POLITECNICO
MILANO 1863

The role of CFD for the design of hydrogen propulsion systems: developments and applications @PoliMi

G. Montenegro

IDROGENO E TECNOLOGIE PER LA GENERAZIONE ENERGETICA E LA PROPULSIONE NEI TRASPORTI GREEN

Genova, 25 Gennaio 2024

Outline

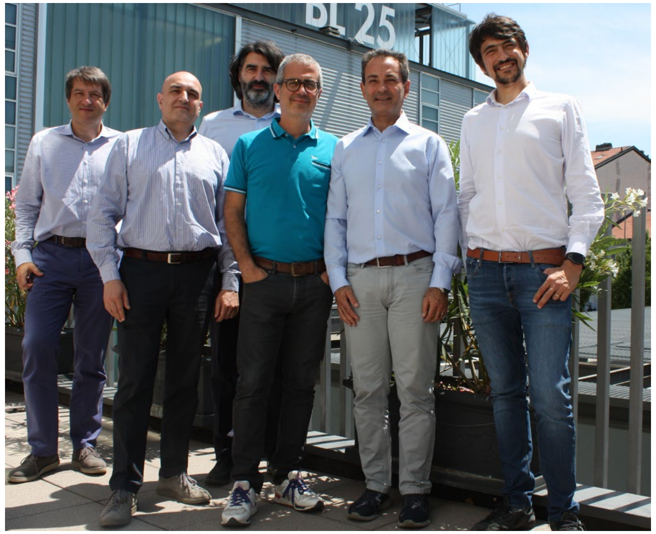
1. ICEGroup
2. 1D and 3D tools developed @PoliMi
3. Applications of CFD in the field of H2 for propulsion systems
    - System modeling (engine/pumping systems)
    - Injection
    - Combustion
    - Aftertreatment
    - Fuel cells

ICE Group @ Polimi Energy Department

ICE Group

- Fundamental and applied research on thermal and fluid-dynamics modeling of energy conversion components
  - IC engines
  - Fluid Machines
  - Electrification
  - Fuel-cells
- 5 professors, 2 assistant professors, 6 PhD students;
- 2-3 visiting Phd students from Europe;
- More than 250 publications in peer-review journals and international conferences;
- Co-founders of the Innovative Spin-off company Sursum-Mi

Sursum-Mi
modeling the future



Industrial collaborations

Ferrari, snam, Eni, LAMBORGHINI, engys, CORNAGLIA MOVING FROM TOMORROW, WIN GD, WÄRTSILÄ

Funded project (national)

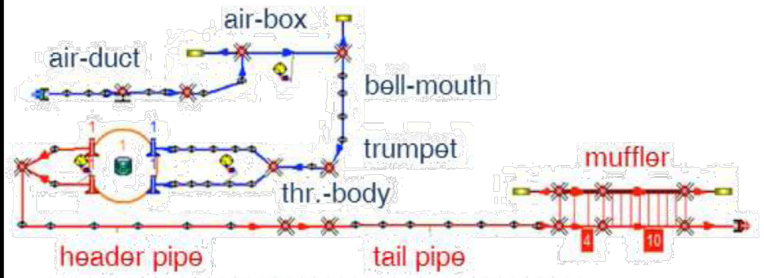
- AMAZING (PoliMI - Stems)
- Flex-Gen (STEMS - PoliMi-PoliTo)
- DHyCE-HD (PoliBa - PoliMi)

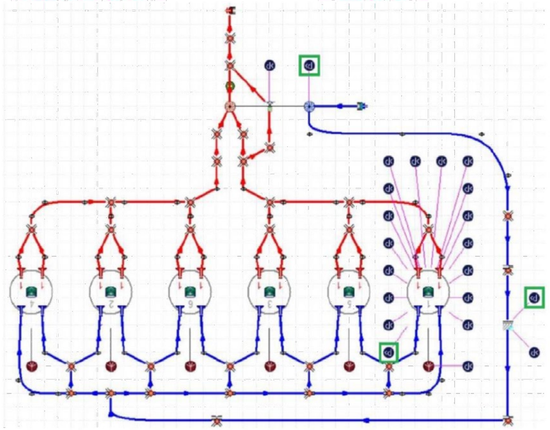
Research activities – numerical modeling

Numerical modeling of IC engines, fluid machines and power systems

Sursum-Mi
modeling the future

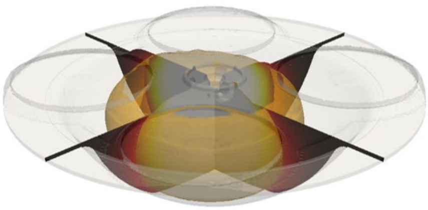
Gasdyn

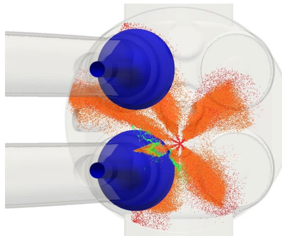


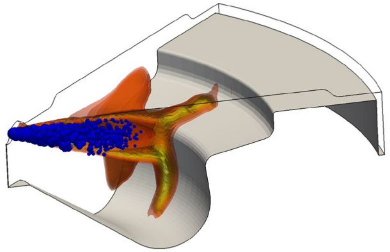


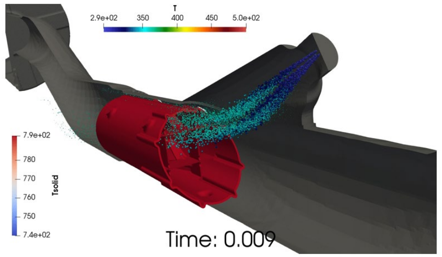
LibICE

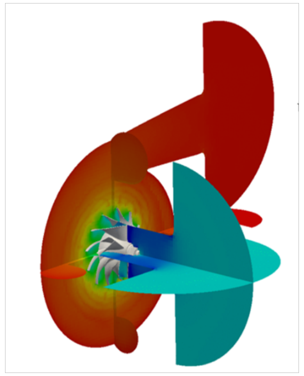
OpenFOAM®

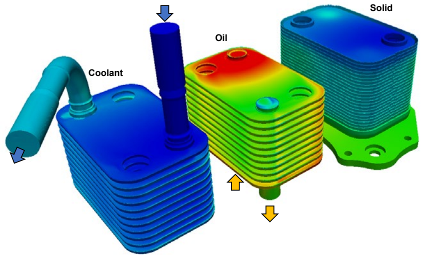








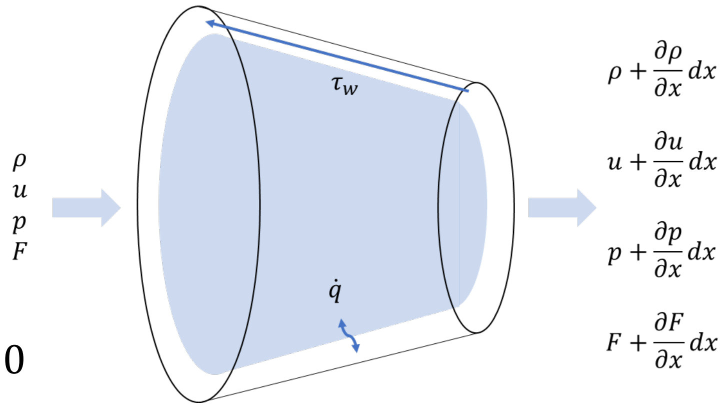




1D simulation methodology

- **One-dimensional, unsteady, compressible**, reacting flow with area variations, friction and heat transfer with the walls

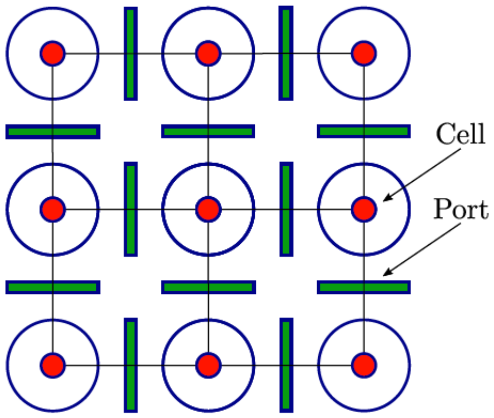
$$
\begin{cases}
\dfrac{\partial(\rho F)}{\partial t} + \dfrac{\partial(\rho u F)}{\partial x} = 0 \\
\dfrac{\partial(\rho u F)}{\partial t} + \dfrac{\partial(\rho u^2 + p)F}{\partial x} - p\dfrac{dF}{dx} + \rho F G = 0 \\
\dfrac{\partial(\rho e_0 F)}{\partial t} + \dfrac{\partial(\rho h_0 u F)}{\partial x} - (\dot{q}\rho + \Delta H_{react})F = 0
\end{cases}
$$



$$
\boldsymbol{W}(x,t) = \begin{bmatrix} \rho F \\ \rho u F \\ \rho e_0 F \\ \rho \boldsymbol{Y} F \end{bmatrix} ; \; \boldsymbol{F}(\boldsymbol{W}) = \begin{bmatrix} \rho u F \\ pF + \rho u^2 F \\ \rho u h_0 F \\ \rho u \boldsymbol{Y} F \end{bmatrix} ;
$$

$$
\boldsymbol{B}(\boldsymbol{W}) = \begin{bmatrix} 0 \\ -p\frac{dF}{dx} \\ 0 \\ 0 \end{bmatrix} ; \boldsymbol{C}(\boldsymbol{W}) = \begin{bmatrix} 0 \\ \rho G F \\ -(\rho\dot{q} + \Delta H_{react})F \\ \rho \dot{\boldsymbol{Y}} F \end{bmatrix} ; \boldsymbol{Y} = \begin{bmatrix} Y_1 \\ \vdots \\ Y_{N-1} \end{bmatrix}
$$

- Finite volume method, explicit **staggered space-time**

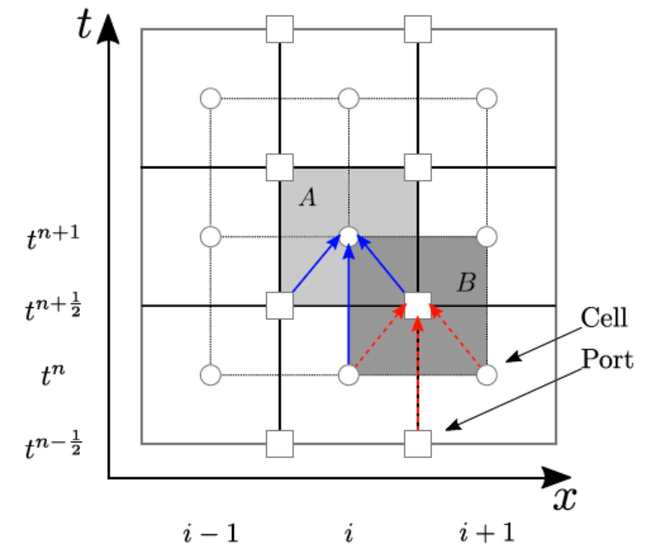


$$
\rho_{cell}^{t+1} = \rho_{cell}^{t} + \frac{\Delta t}{V_{cell}} \sum_{p}^{Nports} (\rho v A)_p^{t+1/2}
$$

$$
(\rho e_0)_{cell}^{t+1} = (\rho e_0)_{cell}^{t} + \frac{\Delta t}{V_{cell}} \sum_{p}^{Nports} (\rho v h_0 A)_p^{t+1/2} + S_e
$$

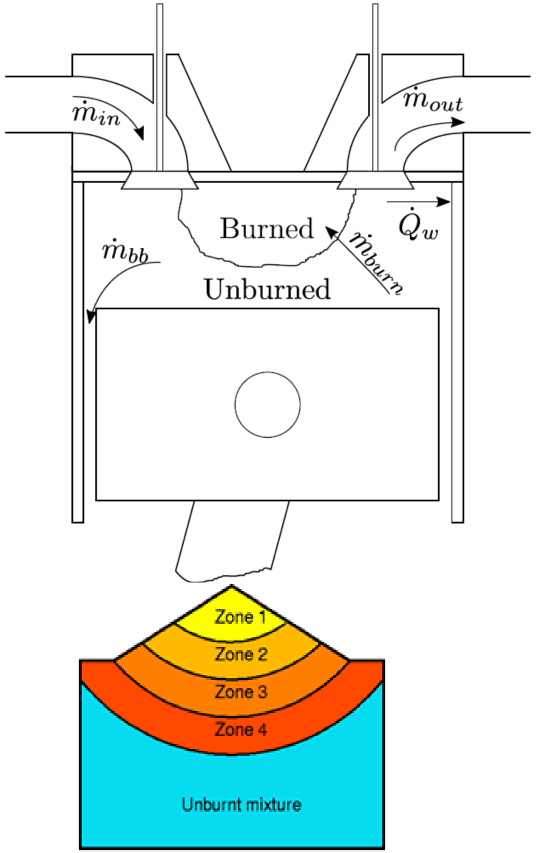
$$
(\rho Y_i)_{cell}^{t+1} = (\rho Y_i)_{cell}^{t} + \frac{\Delta t}{V_{cell}} \sum_{p}^{Nports} (\rho v Y_i A)_p^{t+1/2} + S_{Y_i}
$$

$$
(\rho v A)_{port}^{t+1/2} = (\rho v A)_{port}^{t-1/2} + \frac{\Delta t}{\Delta L_{cell}} \sum_{c}^{Ncells} [(p + \rho v^2)]_c^t \cdot A_p + S_M
$$



