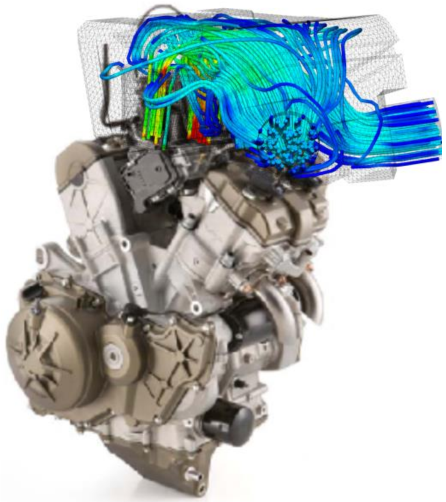
CFD Modeling Techniques for the Design of After-Treatment Systems



A. Onorati, G. Montenegro, A. Della Torre, L. Nocivelli

Internal Combustion Engine Group

Department of Energy, Politecnico di Milano

Background

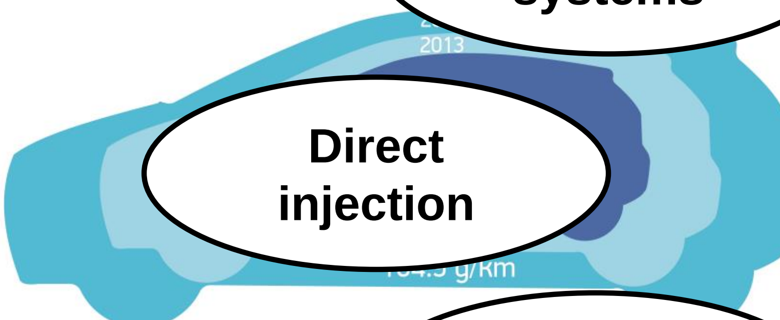
Internal combustion engine development will never stop!

Efficiency increase

Combustion systems

Direct injection

Downsizing

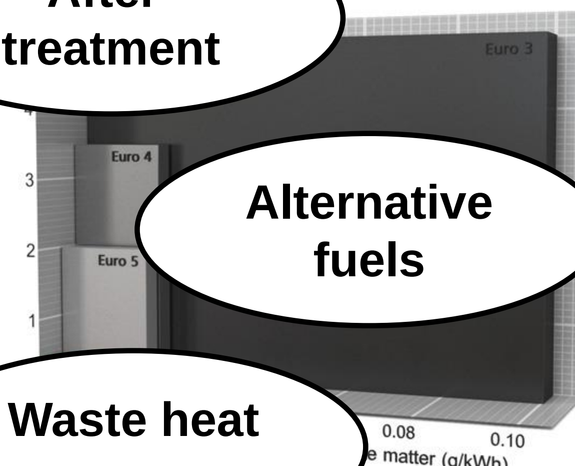


Pollutant emission control

After-treatment

Alternative fuels

Waste heat recovery

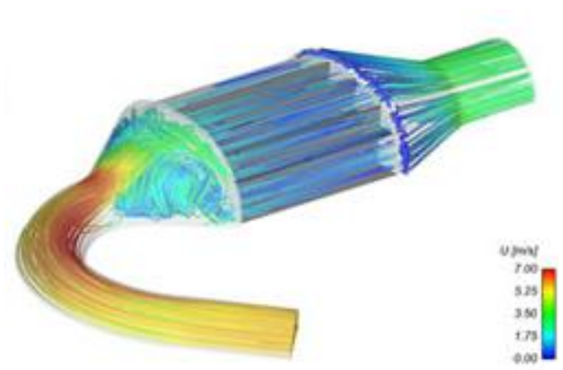


Research arguments at PoliMi

Main research topics

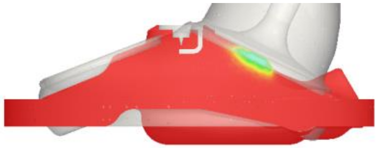
CFD simulation of IC engines:

- combustion and emissions;
- GDI and Diesel sprays;
- alternative fuels for I.C. engines;
- **reacting flows and after-treatment devices (SCR, DPF);**
- Large Eddy Simulation of engine-like geometries;
- integrated 1D-3D fluid-dynamic models;
- 1D thermo-fluid dynamic modeling;
- noise and acoustics.



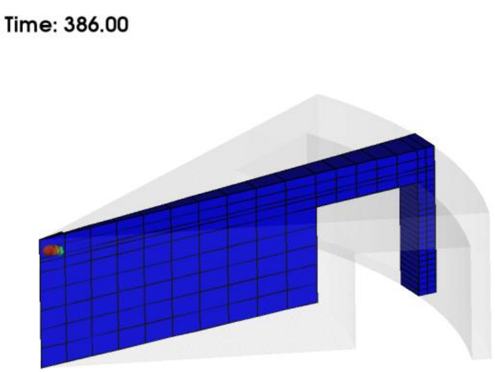
CFD code: OpenFOAM/Lib-ICE

- **OpenFOAM is a free-to-use Open Source numerical simulation software** with extensive CFD and multi-physics capabilities, written in a highly efficient C++ object-oriented programming.



- Free-to-use, allows to exploit high parallelization with only hardware costs.

- Ideal platform for research collaborations.



- Very wide diffusion with 2000 downloads/week.

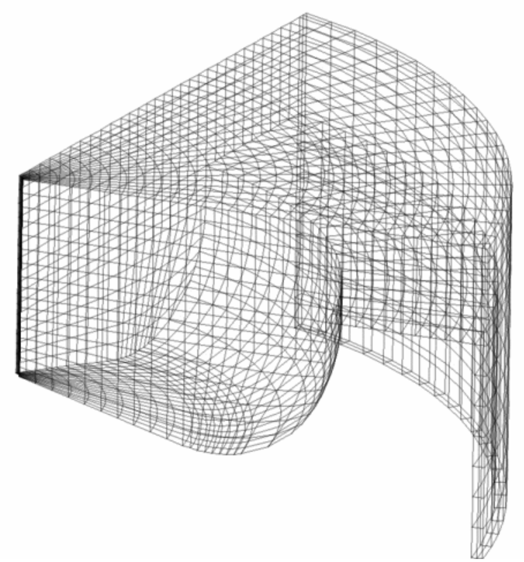
- We started to work with OpenFOAM in 2000. Our group is currently involved in several activities in Europe, concerning **OpenFOAM** development and applications.

