*Second Two-Day Meeting on Internal Combustion Engine Simulations Using the OpenFOAM technology, Milan 26-27th November 2016.*

# In-cylinder flows and combustion modeling: application and validation to real and engine-like configurations

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Politecnico di Milano, Department of Energy

# Topics



In-cylinder flows and combustion modeling using OpenFOAM® technology

OpenFOAM

Lib-ICE

CFD methodologies

Validation

Application

Next steps…

# Lib-ICE

Internal combustion engine modeling using the OpenFOAM technology

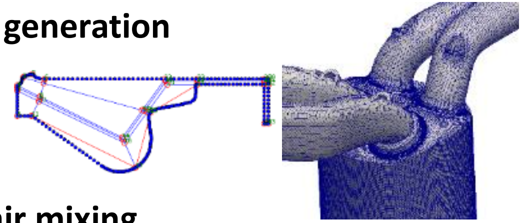
**OpenFOAM-x.x.x**

**Lib-ICE**

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

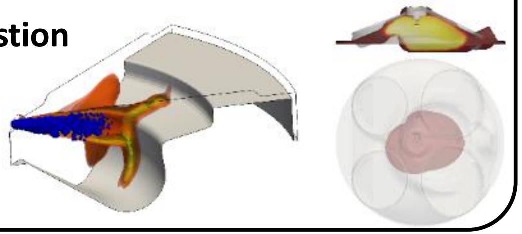
## Engine simulation workflow

**Mesh generation**

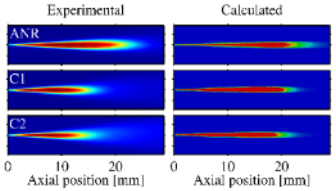


**Fuel-air mixing**

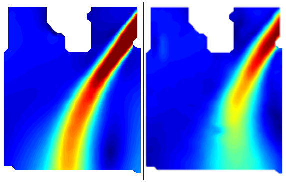
**Combustion**



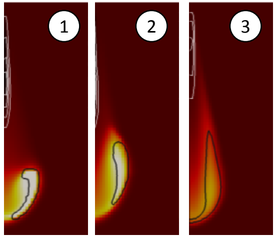
## Development/validation



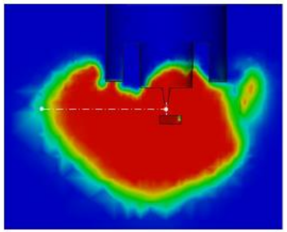

**Spray modeling**



**Engine flows**




**Diesel combustion**



**SI combustion**

# Engine simulation workflow

## Methodology

Diesel engines

SI engines

Mesh management → Cold flow → Fuel-air mixing → Combustion

# Engine simulation workflow



## Methodology

**Diesel engines**

**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

# Engine simulation workflow

## Methodology

Diesel engines

SI engines

Fully integrated approaches ⟷ Open-Source code

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

**Cold flow**
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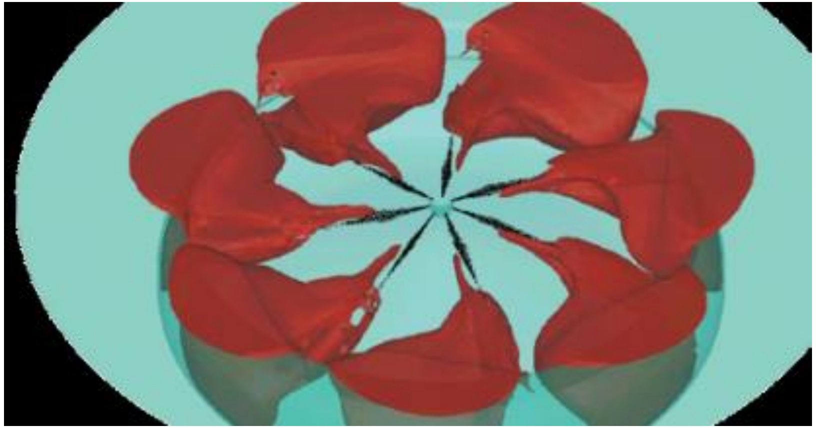
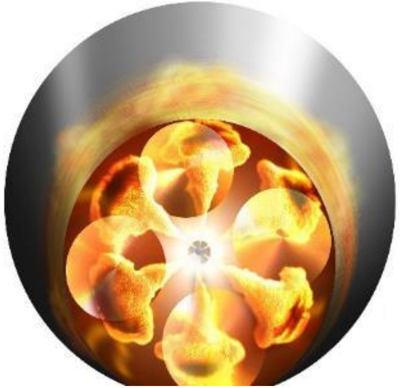
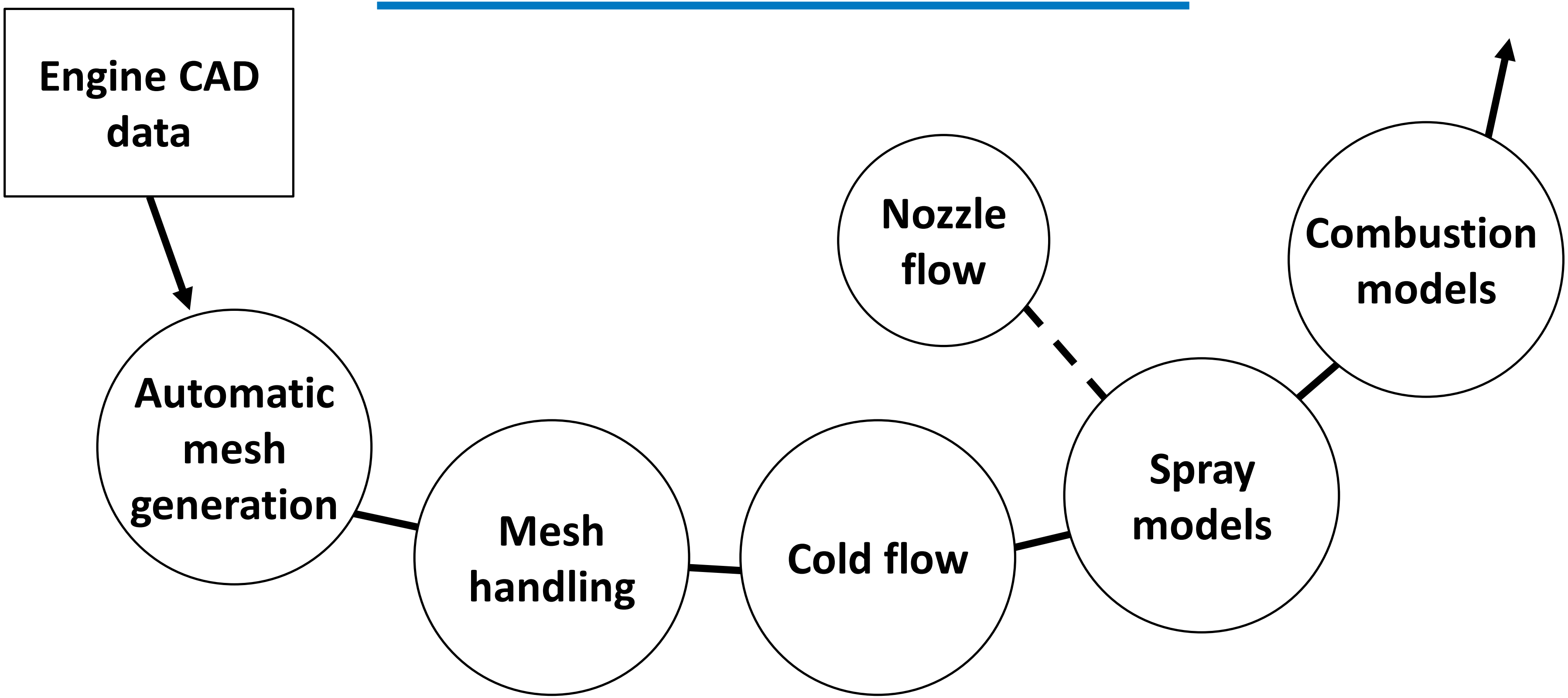




# Diesel Engines

# Diesel engines

## Methodology / model development

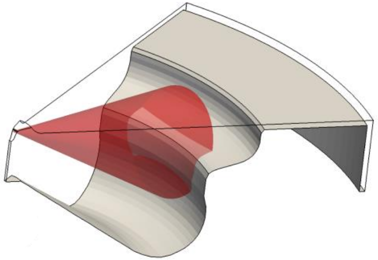


# Diesel engines

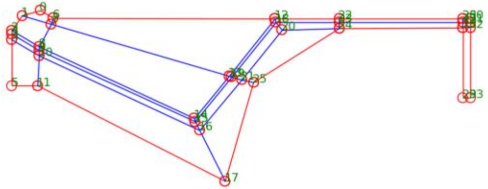
## Mesh management

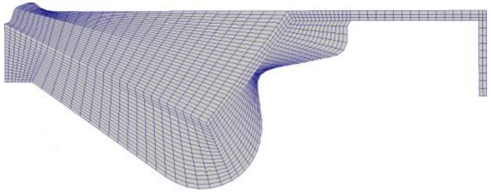
### Automatic mesh generation

**a) Main engine data**

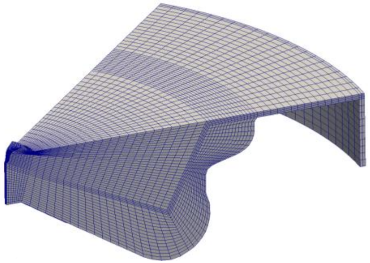


**b) Spray oriented block mesh**





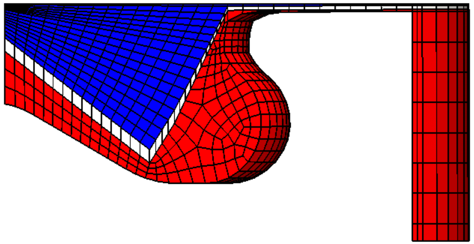
**c) Combustion chamber points fit**



**d) Spray-oriented mesh**

### Mesh handling

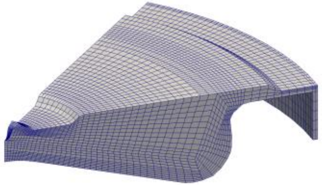
Dynamic layering



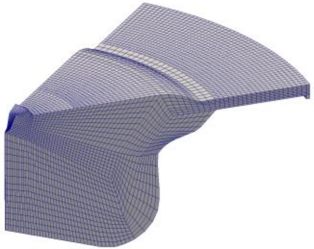
# Diesel engines

## Mesh management

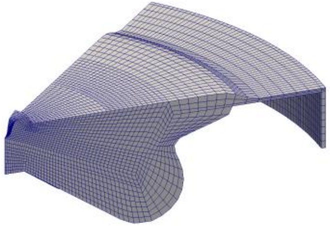
### Automatic mesh generation



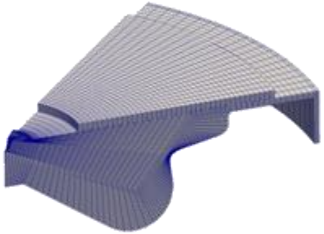
**Bowl #1**



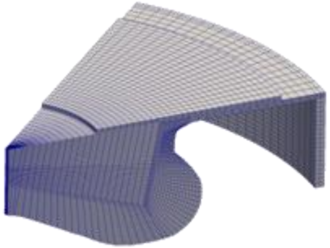
**Bowl #2**



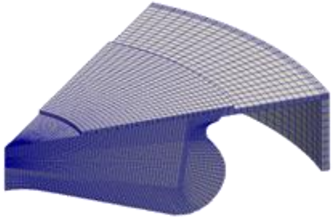
**Bowl #3**



**Bowl #4**



**Bowl #5**

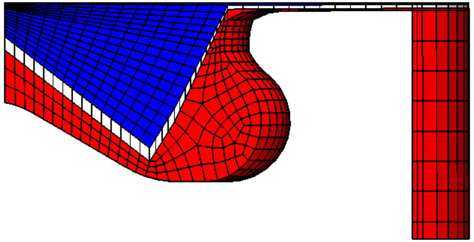


**Bowl #6**

From CAD to SIMULATION: 10 minutes

### Mesh handling

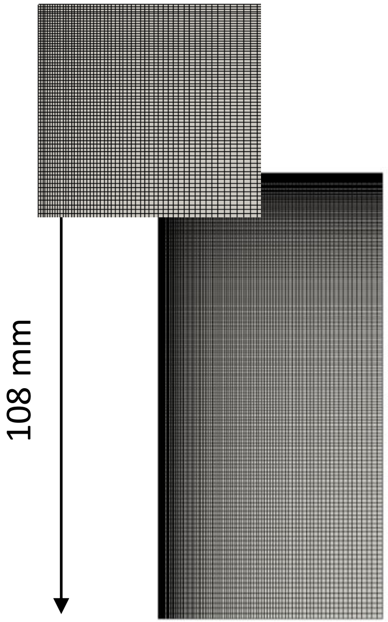
Dynamic layering



# Diesel Engines: spray modeling

## Spray A from Engine Combustion Network

### 2d computational mesh




### Spray model setup

- Injection: blob
- Breakup: KHRT
- Evaporation: Spalding

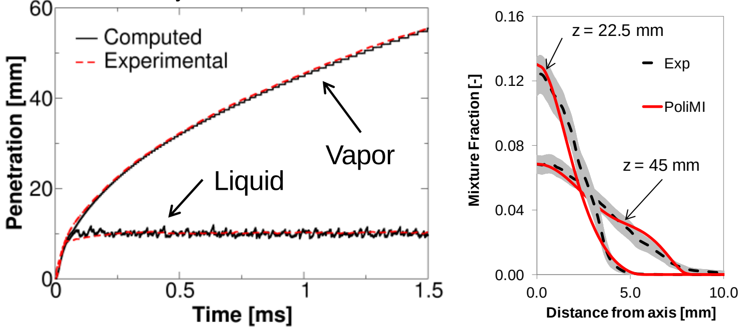
### CFD setup

- Turbulence model: standard k-ε with modified $C_1$

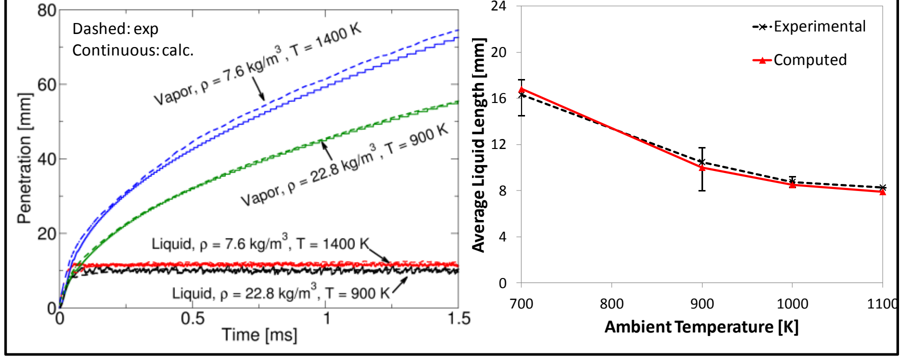
### Test conditions

- Fuel n-dodecane
- Nozzle diameter: 90 μm
- $p_{inj}$: 50-150 MPa
- $T_{amb}$: 700-1200 K
- $\rho_{amb}$ : 7.6 – 22.8 kg/m$^3$

### Baseline ($p_{inj}$ = 150 MPa; $T_{amb}$ = 900 K; $\rho_{amb}$= 22.8 kg/m$^3$)



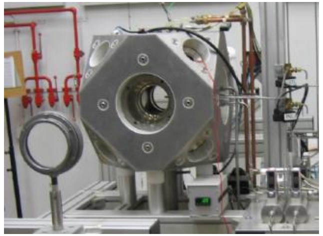

### Parametric variations ($T_{amb}$, $\rho_{amb}$)



# Diesel Engines: spray modeling

FPT C11 Spray (collaboration with TU/e – DI N. Maes and Prof. B. Somers, FPT support)