1D simulation methodology: Combustion prediction

- The in-cylinder phenomena and combustion are modelled by means of **multizone** approach solving the **energy and mass balance** of each sub zone
- Zimont's **correlation** is used to compute **turbulent flame speed** ⇒ $S_t = u'^{3/4} L_i^{1/4} S_l^{1/2} k_u^{-1/4}$

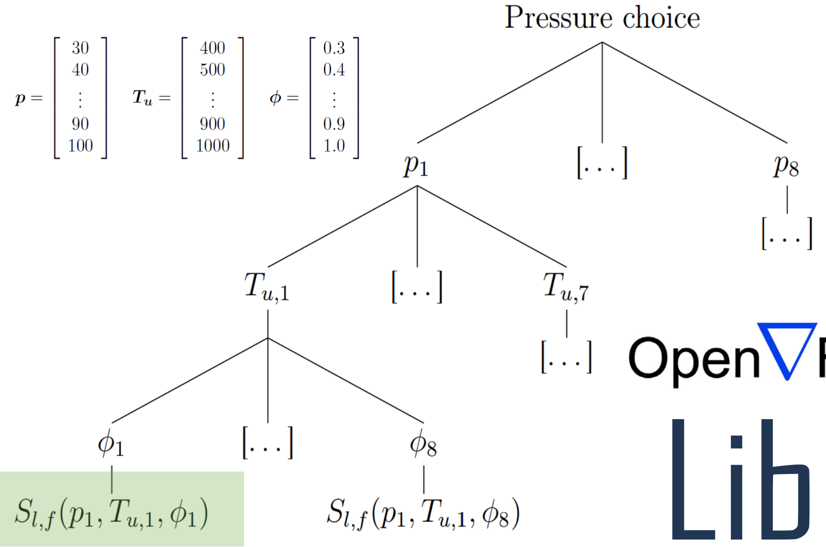


Laminar flame speed evaluation

Old method ⇒ Empirical correlation ⇒ **Strict** validity limits

New method ⇒ Tabulated Kinetic approach ⇒ **Wider** limit ranges

(3D matrix with around 448 values)



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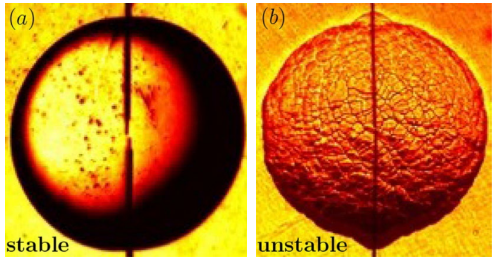
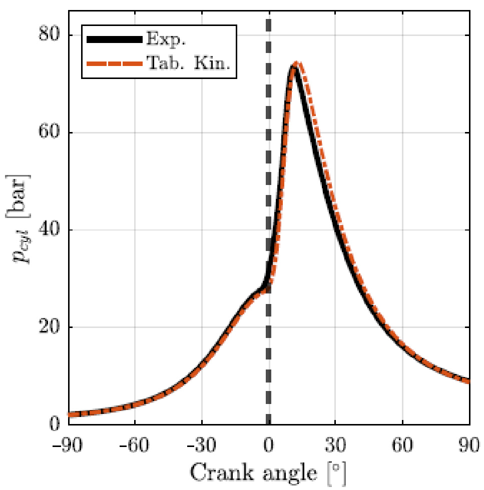
Empirical correction factor for instabilities

$$S_{l,c} = S_l \cdot \left(1 + \left(\left(\frac{S_{l,c}}{S_l}\right)_{ref} - 1\right) \cdot \left(\frac{\phi}{\phi_{ref}}\right)^{\gamma_\phi} \cdot \left(\frac{T_u}{T_{u,ref}}\right)^{\gamma_{T_u}} \cdot \left(\frac{p}{p_{ref}}\right)^{\gamma_p}\right)$$

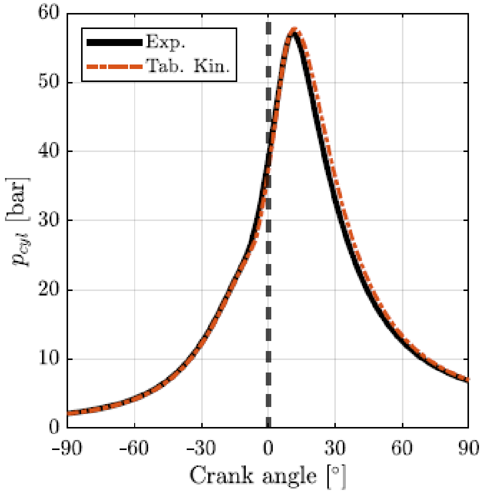
Courtesy of X. Wen, T. Zirwes, A. Scholtissek et al., Flame structure analysis and composition space modeling of thermodiffusively unstable premixed hydrogen flame, https://doi.org/10.1016/j.combustflame.2021.111808



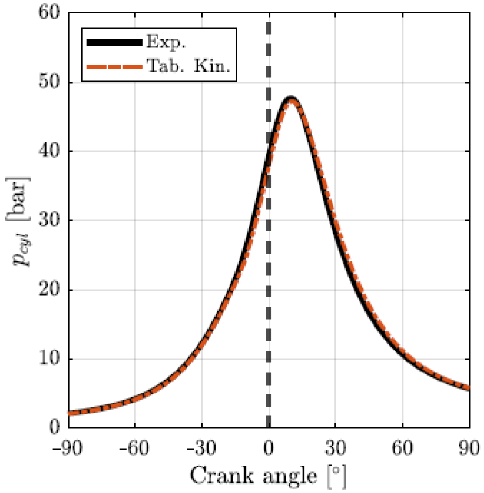
Validation: Single cylinder experimental comparison