ICE GROUP POLITECNICO DI MILANO

CFD code: OpenFOAM/Lib-ICE

The ICE group of Politecnico di Milano has contributed to develop the engine library under **OpenFOAM** technology (Lib-ICE):

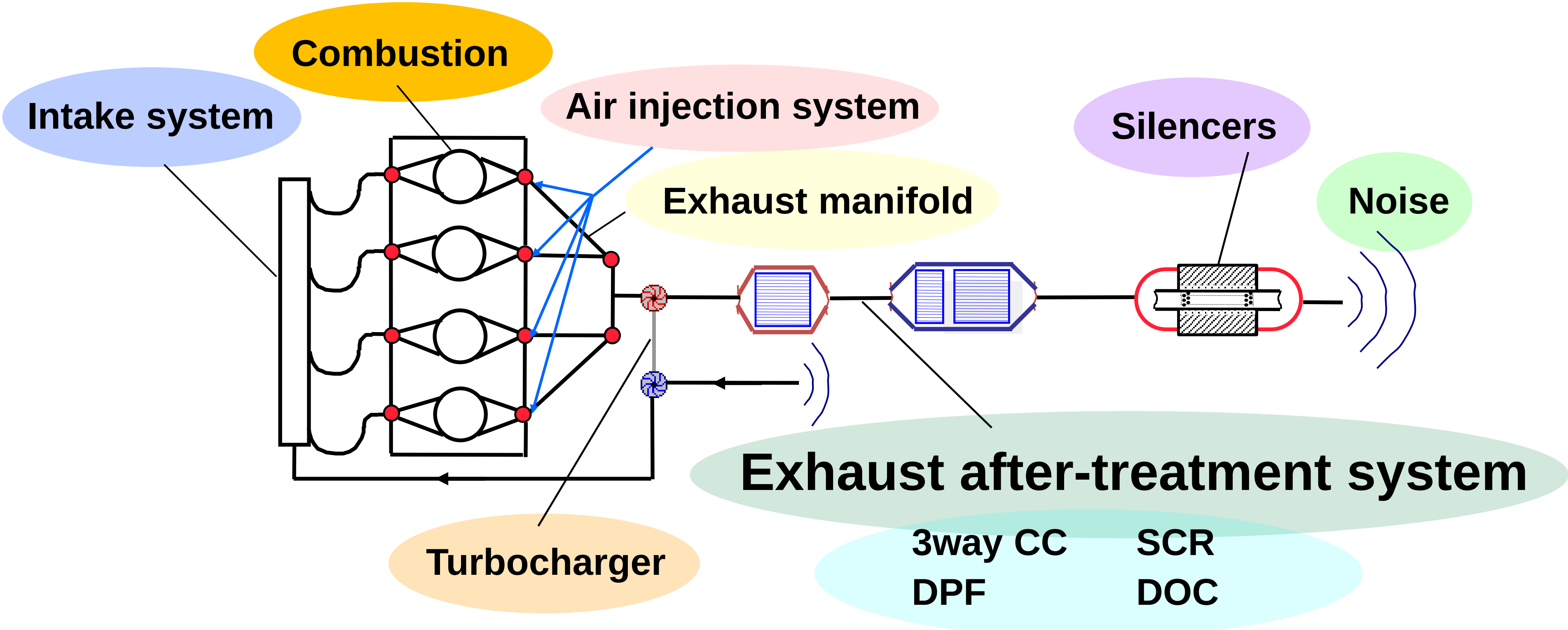
- Moving mesh algorithms
- Spray modeling
- Combustion process modeling
- DPF and SCR modeling
- 1D-3D coupling interface
- Non-linear acoustics modeling



Tool:

