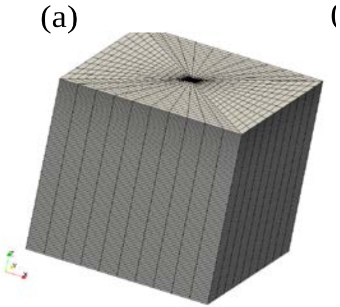
Z0Spray	10	1.0
Z1Spray	7	1.0
R0	10	1.0
R1	40	2.0
ZLayer	2	1.0
ZPistonLayer	2	1.0
ZPiston	7	1.0
RSquish	15	1.0
ZCrevice	7	1.0
RCrevice	3	1.0

version 1.0

Diesel engines: spray modeling

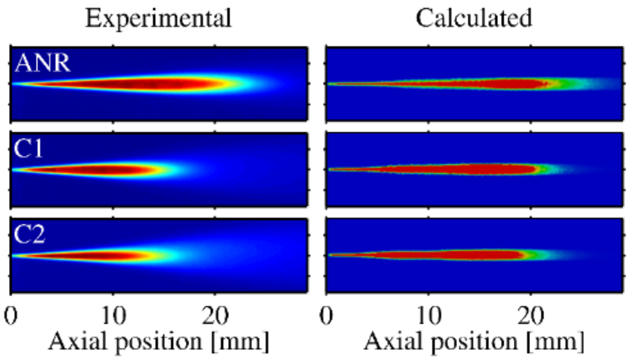
TUE Vessel

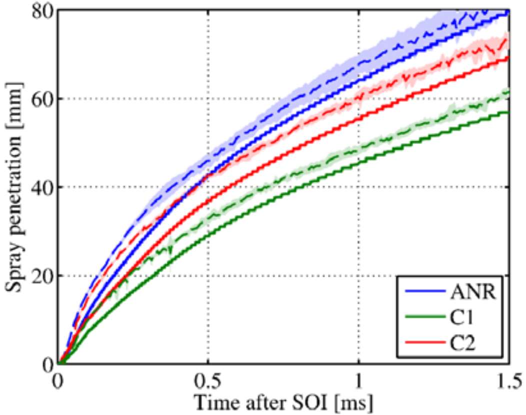
- $d_{inj} = 205\ \mu m$
- 3D mesh
- Huh-Gosman + Pilch Erdman

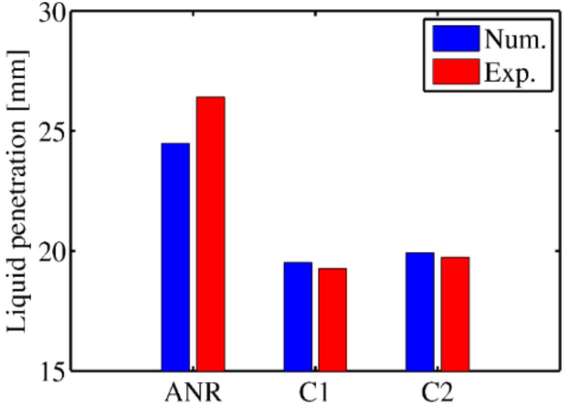


	P_{inj} [MPa]	ρ_{amb} [kg/m³]
ANR	150	22
C1	80	40
C2	150	40

Liquid+vapor penetration



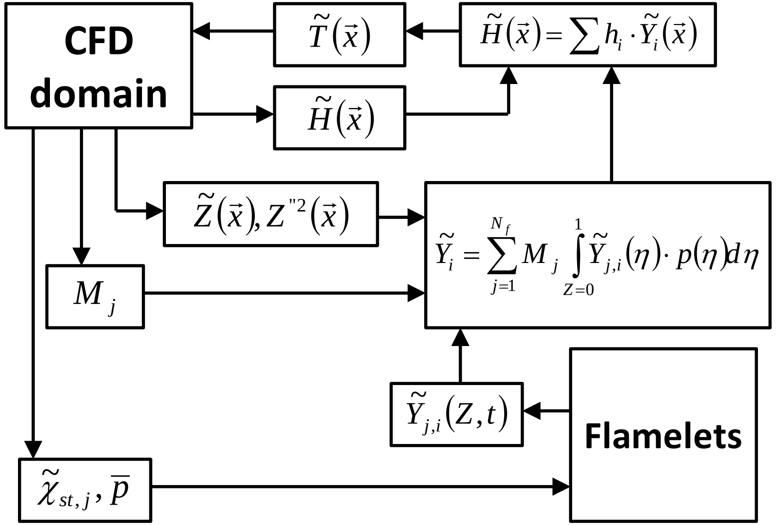




Acknowledgments: B. Somers, N. Maes (TUE), G. Hardy (FPT)

Diesel engines: combustion modeling

RIF: Representative interactive flamelet model



CFD domain

$\tilde{T}(\vec{x})$

$\tilde{H}(\vec{x}) = \sum h_i \cdot \tilde{Y}_i(\vec{x})$

$\tilde{H}(\vec{x})$

$\tilde{Z}(\vec{x}), Z''^2(\vec{x})$

M_j

$\tilde{Y}_i = \sum_{j=1}^{N_f} M_j \int_{Z=0}^{1} \tilde{Y}_{j,i}(\eta) \cdot p(\eta) d\eta$

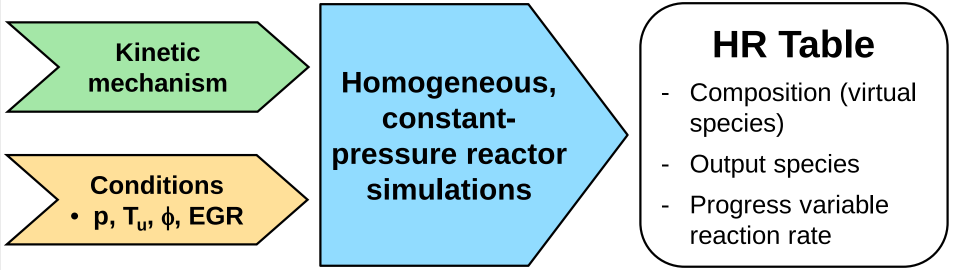
$\tilde{Y}_{j,i}(Z,t)$

Flamelets

$\tilde{\chi}_{st,j}, \bar{p}$

- Flamelet equations solved in the mixture fraction space (`regionModel`)
- Direct-integration of chemistry in Z-space and integration of β-pdf to get the composition in any cell.

Tabulated kinetics



Kinetic mechanism

Conditions
- **p, T_u, ϕ, EGR**

Homogeneous, constant-pressure reactor simulations

HR Table
- Composition (virtual species)
- Output species
- Progress variable reaction rate

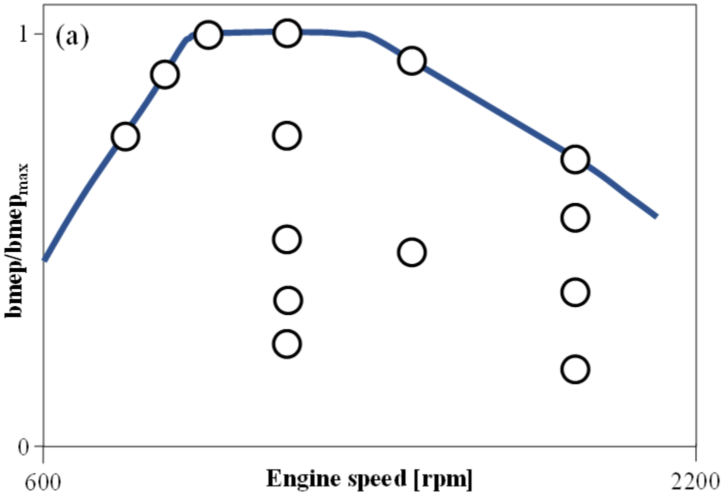
From HR tabulation to more complex flame structures and combustion models for different conditions:

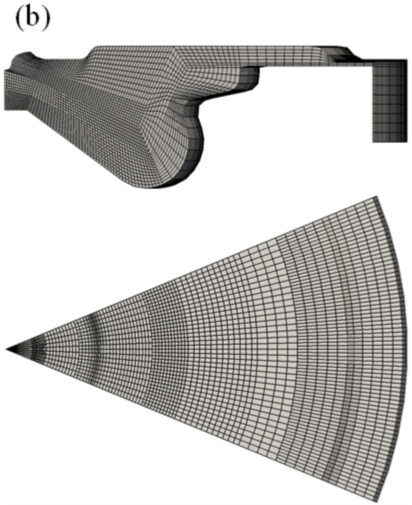
- **TWM** : well mixed (no turbulence chemistry interaction)
- **TPPDF** : presumed pdf
- **TRIF** : RIF model with tabulated reaction rate (from HR)
- **TFPV** : flamelet progress variable model. Reaction rates based on diffusion flame calculations performed with the TRIF model.

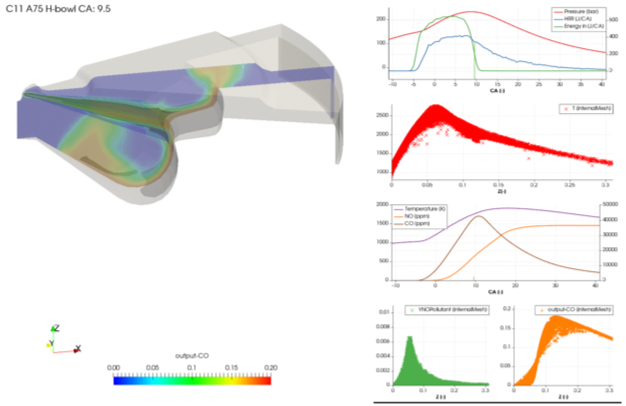
Diesel engines: RIF model

FPT C11 engine

Heavy-duty engine for road transportation







- 14 operating points selected at different loads and speeds
- Spray model constants tuned using results from TUE vessel simulations

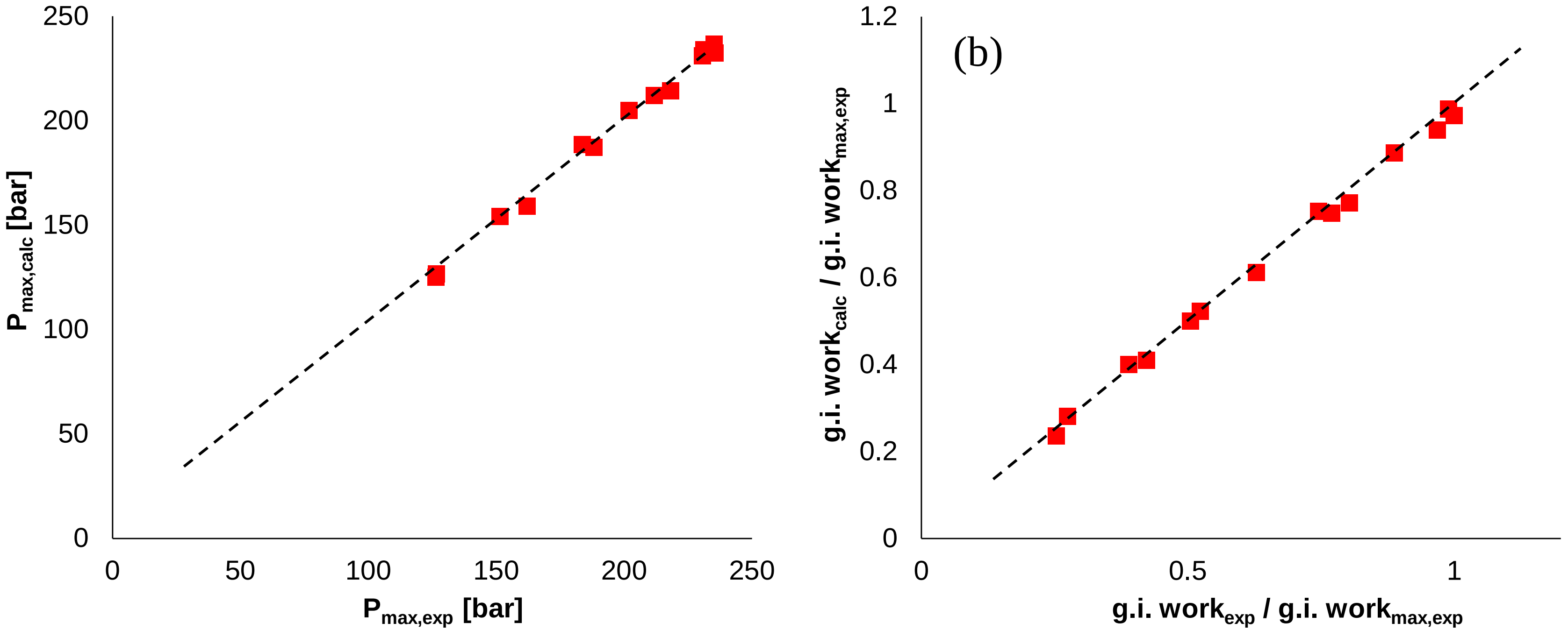
Spray-oriented grid

Acknowledgments: G. Hardy (FPT)

Diesel engines: RIF model

FPT C11 engine

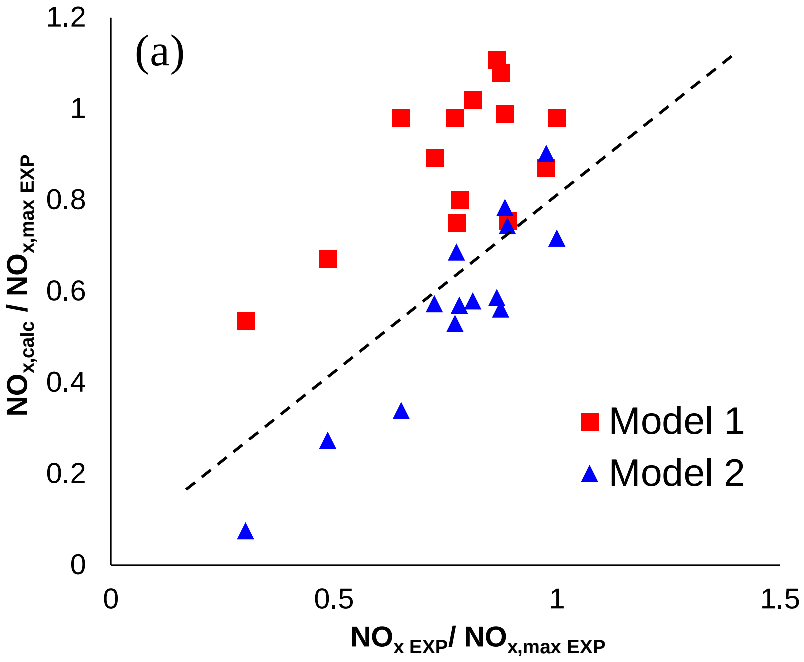
Heavy-duty engine for road transportation: engine performance prediction (pressure and work)

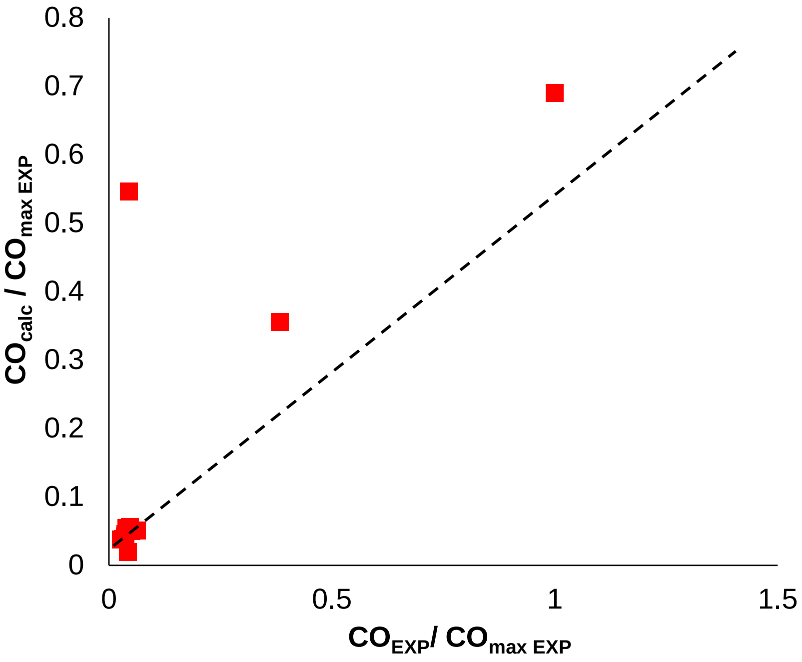


Diesel engines: RIF model

FPT C11 engine

Heavy-duty engine for road transportation: pollutants prediction (NO$_x$ and CO)