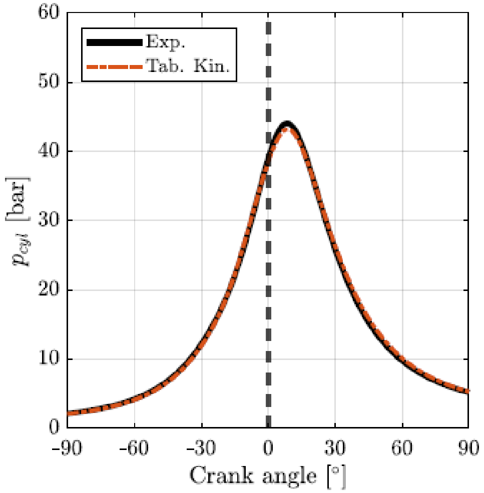
(a) $\lambda = 1.0$



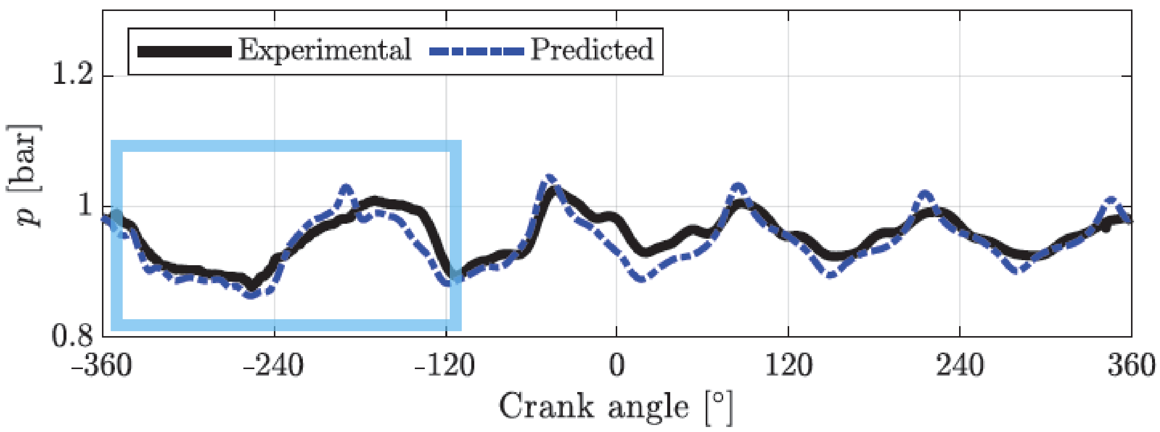
(b) $\lambda = 1.74$



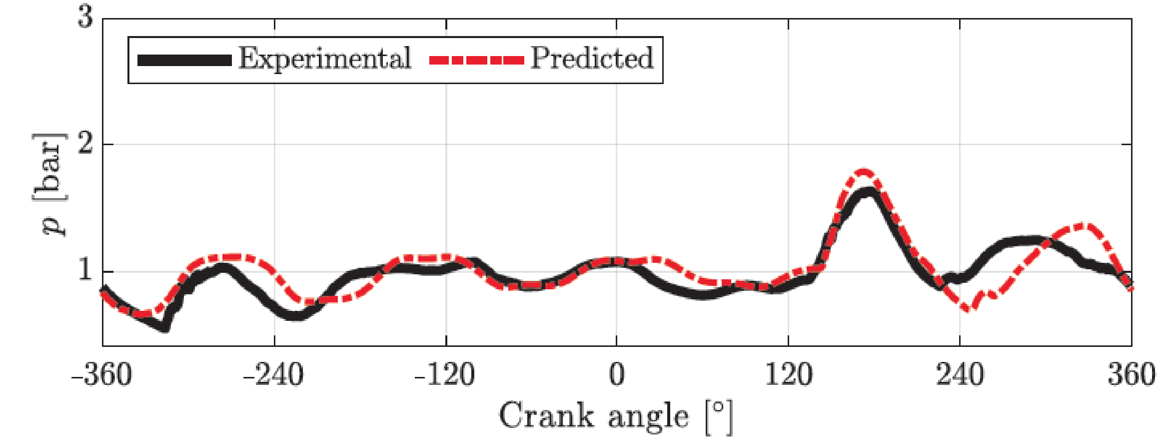
(c) $\lambda = 2.45$



(d) $\lambda = 2.96$



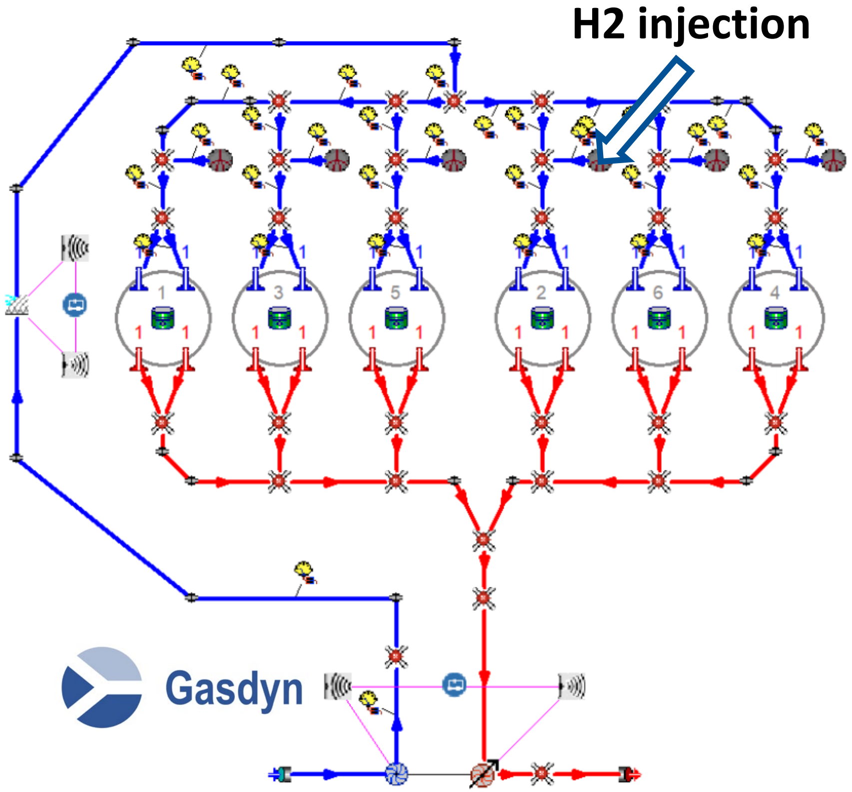
(a) Intake; $\lambda = 1.0$

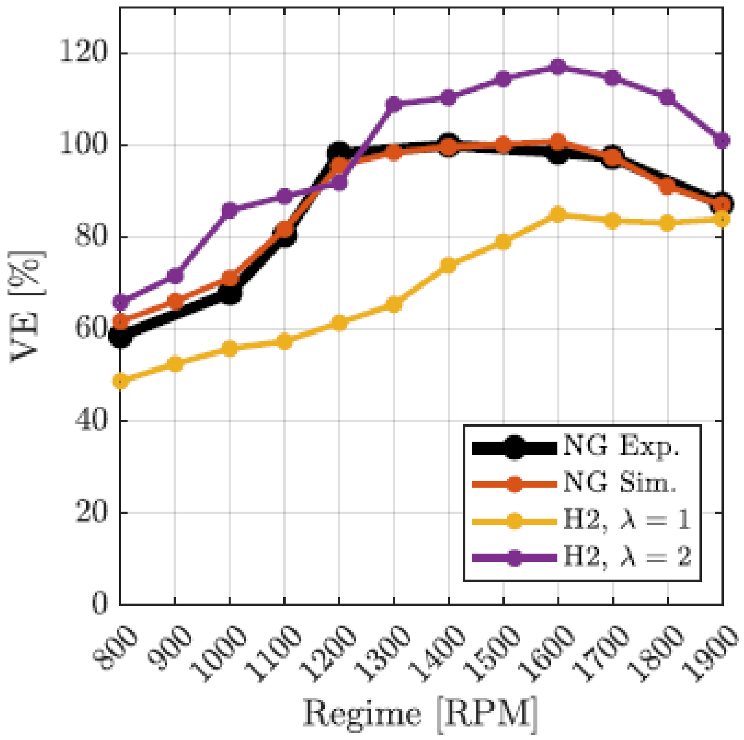


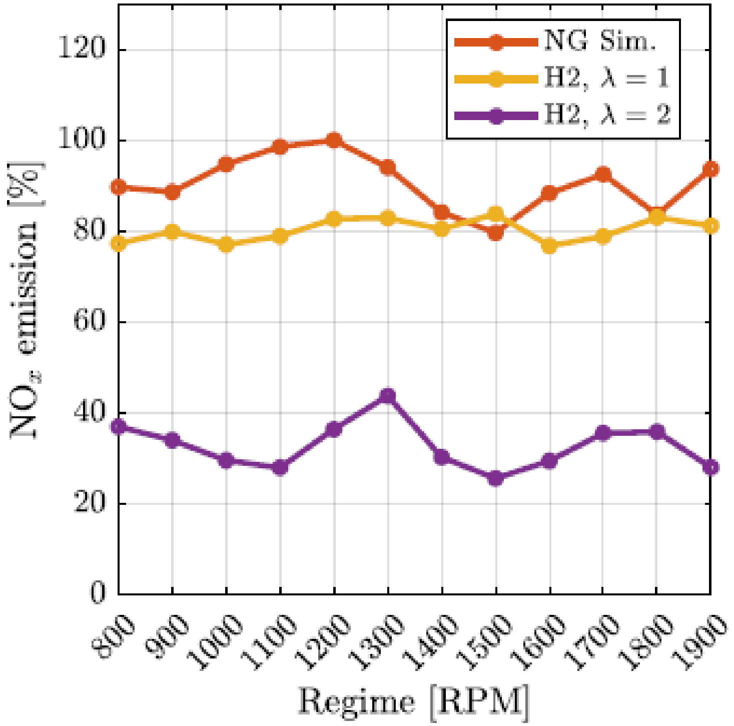
(b) Exhaust; $\lambda = 1.0$

Engine conversion from NG to Hydrogen

- Natural gas fuelled **heavy duty** in-line 6 cylinder featuring a **variable geometry turbine**
- λ =1 and λ =2 feeding conditions have been considered

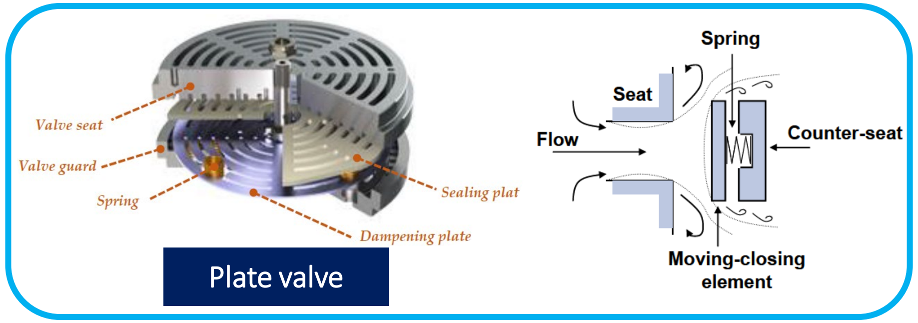




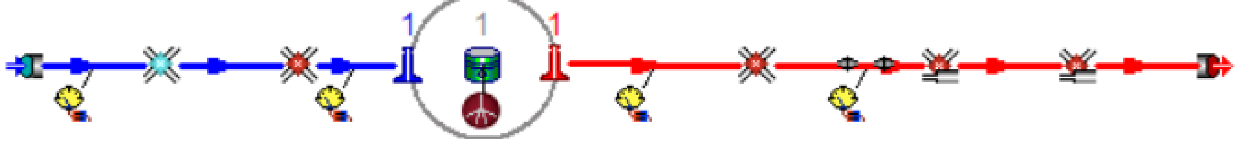


1D Gasdyn model: H2 compression station

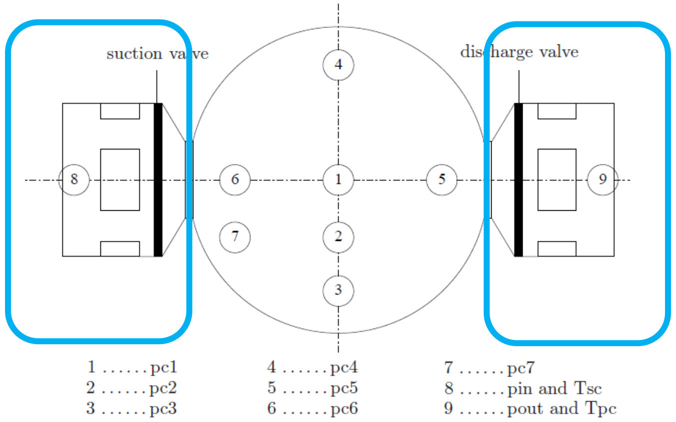
Test case: *Burckhardt compressor 2K90-1A*



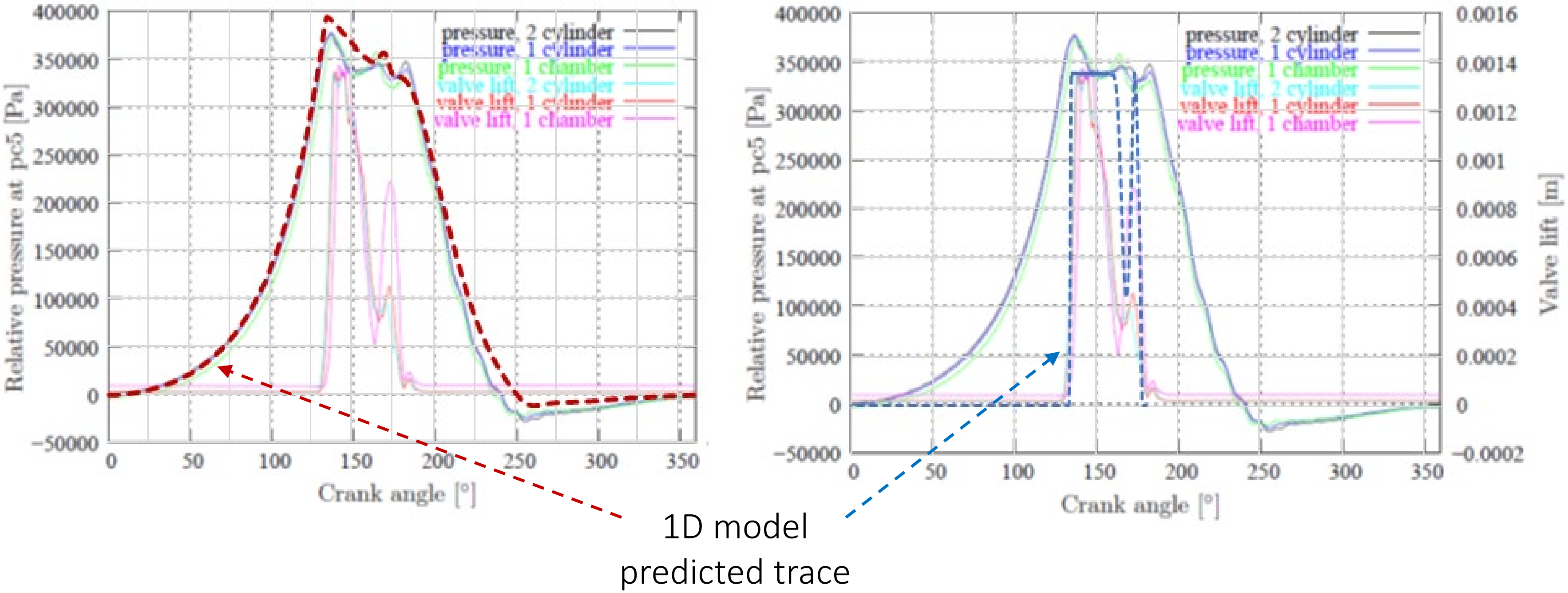
1D Gasdyn model



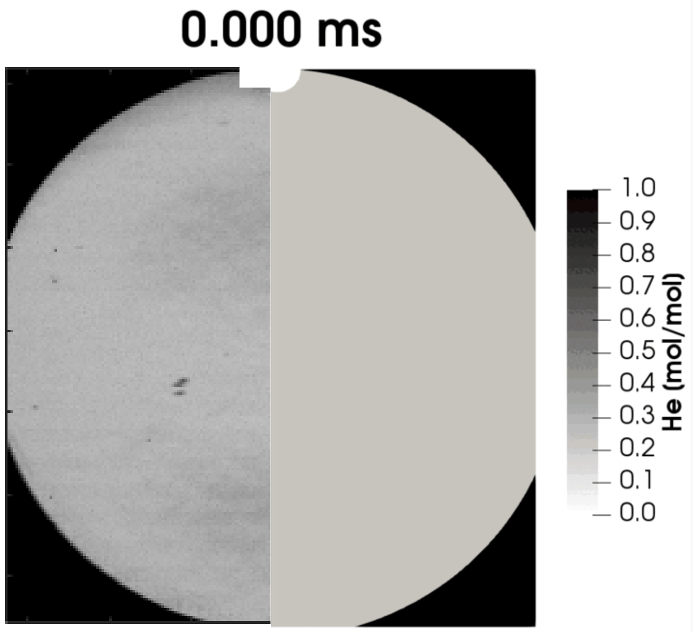
Comparison of relative pressure at pc5 and valve lift at different times t_a, t_b and t_c. Case: p_{out} = 3 bar, c_s =48N/mm , $x_{v,max}$ = 1.35 mm.

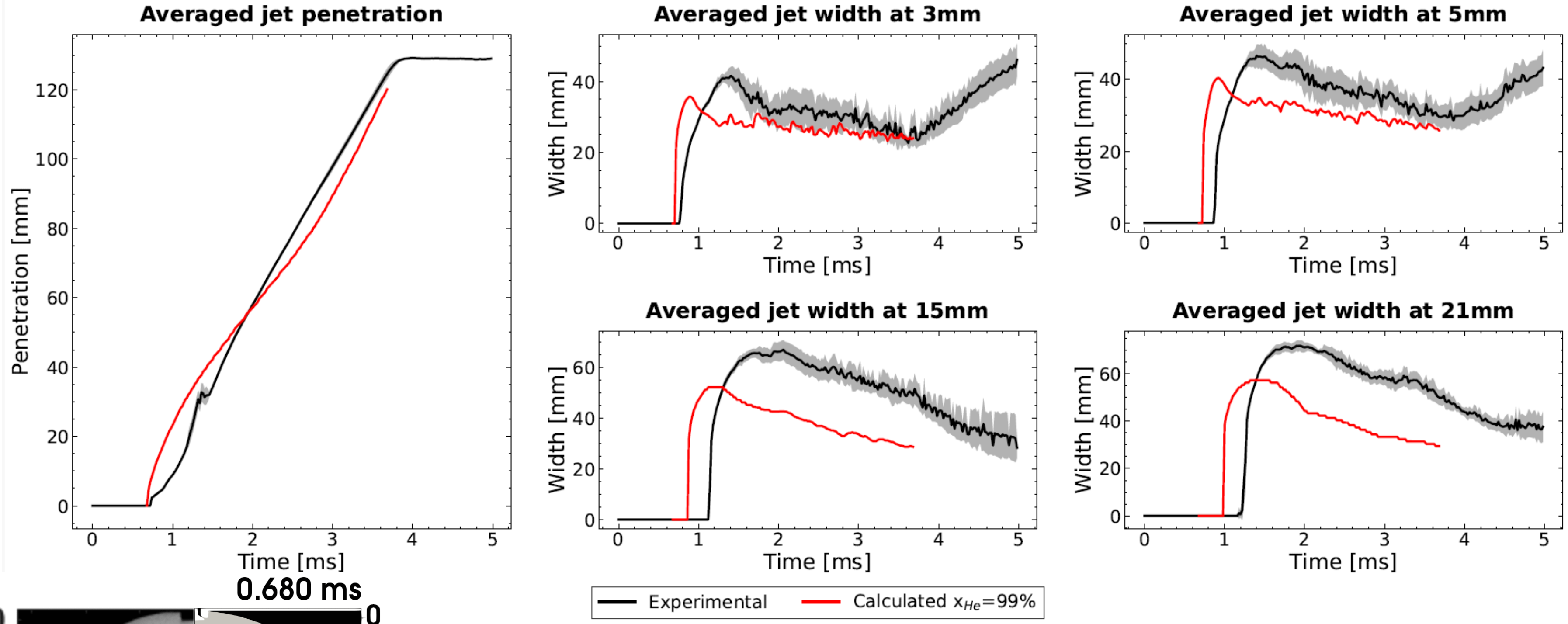


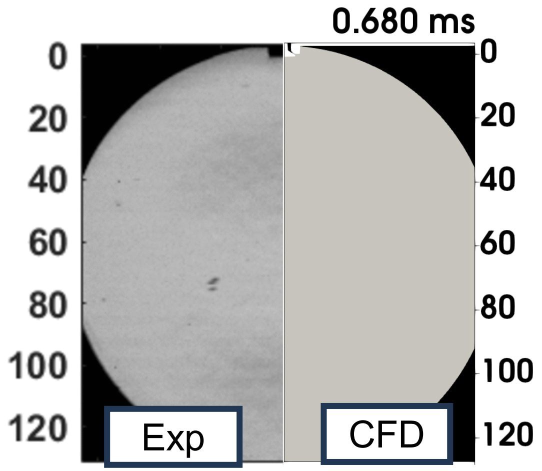
Location of the sensors inside the cylinder 1, the suction and the discharge valve retainer.