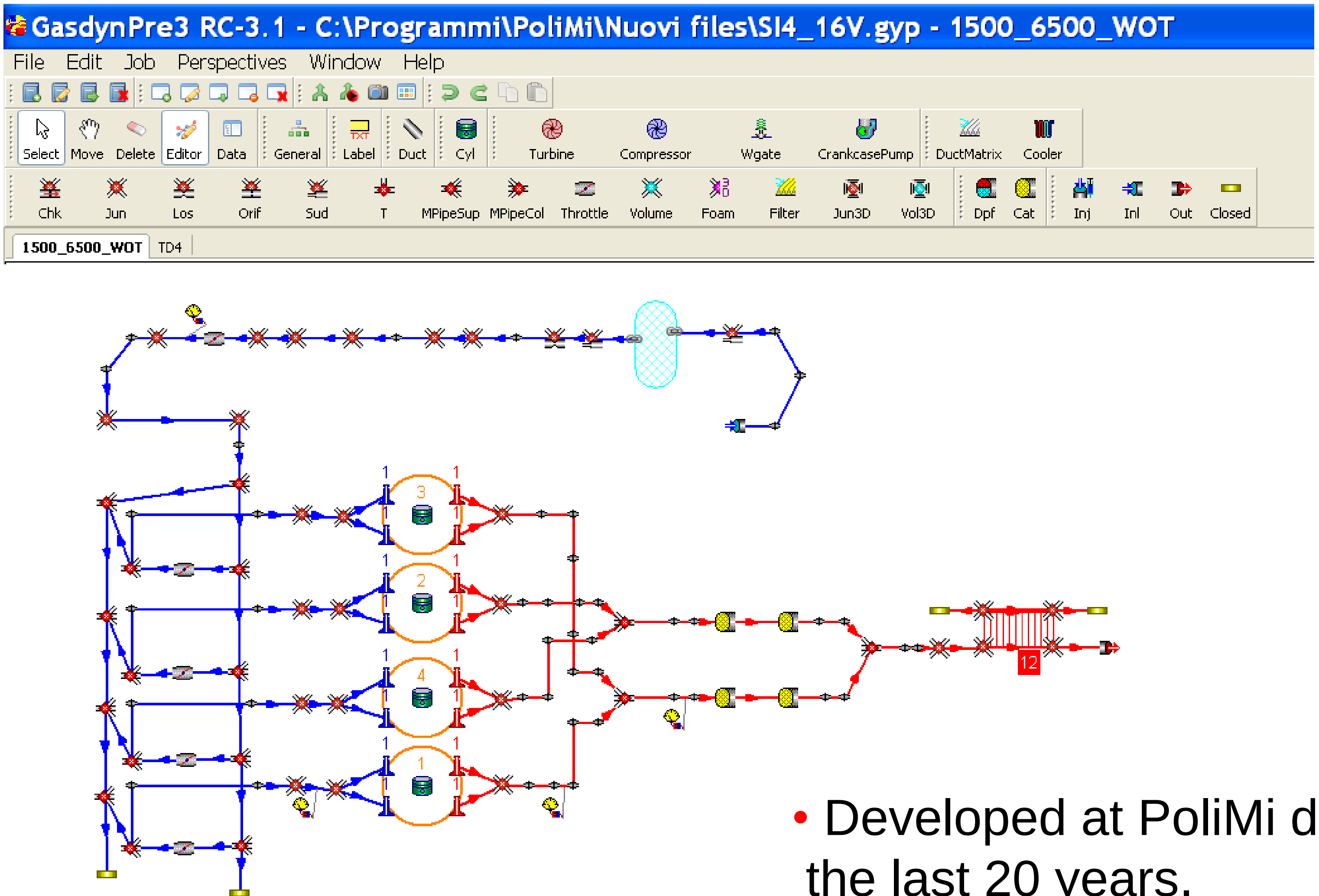
- in-house CFD libraries and solvers (**Lib-ICE**) developed under the **OpenFOAM**® technology.

1D thermo-fluid dynamic modeling of IC engines



- **GASDYN model**: 1D simulation of **wave motion** and **chemical species transport**, with **reactions** in the the **gas** and **solid phase.** Modeling of the main after-treatment devices: **3W catalyst, DPF, DOC, SCR, deNOx trap, secondary air injection**, etc.

1D simulation code: GASDYN



- Developed at PoliMi during the last 20 years.

Fundamental equations

- Fundamental equations in strong conservative form for 1D, unsteady, reacting flows in engine ducts:

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

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

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

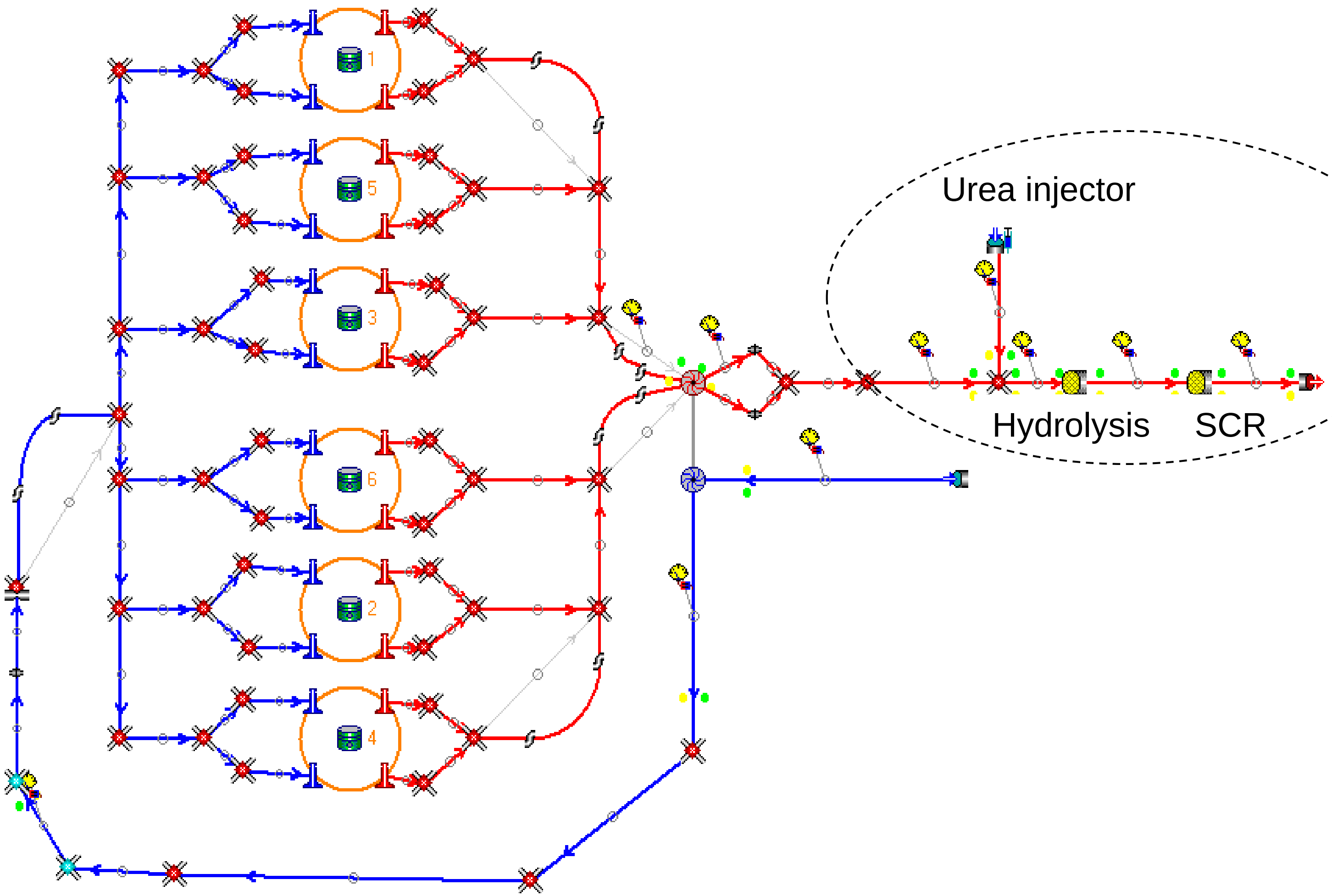
$$Y_i = m_i / m$$

Vector of specie mass fractions

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

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

SCR, 1D modeling: six cylinder Diesel engine

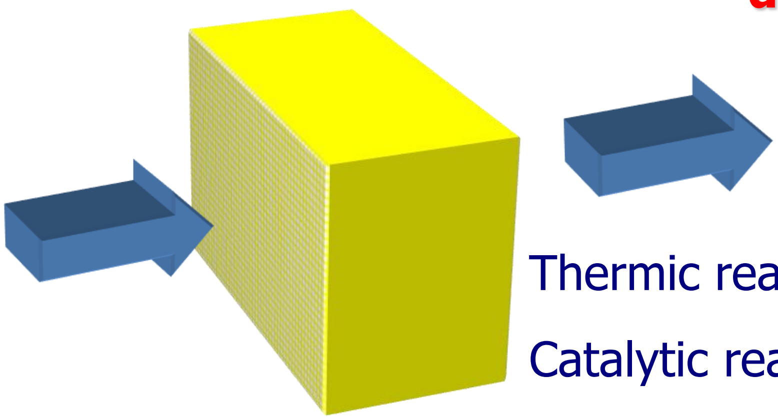


SCR modeling: urea injection and reactions

$$NH_2-CO-NH_2\ (aq.) \rightarrow NH_2-CO-NH_2\ (s) + xH_2O$$

$$NH_2-CO-NH_2\ (s) \rightarrow NH_3 + HNCO$$

Urea thermic decomposition



$$HNCO + H_2O \rightarrow NH_3 + CO_2$$

Isocyanic acid hydrolysis

$$4NH_3 + 4NO + O_2 \rightarrow 4N_2 + 6H_2O$$

"Standard" SCR reaction

$$4NH_3 + 3O_2 \rightarrow 2N_2 + 6H_2O$$

$$8NH_3 + 6NO \rightarrow 7N_2 + 12H_2O$$

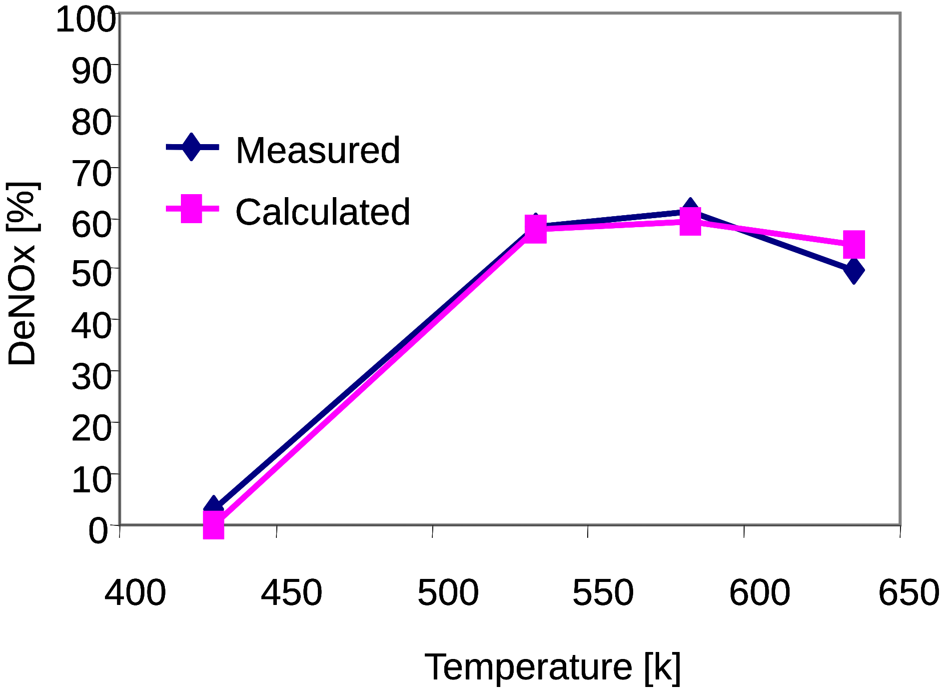
Ammonia Oxidation

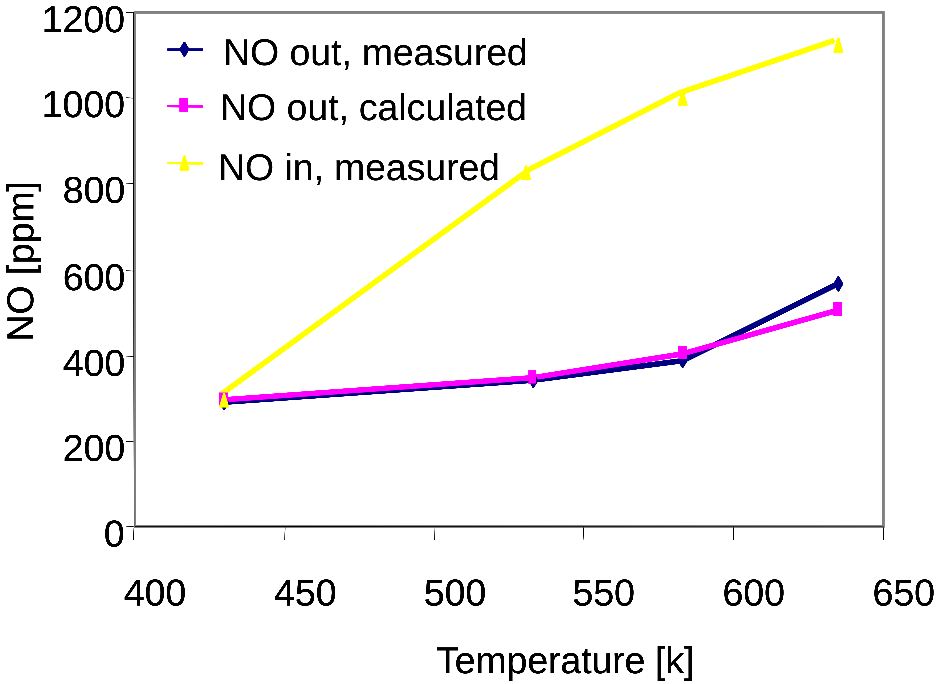
$$4NH_3 + 2NO + 2NO_2 \rightarrow 2N_2 + 6H_2O$$