## TU/e optical vessel



- Liquid penetration: DBI
- Vapor penetration: Schlieren

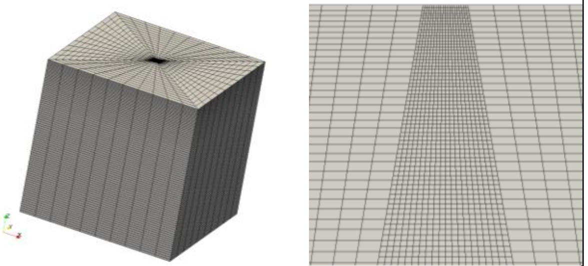
## Operating conditions

- Nozzle diameter: 0.205 mm
- Ambient temperature: 900 K

| | ANR | C1 | C2 |
|---|---|---|---|
| $P_{inj}$ [MPa] | 150 | 80 | 150 |
| $\rho_{amb}$ [kg/m$^3$] | 22.8 | 40 | 40 |

## CFD Setup

### 3D mesh



- Consistent with the engine grid in size and structure

### Spray

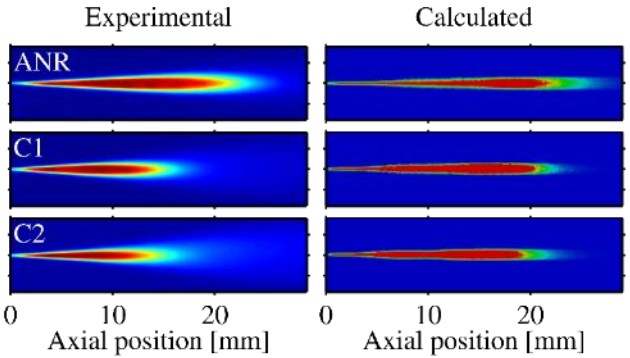
- Huh-Gosman atomization
- Pilch-Erdman breakup

### Turbulence modeling

- k-ε with modified $C_1$

## Validation

- Liquid: exp vs computed extinction profiles



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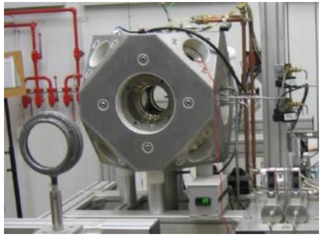

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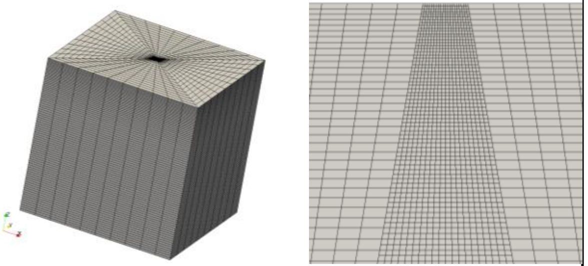

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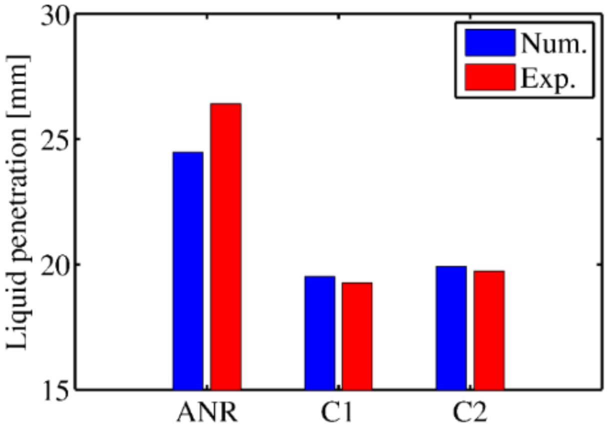

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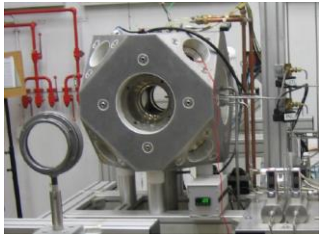

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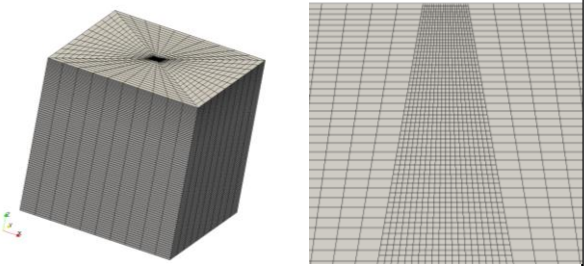

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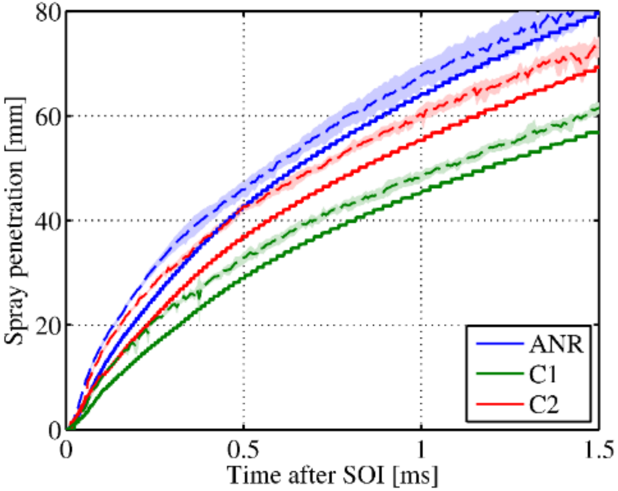
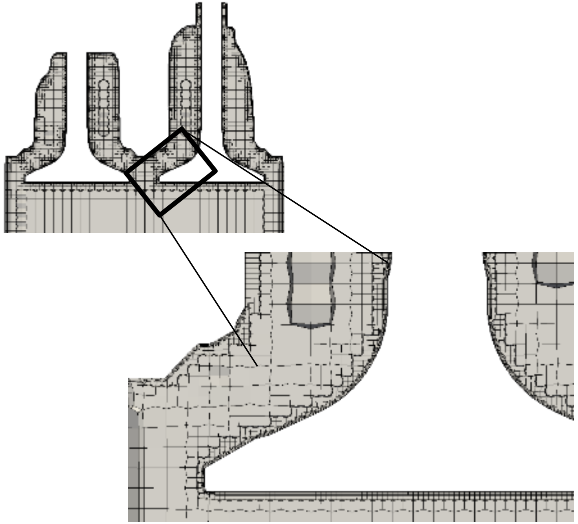



- Vapor: exp (Schlieren), calc. (mixture fraction threshold)

# Diesel Engines: cold flow

## Steady state flow bench simulations (FPT Industrial, Gilles Hardy)

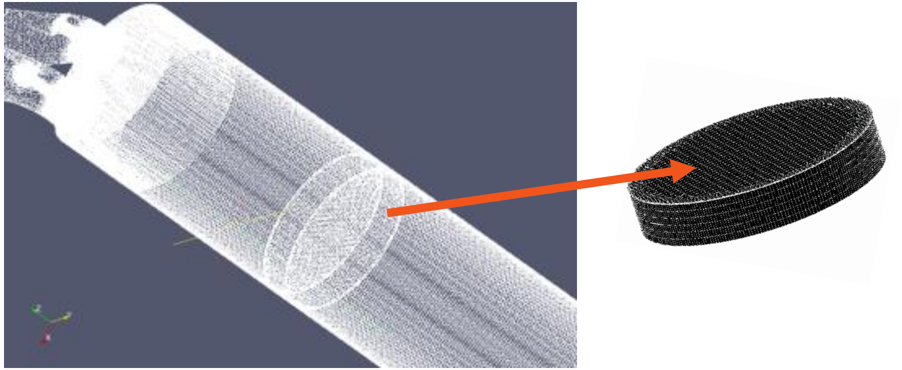
### Mesh generation



Cartesian, body fitted grids with boundary layer generated with `cartesianMesh` (cfMesh) or `snappyHexMesh` (OpenFOAM)

### CFD Setup

- Steady-state flow
- Turbulence model: standard k-ε
- Porous media acts as a flow straigthner in the computational mesh: computation of the swirl torque
- Verification of angular momentum conservation across the mesh boundaries.



# Diesel Engines: cold flow

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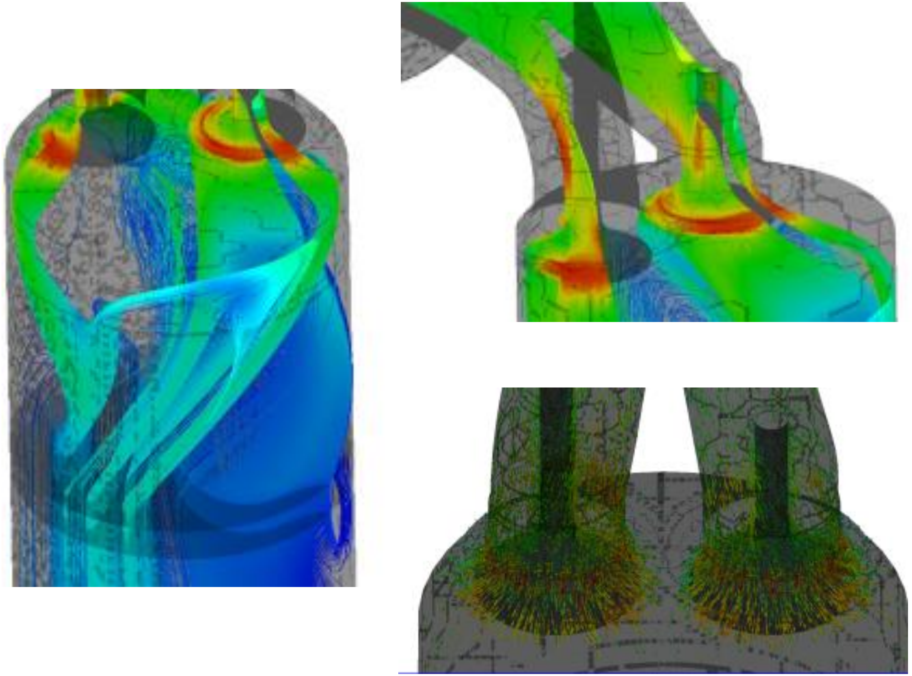
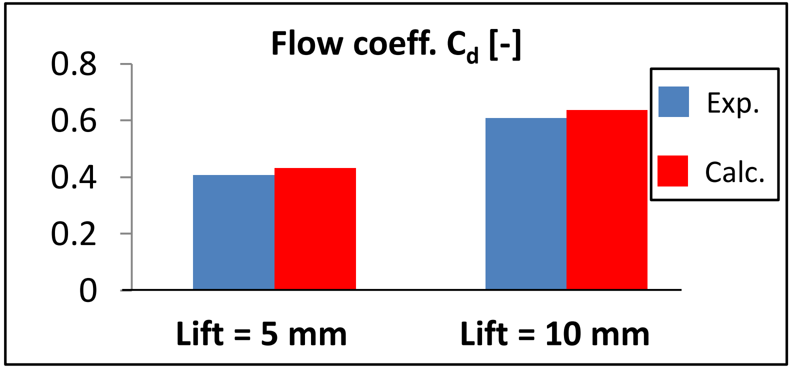
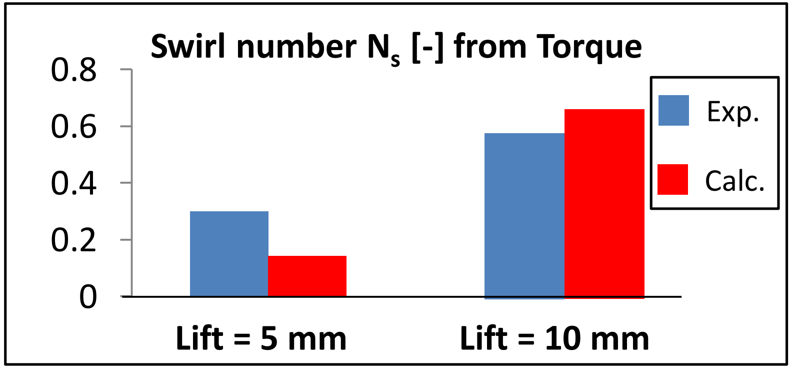
### Computed flow field



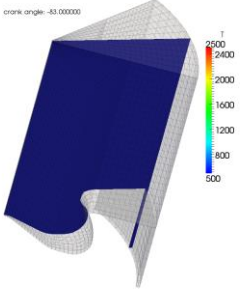


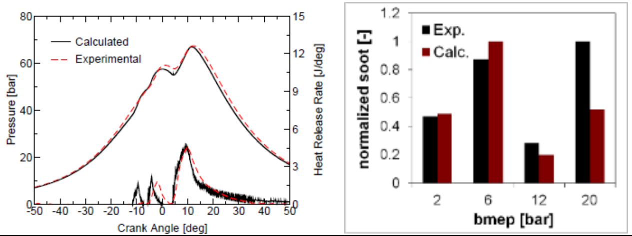
# Diesel Engines

## Combustion modeling

### Characteristic time-scale model (CTC)

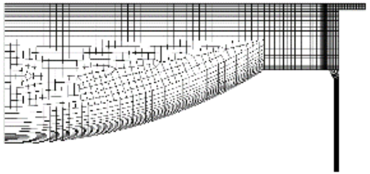


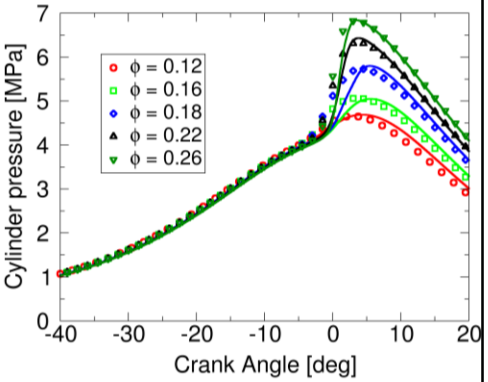
**Passenger-car Diesel engine**




### Well-mixed model

Medium-duty engine operating at low-load with iso-octane fuel.