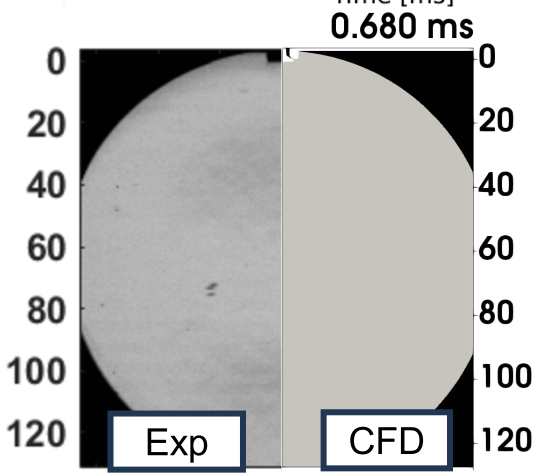


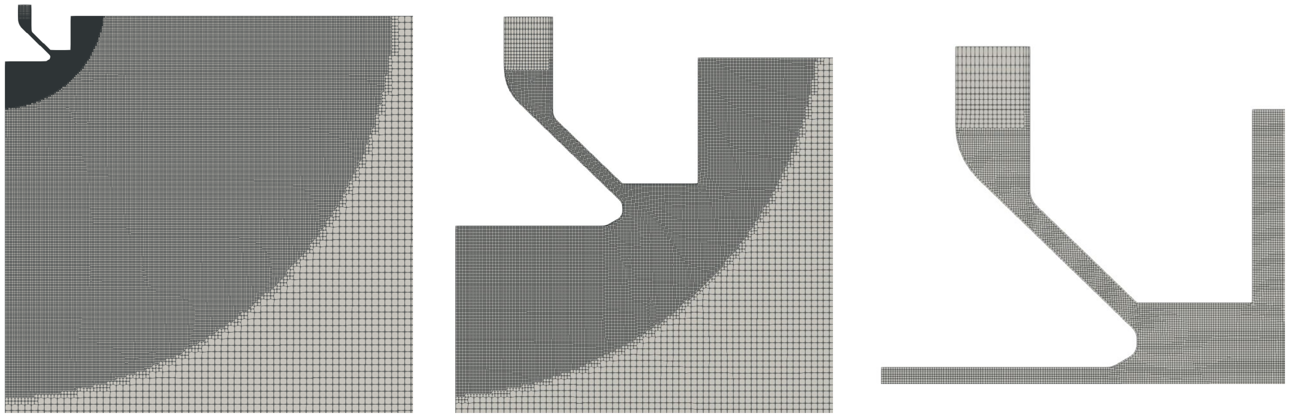
Modeling the H2 injection phase





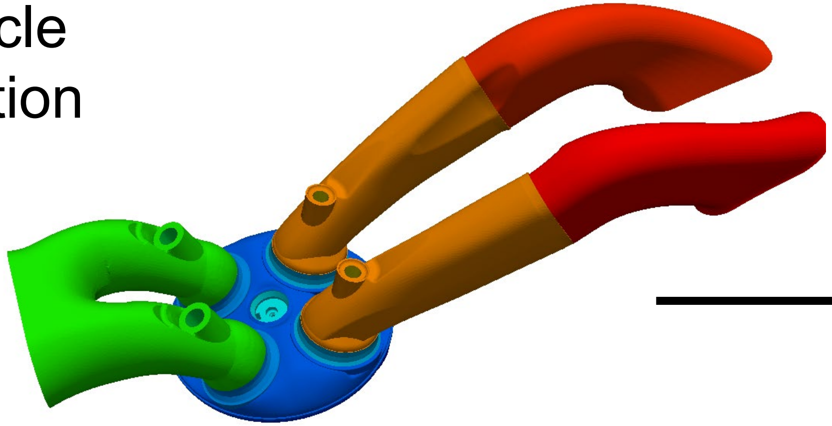


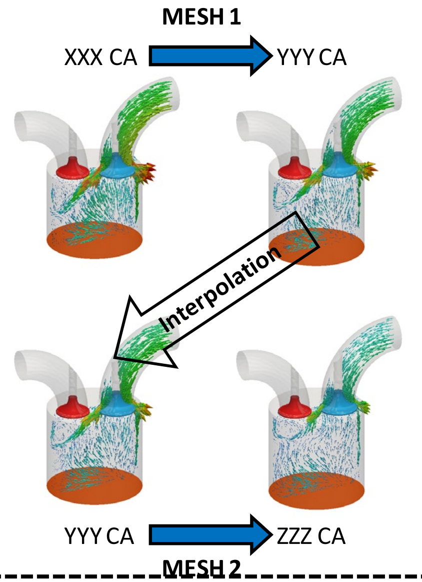


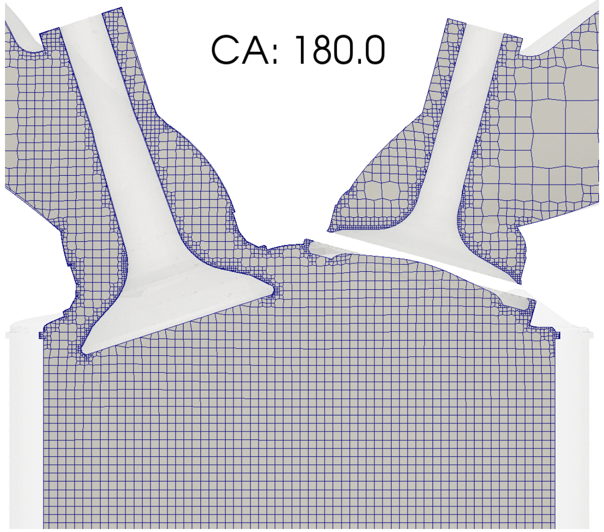


Lib-ICE : mesh management

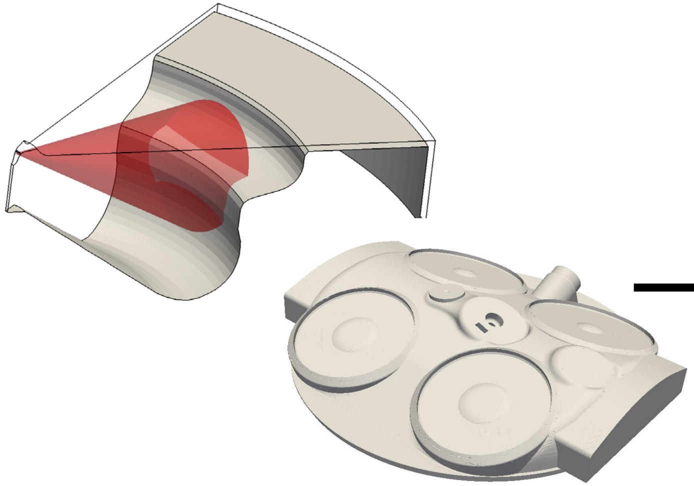
Full-cycle simulation

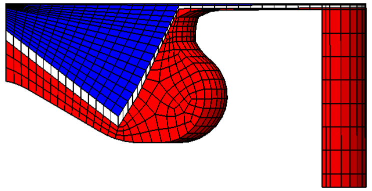






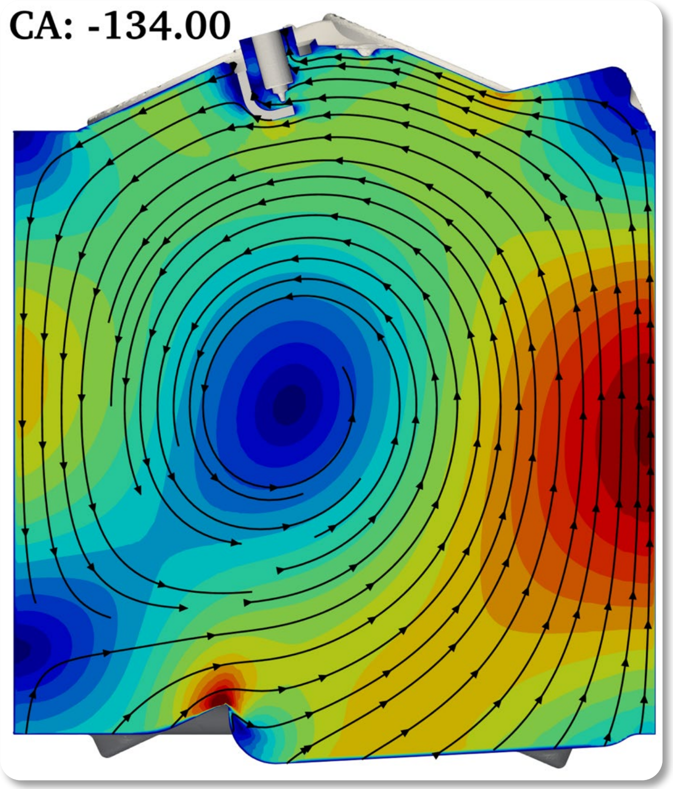
Power-cycle simulation



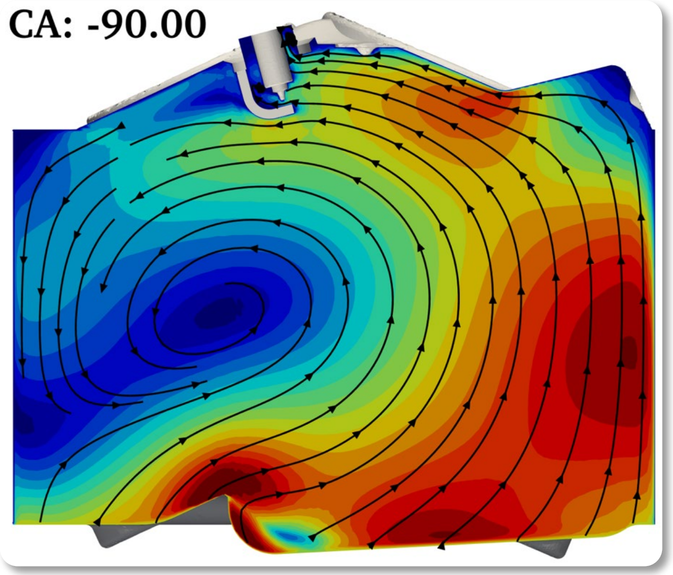


Lucchini, T., Della Torre, et al., *Automatic Mesh Generation for CFD Simulations of Direct-Injection Engines* (2015) **SAE Technical Papers**

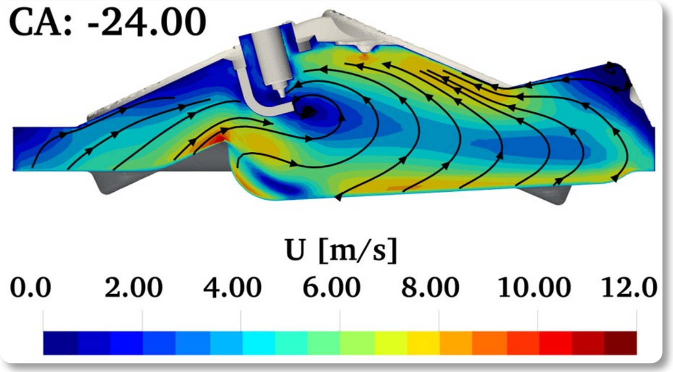
3D-CFD: Compression Stroke

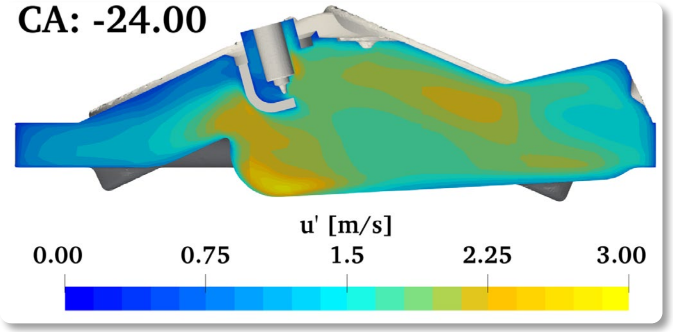


Tumble motion initialized @IVC according to **validated methodology**



Compression stage simulation





Generation of **flow velocity** and **turbulence fields** @SA

Combustion model

- **Spark-ignition combustion**
  - Flame area evolution (FAE) model to predict the **reaction rate**:

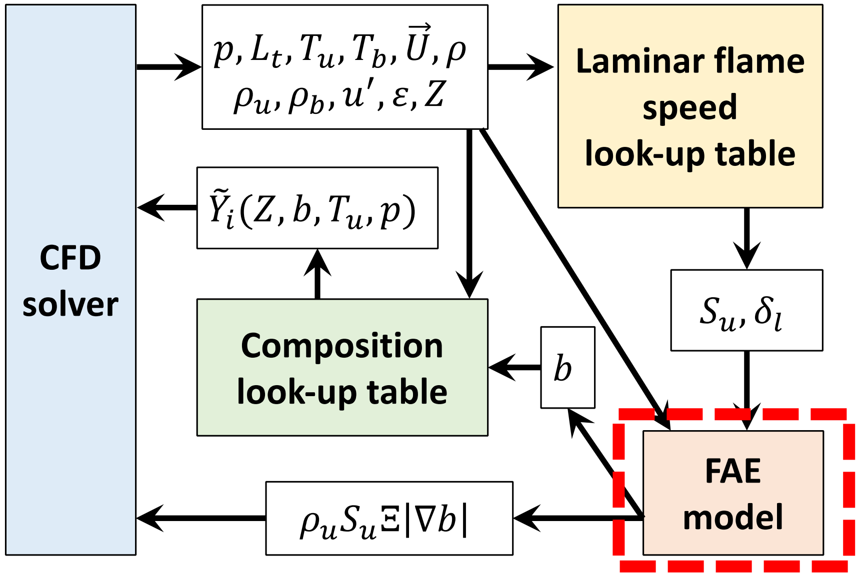
$$\frac{\partial \rho \tilde{b}}{\partial t} + \nabla \cdot (\rho \tilde{\boldsymbol{U}} \tilde{b}) + \nabla \cdot (\mu_t \nabla \tilde{b}) = \rho_u \tilde{S}_u \tilde{\Xi} |\nabla \tilde{b}| + \dot{\omega}_{ign}$$

Turbulent flame propagation

Deposition model

$$\Xi = \frac{S_t}{S_u} = f(\Xi^*_{eq}) \qquad \Xi^*_{eq} = 1 - \frac{a_4 b_3^2}{2 b_1} \frac{L_t}{\delta_l} + \left[\left(\frac{a_4 b_3^2}{2 b_1} \frac{L_t}{\delta_l} \right)^2 + a_4 b_3^2 \frac{u'}{S_u} \frac{L_t}{\delta_l} \right]^{1/2}$$

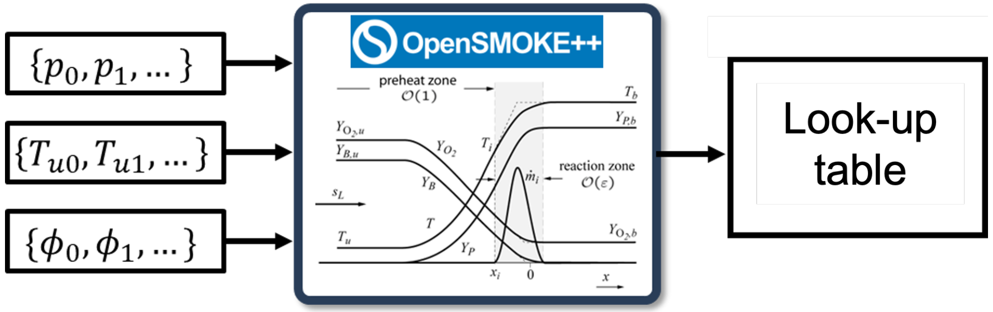
$$Y_i = b\, Y_{u,i} + (1 - b)\, Y_{b,i}$$



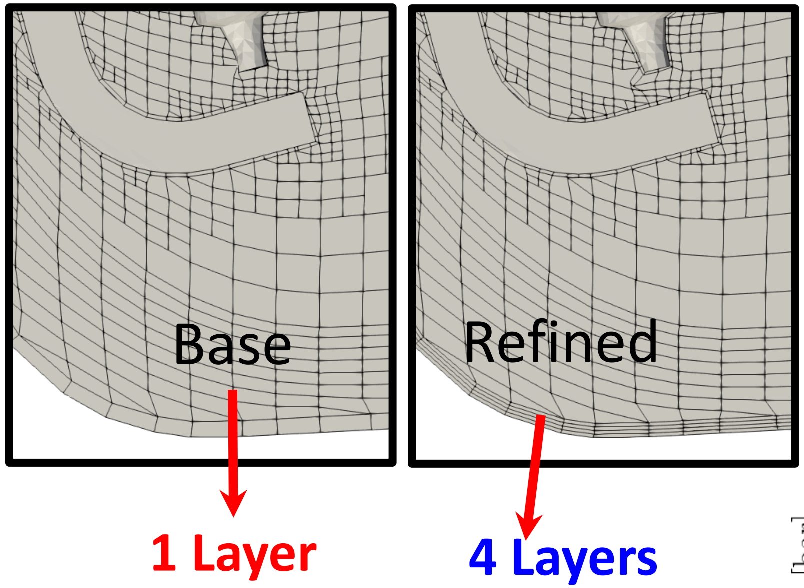
- **Tabulated kinetics** generated with Kéromnès mechanism

- **Laminar flame speed S_u**

$$S_u = C_0\, S_{u0} \qquad C_0 = 1 + \left(\frac{S_u}{S_{u0}} \bigg|_r - 1 \right) \left(\frac{\phi}{\phi_r} \right)^{\gamma_\phi} \left(\frac{T_u}{T_{u,r}} \right)^{\gamma_{T_u}} \left(\frac{p}{p_r} \right)^{\gamma_p}$$



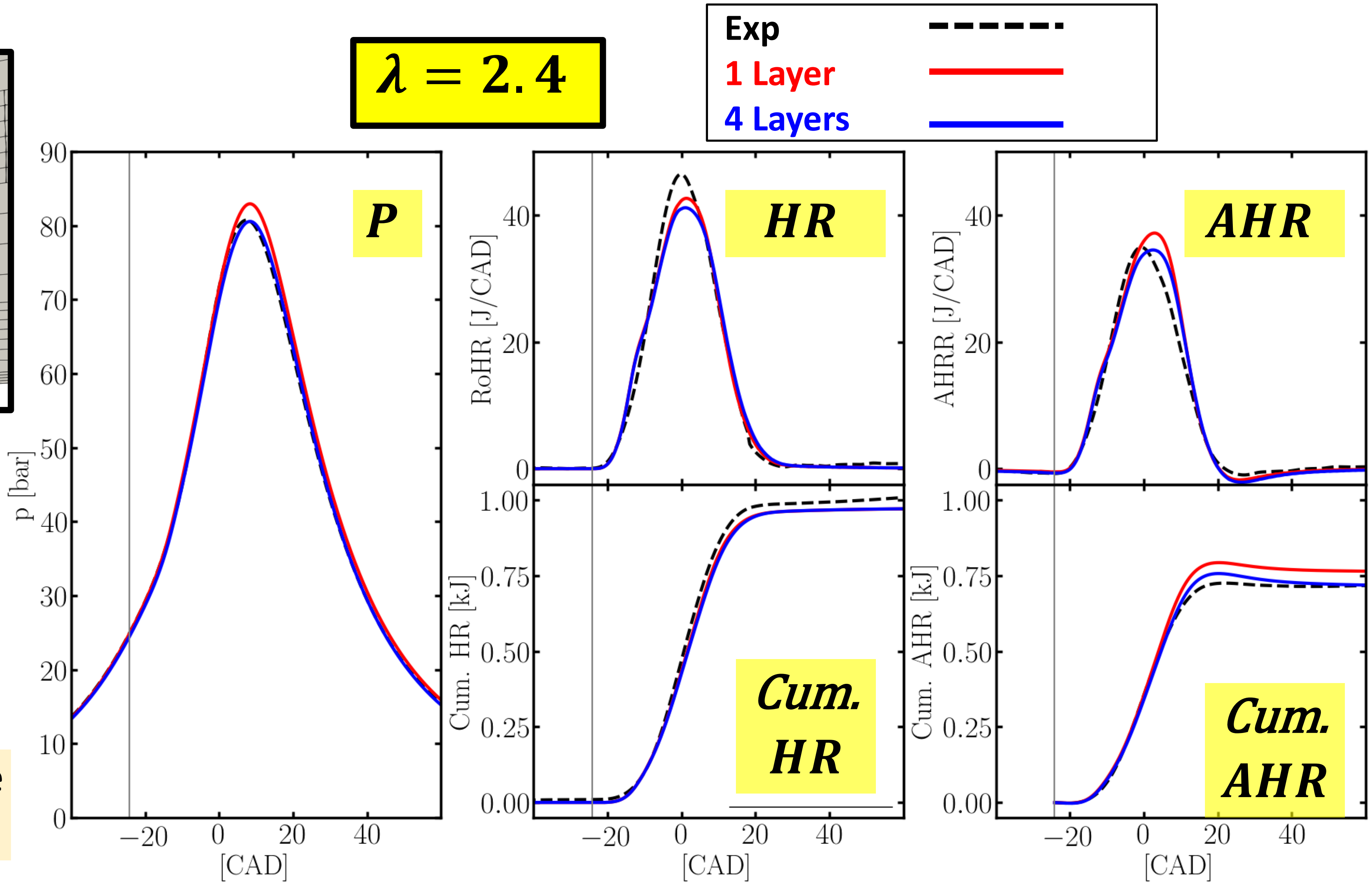
PFI results: flame-wall interaction effect



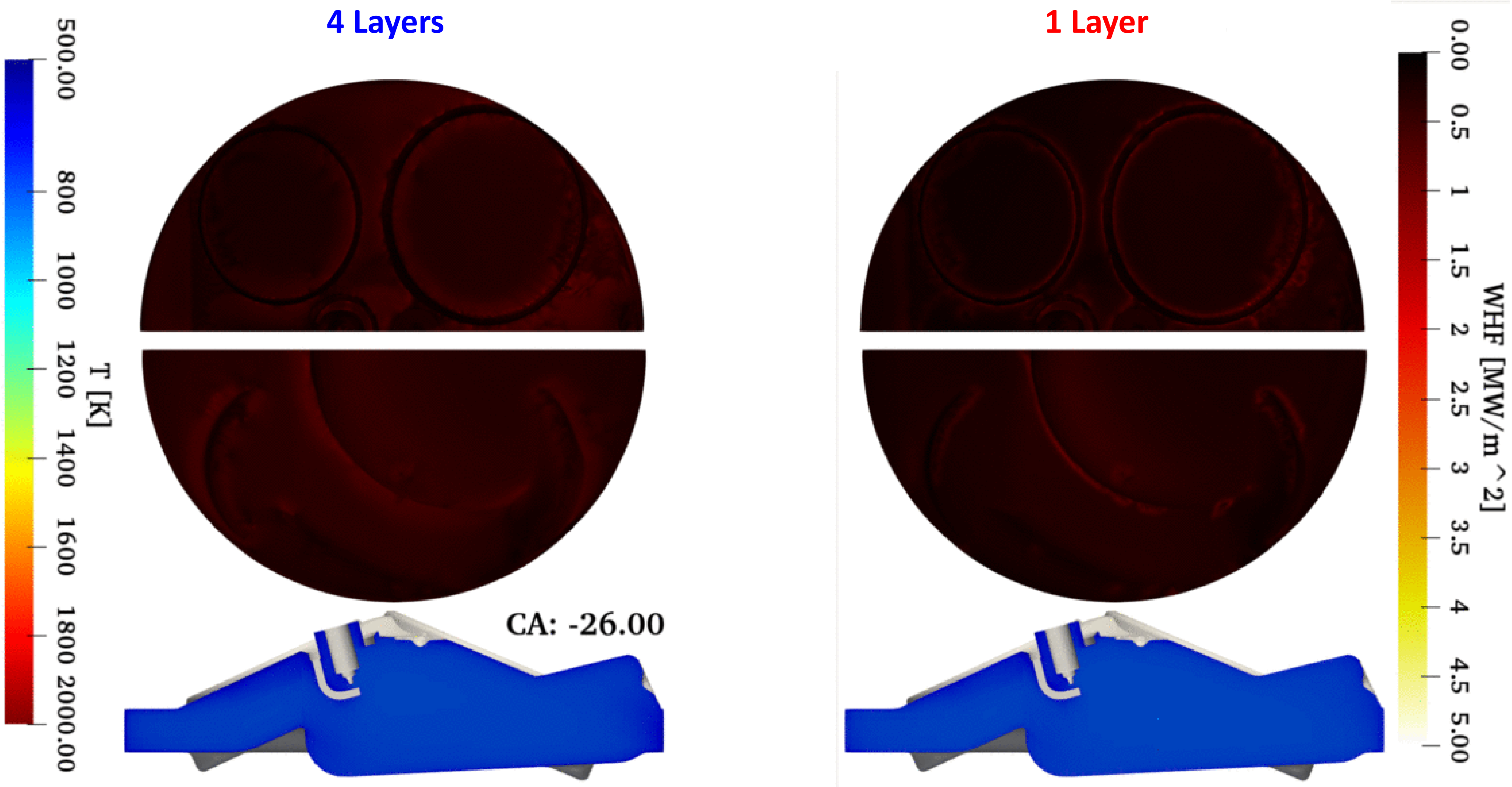
- ↑ n. layers:
  - ↑ **wall heat fluxes**

    ↓ $AHRR$ peak value

    ↓ $RoHR$ peak due to flame quenching at walls



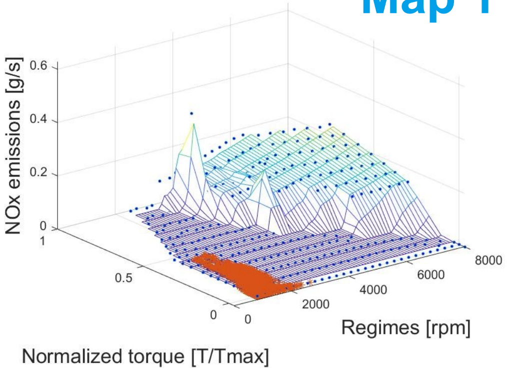
PFI results: flame-wall interaction effect