"Fast" SCR reaction

SCR modeling: urea injection and reactions

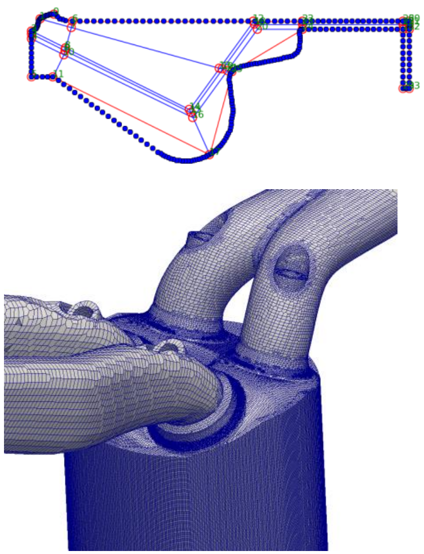
Calculated and measured de-NO_x efficiency and NO emission level versus catalyst temperature at 2200 rpm.





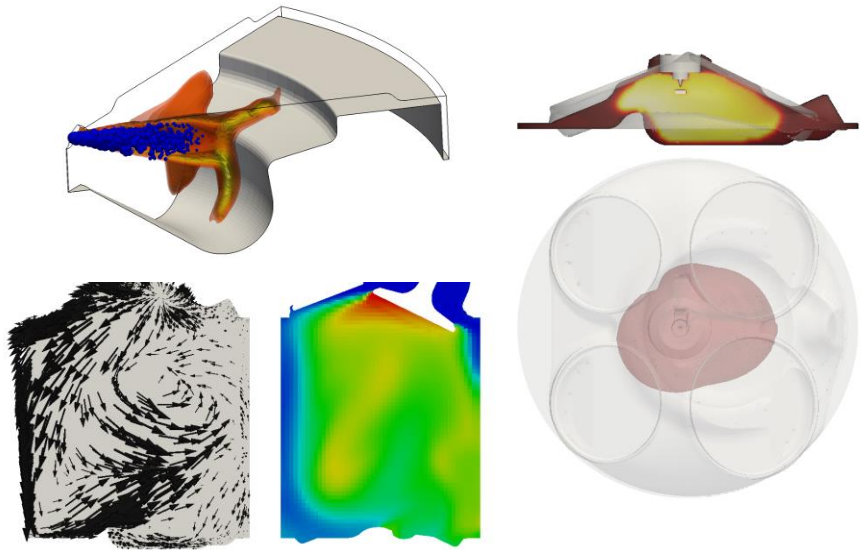
OpenFOAM at PoliMi (Lib-ICE)

Pre-Processing



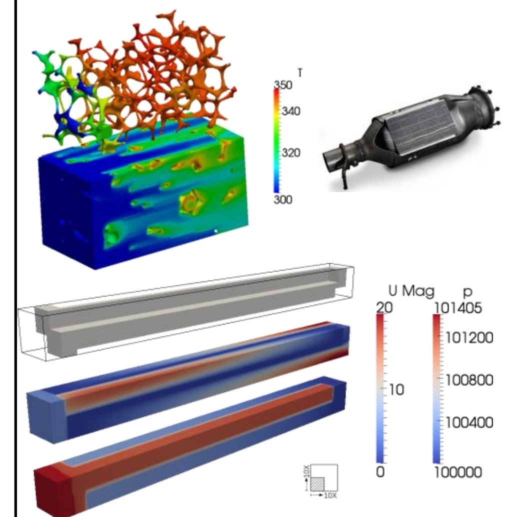
Automatic mesh generation

In-cylinder flows & combustion



Gas exchange, fuel air mixing
SI, CI, PCCI, HCCI combustion

After-treatment



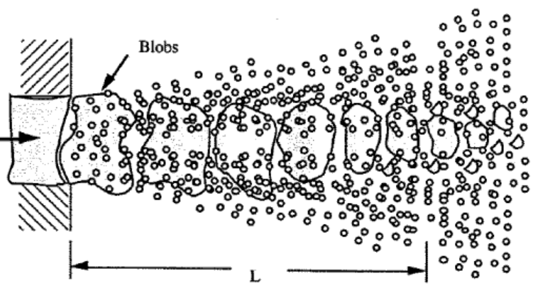
After-treatment modeling
SCR, DPF, TWC, DOC

Spray and wall-film modeling

New sub-models for multi-hole nozzles

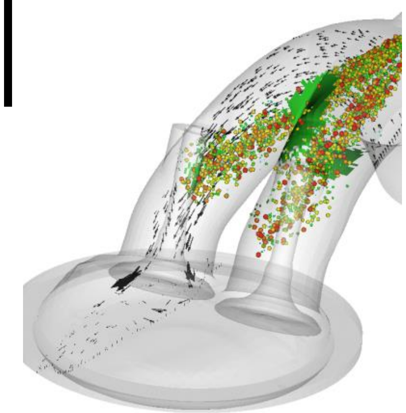
- **Injection**: Huh, Reitz-Bracco, Nurick
- **Atomization** : Huh-Gosman, Bianchi
- **Breakup**: KHRT
- **Wall-interaction**: Bai and Gosman, Stanton and Rutland
- **Evaporation**: based on Spalding mass number