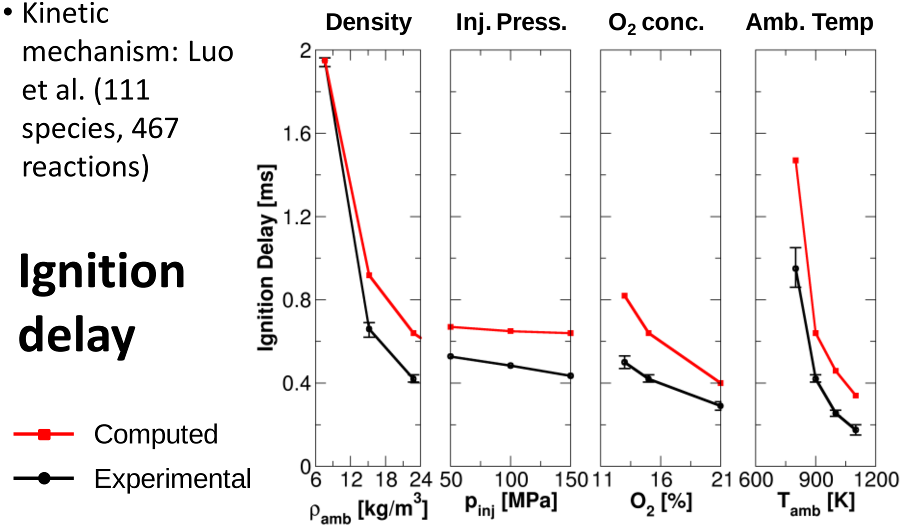





### mRIF model

- N-dodecane spray combustion at constant volume conditions
- ECN Spray-A experiment
- Variation of ambient temperature, density, oxygen and injection pressure
- Kinetic mechanism: Luo et al. (111 species, 467 reactions)

**Ignition delay**



# Diesel Engines

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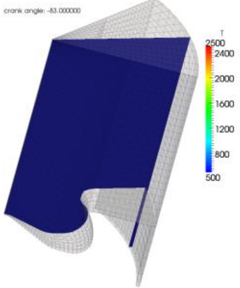


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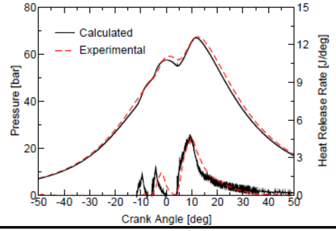


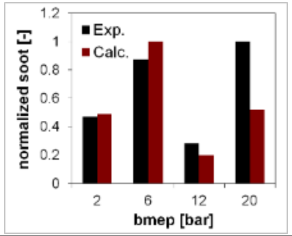


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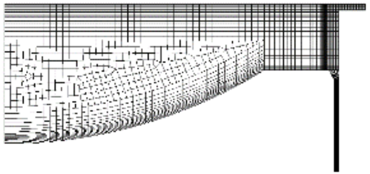

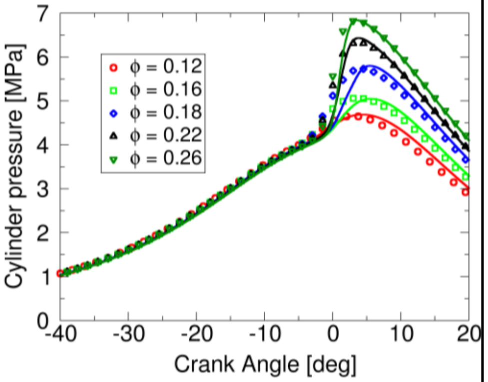


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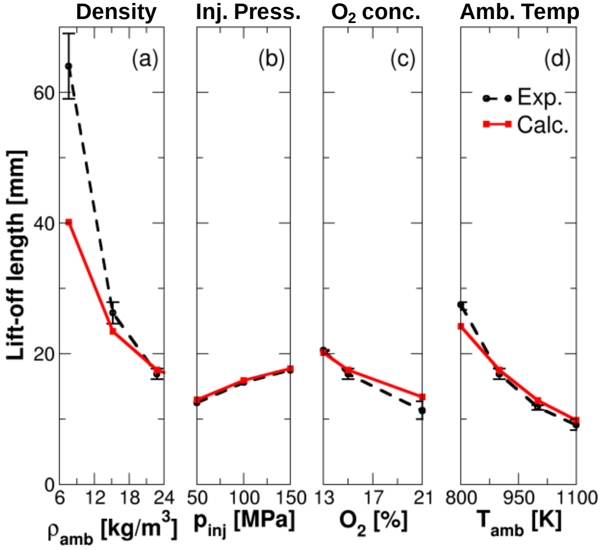
**Flame lift-off**



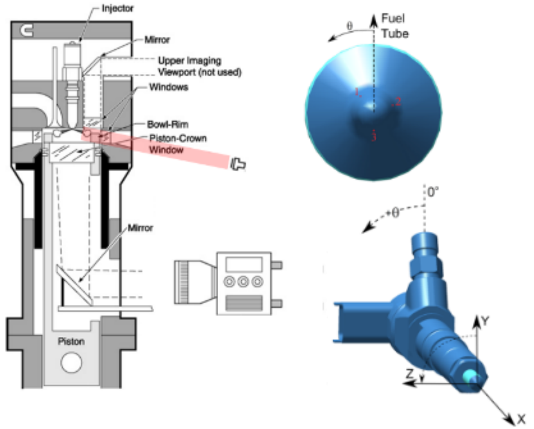

Computed

Experimental

# Diesel Engines: validation

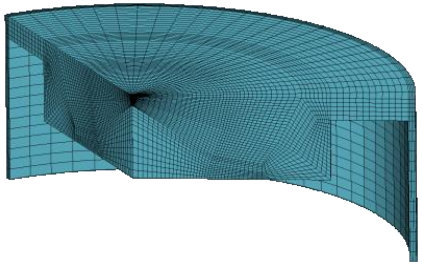
Spray B in Engines (from ECN, collaboration with Dr. Eagle, Dr. Malbec, Dr. Musculus)

## Optically accessible engine with three hole injector




Nozzle design very similar to spray A: possibility to perform same studies in engine and constant-volume vessel.

## CFD setup and tested points



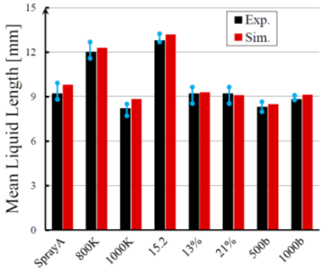
- Same CFD setup used in Spray A simulations, two different combustion models tested: mRIF and well-mixed.

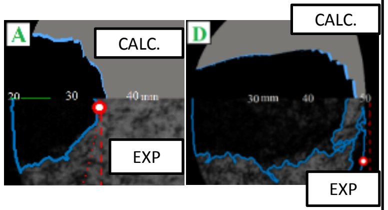
### Tested conditions

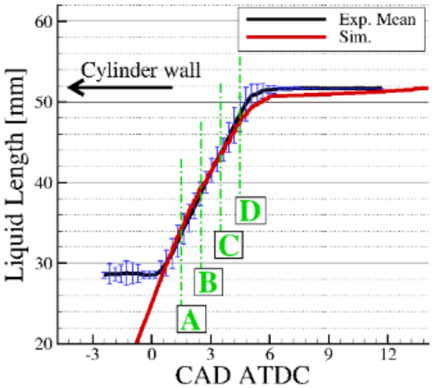
- T@SOI: 800-1000 K
- $P_{inj}$ [bar]: 500 – 1500 bar
- $O_2$ [%]: 13-21 %
- $\rho$ @ SOI: 15.2 – 22.8 kg/$m^3$

Fuel: n-dodecane

## Validation: non reacting



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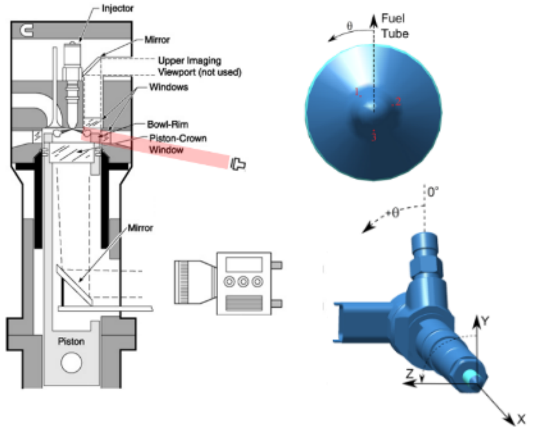
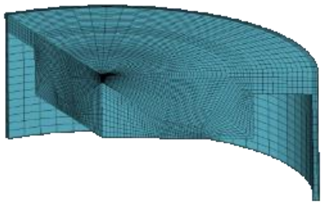



Nozzle design very similar to spray A: possibility to perform same studies in engine and constant-volume vessel.

## CFD setup and tested points



Automatically generated grid

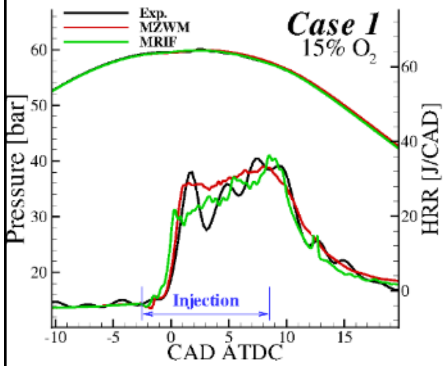
- Same CFD setup used in Spray A simulations, two different combustion models tested: mRIF and well-mixed.

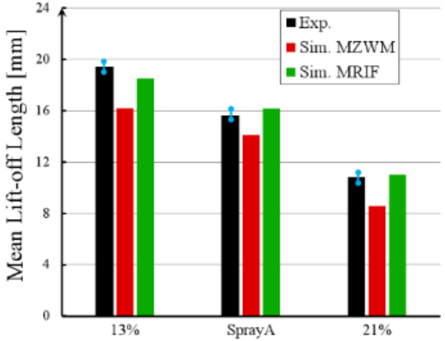
## Tested conditions

- T@SOI: 800-1000 K
- $P_{inj}$ [bar]: 500 – 1500 bar
- $O_2$ [%]: 13-21 %
- ρ @ SOI: 15.2 – 22.8 kg/m$^3$

Fuel: n-dodecane

## Validation: reacting



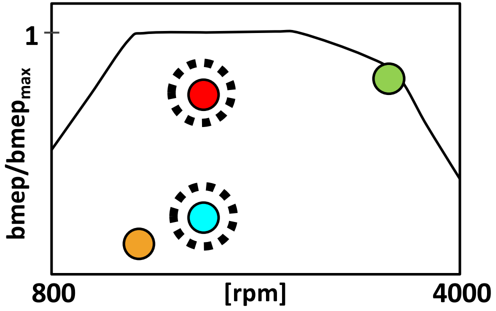



# Diesel Engines: validation

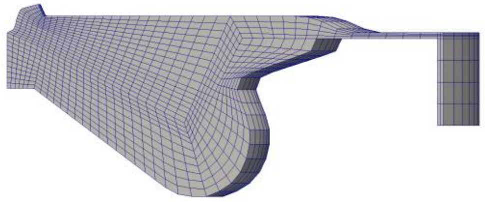


EU 6 FPT Engine MD (support from FPT, DI Gilles Hardy)

## Five operating points: with different EGR levels



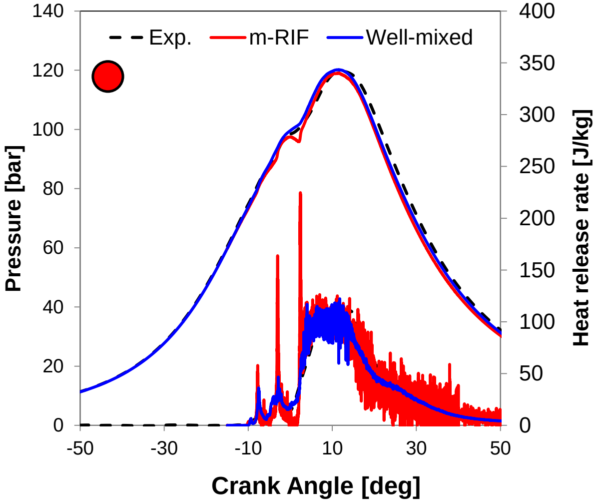

## Grid automatically generated



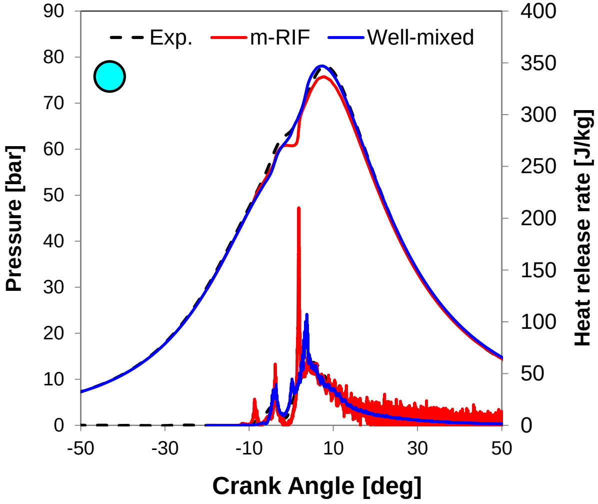
- Initial conditions from 1D simulations

## Cylinder pressure validation (mRIF and well-mixed)

**75% load, 15% EGR, 2 injections**




**25% load, 20% EGR, 3 injections**

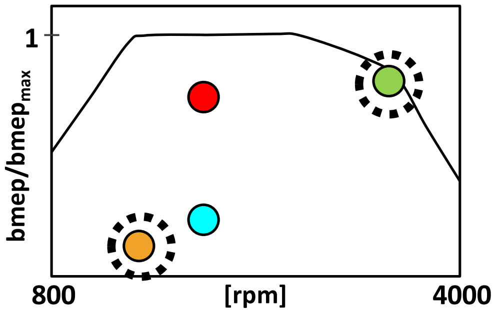


# Diesel Engines: validation

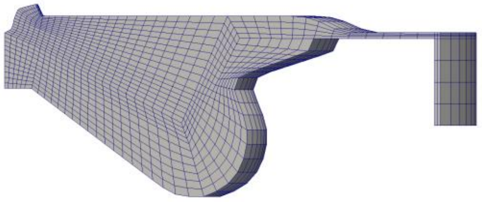


EU 6 FPT Engine MD (support from FPT, DI Gilles Hardy)

## Five operating points: with different EGR levels

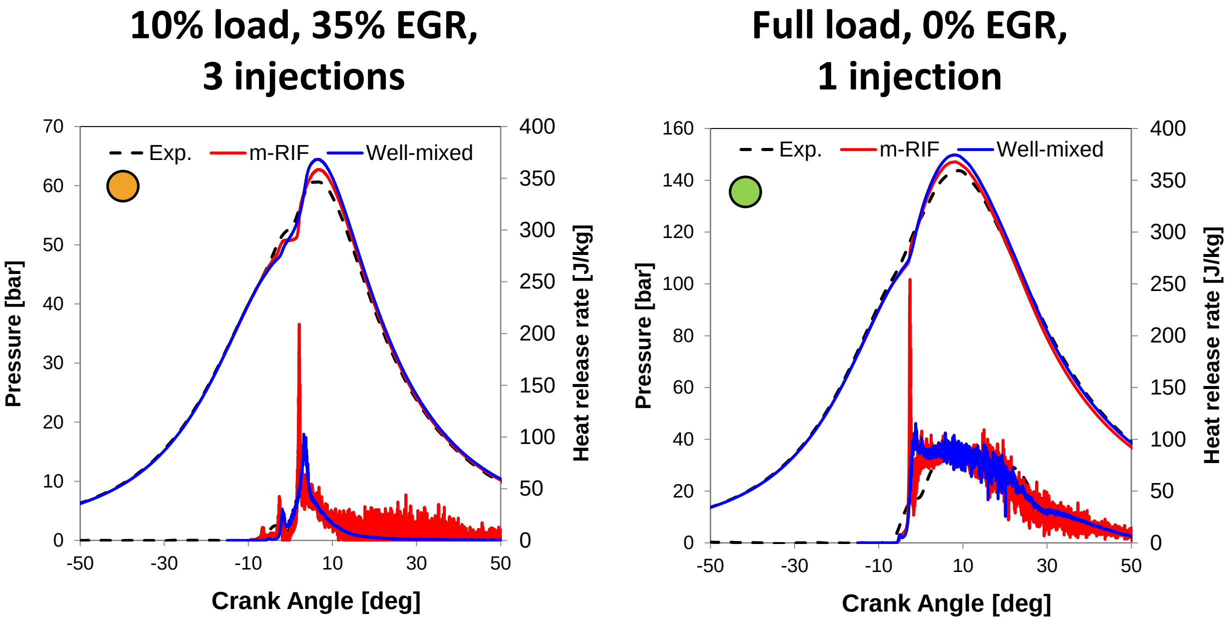



## Grid automatically generated



- Initial conditions from 1D simulations

## Cylinder pressure validation (mRIF and well-mixed)



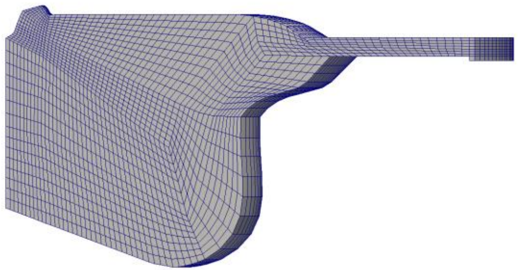
# Diesel Engines: validation

## PCCI engine (support from FPT, DI Gilles Hardy)

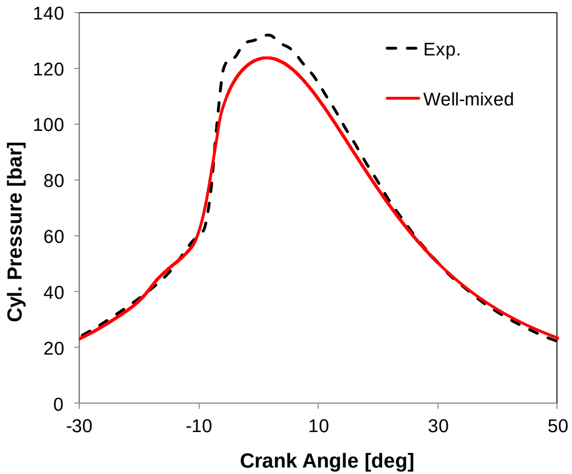
**PCCI combustion conditions**

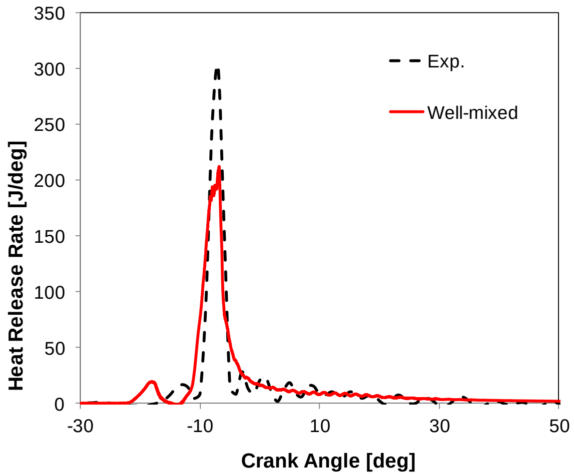
- **High EGR rate (50%)**
- **3000 rpm**