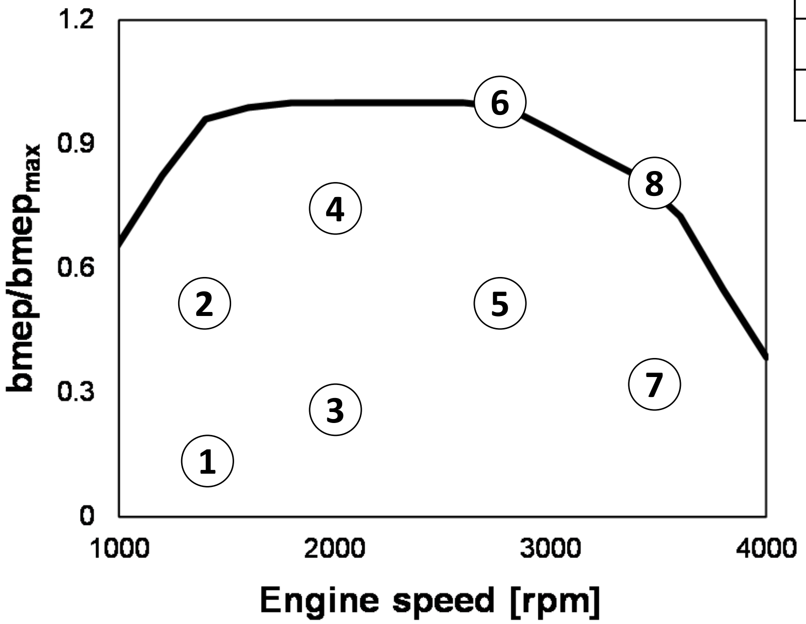
Diesel engines: tabulated kinetics

FPT F1C engine

Light-duty engine for road transportation

Compr ratio	18
IVC	-145 deg
EVO	110 deg

Nozz hole di	
Hom	



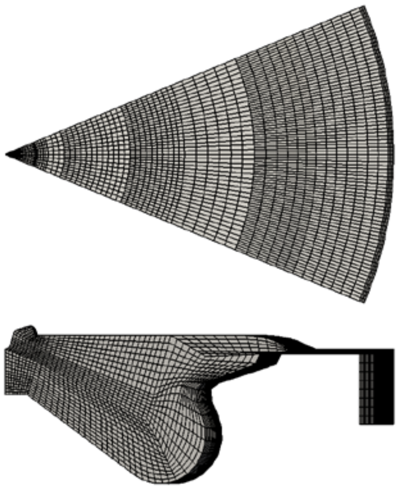
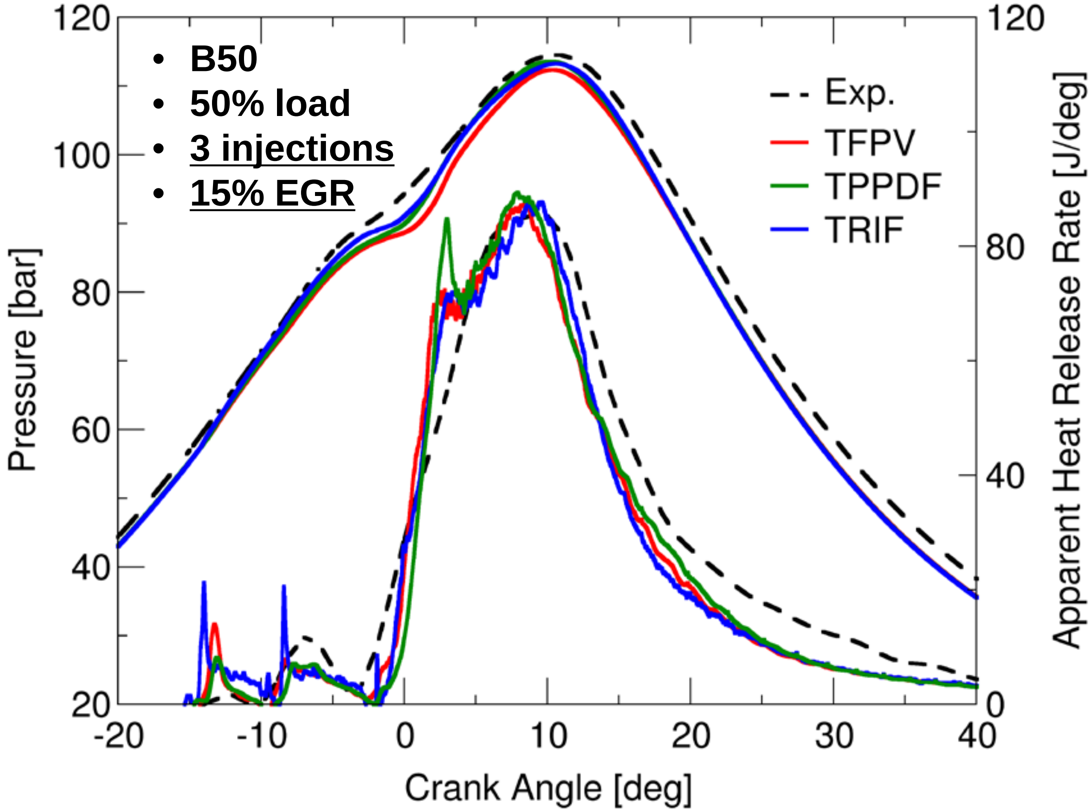


Table discretization

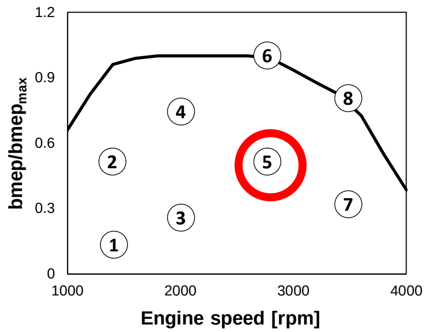
Temperature [K]	600 – 1300
Pressure [bar]	30 - 200
Equivalence ratio	0 – 3
Mixture fraction segregation	0.0 - 1.0
Scalar dissipation rate χ_{st} [1/s]	0 – 55

- **TPPDF, TRIF, TFPV**
  - ⇨ TCI included

Diesel engines: tabulated kinetics

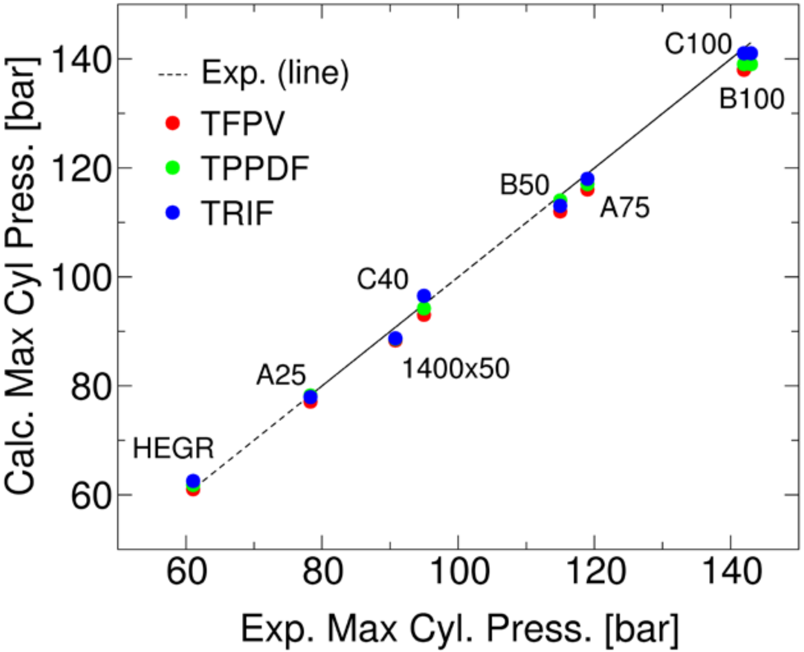


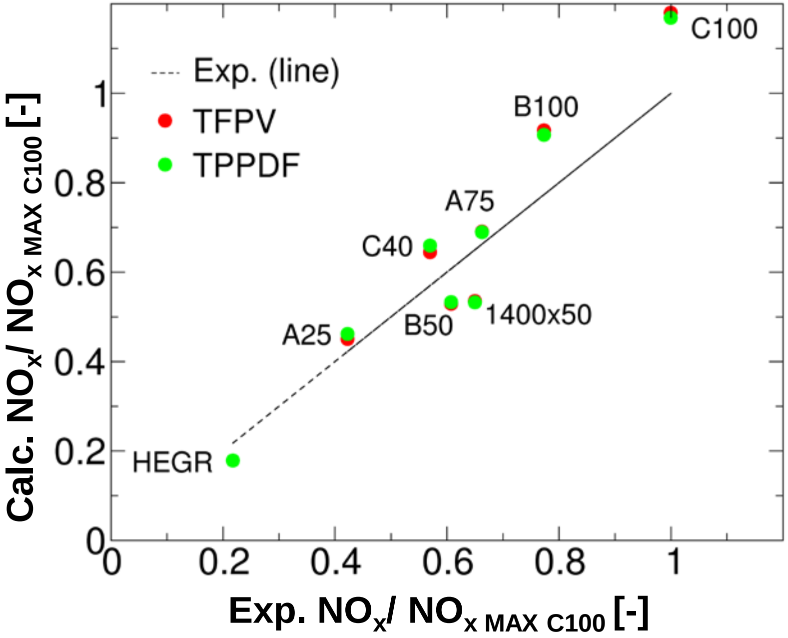
- **B50**
- **50% load**
- **3 injections**
- **15% EGR**



- Similar heat release rate during main combustion
- **Ignition delay:**
  - ➪ TFPV ignites earlier than TRIF and TPPF during second and main injection events.

Diesel engines: tabulated kinetics

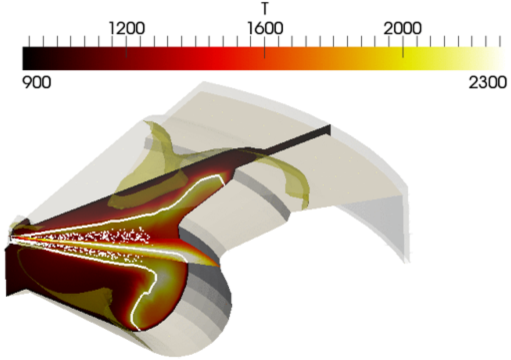




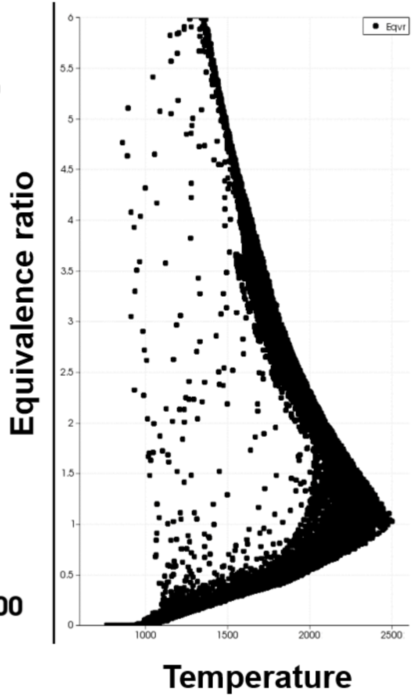
- All the models are able to capture in-cylinder pressure peak and NOx
- CPU time: 15 hours on a 8 core machine for a power-cycle (dual-core, eight processor Intel Xeon E5- 2630 v3 2.40GHz)