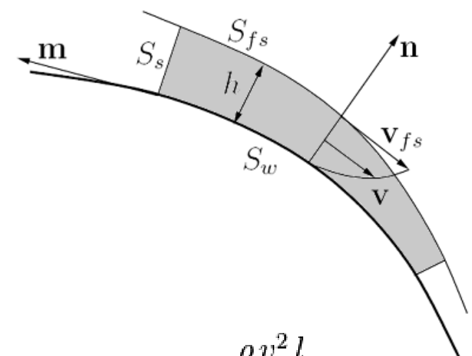
Blob injection



Wall-film model (finite-area)

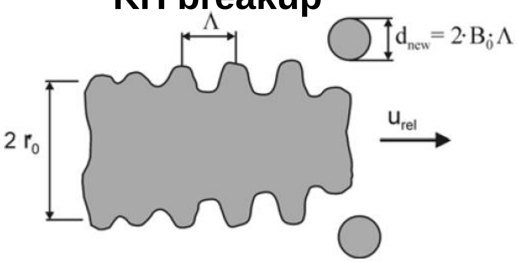
- Mass, momentum and energy equations for the liquid film solved on mesh boundary.



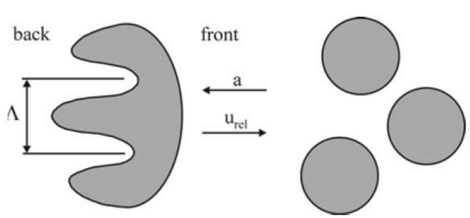


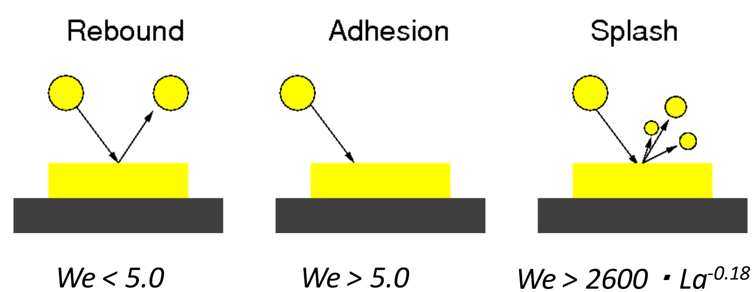
$$\mathrm{We} = \frac{\rho v^2 l}{\sigma}$$

KH breakup



RT breakup





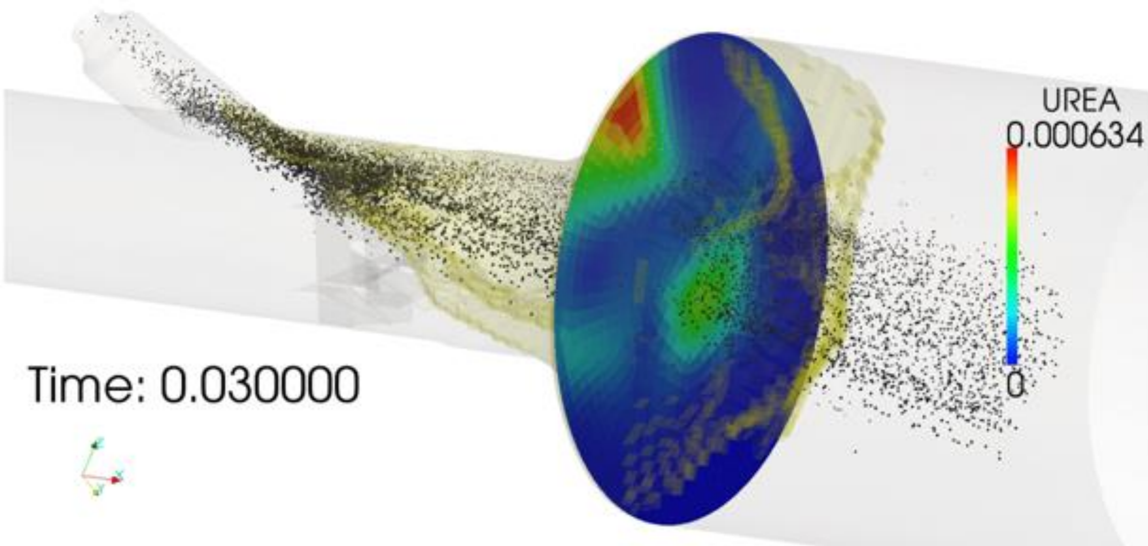
GDI engine simulations

Full-cycle simulation of GDI engines

This work was sponsored and carried out in collaboration with

After-treatment: SCR

- **Unsteady flow solver** with Lagrangian tracking of particles.
- **Multi-component liquid mixture** and homogeneous chemical reactions (urea thermal decomposition).
- **Wall film** formation and evaporation.