**Computational mesh generated automatically with the Polimi tool**



**Combustion model: Well-mixed**




**Diesel fuel: n-dodecane**

**Kinetic mechanism: Faravelli et al. (110 species, 300 reactions)**

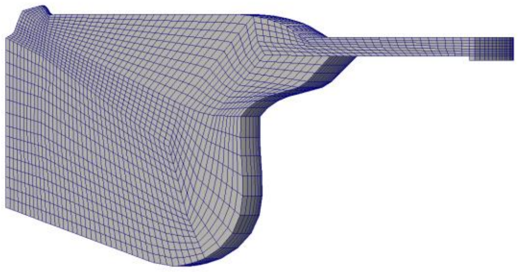
# Diesel Engines: validation

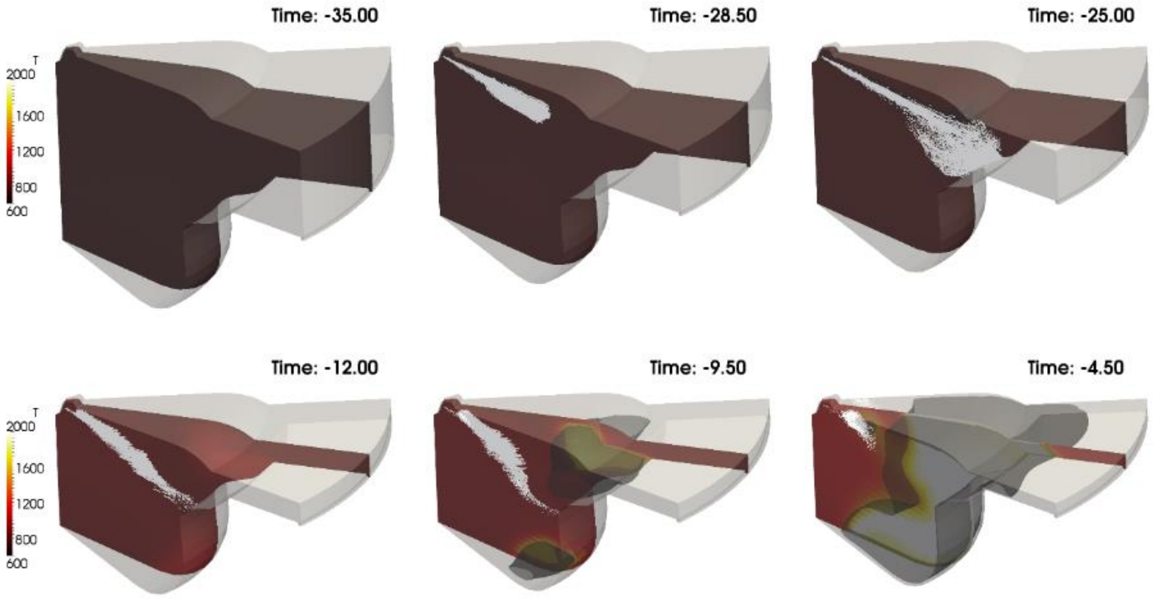
PCCI engine (support from FPT, DI Gilles Hardy)

**PCCI combustion conditions**

- **High EGR rate (50%)**
- **3000 rpm**

**Computational mesh generated automatically with the Polimi tool**

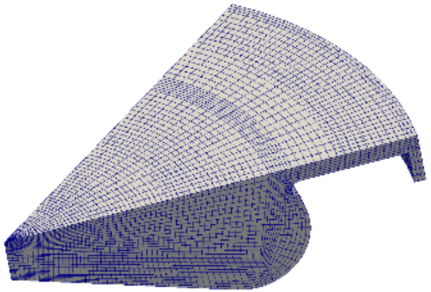




# Diesel Engines: validation

Heavy Duty engines (support from GE Global Research, Dr. Pasunurthi)

## Automatic mesh generation



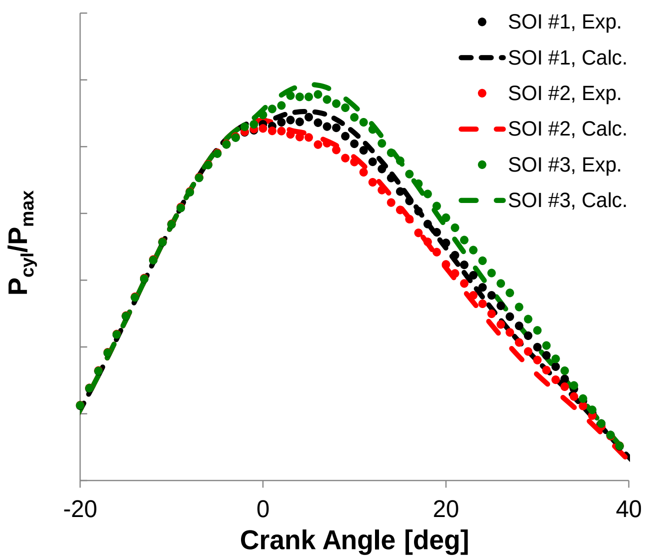
## Operating conditions

- SOI variation
- Soot/$NO_x$ trade-off
- Dual-fuel combustion

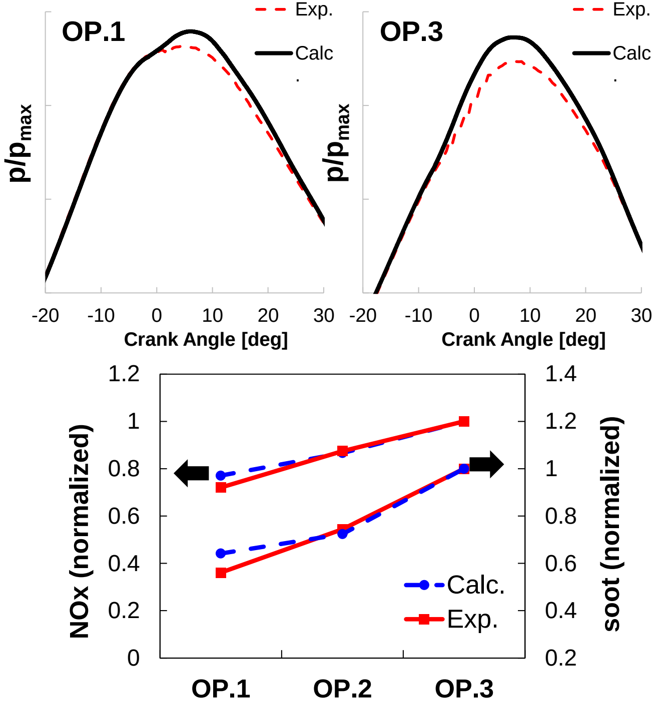
➢Diesel: **mRIF**
➢Dual-fuel: **PaSR**
➢NOx: **Zeldovich**, soot: **Moss**

## Conventional Diesel Combustion

### Engine 1: SOI variation




## Engine 2: pollutant prediction



# Diesel Engines validation



Heavy Duty engines (support from GE Global Research, Dr. Pasunurthi)

## Setup

- Reduced mechanism for Diesel ($C_7H_{16}$) and natural gas
- Combustion model: PaSR

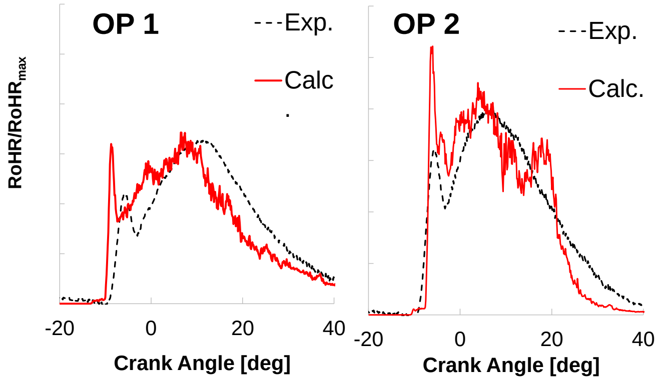
$$k = \frac{t_c}{t_c + t_{mix}} = \frac{\min\left(-\left.\frac{\rho Y_i}{\omega_i}\right|_{\omega_i<0}\right)}{\min\left(-\left.\frac{\rho Y_i}{\omega_i}\right|_{\omega_i<0}\right) + C_{mix}\frac{k}{\varepsilon}}$$

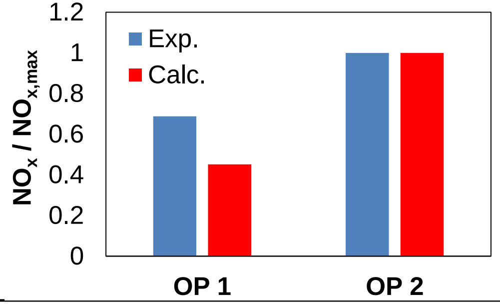
- Pollutants
  - $NO_x$ : Zeldovich
  - Soot: Moss

- Two operating points: same air/fuel ratio, different amount of injected Diesel fuel

## Dual-fuel combustion


## Validation



# Diesel Engines

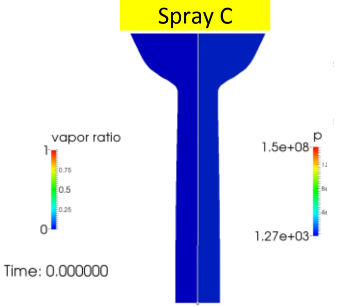


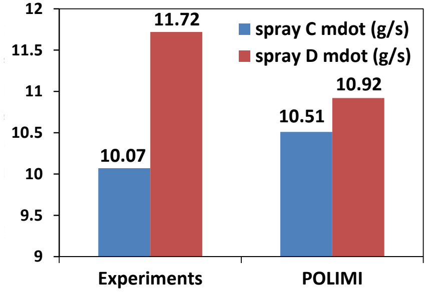
## Next steps...

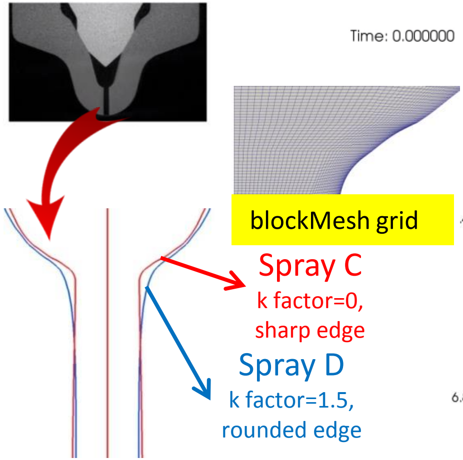
### Internal nozzle flow modeling (RANS, cavitation)

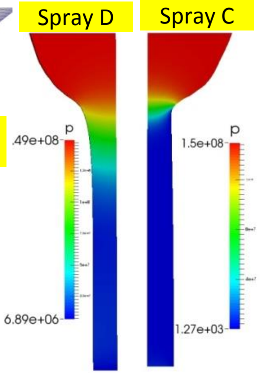
**Spray C & Spray D**

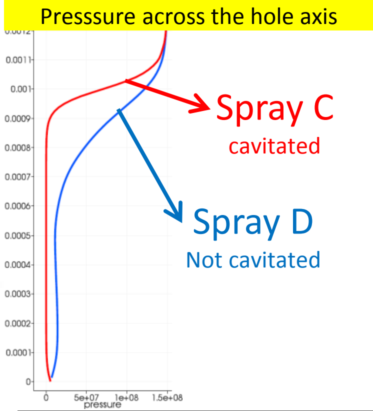
These two single hole injectors are defined by ECN to compare the effect of geometry on flow behavior.




### ...and more...

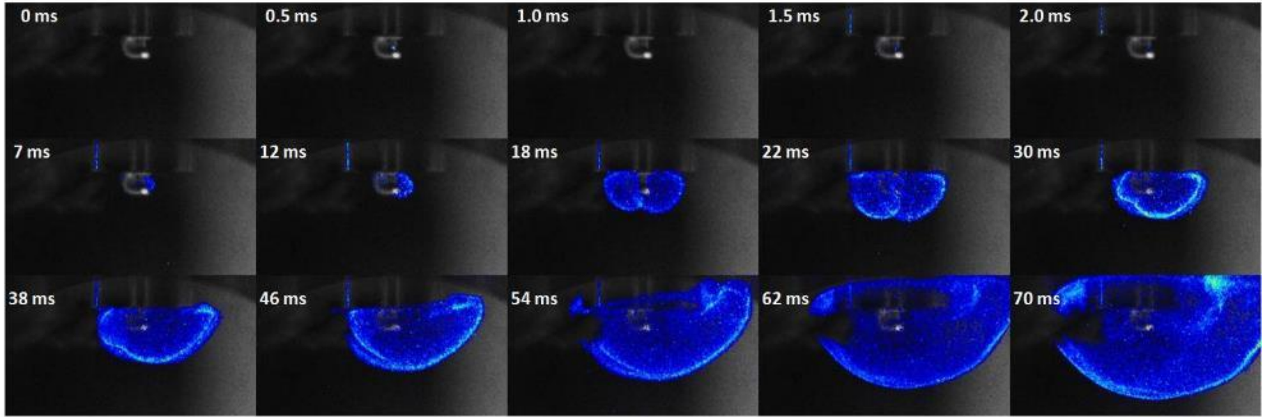
- mRIF with multiple injections

Tabulated kinetics:

- Homogeneous reactors
- Unsteady RIF

Transported PDF combustion modeling:

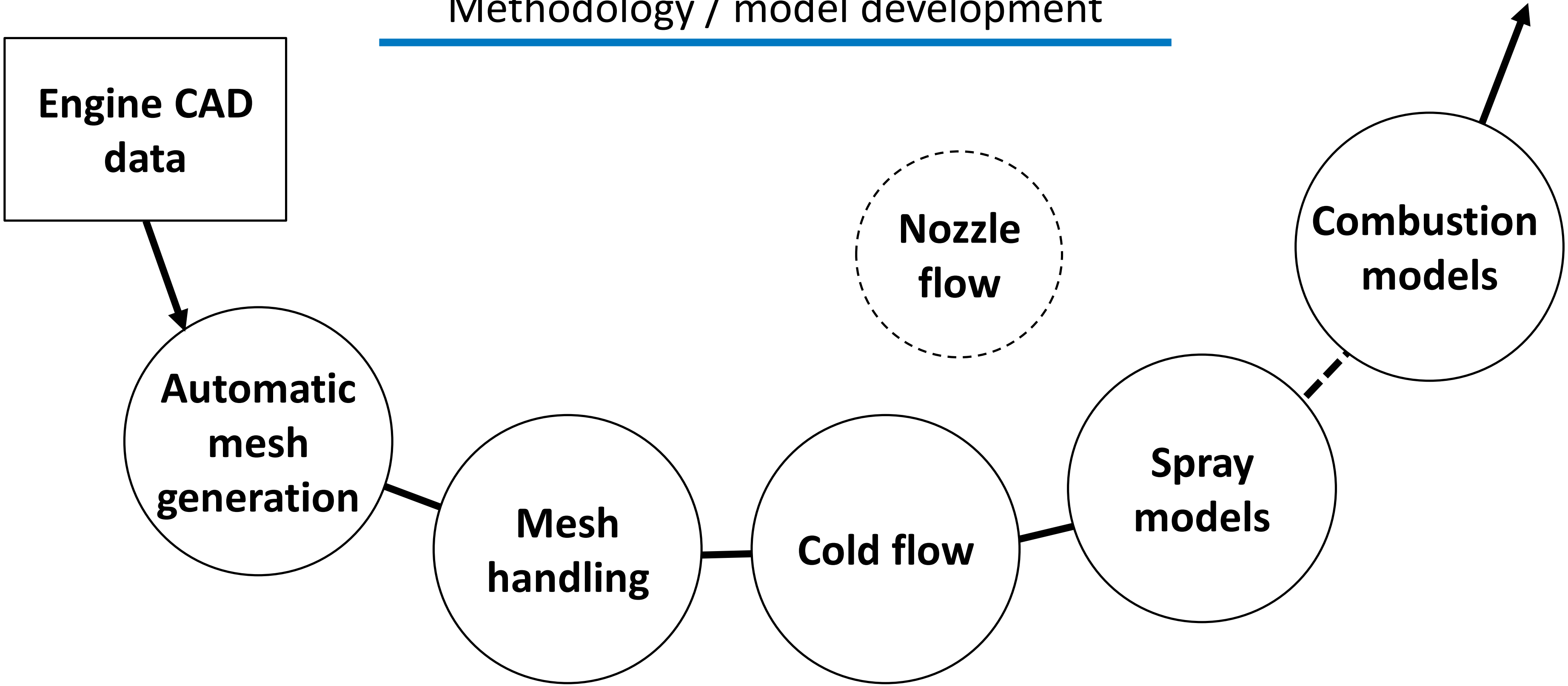
- Eulerian Stochastic fields with tabulated kinetics!