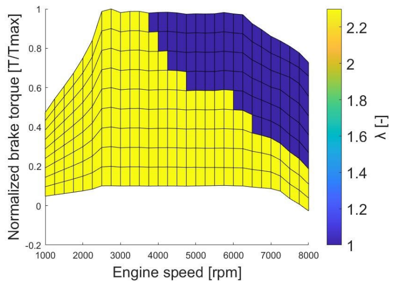


ATS design for H2 engines

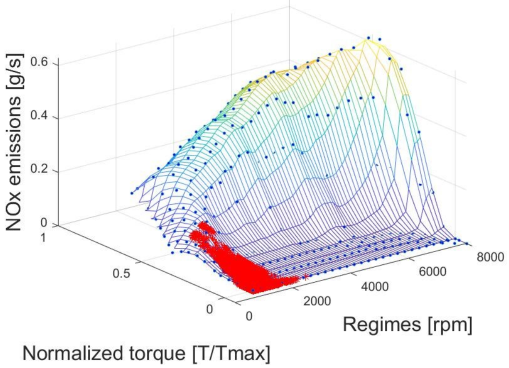
ATS for H2 high-performance engine: coupling engine strategies and ATS design

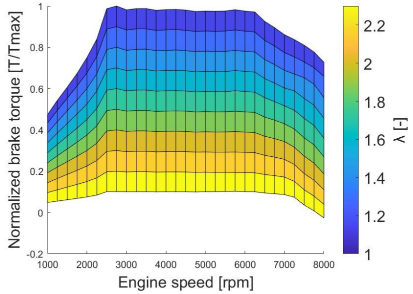
Map 1

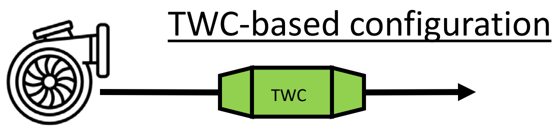


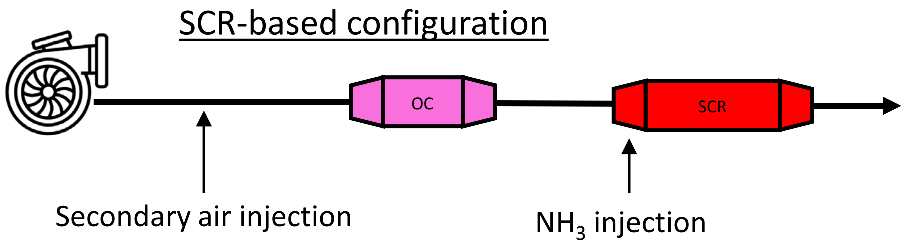


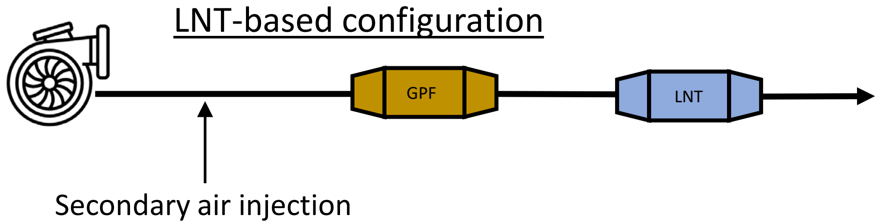
Map 2







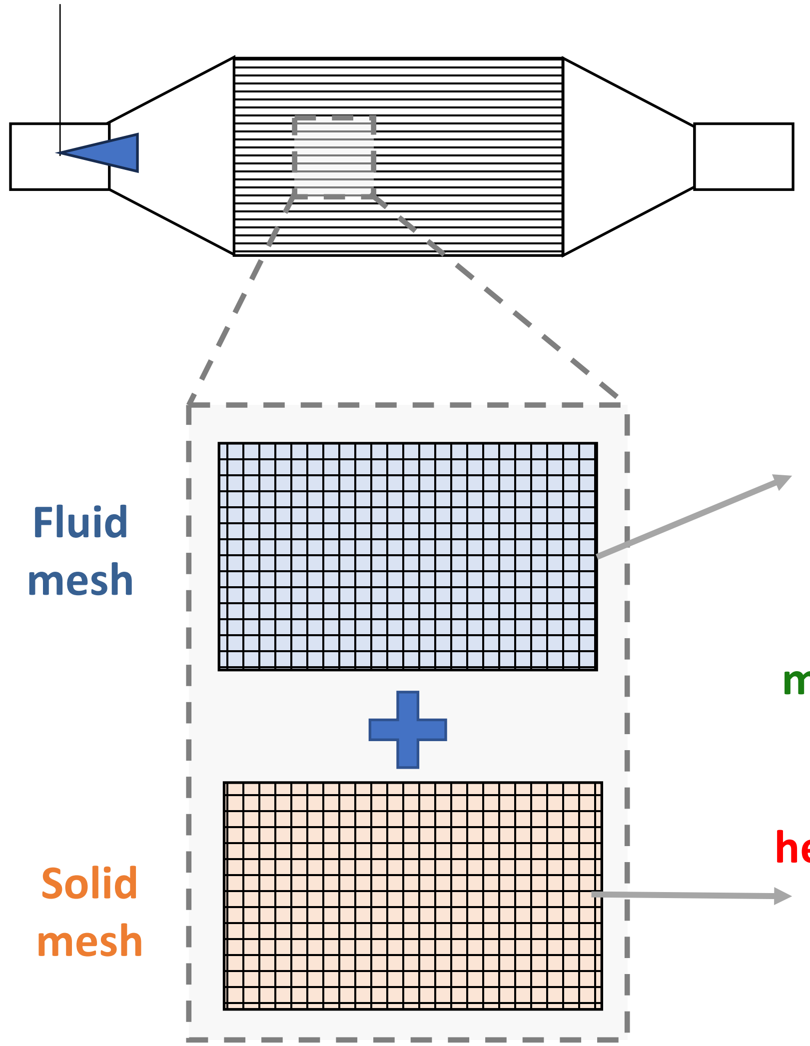


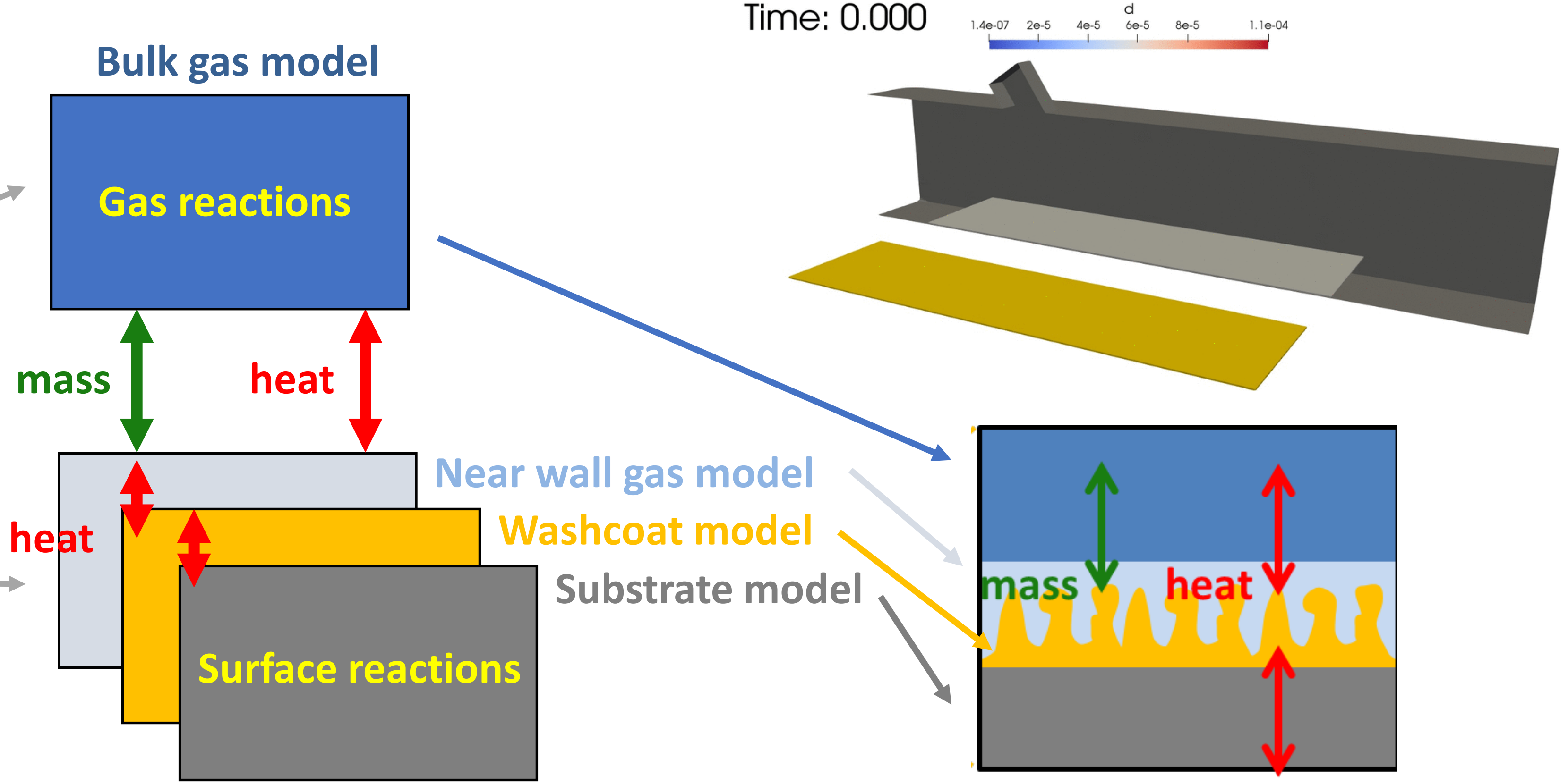


Bulgarini, M., Della Torre, A., Montenegro, G., Onorati, A., Gullino, F., Tonelli, R. «Towards H2 High-Performance IC Engines: Strategies for Control and Abatement of Pollutant Emissions» (2023) SAE Technical Papers, (2023)

CFD macro-scale model for ATS simulations

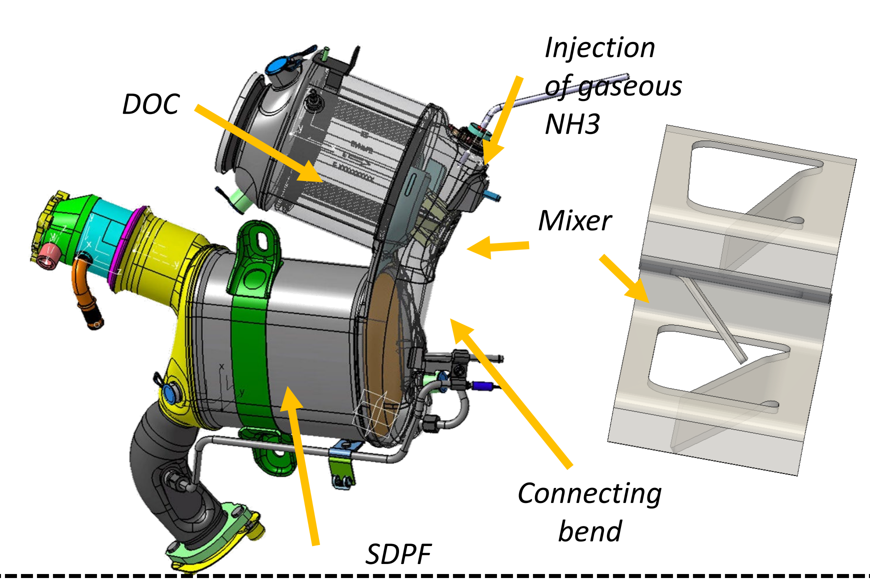
- Overlapping fluid and solid FV meshes
- Solid mesh support the modelling of different zones
- Coupling with lagrangian and eulerian models for tracking of droplets and liquid film