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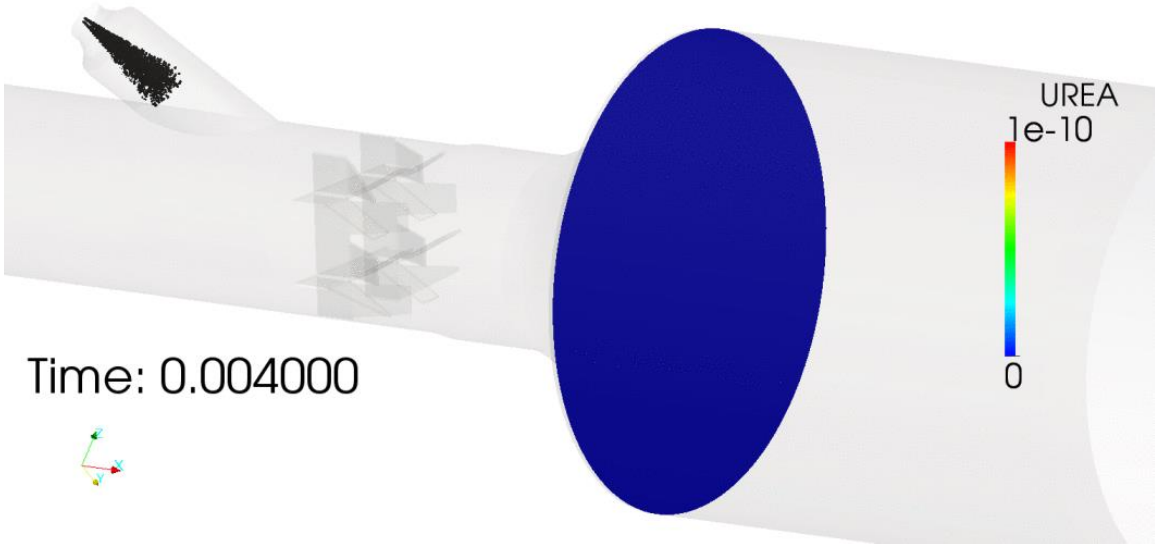
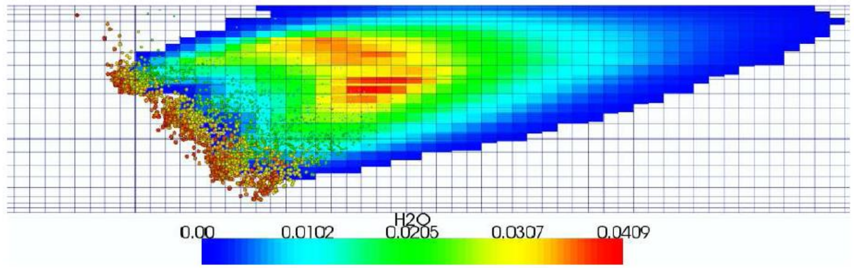
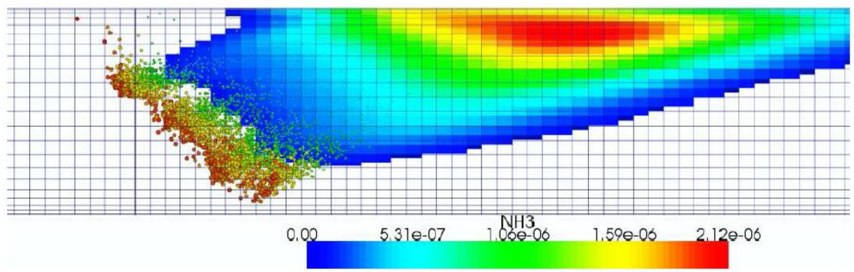


Urea spray in a duct



H_2O distribution



NH_3 distribution

- Liquid urea properties have been added in order to account for AdBlue or urea solutions.
- Inclusion of chemistry to model the thermal decomposition of urea particles into HNCO and NH_3 .

Selective Catalytic Reduction (SCR)

The chemical and physical processes to be taken into account are:

- the injection and evaporation of urea solution;
- the thermal decomposition of urea in gas phase;
- the hydrolysis of isocyanic acid generated during the urea thermal decomposition process;
- the reactions of NOx reduction (fast and standard) occurring onto the catalytic bed:

$$
\begin{aligned}
NH_2 - CO - NH_2 \quad &\rightarrow \quad NH_3 + HNCO \\
HNCO + H_2O \quad &\rightarrow \quad NH_3 + CO_2 \\
2NH_3 + 2NO + 0.5O_2 \quad &\rightarrow \quad 2N_2 + 3H_2O \\
2NH_3 + NO + NO_2 \quad &\rightarrow \quad 2N_2 + 3H_2O \\
2NH_3 + 1.5O_2 \quad &\rightarrow \quad N_2 + 3H_2O
\end{aligned}
$$

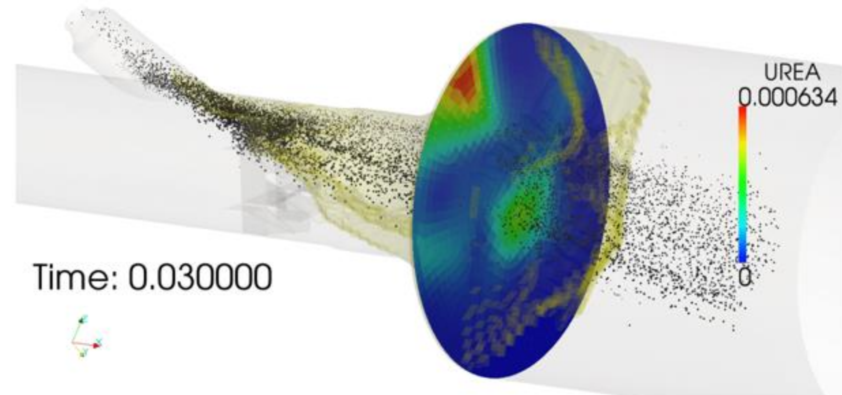
Injection of urea-water solution and solid deposits

Wall impingement can be a paramount parameter to be taken into account in the generation of an uniformly distributed gaseous mixture.