0 ms
0.5 ms
1.0 ms
1.5 ms
2.0 ms
7 ms
12 ms
18 ms
22 ms
30 ms
38 ms
46 ms
54 ms
62 ms
70 ms

# SI Engines

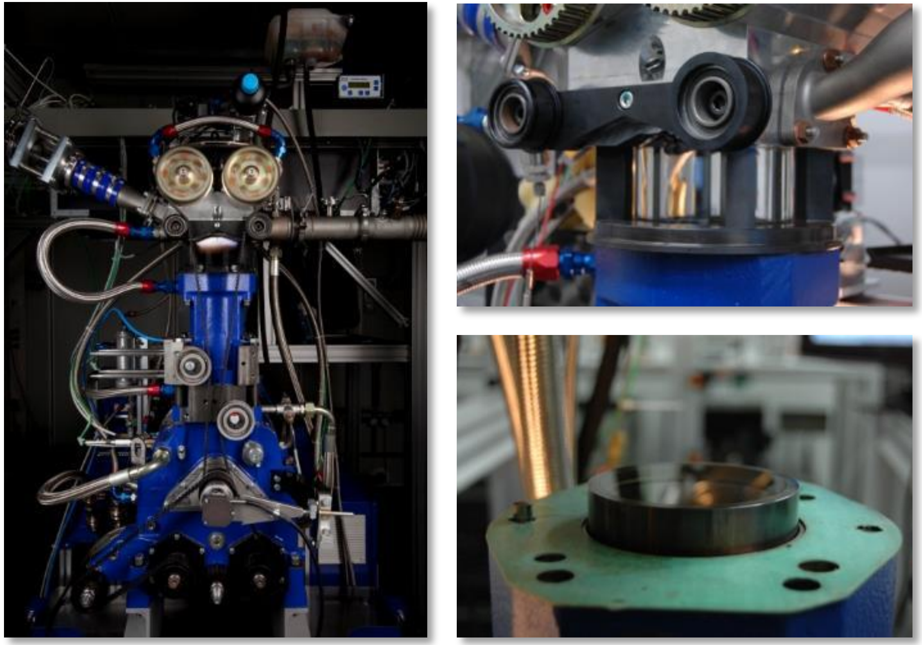
# SI Engines

## Methodology / model development

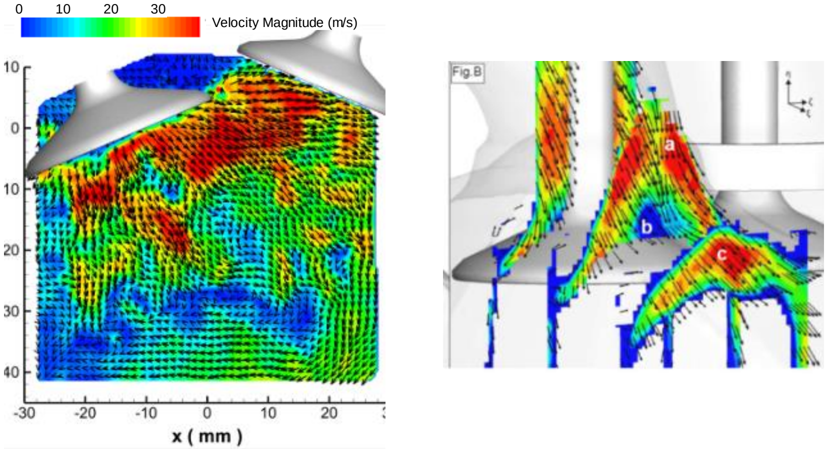


# SI Engines: cold flow

## Darmstadt optical engine (collaboration with Dr. B. Bohm and DI C. P. Ding)



Four-valve engine, fully optically accessible



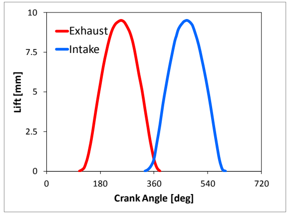

PIV measurement techniques:

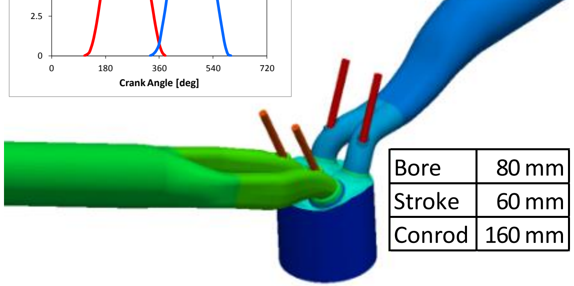
- low repetition rate planar PIV
- high-speed PIV (HS-PIV)
- stereoscopic PIV (SPIV)
- tomographic PIV (TPIV).

# SI Engines: cold flow

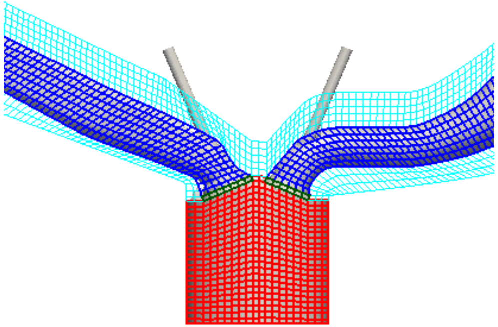
## Full cycle SI: Darmstadt optical engine – automatic mesh generation

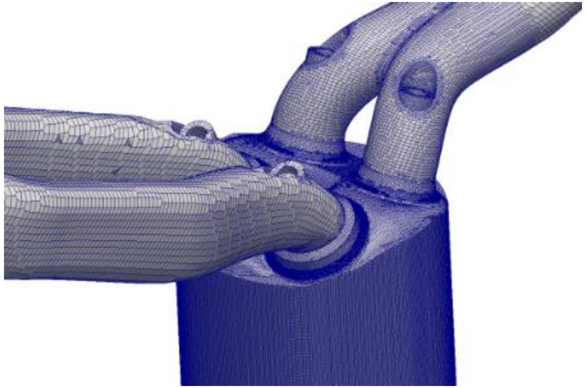
STL + data → Geometry-oriented block structured mesh → **snappyHexMesh**



| | |
|---|---|
| Bore | 80 mm |
| Stroke | 60 mm |
| Conrod | 160 mm |

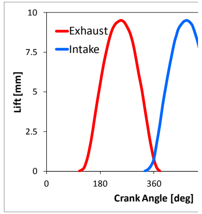


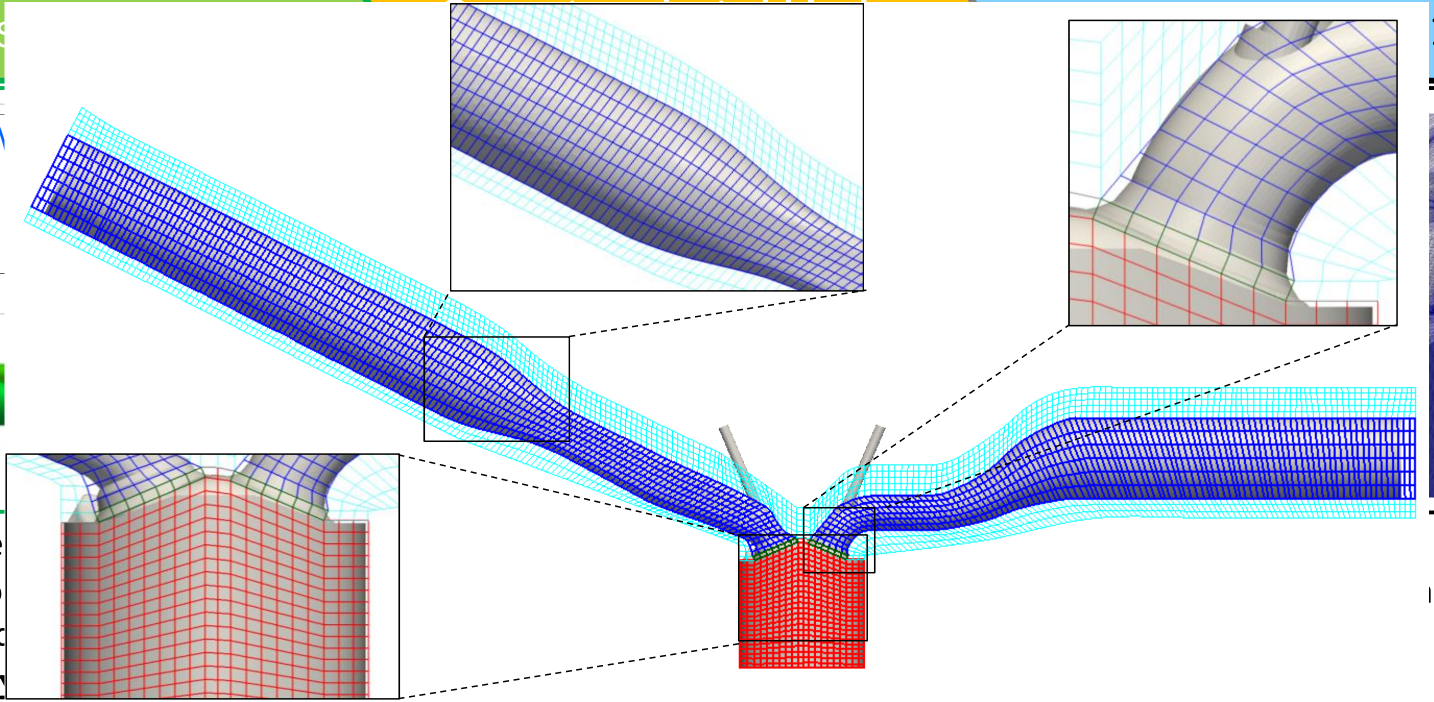


- The user provides combustion chamber geometry and data (bore, stroke, valve lifts)
- A python program automatically recognizes the direction of ducts, cylinder and valves and generates a geometry-oriented background grid
- **snappyHexMesh** is then run using the geometry-oriented background mesh

# SI Engines: cold flow

## Full cycle SI: Darmstadt optical engine – automatic mesh generation



- The use
- A pytho … geometry-oriented
- **snappy**

# SI Engines: cold flow

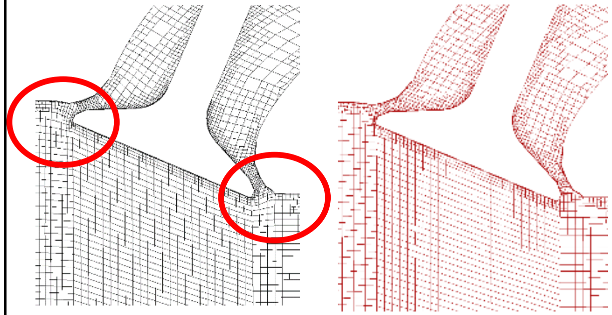
## Full cycle SI: Darmstadt optical engine – mesh management

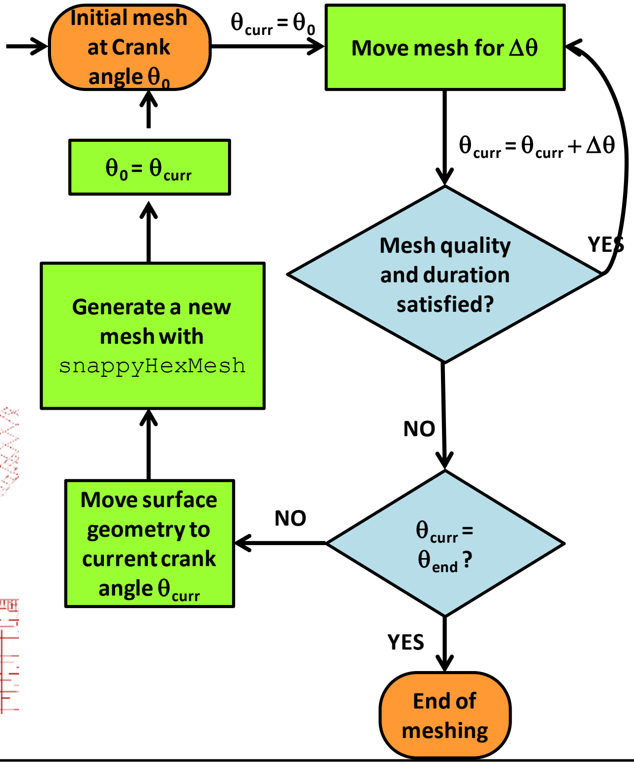
**Full-cycle simulations:**

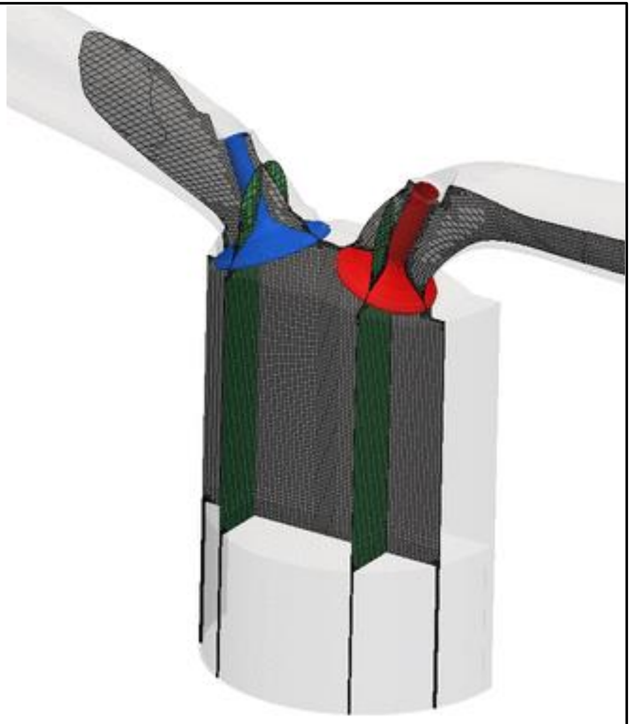
- **Multiple meshes**
- **Mesh to mesh interpolation strategy.**

**Duration of each mesh:**

- **User defined + quality criteria**





# SI Engines: cold flow

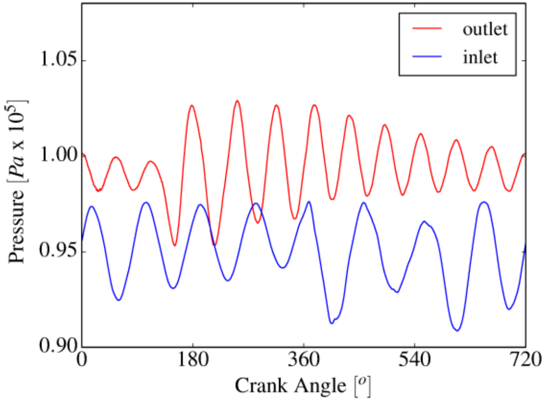
## Full cycle SI: Darmstadt optical engine – case setup

### Models and boundary conditions

#### Engine geometry data

| | |
|---|---|
| Bore | 86 mm |
| Stroke | 86 mm |
| Compression ratio | 8.5 |
| IVO | 325 CAD |
| IVC | 485 CAD |
| EVO | 105 CAD |
| EVC | 345 CAD |
| **Speed** | **850 rpm** |
| Combustion | no |

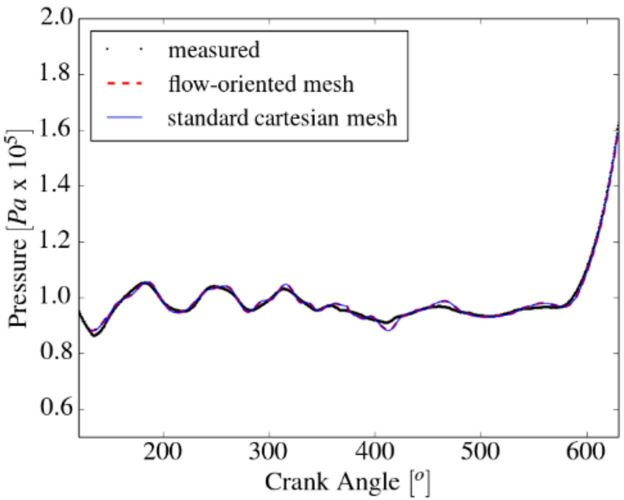
#### Boundary conditions




- Unsteady boundary conditions (from exp. data) imposed at inlet and outlet ports.