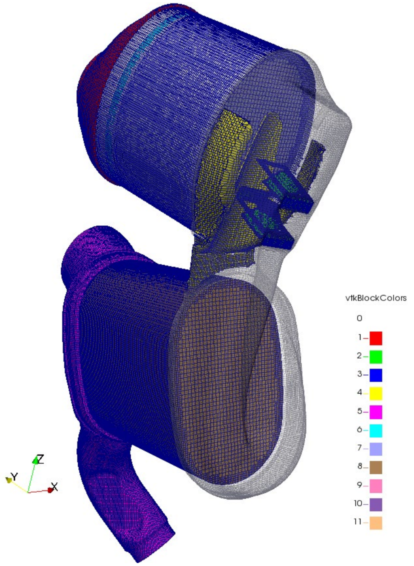


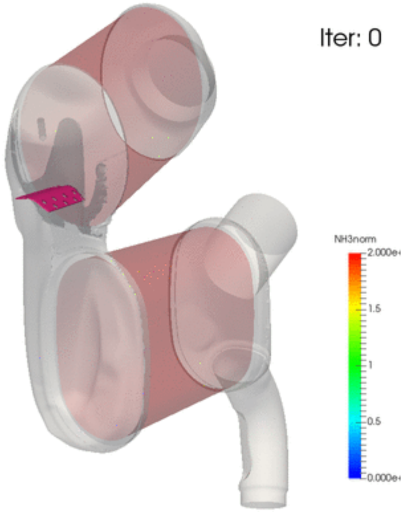


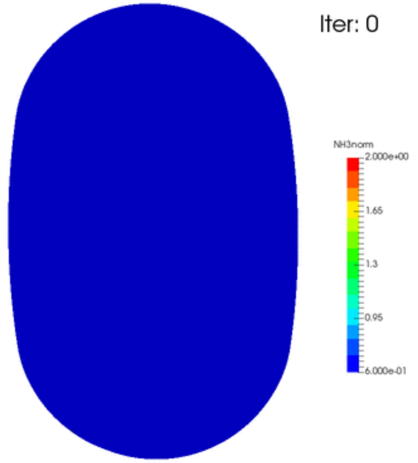
DeNOx technology for ATS of H2 engines

GASEOUS NH3

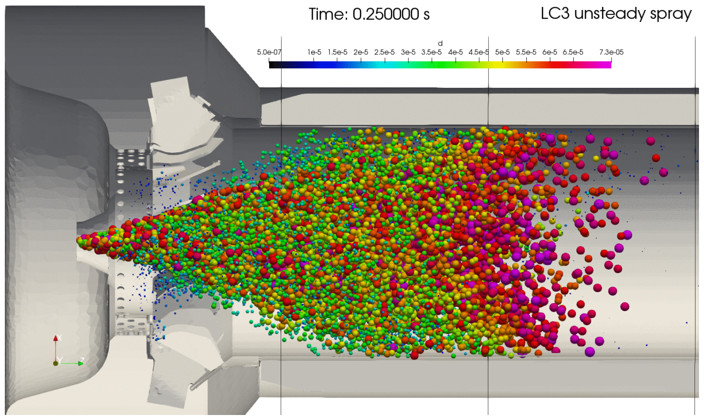


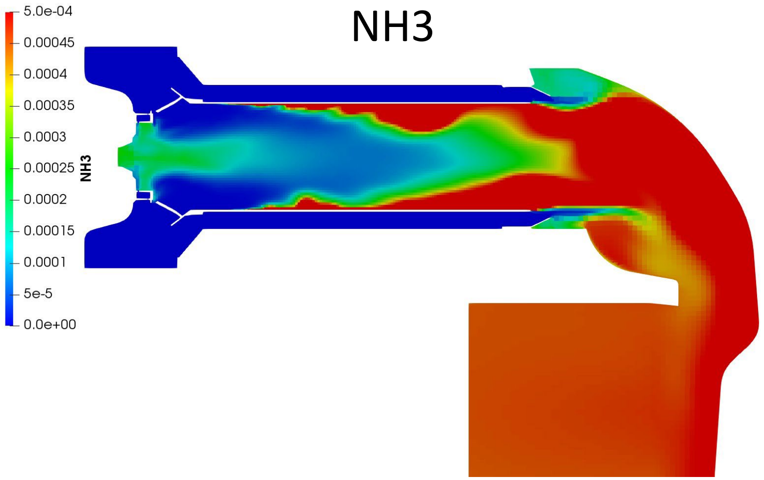


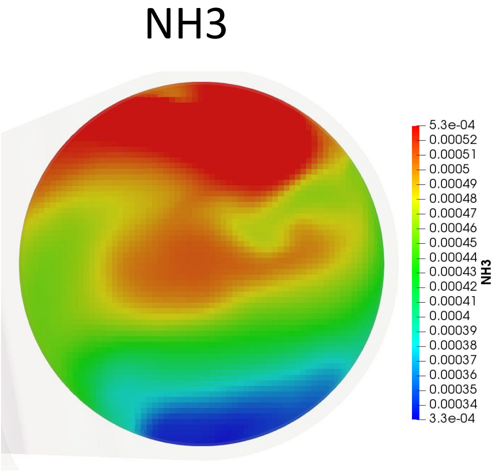




UWS NH3 CARRIER

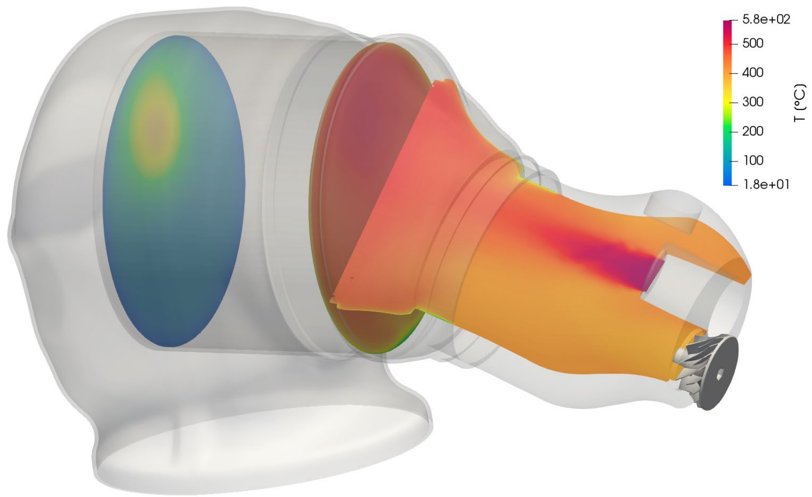


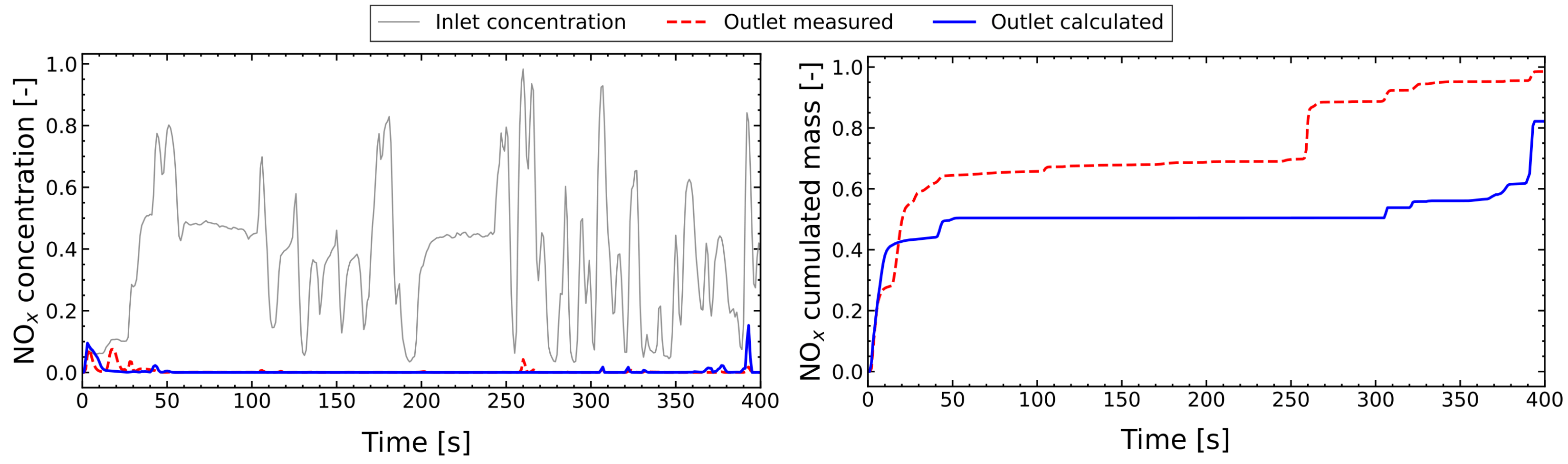


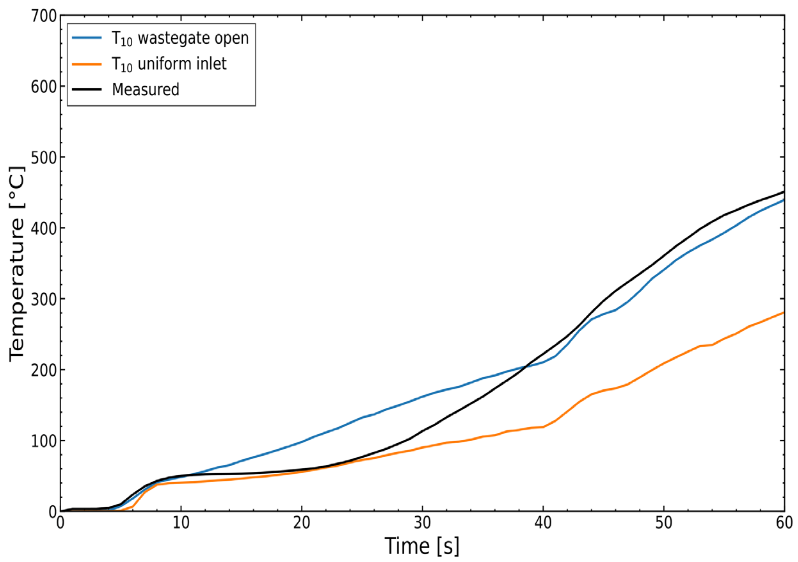


Della Torre, A., Montenegro, G., Onorati, A., Cerri, T., Tronconi, E., Nova, I. Numerical Optimization of a SCR System Based on the Injection of Pure Gaseous Ammonia for the NOx Reduction in Light-Duty Diesel Engines (2020) SAE Technical Papers,

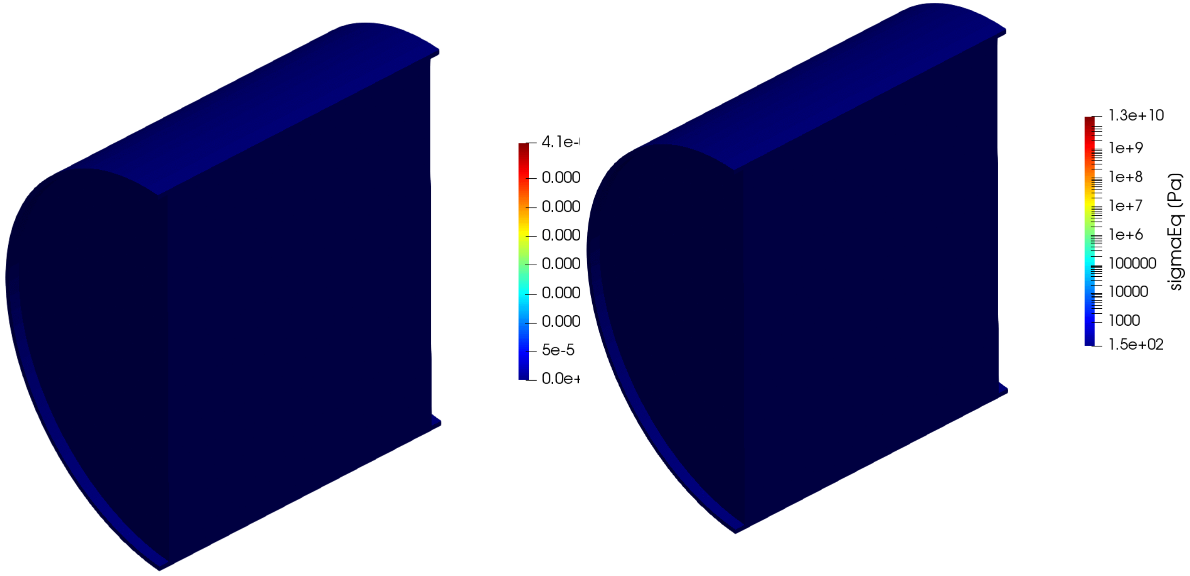
TWC/LNT technology for ATS of H2 engines







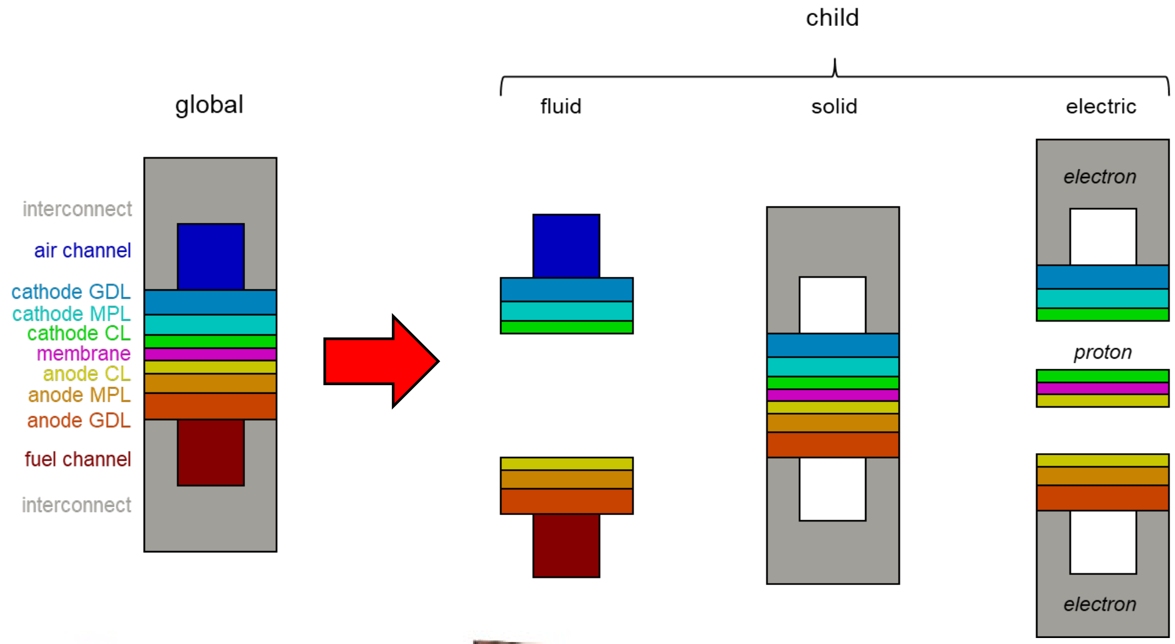
- Water condensation and evaporation submodel
- Stress and deformation caused by temperature gradients