Diesel engines: alternative combustion modes

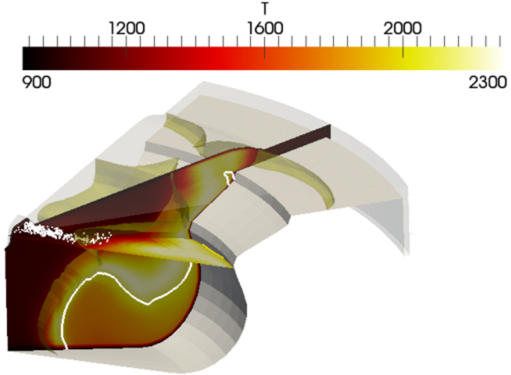
Conventional Diesel combustion



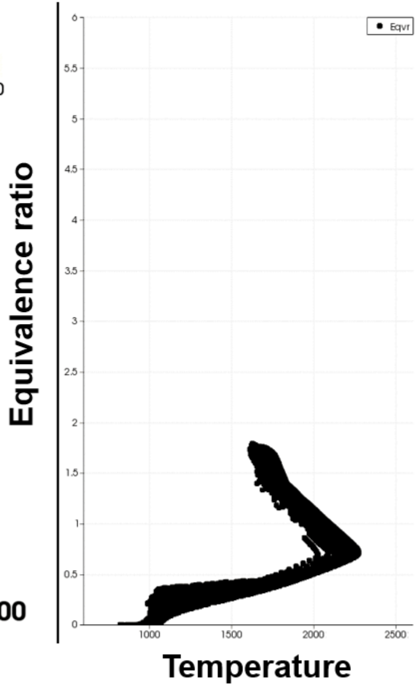
Time: 6.00



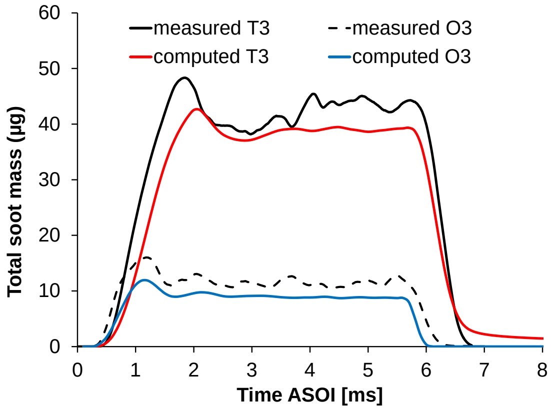
PCCI combustion



Time: -9.00



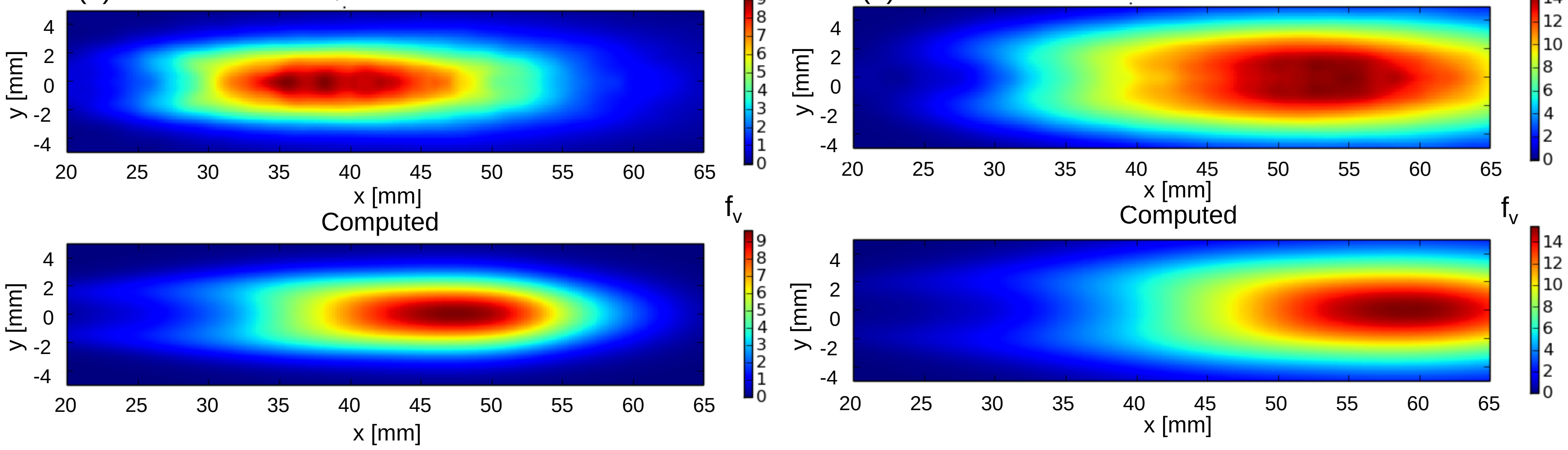
Diesel engines: soot prediction



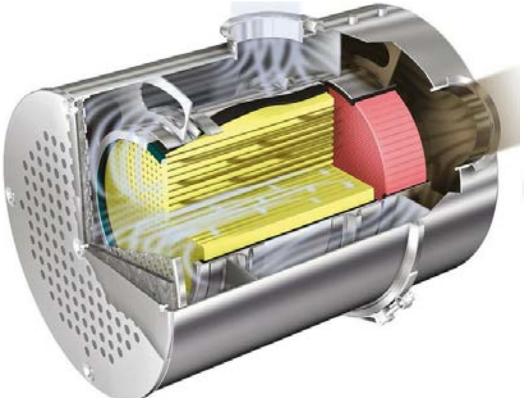
Leung-Lindsted and Jones model

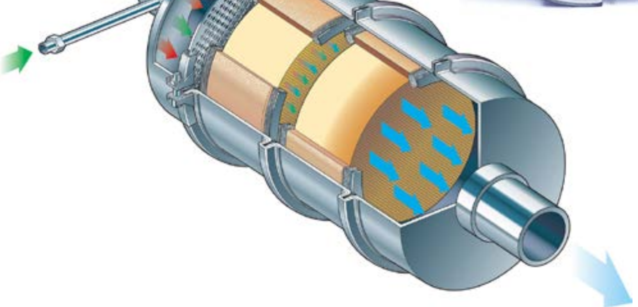
- Two equation approach solving for f_v and N_p using C_2H_2 as precursor

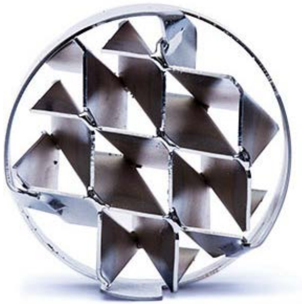
Soot distribution



After-treatment

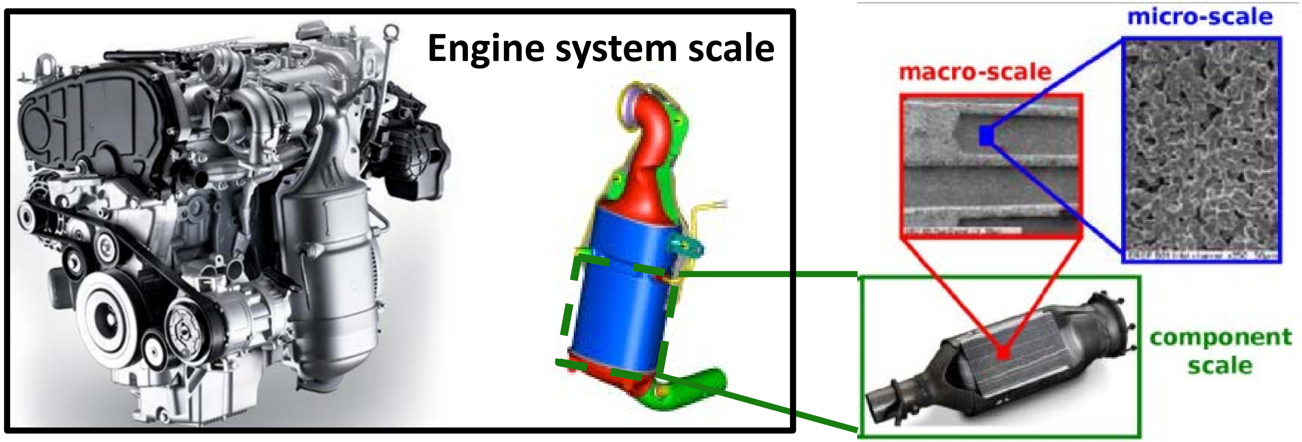




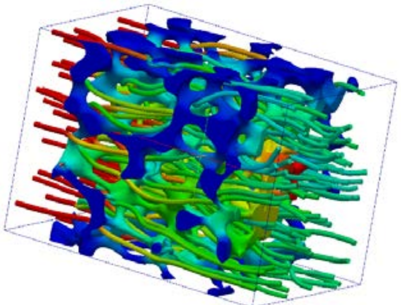


After treatment

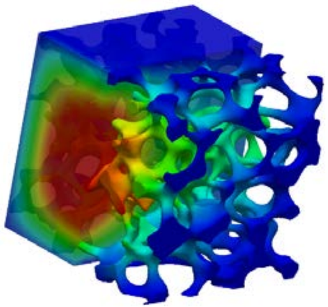
Overview of the physical scales of the problem
&
CFD modelling approaches



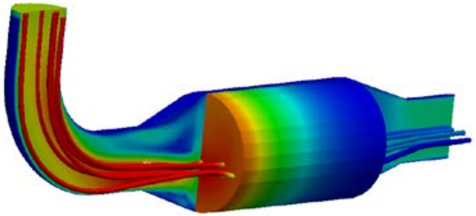
Micro-scale



Macro-scale



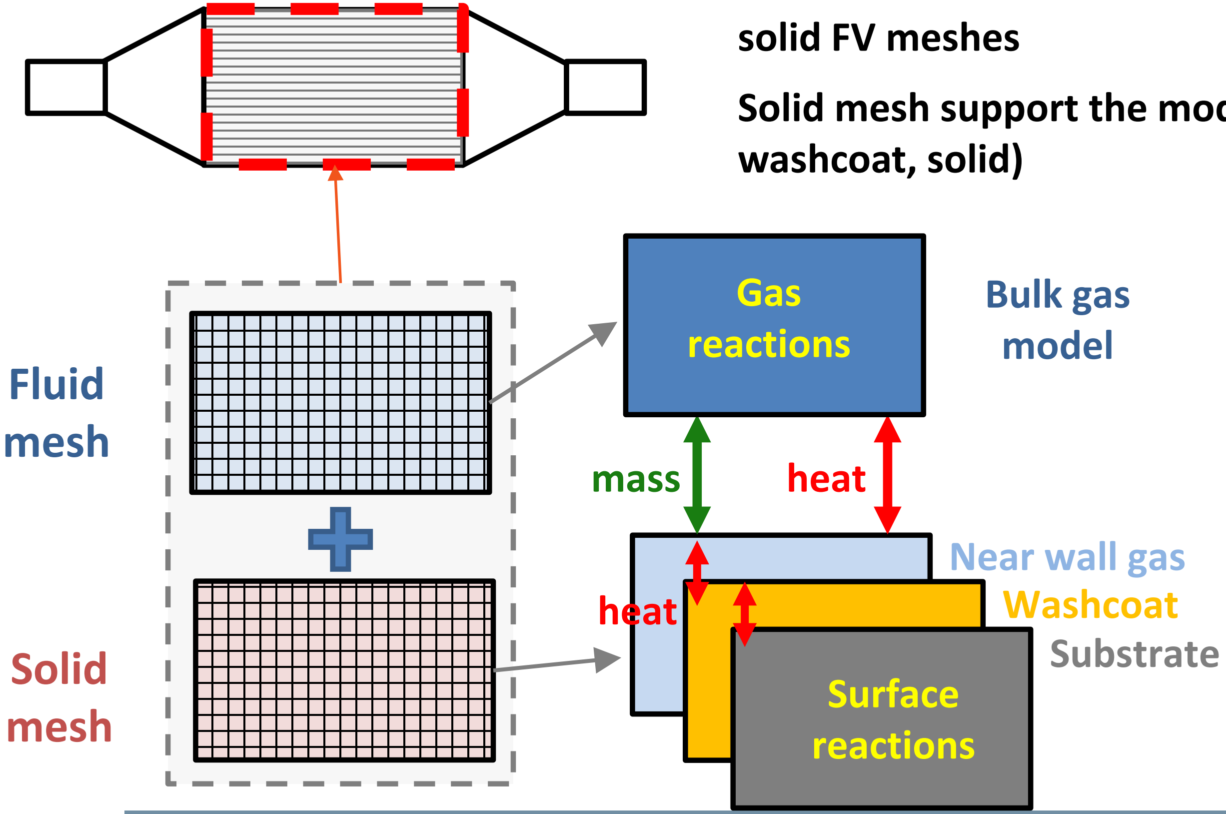
Component scale



After treatment: computational model

Macro-scale model is defined on two overlapping fluid and solid FV meshes

Solid mesh support the modelling of different zones (gas, washcoat, solid)

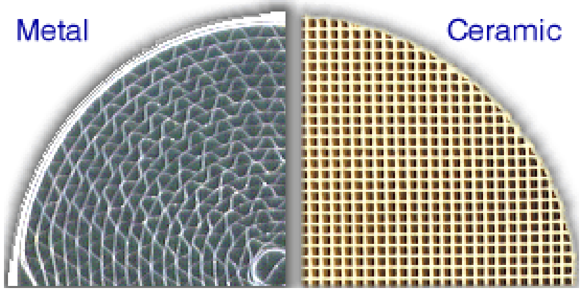


Coupling between fluid and solid regions requires specific models (*Geometry, Permeability, Heat transfer, mass transfer, reaction)*

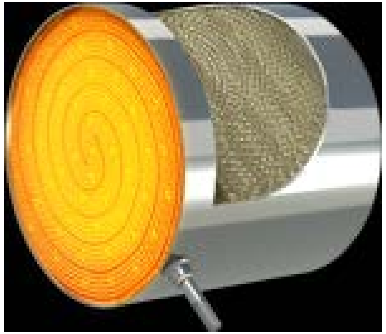
Information for the setup of the models are obtained by micro-scale simulations or experimental correlations.