#### CFD models

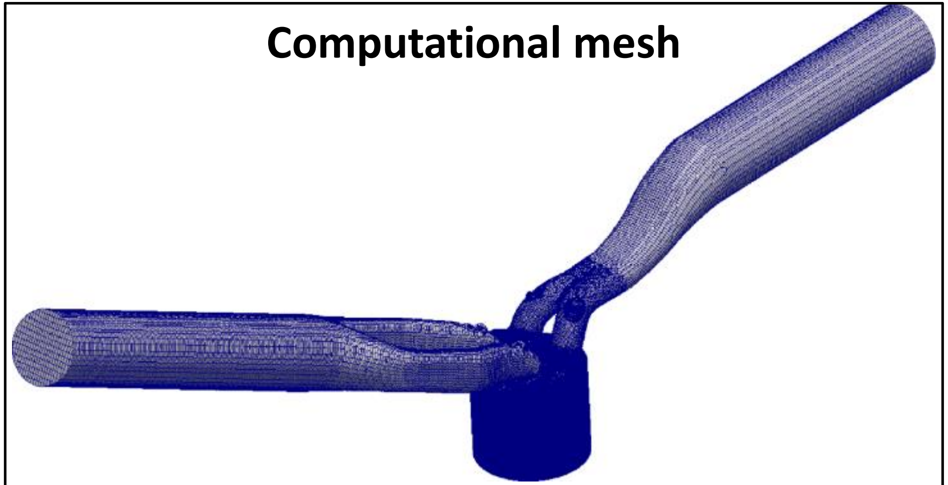
- Second-order discretization (TVD)
- Turbulence model: standard k-ε



# SI Engines: cold flow

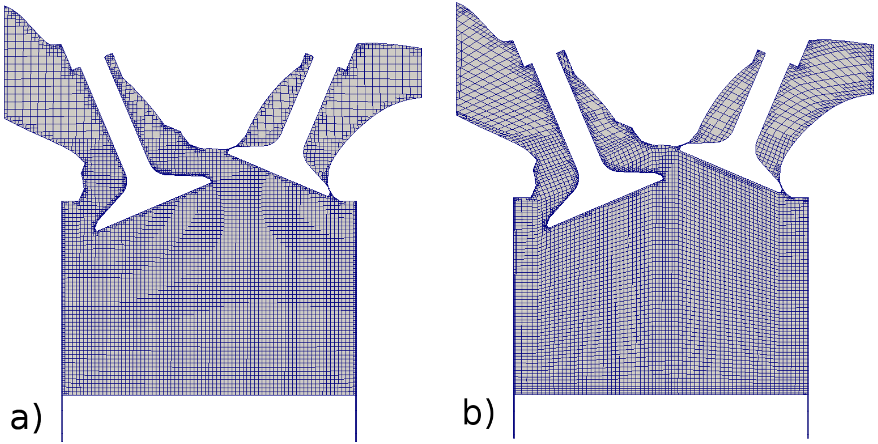
## Full cycle SI: Darmstadt optical engine – case setup

### Computational mesh



- 4 mm mesh size in the ducts region;
- 2 mm mesh size in the cylinder and valve region;
- local refinement up to 1 mm close to cylinder head, piston and liner boundaries;
- local refinement up to 0.25 mm close to the valves boundaries.

### Mesh layouts



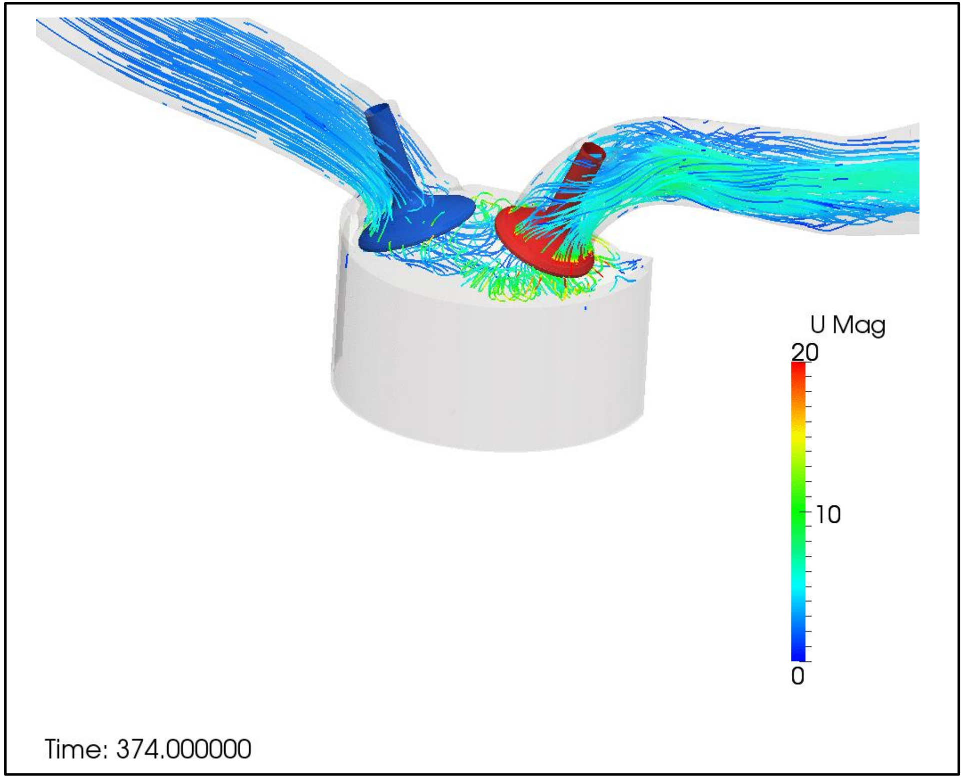

a) Cartesian mesh (automatically generated + snappyHexMesh)

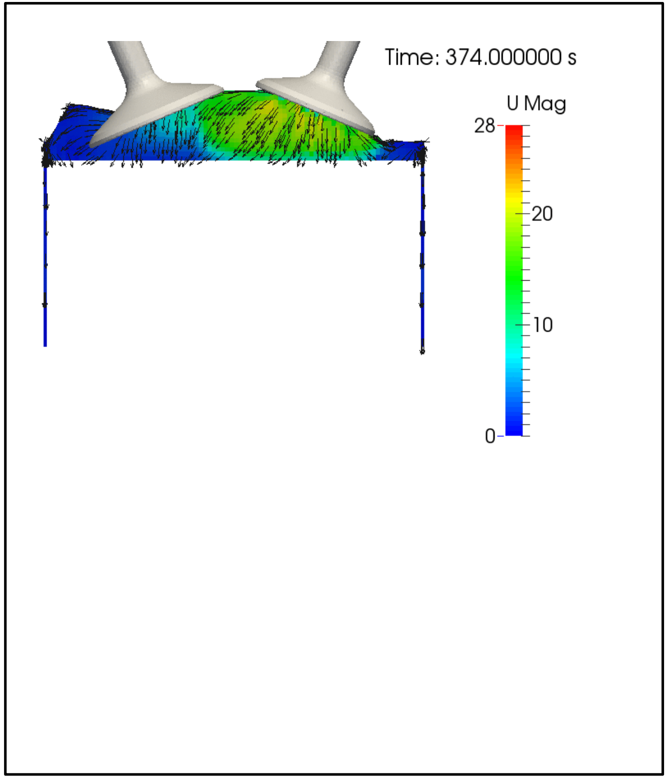
b) Flow-oriented mesh (automatically generated + Polimi tool + snappyHexMesh)

# SI Engines: cold flow



## Full cycle SI: Darmstadt optical engine – validation

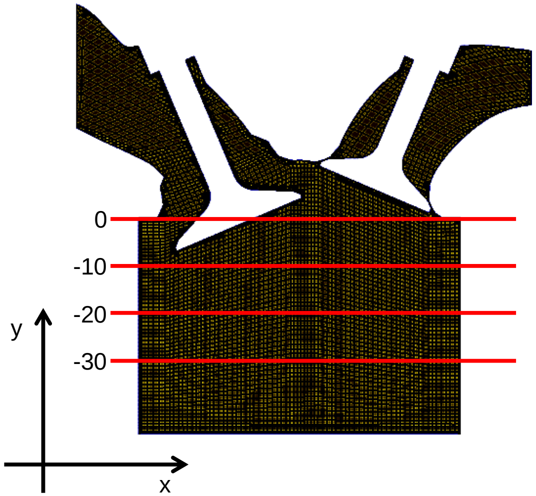


# SI Engines: cold flow

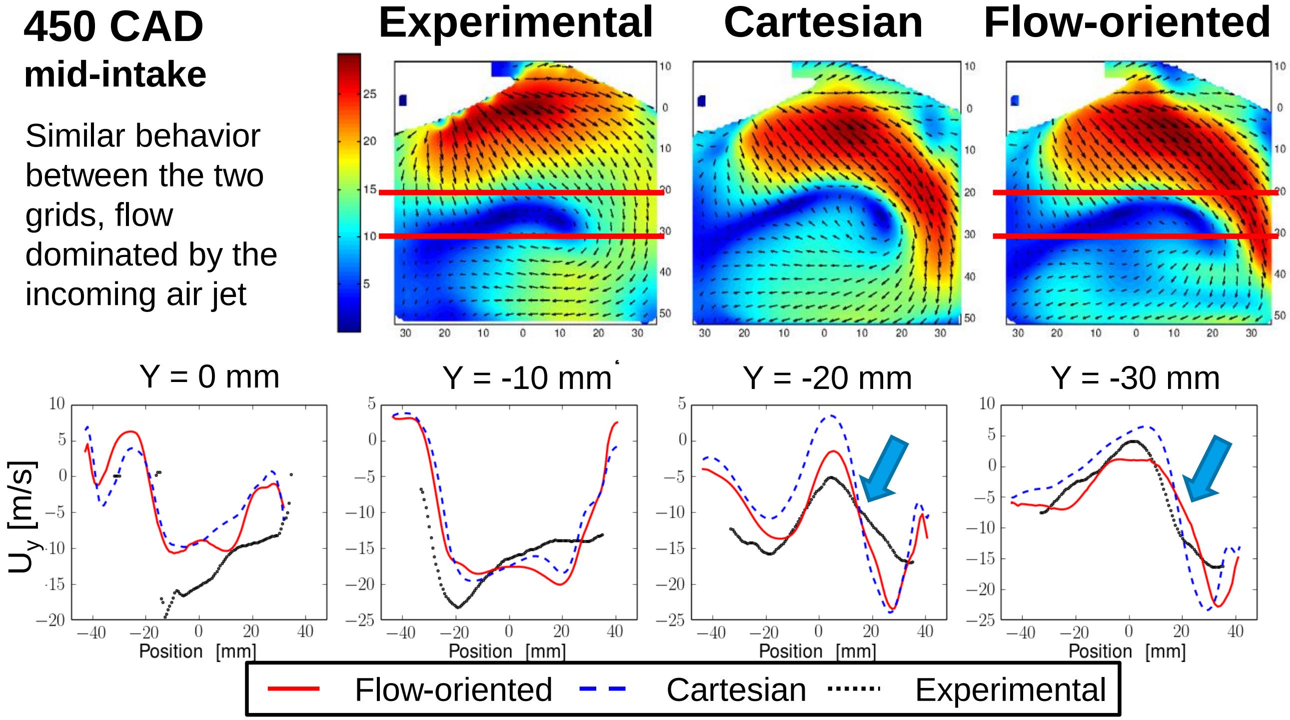
## Full cycle SI: Darmstadt optical engine – validation

x and y velocity components along four different measurement lines located at different distances from the cylinder head.