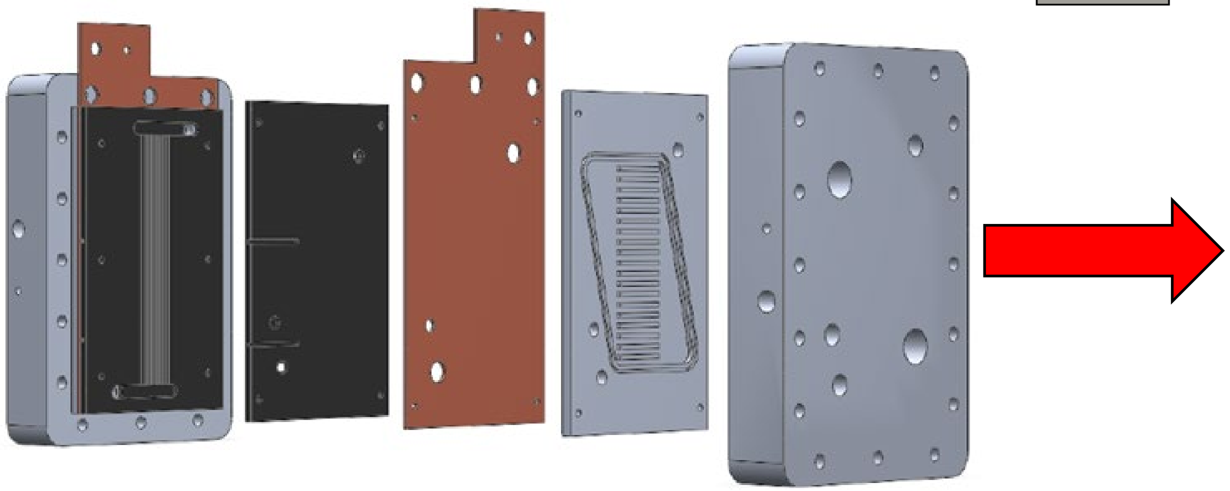
Displacement field

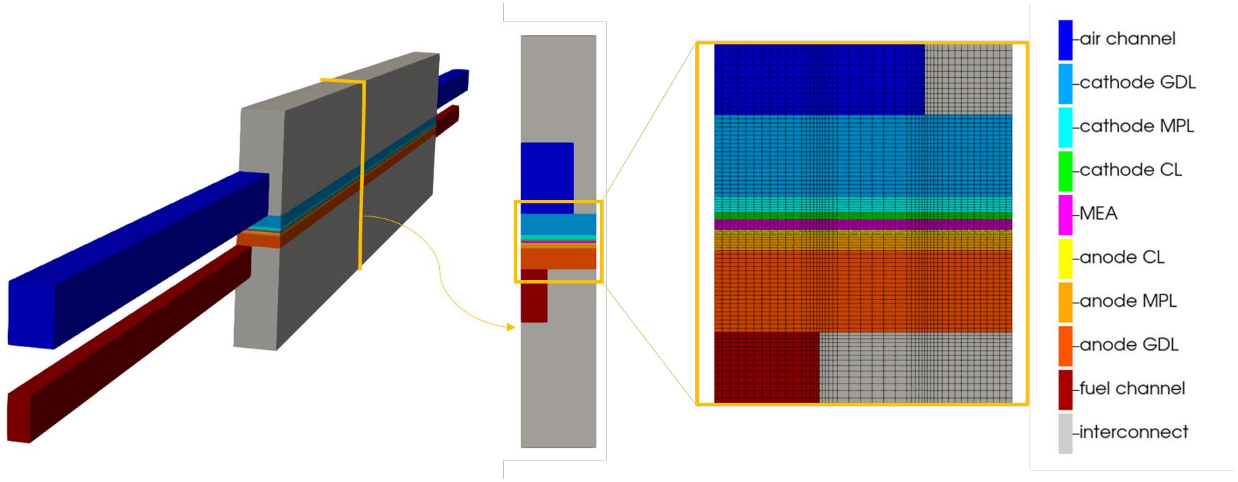
Equivalent stress

Fuel Cell Simulation



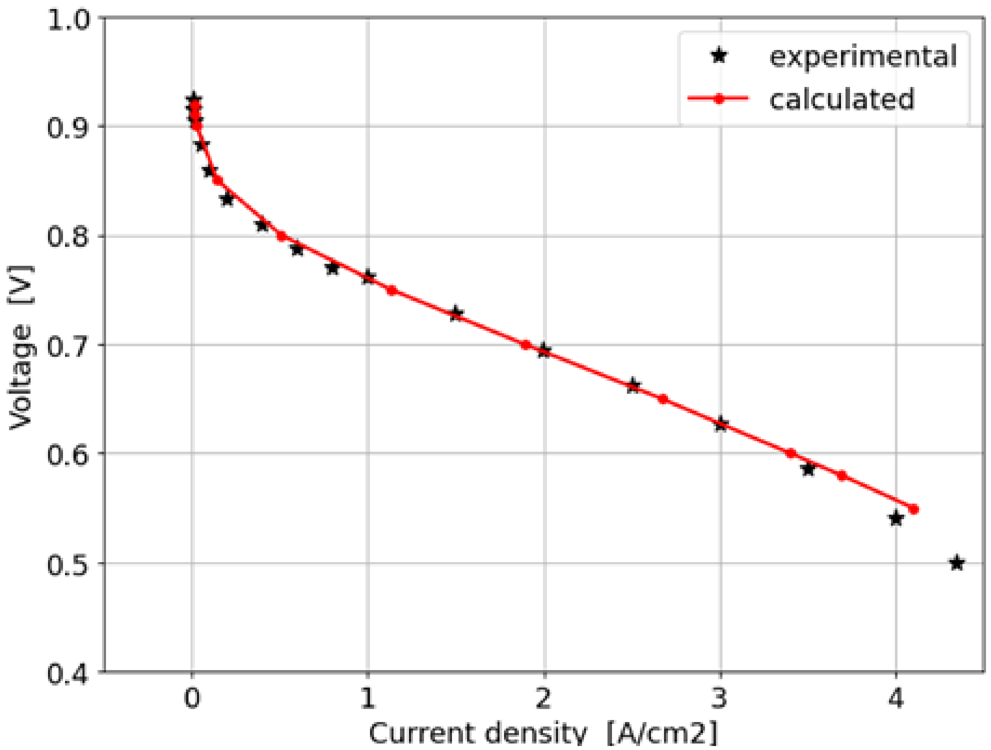
- The model was originally developed by Weber et al. (Juelich) based on the OpenFOAM technology and released under GPL2
- It is based on a multi-region aproach for the modeling of fluid, solid and electric region
- Modeling at the channel scale and device scale of PEM fuel cells and electrolyzers
- At PoliMI: implementation of novel models (reaction kinetics, water management) aimed at the study of degradation





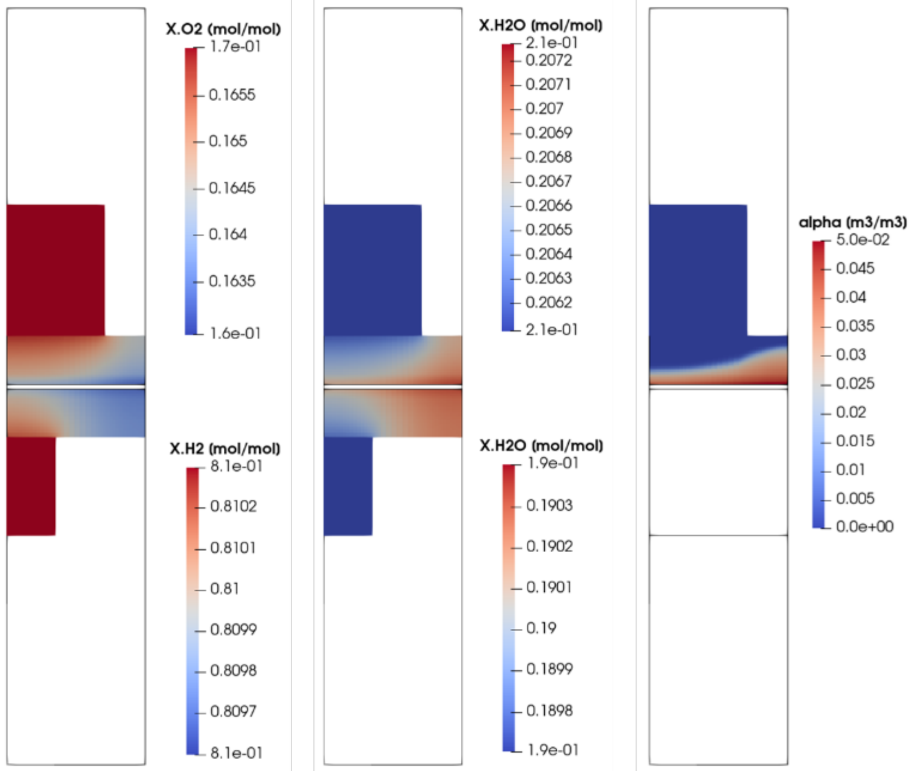
Fuel Cell Simulation

Validation: polarization curve



- Calculation of the polarization curve: the implemented PtOx model improve the prediction in the kinetic region (low current density)

Detailed analysis of reactants distribution



- Prediction of reactants distribution, water formation and liquid distribution in the GDL / MPL zones

Aknowledgments

- This presentation has collected the results of the whole research group ICEGroup at PoliMi:

Prof. Angelo Onorati
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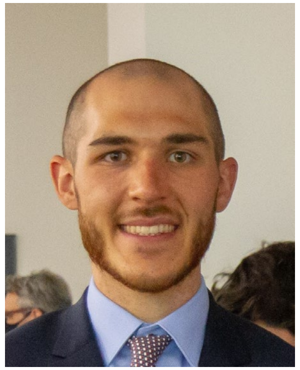
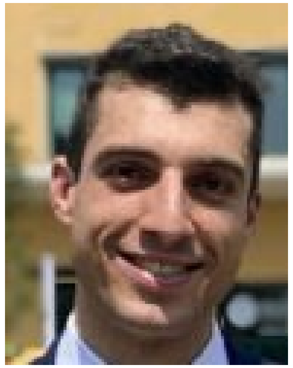
Dr. Giovanni Gianetti
Dr. Andrea Marinoni
Ing. Loris Barillari
Ing. Federico Ramognino
Ing. Alberto Ballerini
Ing. Alessandro Nodi
Ing. Andrea Sartirana
Ing. Margherita Bulgarini





6th Two Day Meeting (Milan, 11-12 March 2024)

The sixth edition of the "Two Day Meeting on Propulsion Simulations using OpenFOAM Tecnology" co-organized by the Internal Combustion Engine Group at Politecnico di Milano and the STFS group at TU Darmstadt will be held at Department of Energy of Politecnico di Milano on 11th and 12th March 2024.

This Two-Day Meeting is aimed at engineers and researchers who use OpenFOAM technology to simulate propulsion systems. Similar to previous events, the primary focus is on internal combustion engines, with an emphasis on alternative and sustainable fuels. Furthermore, a new session on fuel cells and BEV has been added. Presentations from universities, research institutes and industries will address the state of the art, real applications and specific developments related to:

- in-cylinder flows: gas exchange, fuel-air mixing, combustion, pollutant formation;
- intake and exhaust systems: after-treatment, unsteady flows, silencers;
- fuel cells and BEV powertrain cooling modeling.

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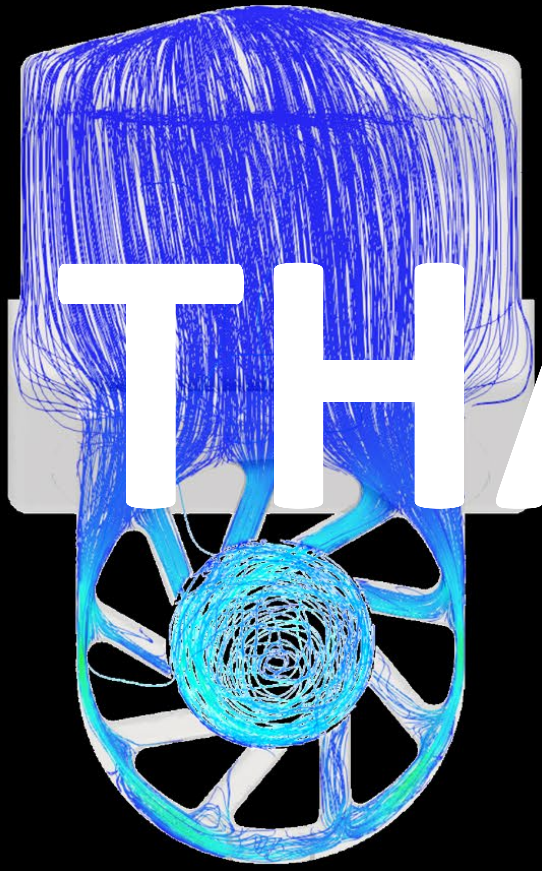

THANK YOU

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