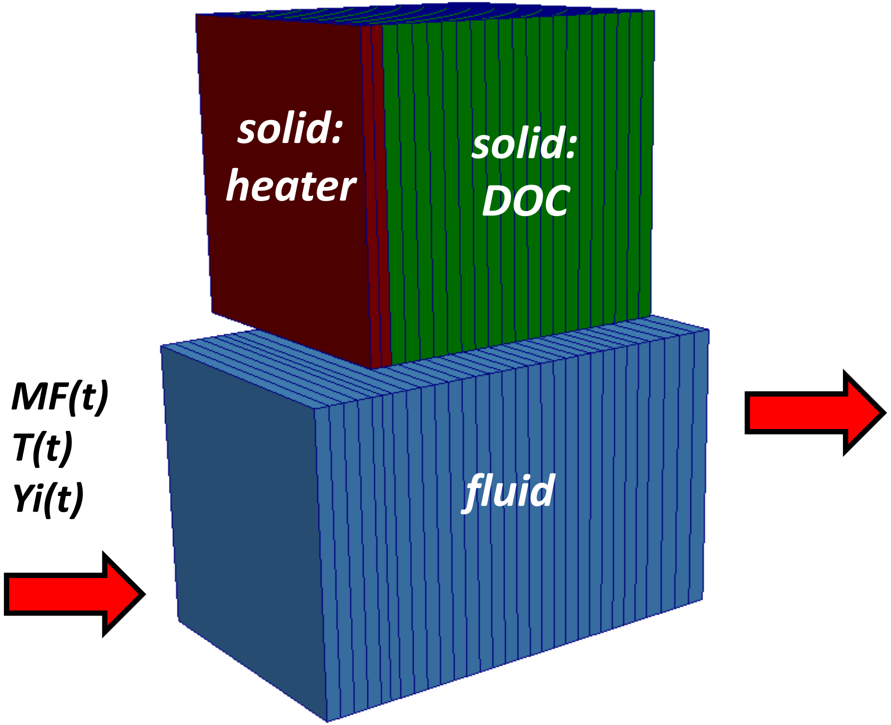
After treatment: DOC simulation

DOC modelling: preliminary validation case



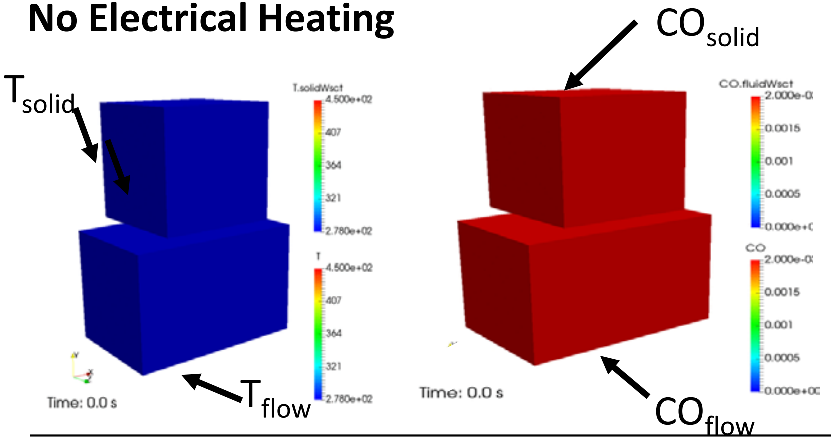
Electrical
heated

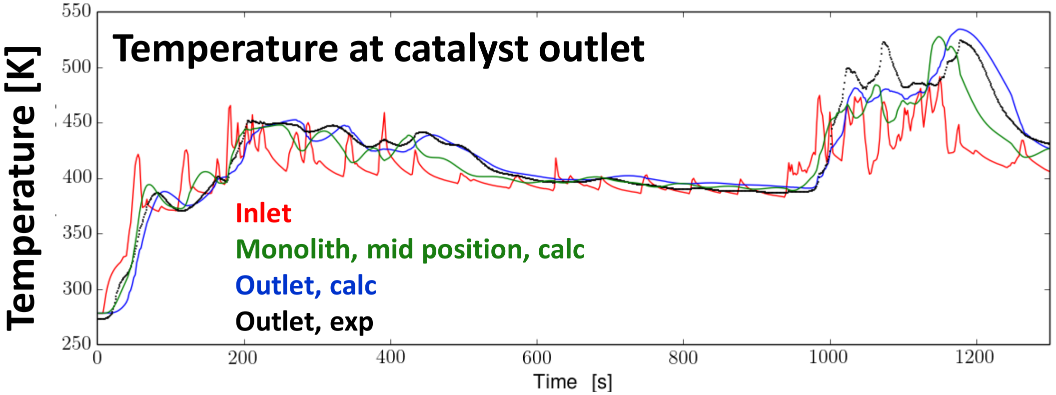




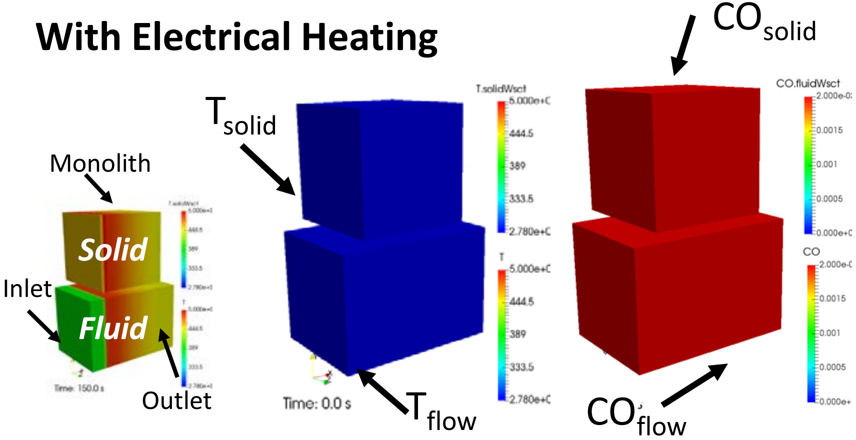
After treatment: DOC simulation

No Electrical Heating

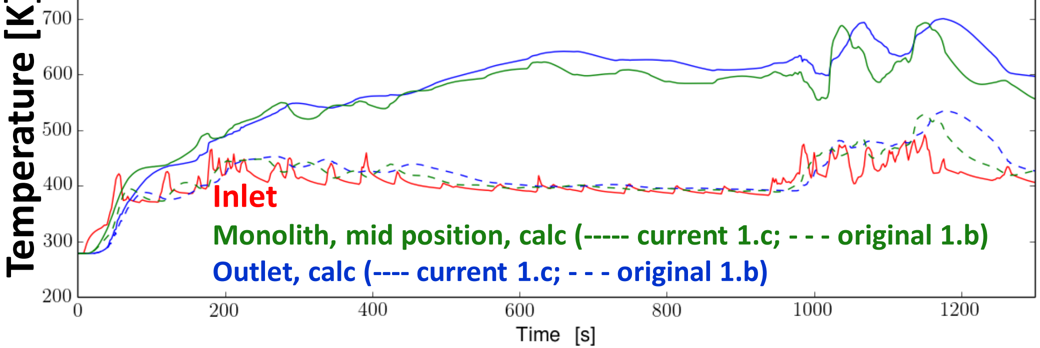




With Electrical Heating

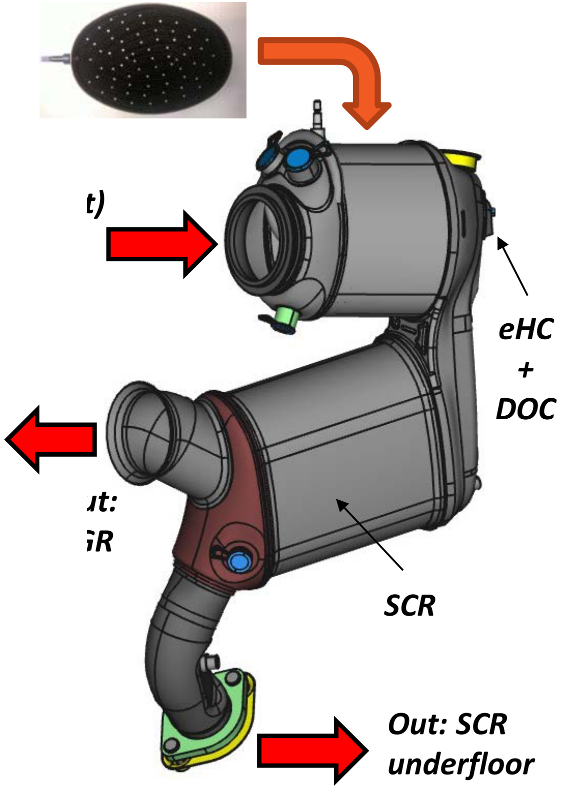


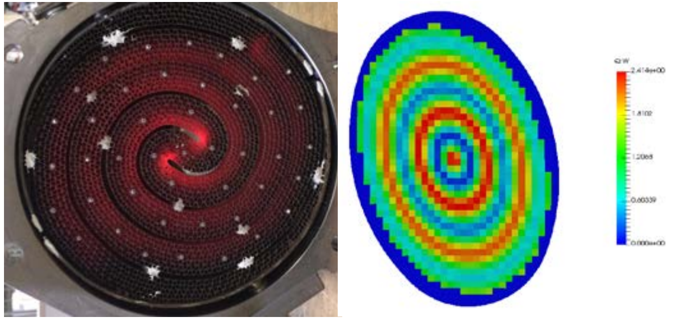
- Ceramic substrate (1.b)
- Metallic substrate (1.c), <u>with electrical heating P$_{el}$ = 1kW</u>



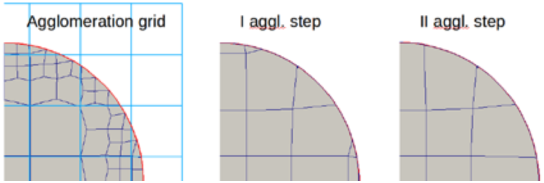
After treatment: DOC simulation

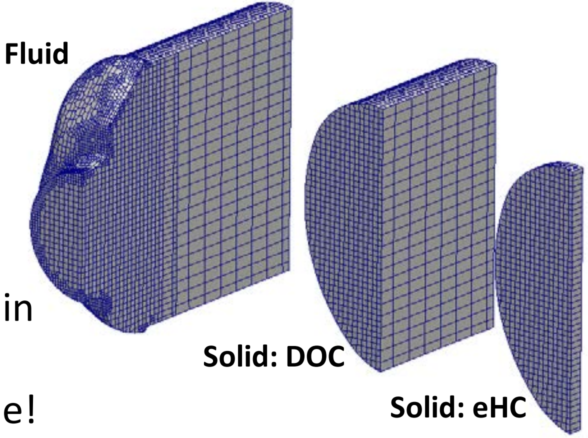
Full-scale 3D case including DOC monolith and electrical heating





Semi-empirical model to describe electrical heating based on assumed temperature distribution





- Cell agglomeration after meshing
- Different maximum Courant numbers in different zones

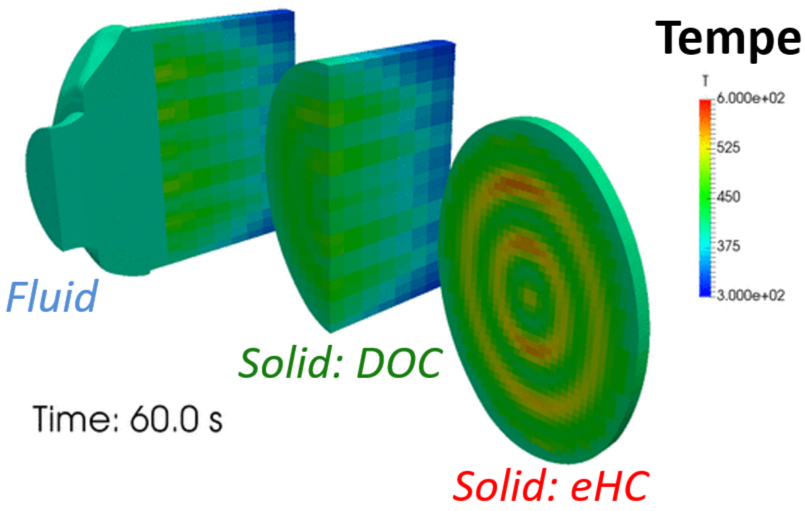
⇨ CFD Modeling of RDE Cycle is possible!

After treatment: DOC simulation

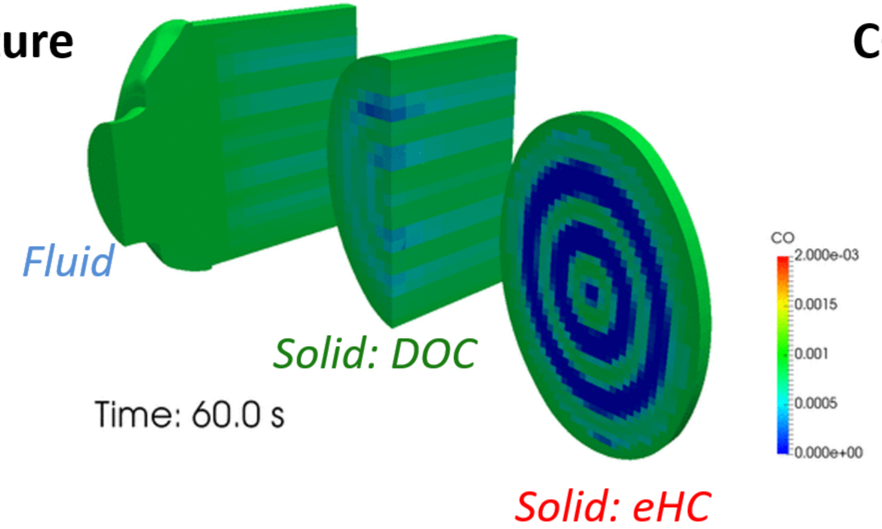
Non-uniform heating
P_{el} = 1 kW : 0-100 s
P_{el} = 0.5-0.2 kW : 100-300 s

Non-uniformity of the heating generates hot spots
→ **earlier light-off**

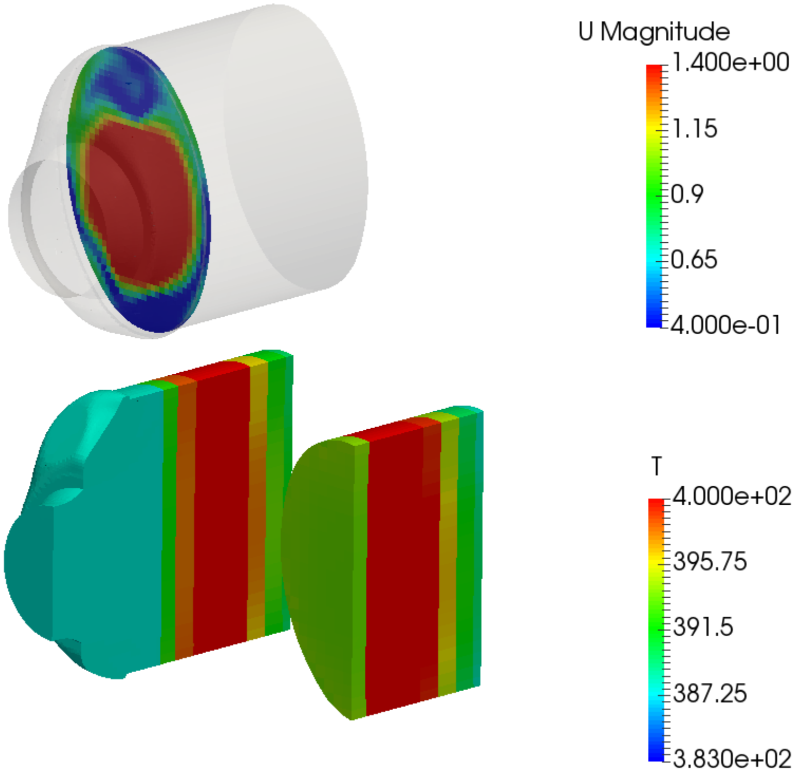
Temperature



CO

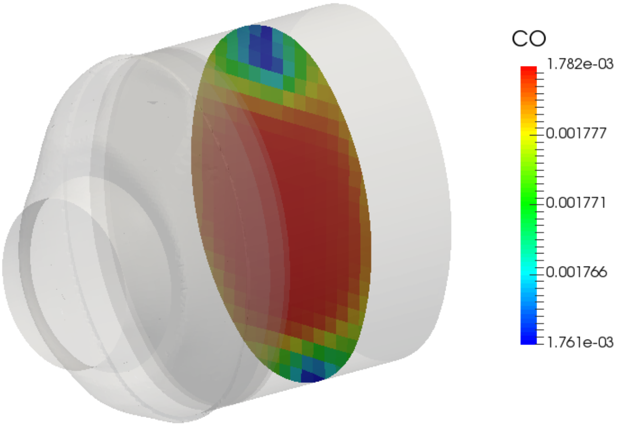


After treatment: DOC simulation

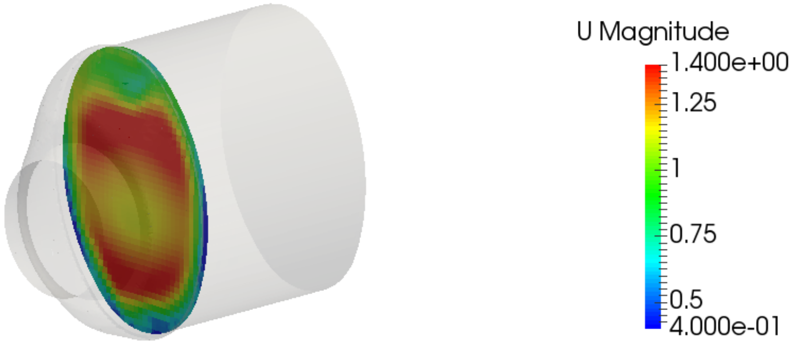


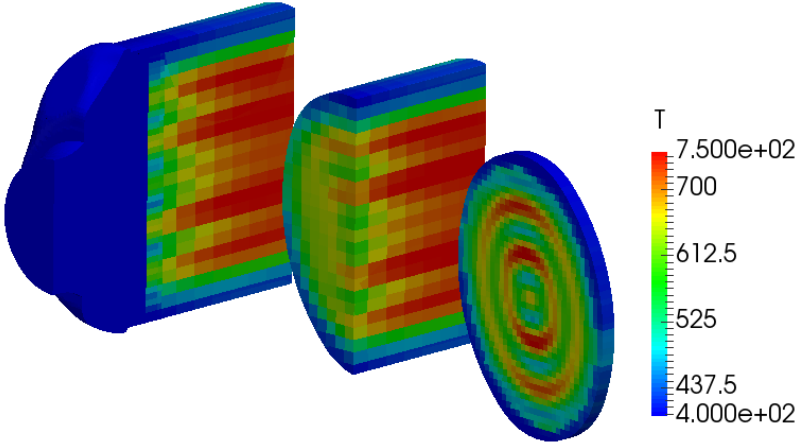
Non-heated DOC configuration

Time = 140 s



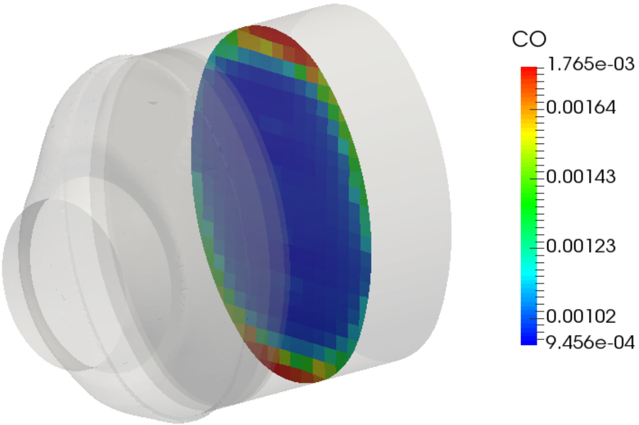
After treatment: DOC simulation





DOC configuration with non-uniform heating (Pel = 1 kW)