**450 CAD**
**mid-intake**

Similar behavior between the two grids, flow dominated by the incoming air jet



# SI Engines: cold flow



## Full cycle SI: Darmstadt optical engine – validation

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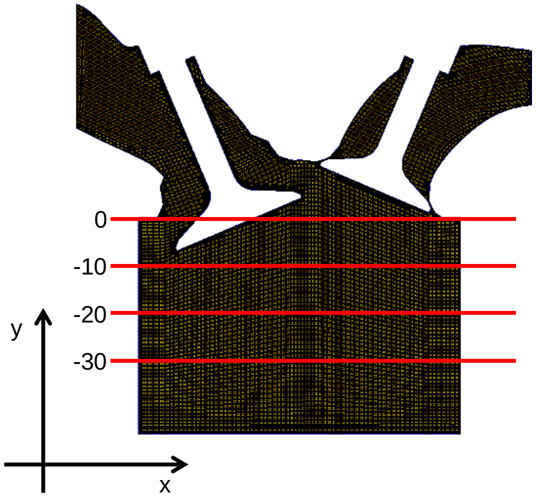


**450 CAD**
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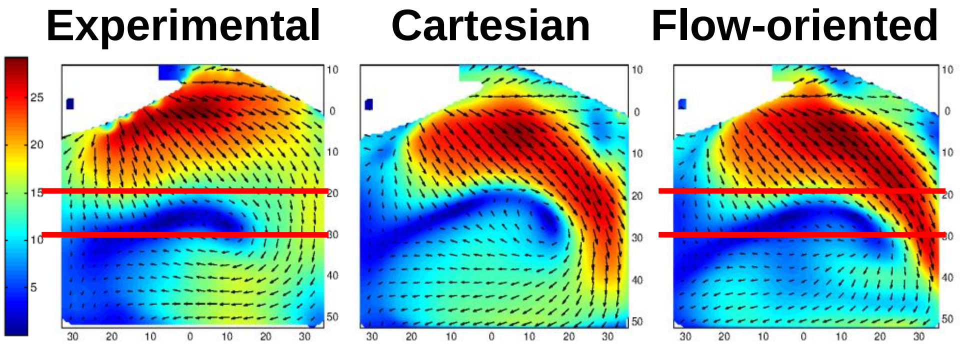


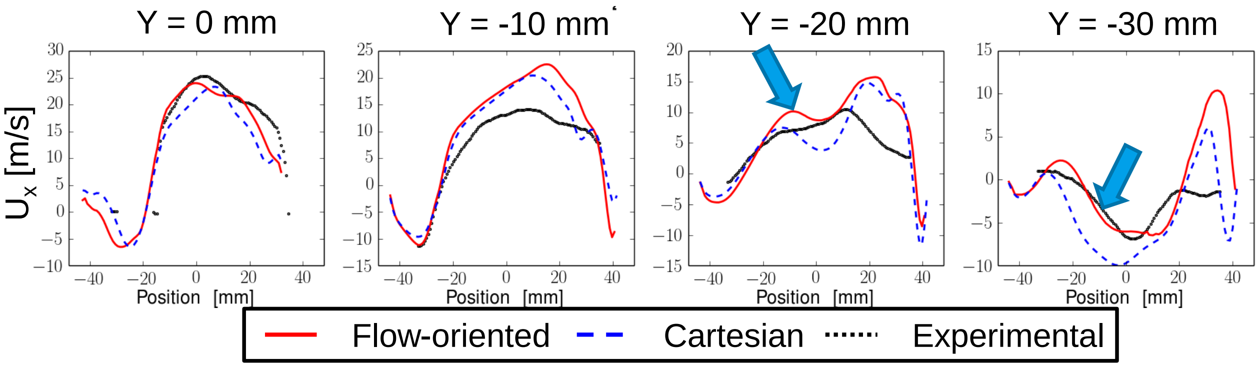

# SI Engines: cold flow

## Full cycle SI: Darmstadt optical engine – validation

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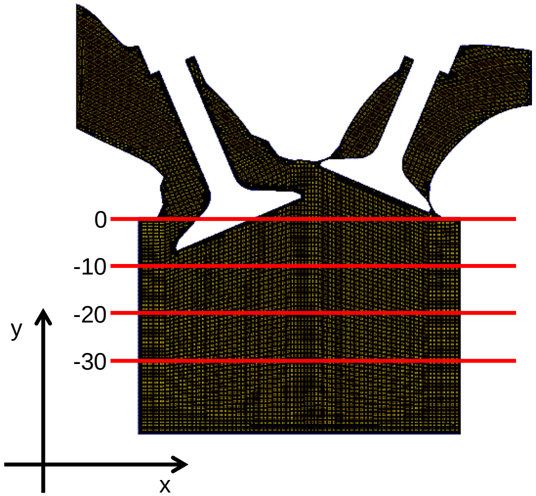
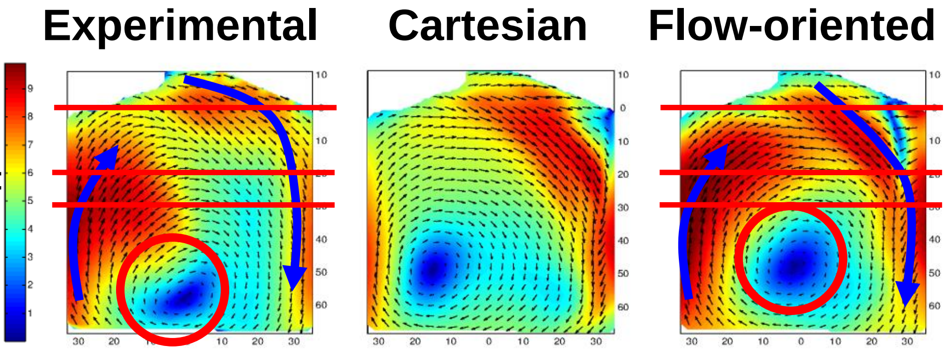
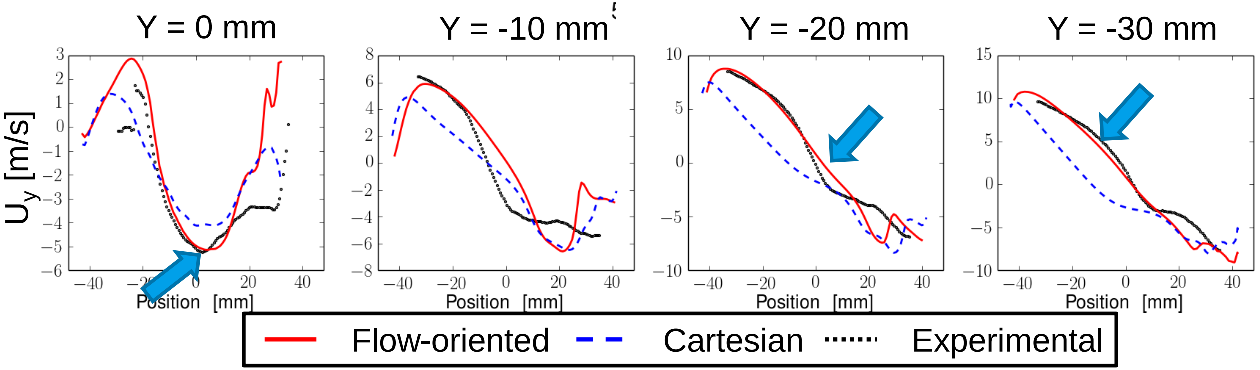



**540 CAD**
**BDC, intake**

Better prediction of the flow oriented grid: Vortex location, distribution of the two main streams

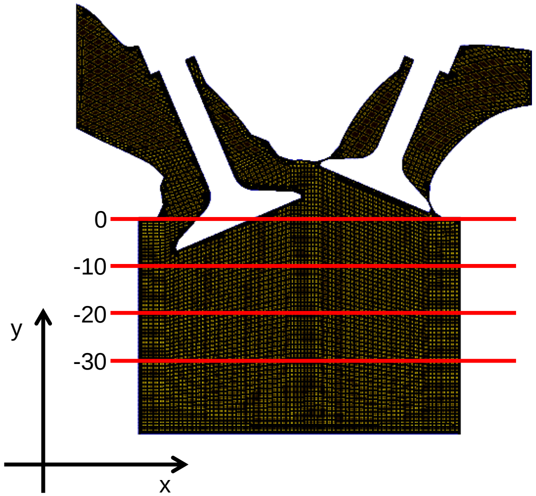


# SI Engines: cold flow

## Full cycle SI: Darmstadt optical engine – validation

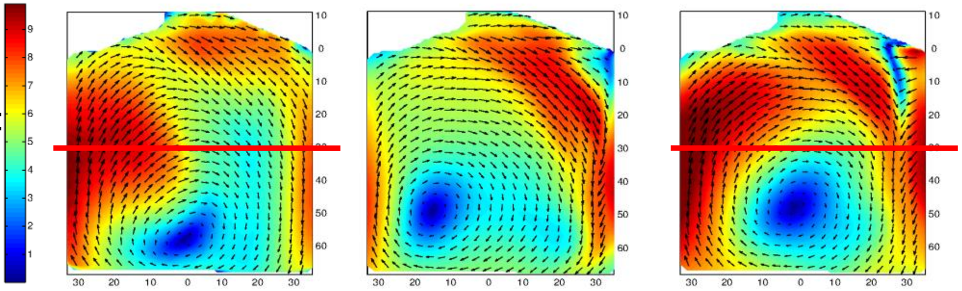
x and y velocity components along four different measurement lines located at different distances from the cylinder head.

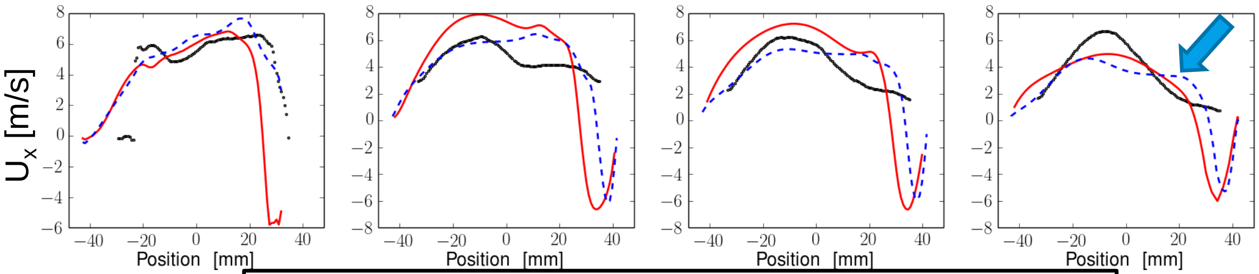



**540 CAD**
**BDC, intake**

Better prediction of the flow oriented grid: Vortex location, distribution of the two main streams

**Experimental** **Cartesian** **Flow-oriented**



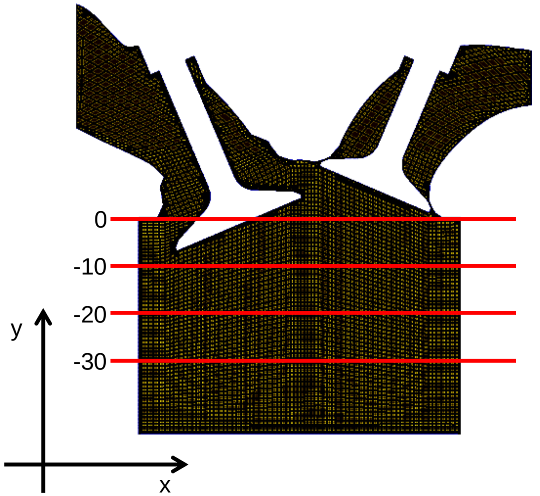



Flow-oriented — Cartesian - - Experimental ·······

# SI Engines: cold flow

## Full cycle SI: Darmstadt optical engine – validation

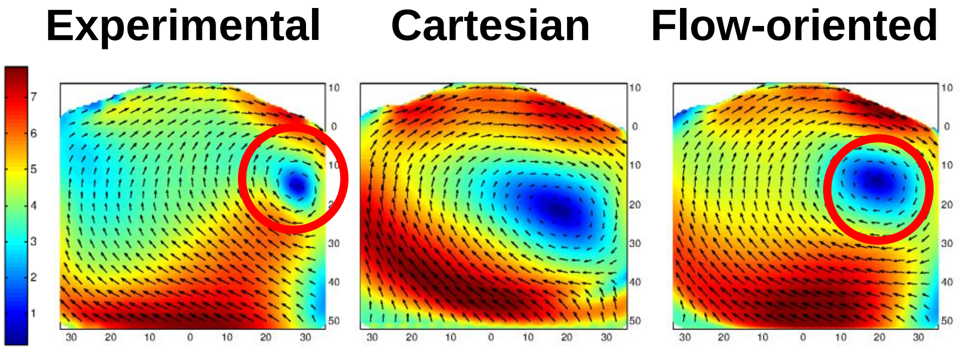
x and y velocity components along four different measurement lines located at different distances from the cylinder head.

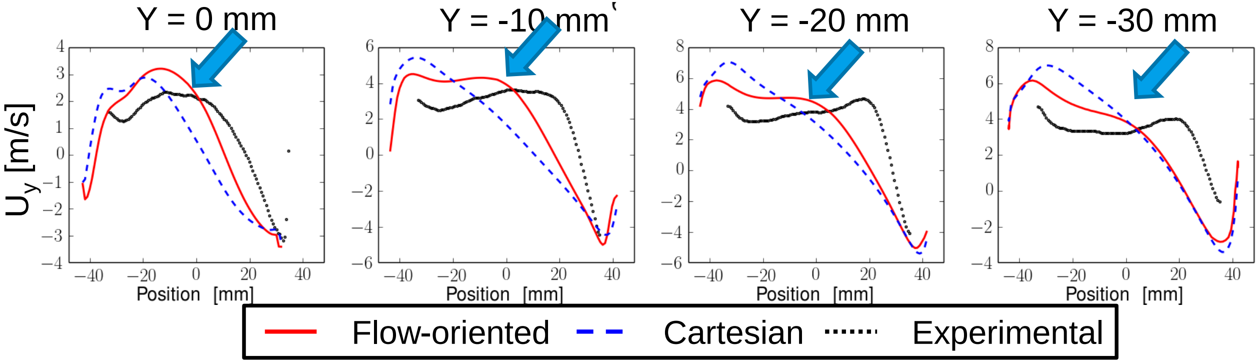



**660 CAD**

**mid-compression**

Flow-oriented grid better describe the tumble vortex structure

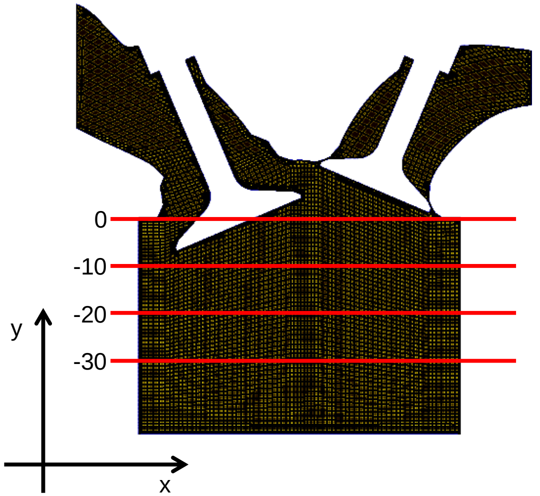


# SI Engines: cold flow

## Full cycle SI: Darmstadt optical engine – validation

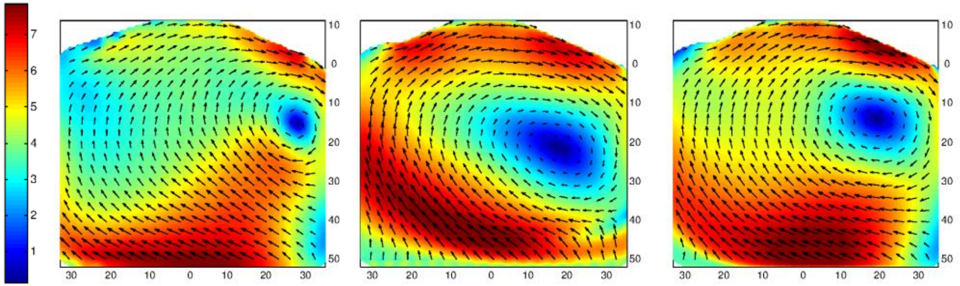
x and y velocity components along four different measurement lines located at different distances from the cylinder head.