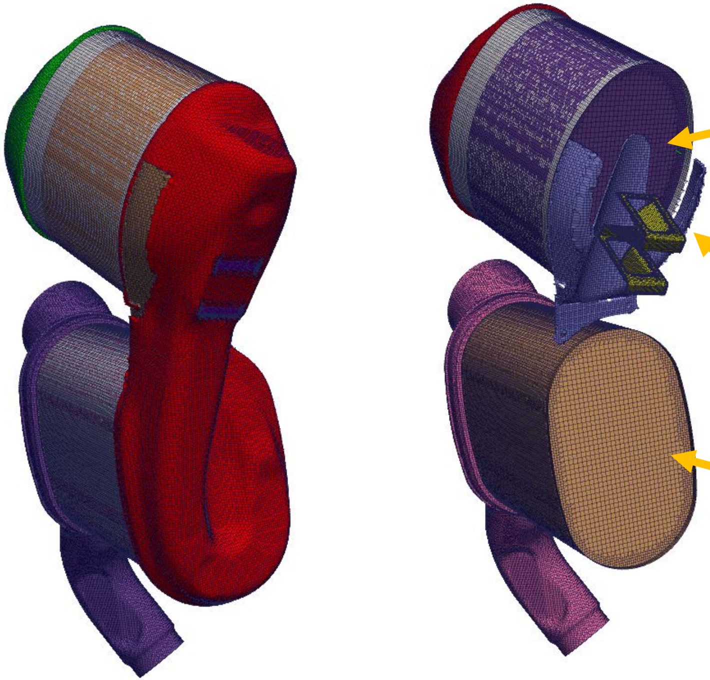
Time = 140 s



After treatment: SCR mixer optimization

Optimization of the mixer geometry

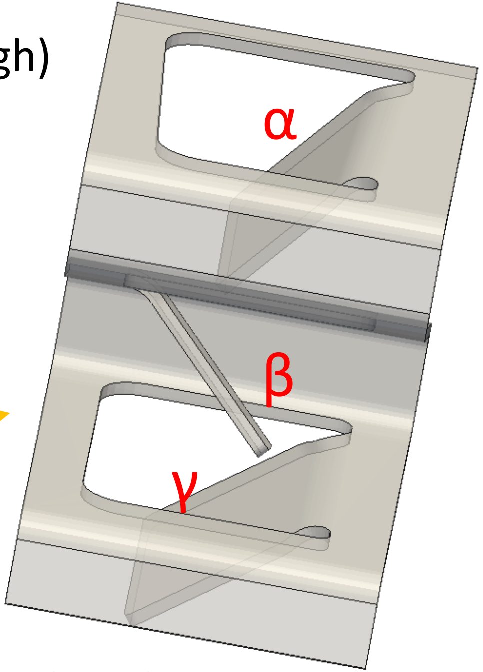
- <u>Variables</u>: angles α, β, γ of the mixer blades
- <u>Function objects</u>: Δp_{mix}, $UI(NH_3)\ _{SCR,inl}$ x 2 MF (low and high)



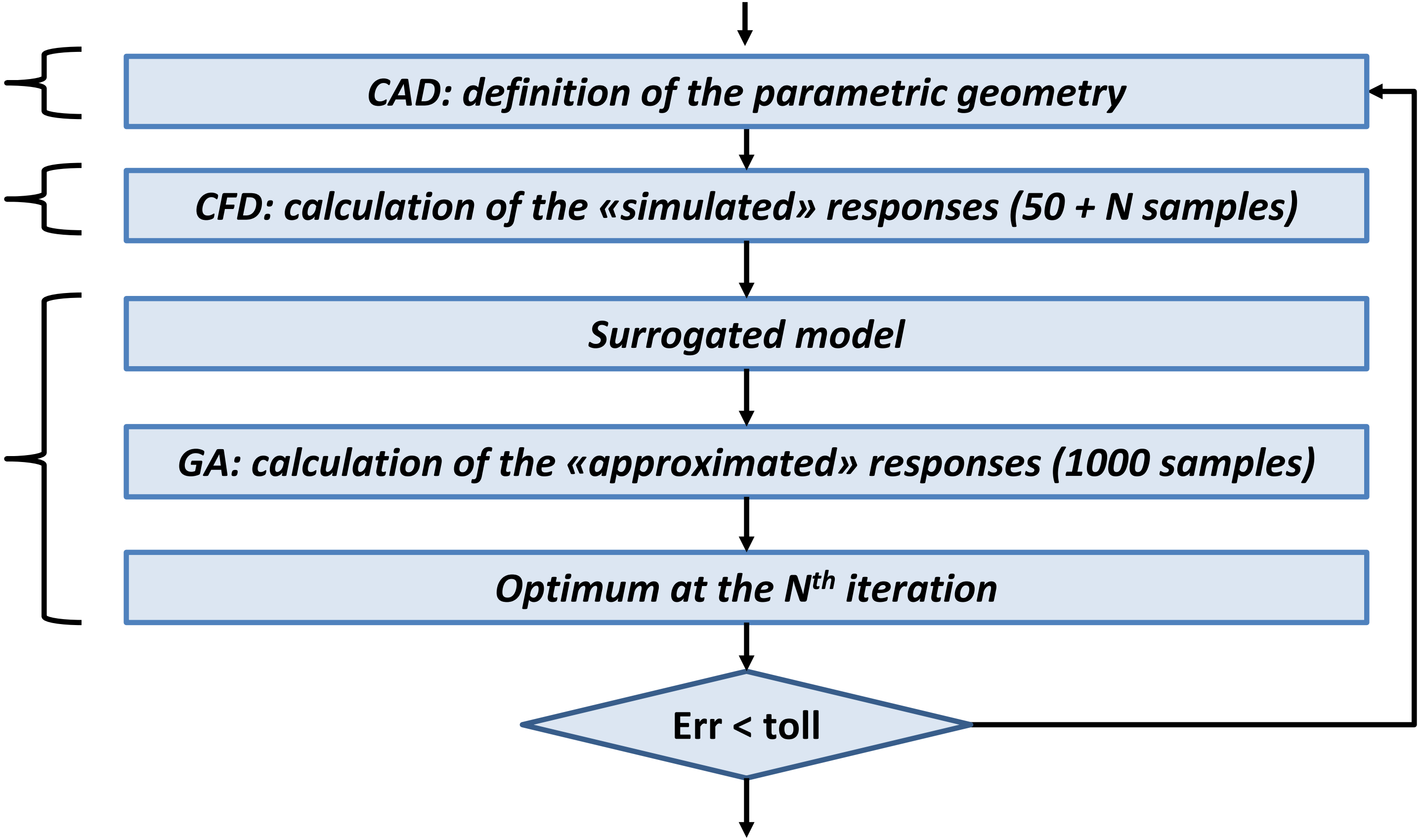
Injection of gaseous NH3

Mixer

Evaluation of the $UI(NH_3)$ on the SRC inlet plane



After treatment: optimization procedure



CAD: definition of the parametric geometry

CFD: calculation of the «simulated» responses (50 + N samples)

Surrogated model

GA: calculation of the «approximated» responses (1000 samples)

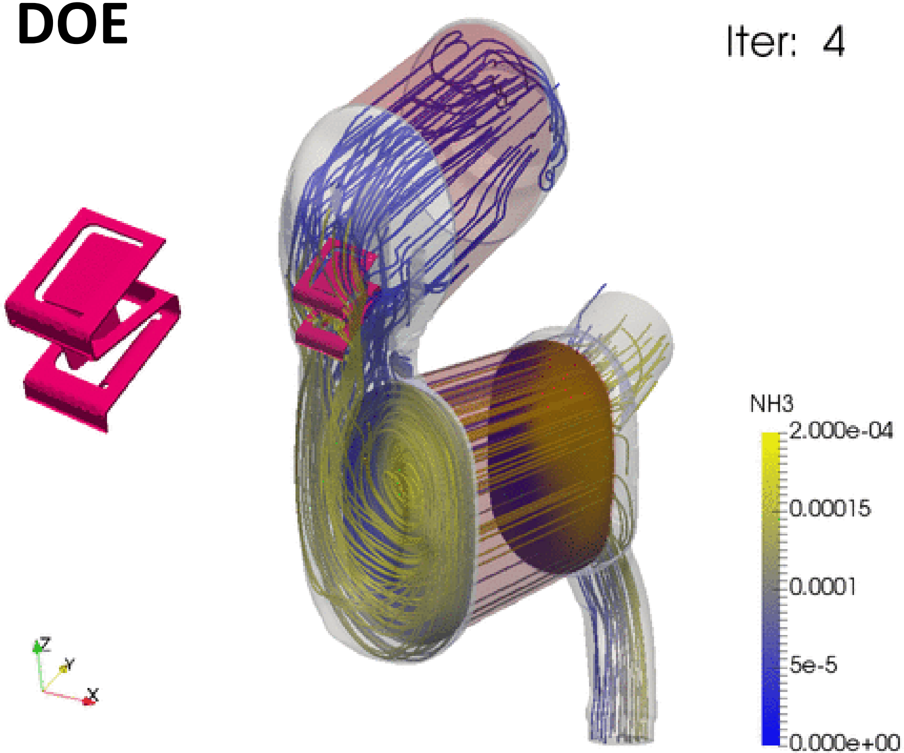
Optimum at the Nth iteration

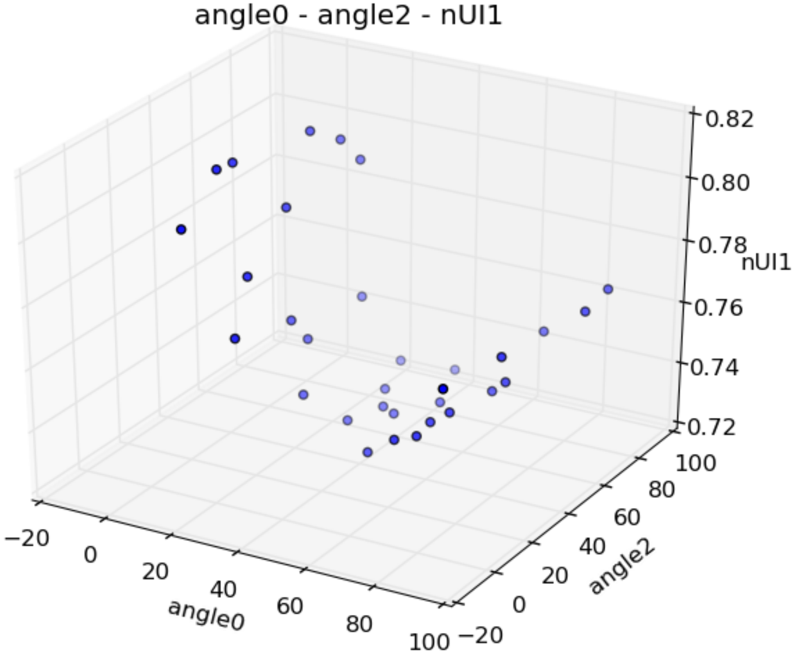
Err < toll

(c) Dakota®.

After treatment: SCR mixer optimization

DOE





Conclusions on LibICE activities

OpenFOAM for IC Engine simulations

Ideal platform to develop advanced models to simulated complex problems in real geometries including:

- Turbulent and multiphase flows
- Chemical reactions
- Moving boundaries

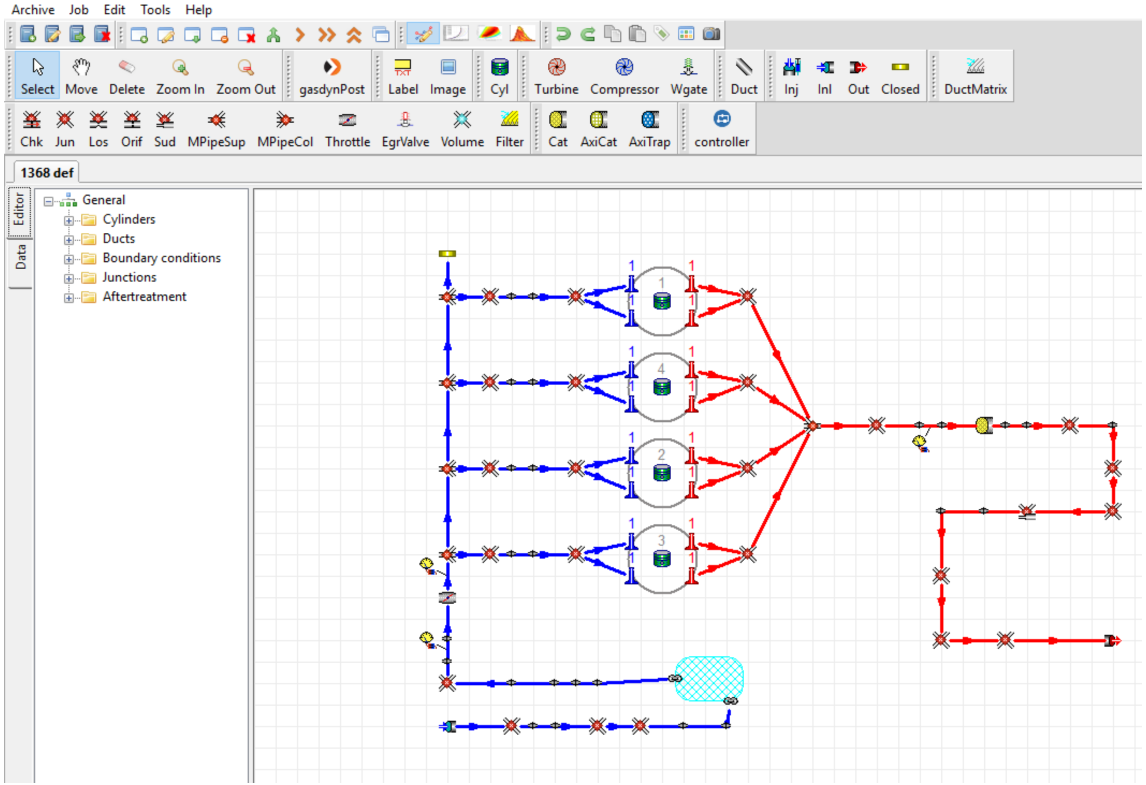
OpenFOAM + LibICE: consolidated tool for engine design, optimization and analysis:

- In-cylinder flows
- Combustion and pollutant emissions
- After-treatment devices

Next directions

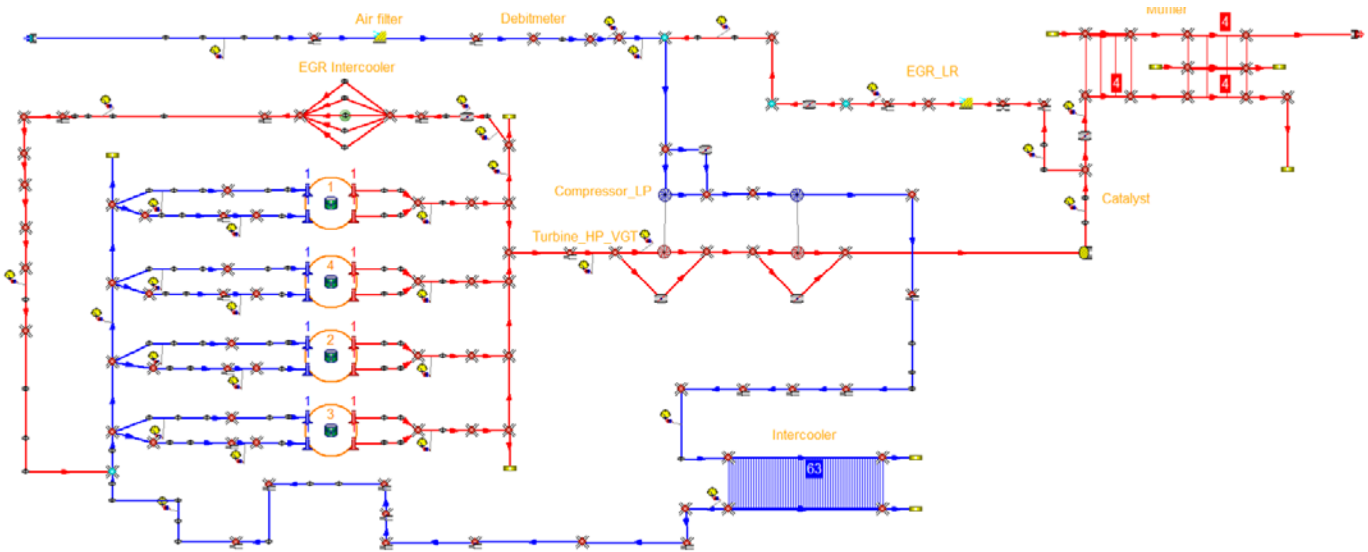
- Advanced combustion modes (RCCI, PCCI, dual fuel)
- Flash boiling and new wall film model (Lagrangian)
- Models for sophisticated after-treatment devices operating under RDE conditions.

1D simulation code: GASDYN



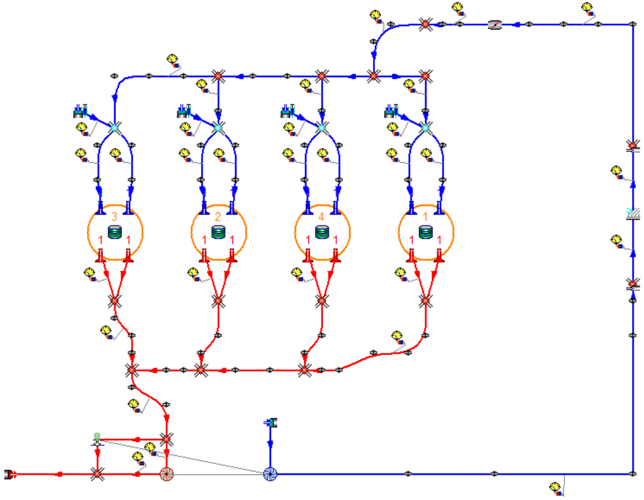
Developed at PoliMi during the last 20 years, now co-developed with Exothermia. GASDYN is also coupled to the AXISUITE simulation code, for the simulation of the complete after-treatment system.

1D simulation code: GASDYN

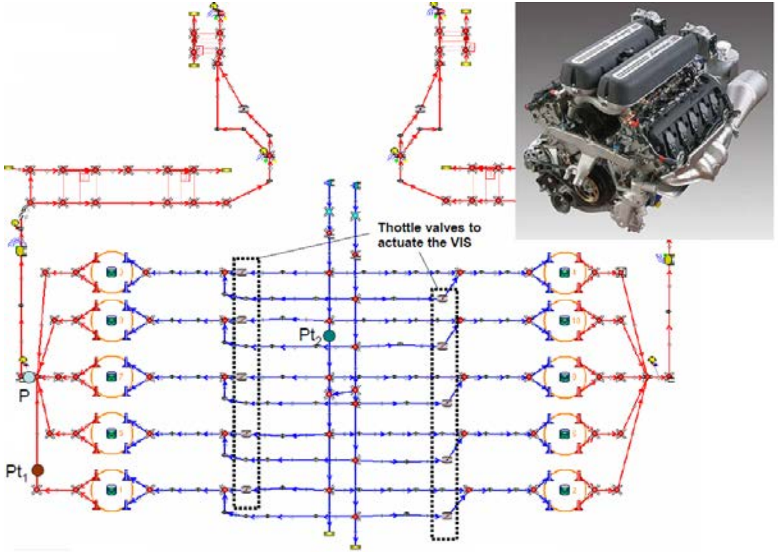


- **Strong partnership** between **PoliMi, Exothermia** and **Aristotle University** on this research topic, for further developments and applications of GASDYN.

1D simulation code: GASDYN



L4 turbo-charged, natural gas SI engine with complete intake and exhaust systems.



V10 NA SI high-speed engine with Variable Intake System (VIS)

1D simulation code: GASDYN

Conservation equations for mass, momentum and energy in 1D:

$$\frac{\partial \mathbf{W}(x,t)}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{W})}{\partial x} + \mathbf{B}(\mathbf{W}) + \mathbf{C}(\mathbf{W}) = 0$$

$$\mathbf{W}(x,t) = \begin{bmatrix} \rho F \\ \rho u F \\ \rho e_0 F \\ \rho \mathbf{Y} F \end{bmatrix} \quad \mathbf{F}(\mathbf{W}) = \begin{bmatrix} \rho u F \\ \rho u^2 F + pF \\ \rho u h_0 F \\ \rho u \mathbf{Y} F \end{bmatrix} \quad \mathbf{B}(\mathbf{W}) = \begin{bmatrix} 0 \\ -p\frac{dF}{dx} \\ 0 \\ 0 \end{bmatrix}$$

$$\mathbf{C}(\mathbf{W}) = \begin{bmatrix} 0 \\ \rho G F \\ -\rho(q + q_{re})F \\ \rho \dot{\mathbf{Y}} F \end{bmatrix} \quad \mathbf{Y} = \begin{bmatrix} Y_1 \\ \vdots \\ Y_{N-1} \end{bmatrix}.$$

$$Y_i = m_i / m$$

Vector of specie mass fractions

Reactions of species in the flow (exhaust manifold and catalysts).

$$\mathbf{Y} = \begin{bmatrix} O_2 \\ N_2 \\ Ar \\ CO_2 \\ H_2O \\ H_2 \\ CO \\ NO \\ C_3H_6 \\ C_3H_8 \\ . \\ . \\ . \end{bmatrix}$$

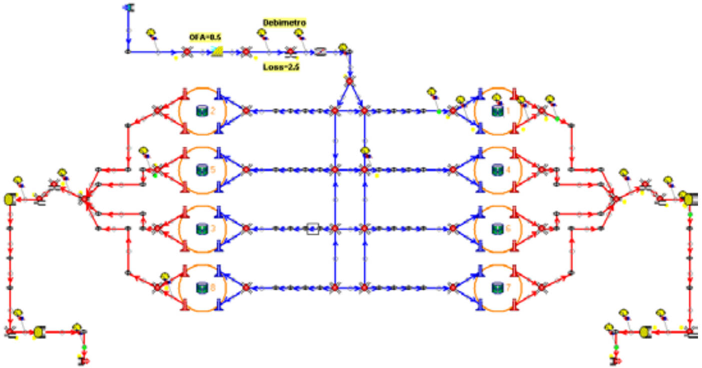
1D simulation code: GASDYN

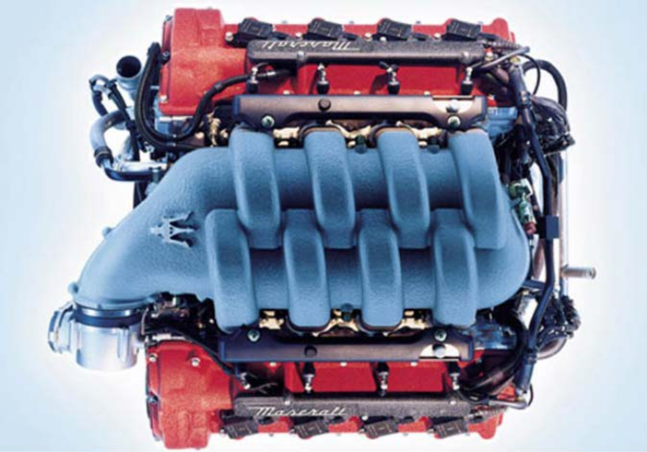
Model application: Ferrari-Maserati V8 Engine

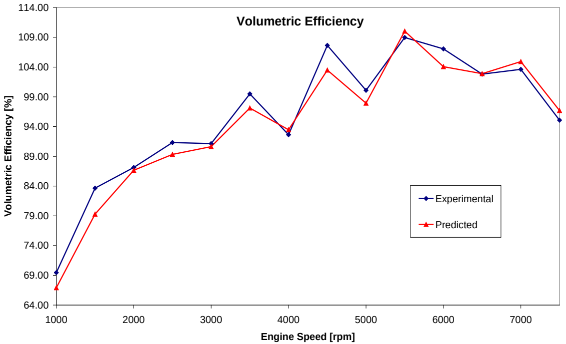
Swept volume: 4244 cm^3

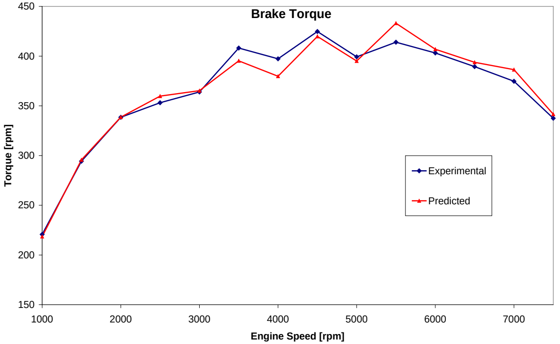
Max. Power: 287 kW @ 7000 rpm

Max. Torque: 451 Nm @ 4500 rpm

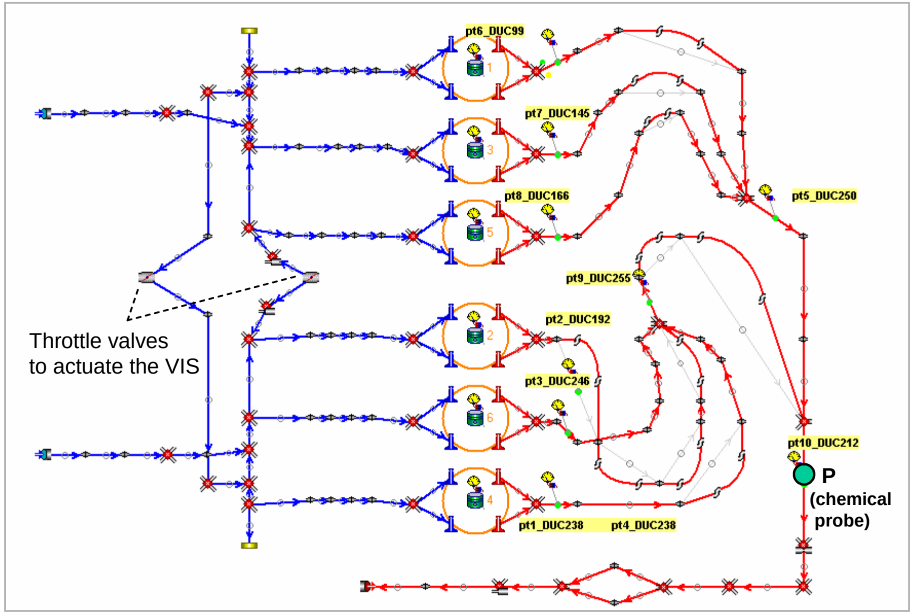


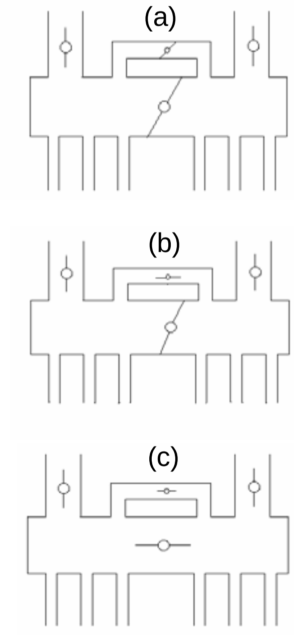


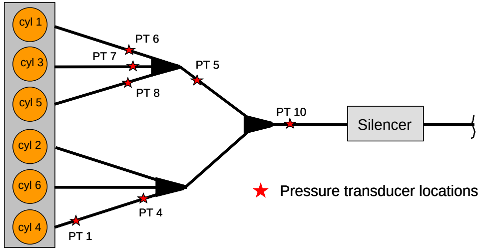




1D simulation code: GASDYN



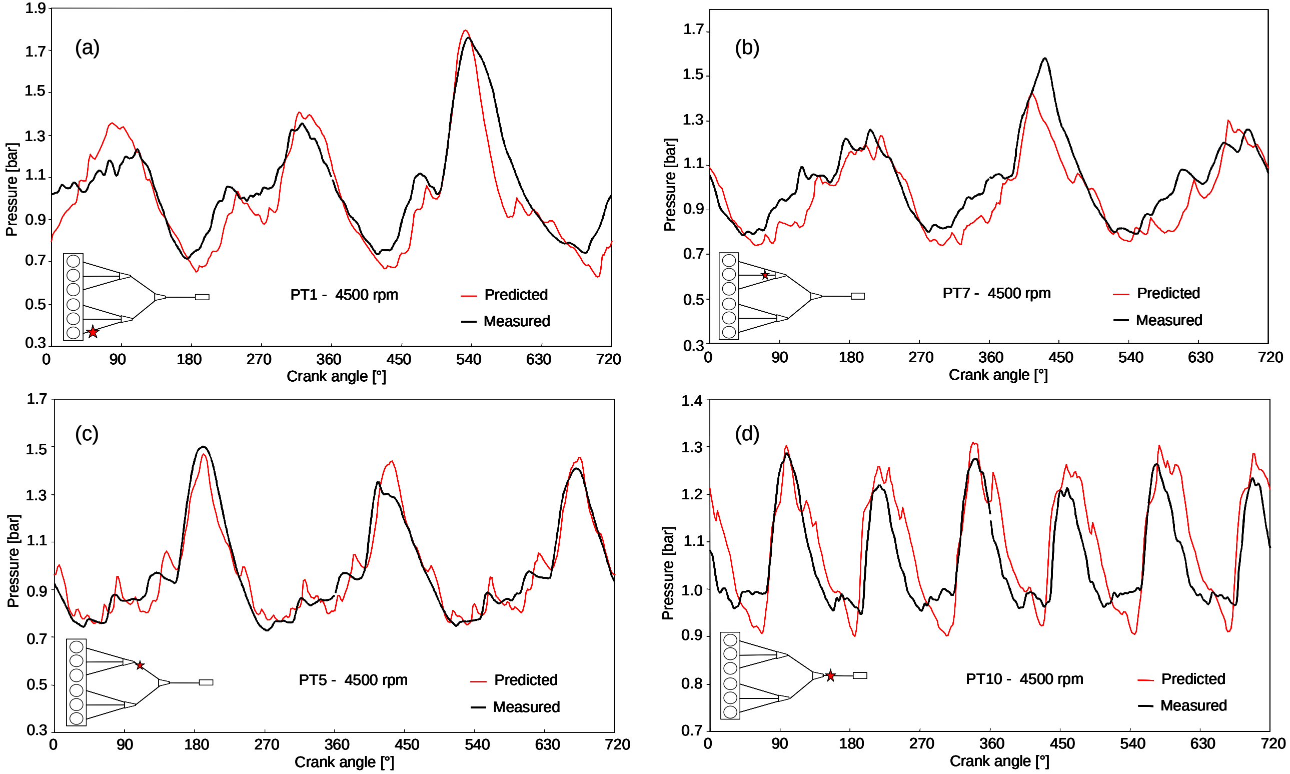




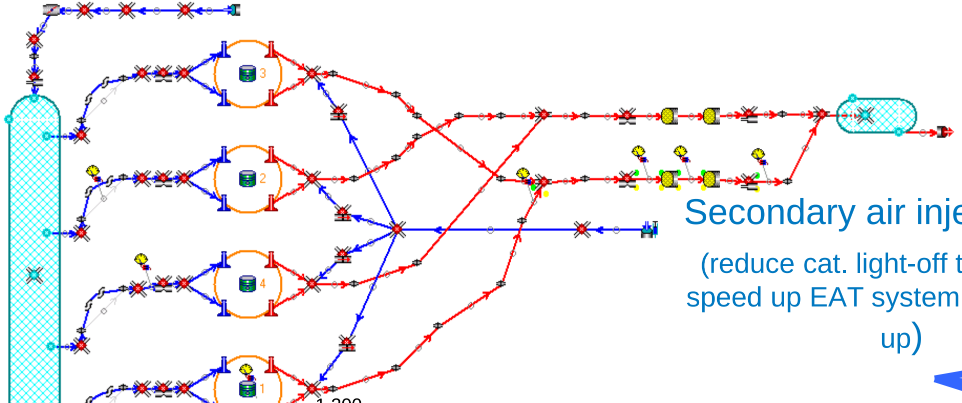
- 12 Cylinders, V60, 6.2 liters, Variable Intake System, intake and exhaust VVT, 650 Nm@5400 rpm, 426 kW@7500 rpm