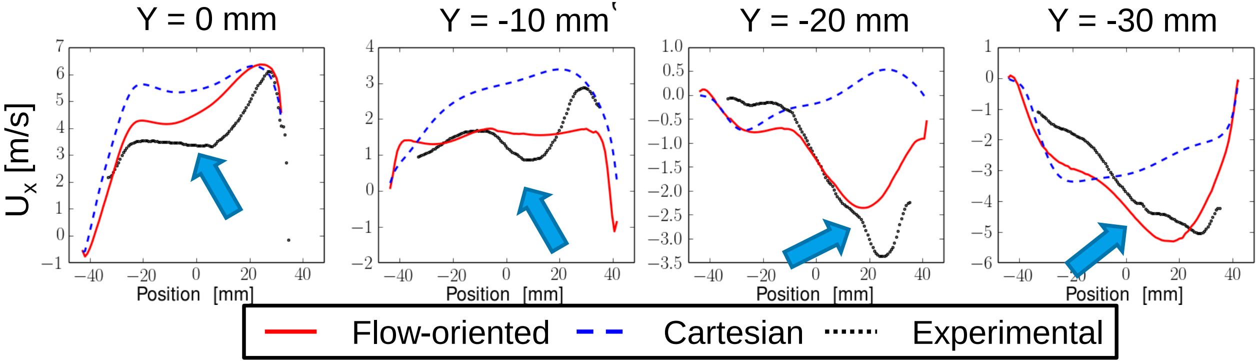



**660 CAD**
**mid-compression**

Flow-oriented grid better describe the tumble vortex structure

**Experimental** **Cartesian** **Flow-oriented**



# SI Engines: GDI fuel-air mixing

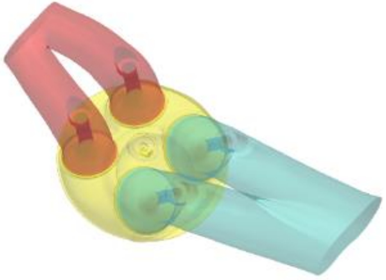
Stratified engine (collaboration with IM-CNR, Ing. Sementa, Ing. Montanaro)

## Optically accessible GDI engine

### Operating points

| | Injection pressure [bar] | SOI [° BTDC] | Charge stratification |
|---|---|---|---|
| **1** | 100 | 60 | **High** |
| **2** | 100 | 110 | **Low** |
| **3** | 60 | 60 | **High** |
| **4** | 60 | 120 | **Low** |

bmep = 7.2 bar, SA = 13 BTDC; $\lambda$ = 1.15 (lean)



# SI Engines: GDI fuel-air mixing

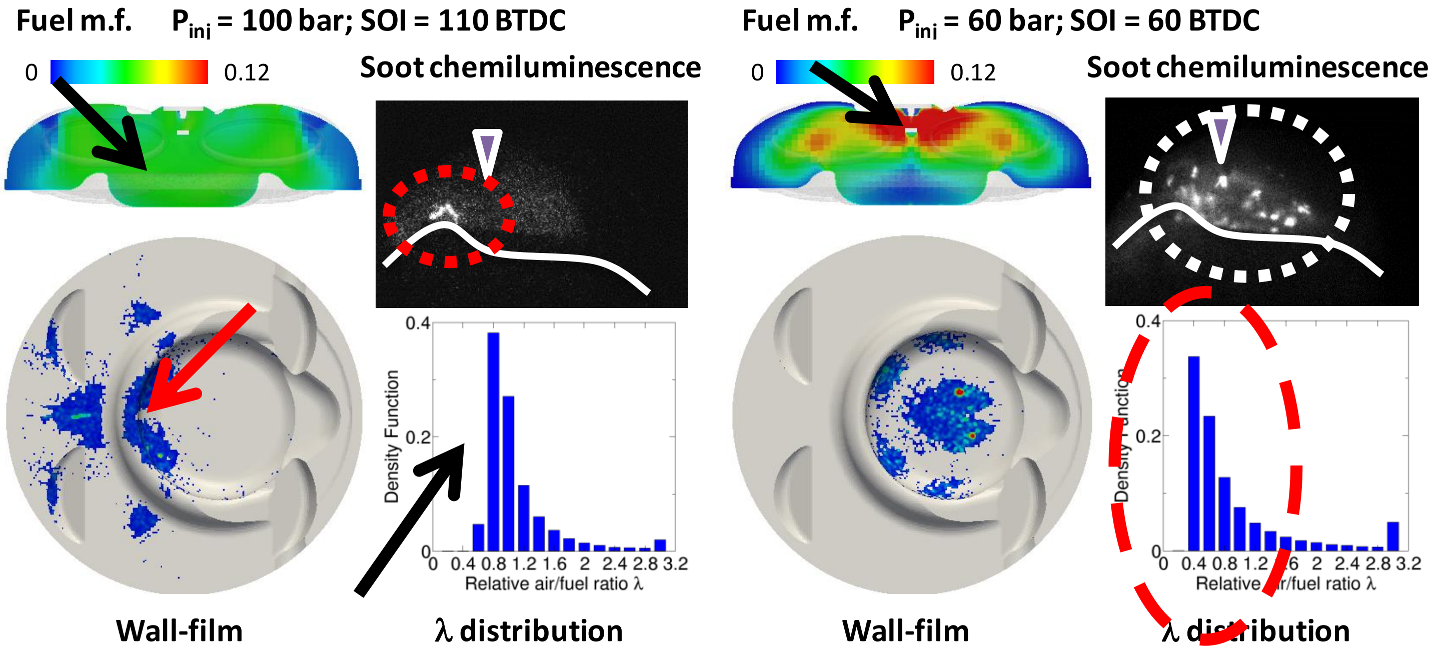
## Stratified engine

### Optically accessible GDI engine: optical/computed data correlation

**Possible sources of soot:**

- **Rich pockets**
- **Wall-film**

**Correlated with optical soot chemiluminescence**



# SI Engines: combustion

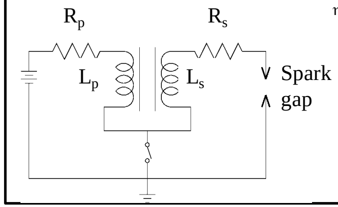
## Modeling

### Comprehensive combustion model

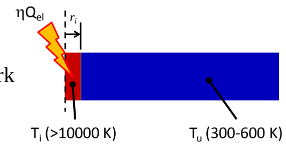
- Detailed description of the flame kernel growth process via Lagrangian approach and suitable sub-models (breakdown, electrical circuit, wrinking)
- Coherent flamelet model for flame propagation in the Eulerian phase (gas)
- Strict coupling between Eulerian and Lagrangian phases

### Sub-models

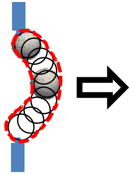
**Secondary circuit energy transfer**




**Breakdown**

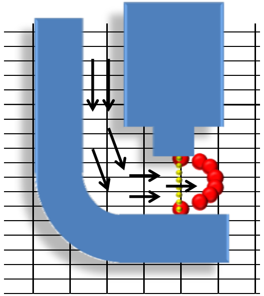



**Flame surface density**

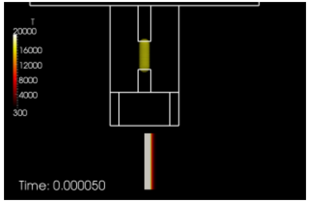


$$\Sigma_{spk} = \frac{\sum_{i=1}^{N_f} \Xi_i \cdot S_i}{V_{cell}}$$

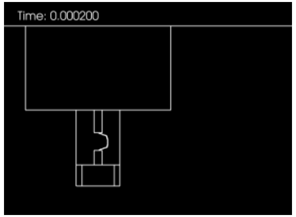
**Lagrangian particles for the spark-channel**

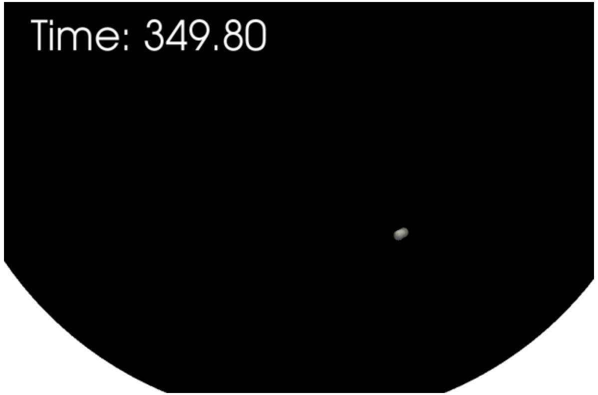


**Mass and energy equations solved for the flame kernel particles**




**Particles convected by the flow, possibility to predict restrike**



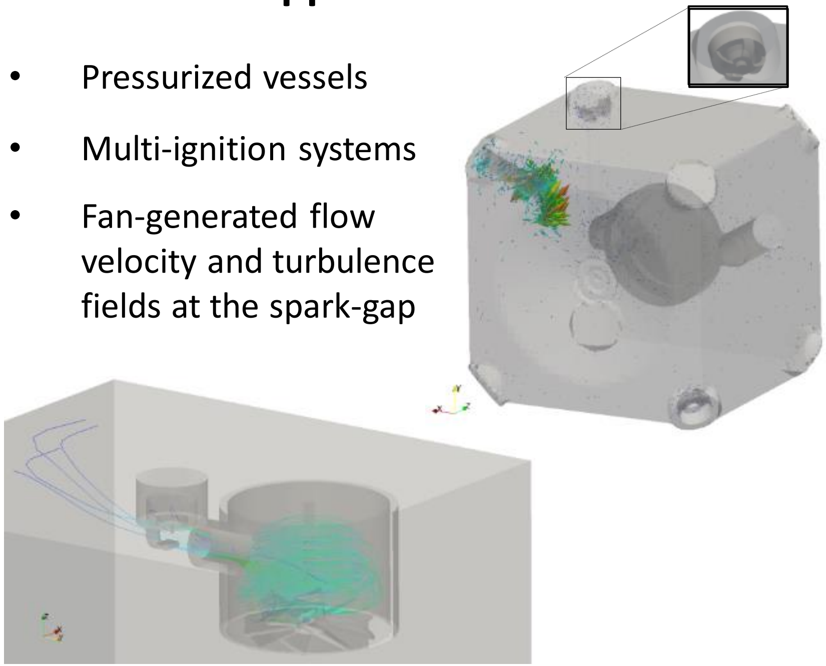

Possibility to predict the effects of local flow, mixture conditions, turbulence, electrical circuit properties (voltage, current). Prediction of misfire also possible.

# SI Engines: combustion

## Assessment and validation

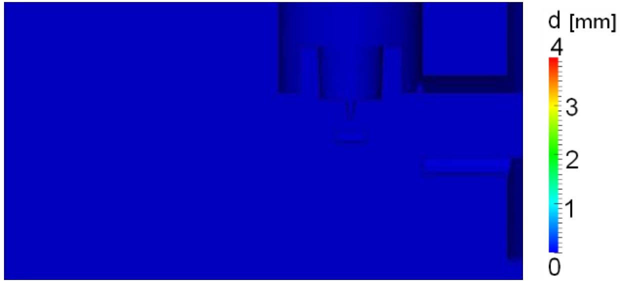
### Applications

- Pressurized vessels
- Multi-ignition systems
- Fan-generated flow velocity and turbulence fields at the spark-gap

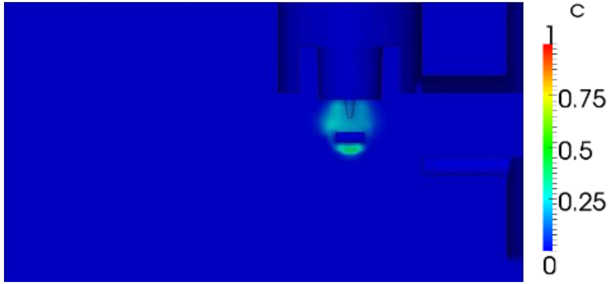


### Results

Initial combustion stage
(Lagrangian – Eulerian coupling)



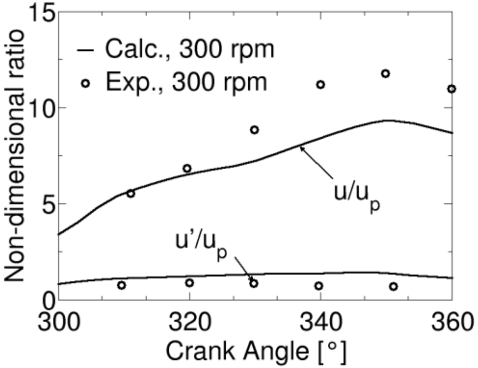

Fully turbulent flame
(Eulerian model only)

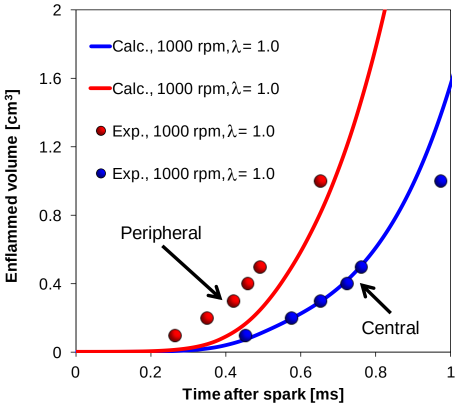


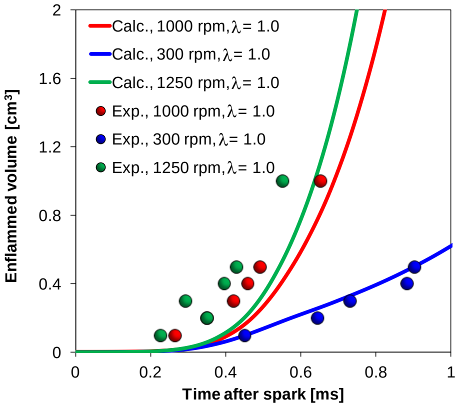
# SI Engines: combustion



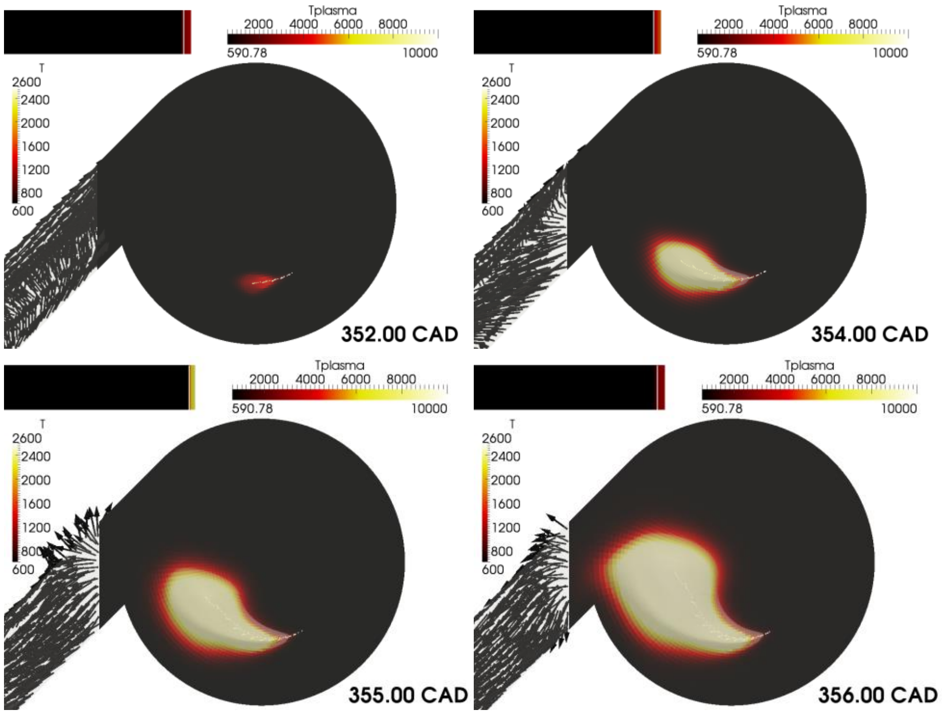
## Experimental validation: Herweg and Maly Engine




**Flow field, flame propagation and plasma temperature details**




**This work is part of Lorenzo Sforza PhD project**

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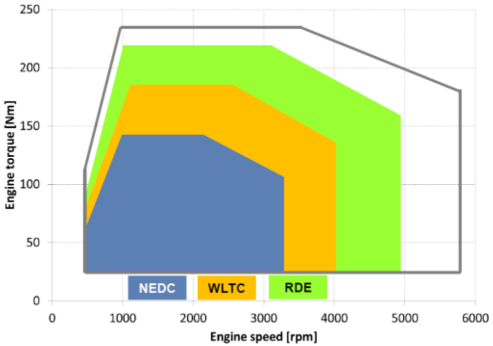
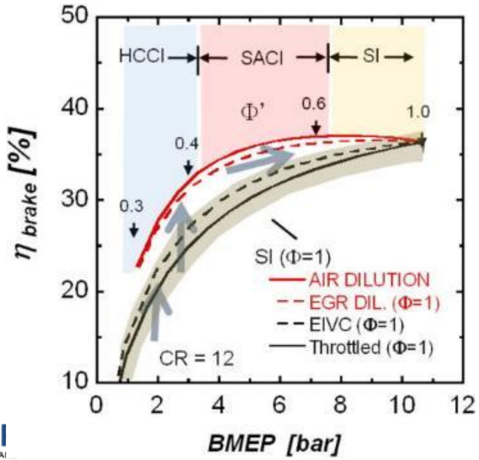
# Conclusions

## CFD modeling of in-cylinder phenomena at Polimi with OpenFOAM

- Detailed models continuously validated and improved:
  - Fundamental studies
  - Applied research
- Consolidated methodologies, currently applied in the context of industrial collaborations
- **…but there is still a lot to do!**

Thanks for your attention!