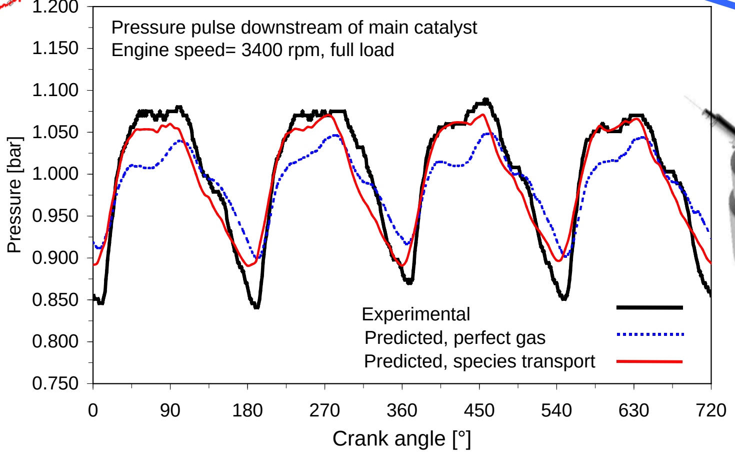
1D simulation code: GASDYN

Pressure pulses in the exhaust system



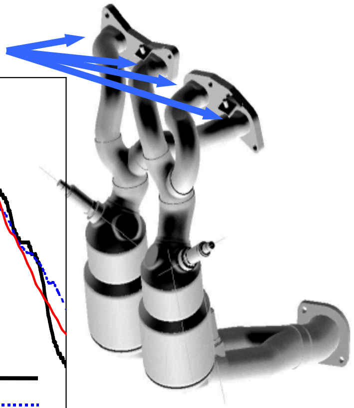
1D simulation code: GASDYN





Secondary air injection

(reduce cat. light-off time – speed up EAT system warm-up)

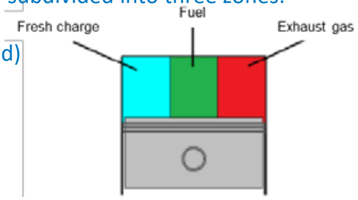


- 10 species (or more) can be transported along the duct system with eventual reactions (**unsteady reacting flows**)
- (e.g. O_2, N_2, Ar, CO_2, H_2O, H_2, CO, NO, C_3H_6, C_3H_8)

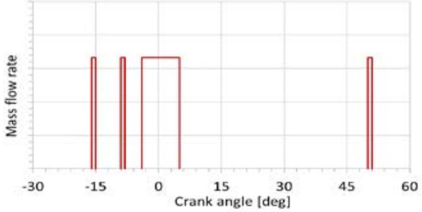
Gasdyn MDW3Z Model

Multiple Double-Wiebe 3-Zone Combustion Model

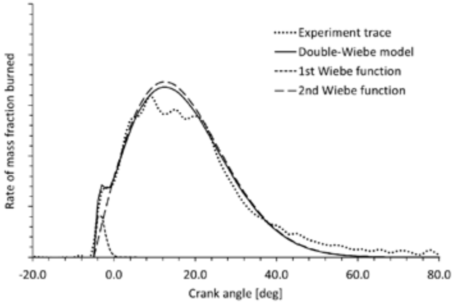
- Combustion model developed by ICEgroup
  - Designed to handle modern multi-pulse injection
  - Combustion chamber subdivided into three zones:
    - Fresh charge
    - Fuel (vaporized)
    - Exhaust gas



- Combustion rate imposed by means of multiple double-Wiebe law taking account the in-cylinder conditions
  - Pressure and temperature
  - Mixture composition (fresh charge, fuel, EGR)
  - Injection timings
- Fast run time
- Injection
  - Each discrete injection event is defined as a pulse
  - Up to 4 number of pulses



- Double Wiebe function
  - Each pulse burns with a rate defined by the following expression



$$x_b = \underbrace{p\left(1-\exp\left[-\left(\frac{\theta-\theta_o}{\alpha_1}\right)^{\beta_1}\right]\right)}_{\text{1st Wiebe function (premixed combustion)}} + \underbrace{(1-p)\left(1-\exp\left[-\left(\frac{\theta-\theta_o}{\alpha_2}\right)^{\beta_2}\right]\right)}_{\text{2nd Wiebe function (diffusive combustion)}}$$

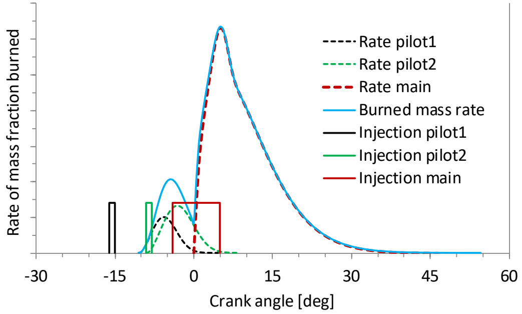
- Ignition
  - Ignition delay calculated as

$$\tau_{ign} = C_{ign}\rho^{C_{ign2}} \exp\left(\frac{C_{ign3}}{T}\right) f(\text{EGR})$$

- Ignition occurs when

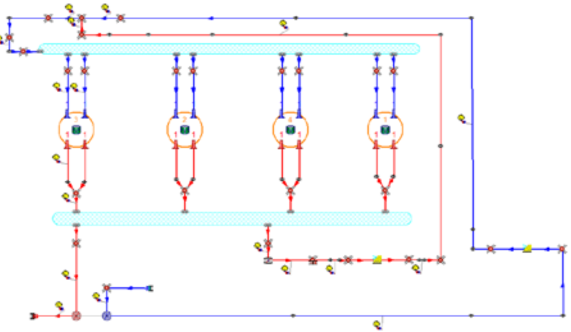
$$\int_{t_0}^{t_{ign}} \frac{1}{\tau_{ign}} dt = 1$$

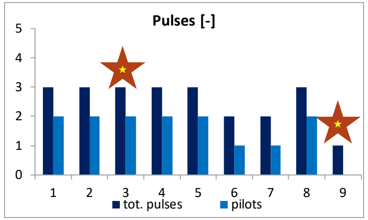
- NOx
  - Extended Zeldovich mechanism
- CO
  - Equilibrium approach
- Soot
  - Semi-empirical Hiroyasu model predicts the soot formation rate
  - Semi-empirical Nagle Strickland predicts the oxidation soot step
- Combustion model
  - HRR calculated separately for each pulse
  - Different Wiebe coefficients for each pulse
  - Wiebe coefficients parametrized as a function of in-cylinder residuals

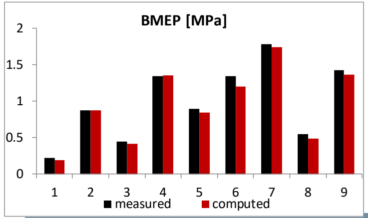


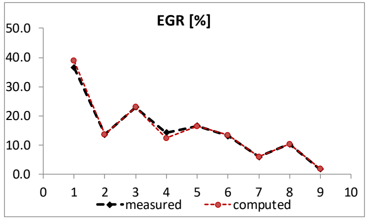
Gasdyn MDW3Z Model

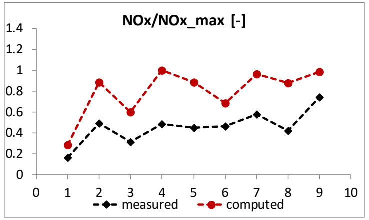
Case Study: Four Cylinders, Turbo-Charged, DI Diesel Engine

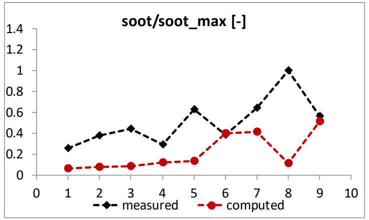


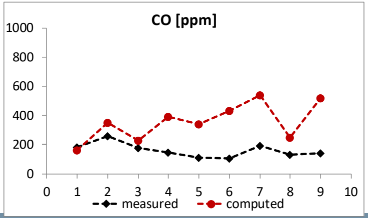




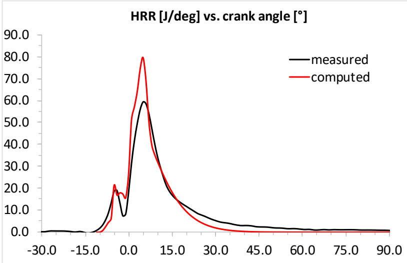


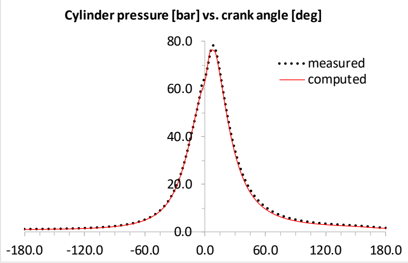




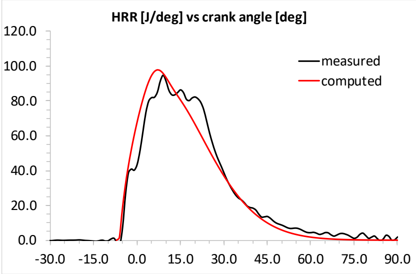


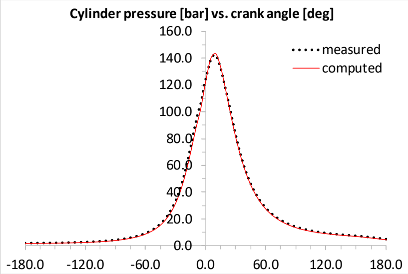
- Operating point #3
  - 25% load, 2000 rpm, three injections: 2 pil. + main





- Operating point #9
  - 100% load, 3500 rpm, only main injection

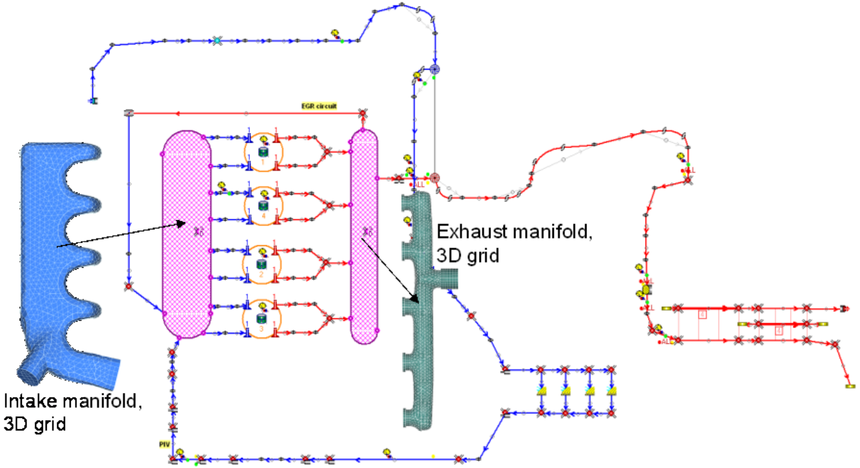


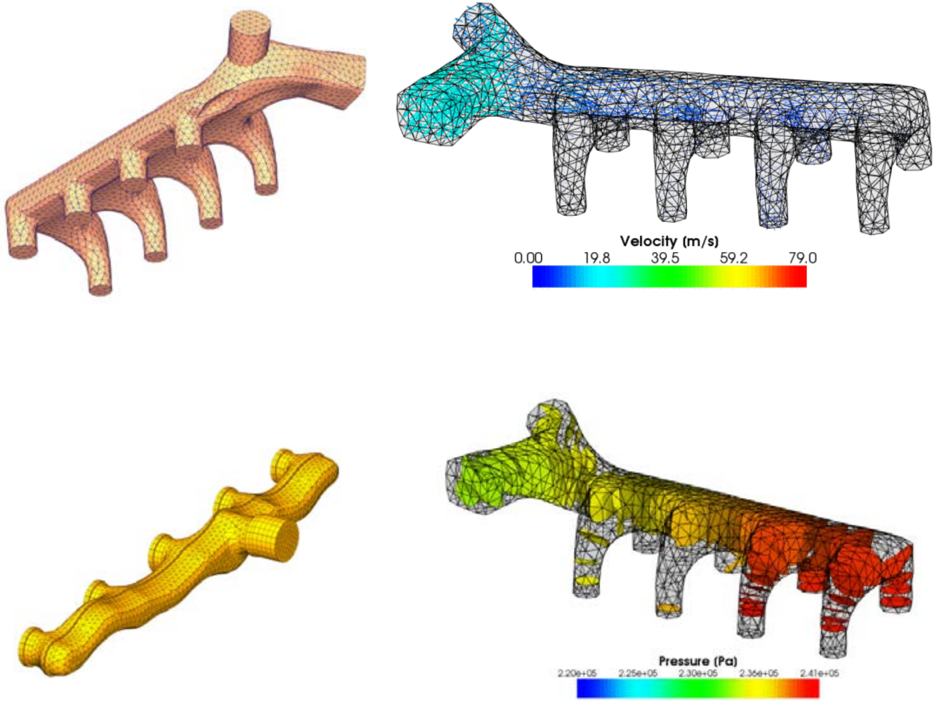


★ Operating points used to tune the combustion model

Coupled 1D-3D simulations

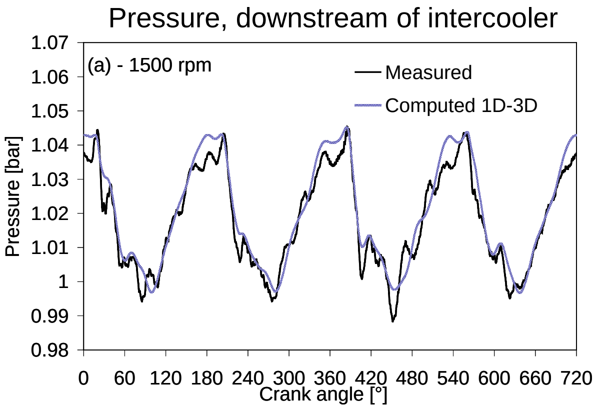
Unsteady flows in intake and exhaust systems: 1D-3 coupling

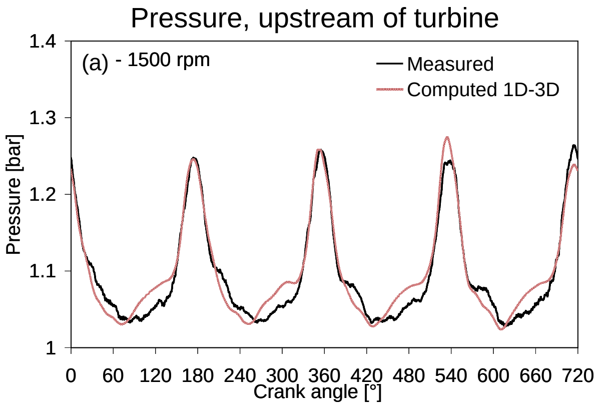


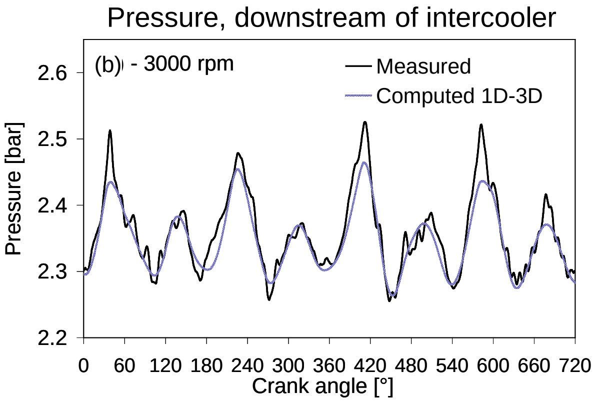


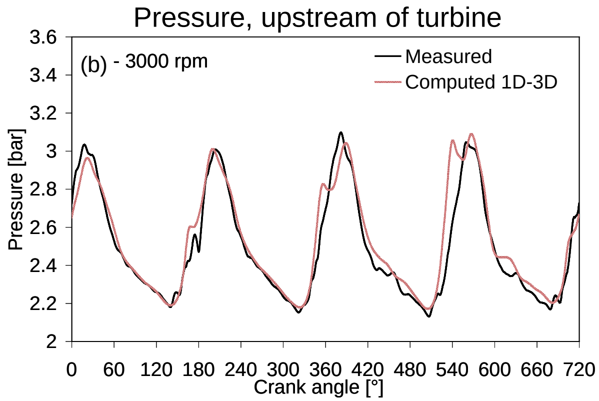
Pressure wave validation, 1D-3D simulations

1500 rpm – 40 Nm, 3000 rpm – 220 Nm


Pressure, downstream of intercooler

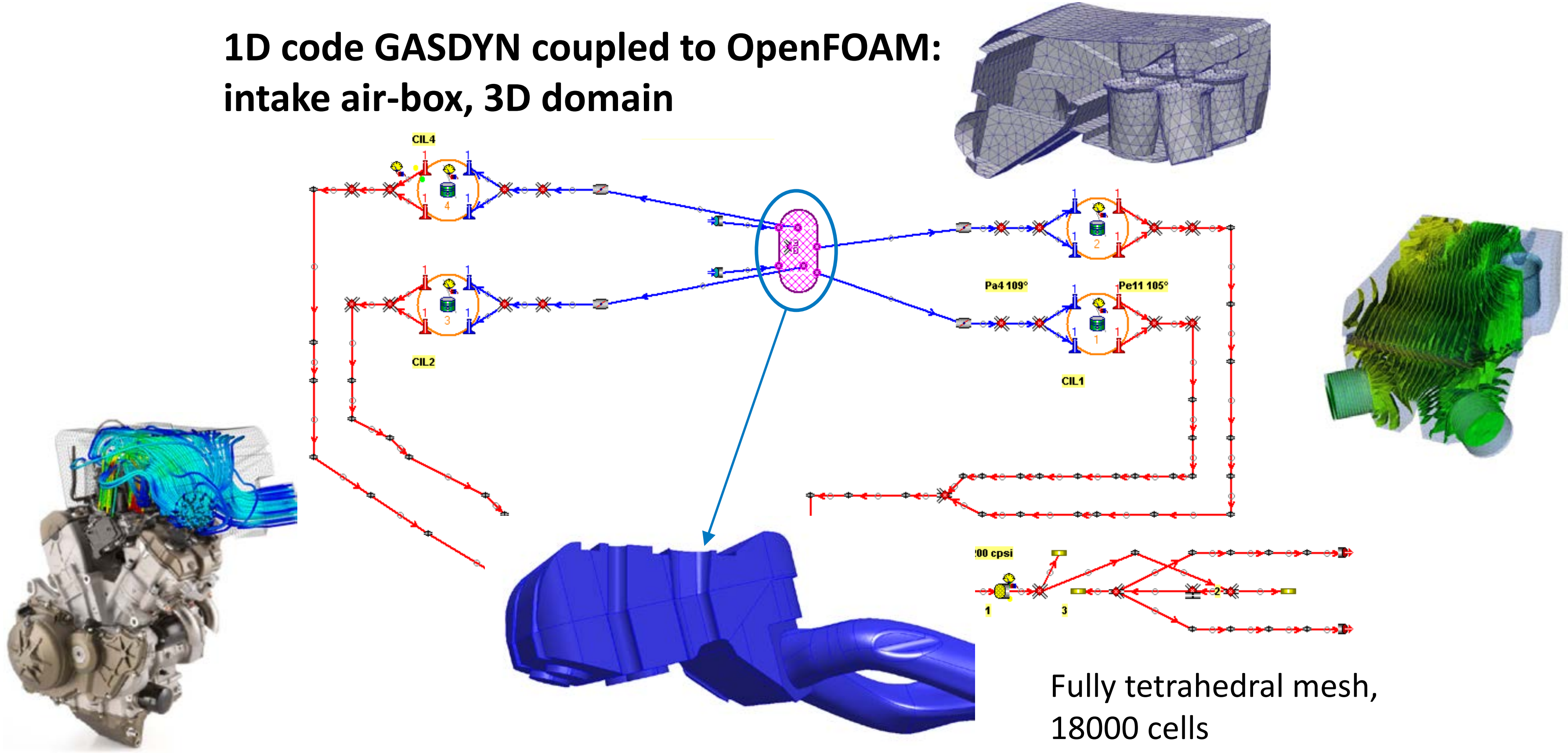

Pressure, upstream of turbine


Pressure, downstream of intercooler


Pressure, upstream of turbine

1D-3D simulation of an Aprilia V4 engine

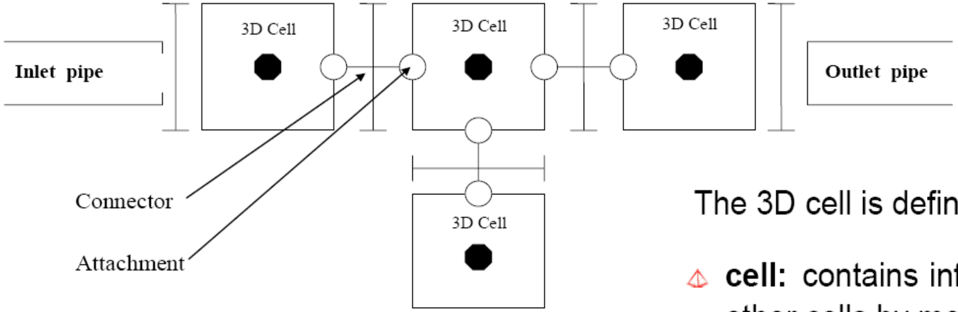
1D code GASDYN coupled to OpenFOAM: intake air-box, 3D domain

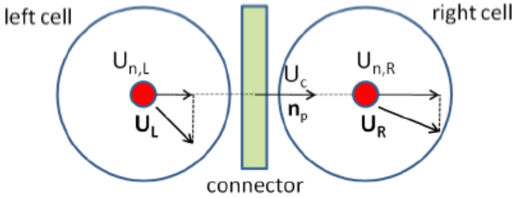


Fully tetrahedral mesh, 18000 cells

3Dcell approach

- A quasi-3D method (**3Dcell approach**) has been developed and validated as a compromise between the time-demanding 3D CFD analysis and the fast 1D approach, resorting to a 3D grid of 0D elements (coarse grid: 1-2 cm).

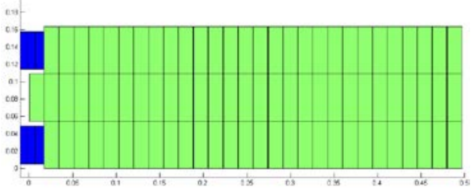




The 3D cell is defined by means of two fundamental elements:

- **cell:** contains information about the volume of the element and is connected to other cells by means of connectors
- **connector:** contains information about the cell connectivity, the distance from the center of the neighboring cells and has its own momentum

- Unviscous gas: Euler equations

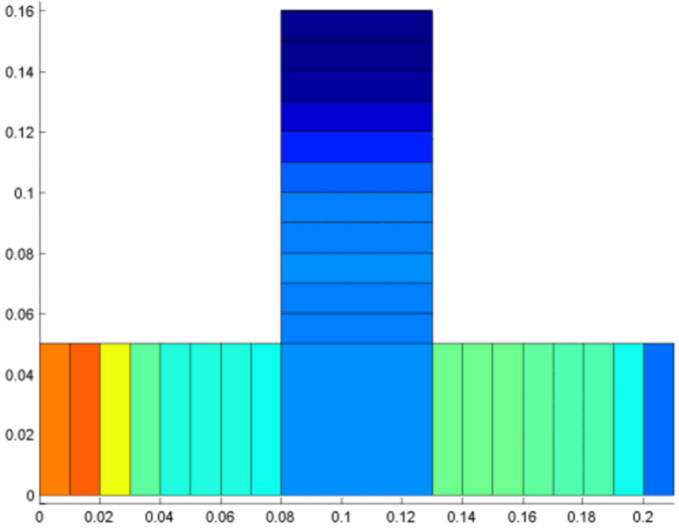


The model is based on a staggered grid approach

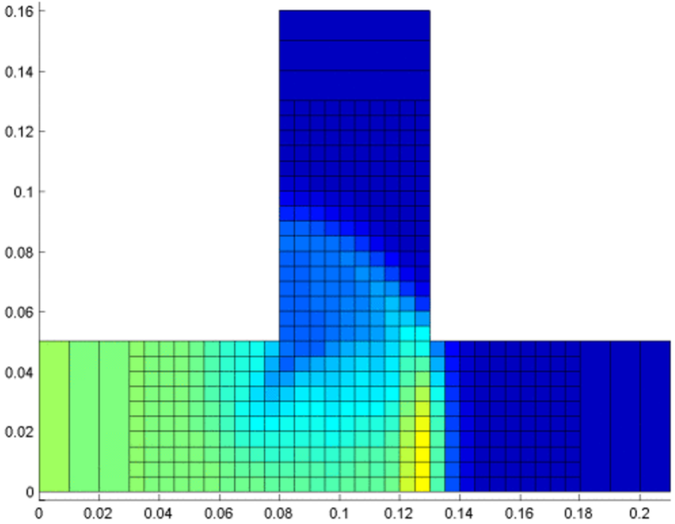
Explicit time marching method

3Dcell approach

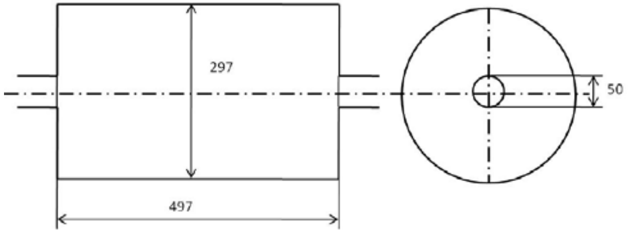
90° T junction: simulation (coarse grid)

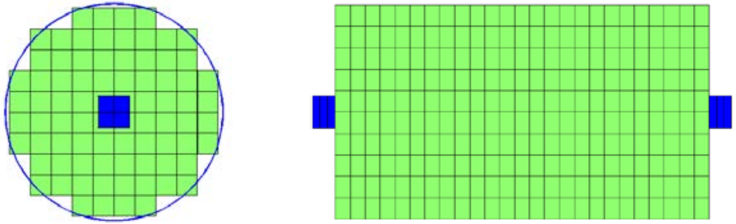


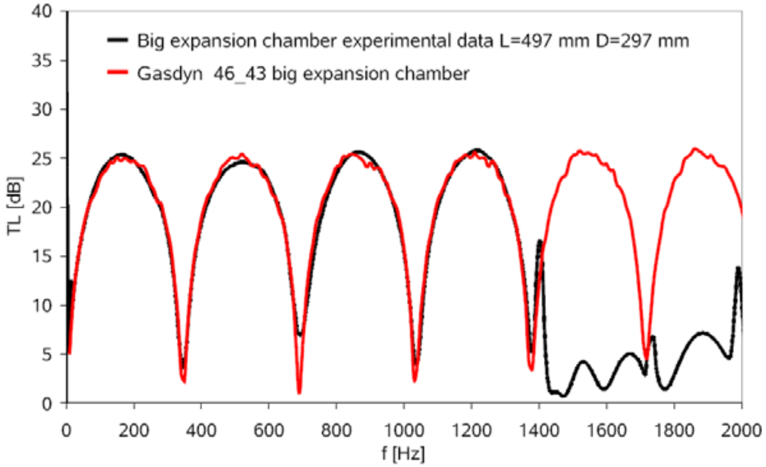
90° T junction: simulation (fine grid)

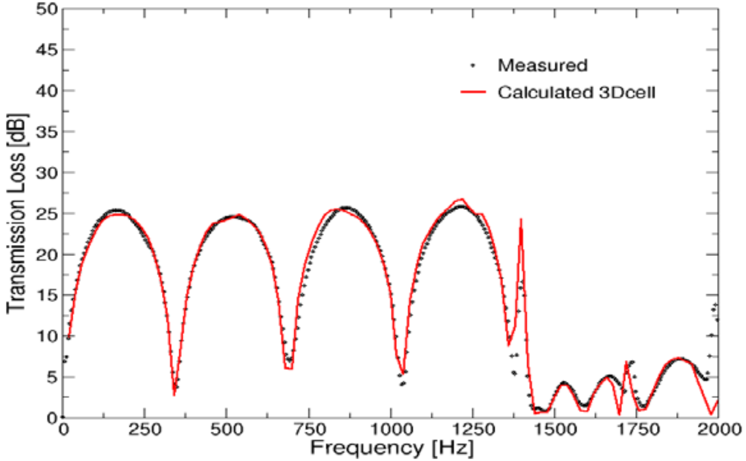


Simple expansion chamber:
1D model vs 3D cell prediction

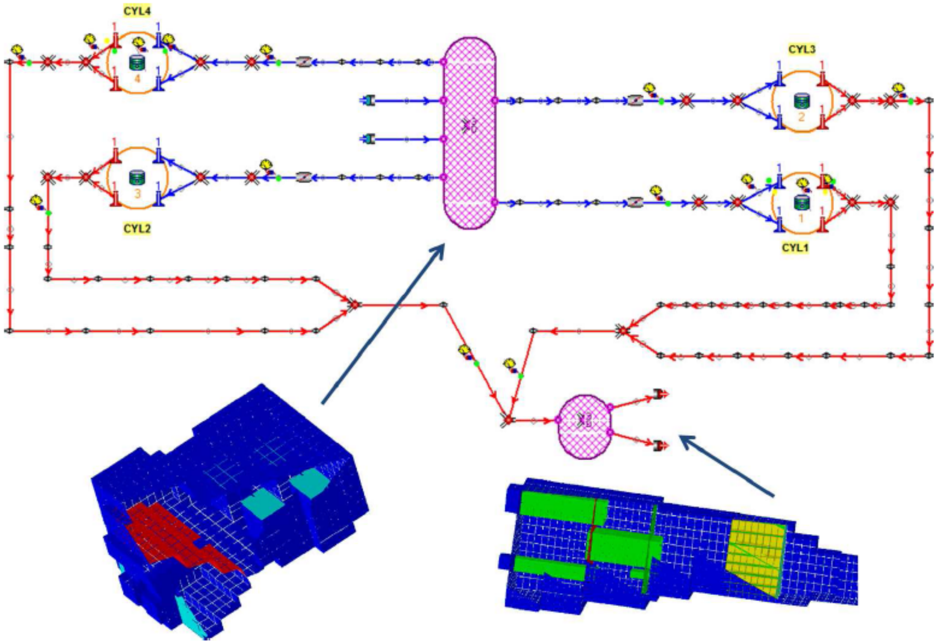








1D-quasi3D integrated model



- Fully coupled simulation with 1D code (GASDYN)
- The same numerical method is applied to 1D pipes and 3D components

Air-box and silencer modeling

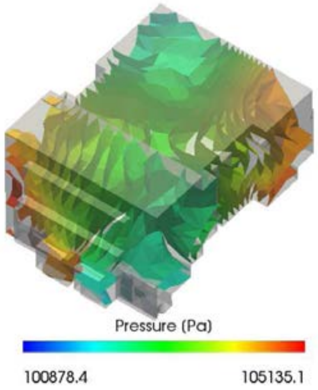
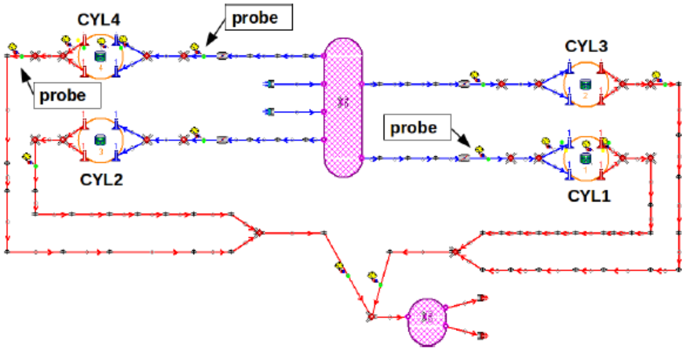


FIGURE 25. Pressure field inside the airbox.



- Pressure pulses in three different locations
- Pulses in the intake runners are strongly influenced by the interference between the cylinders