Direct injection of urea-water solution in the pre-catalytic section:

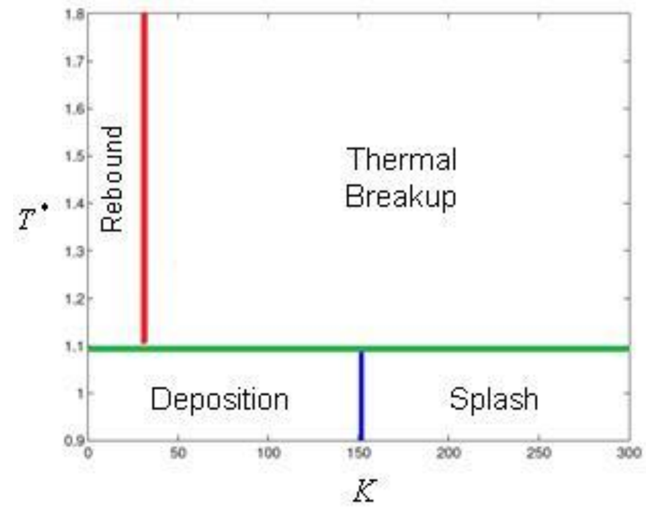
- **Low pressure injection.**
- **No secondary breakup.**
- **Slow urea thermal decomposition.**

Possible solid urea byproduct deposition



SCR modeling: injection of AdBlue

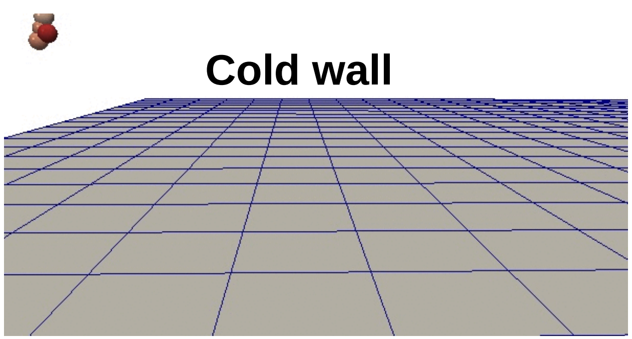
- **Multi-component liquid mixture** customized properties for urea along with multi-component liquid film.
- Temperature dependence of the spray-wall interaction and wall cooling effect.



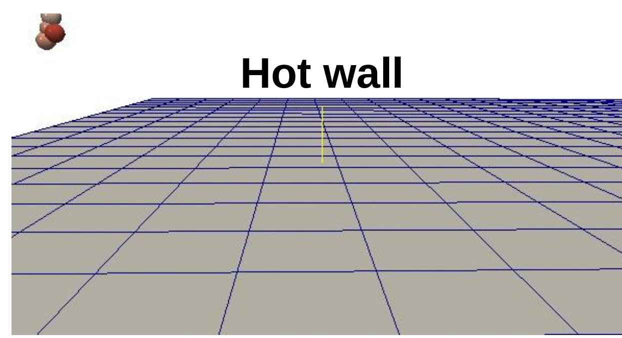
Absolute We = 264
Normal We = 137

$$K = We^{5/8} La^{1/8}$$

Cold wall



Hot wall



T* = 0.8

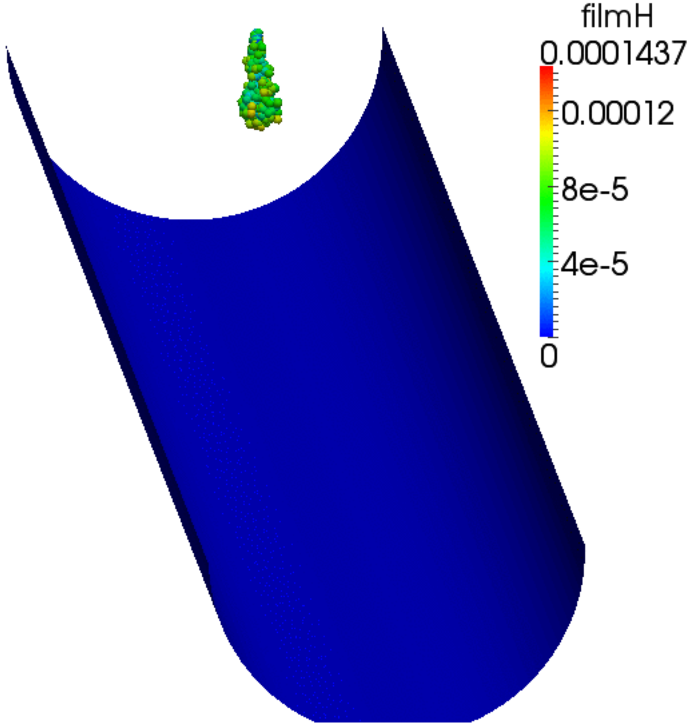
T* = 1.2

$T^* = T_{wall} / T_{sat}$

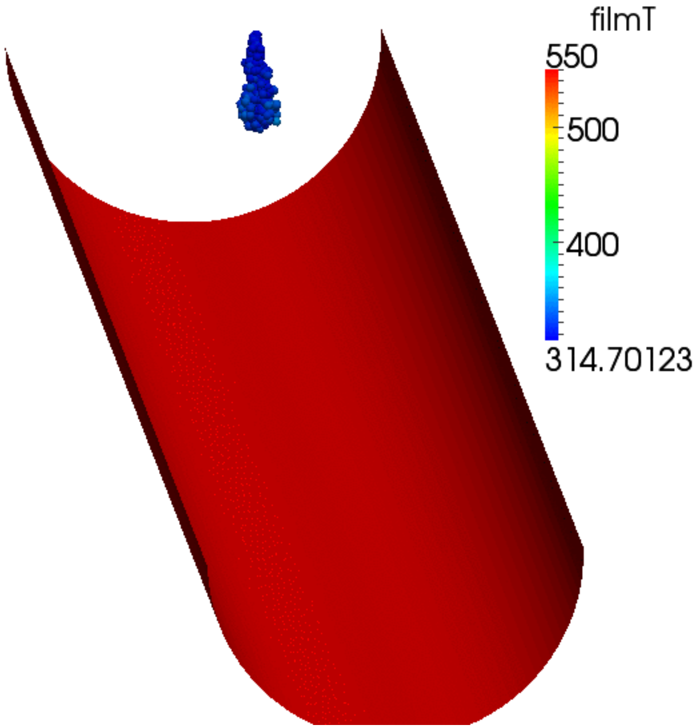
(In collaboration with **EMPA**, Dr. P. Dimopoulos and **Fiat Industrial - CNH**)

SCR: wall film modeling

Film thickness

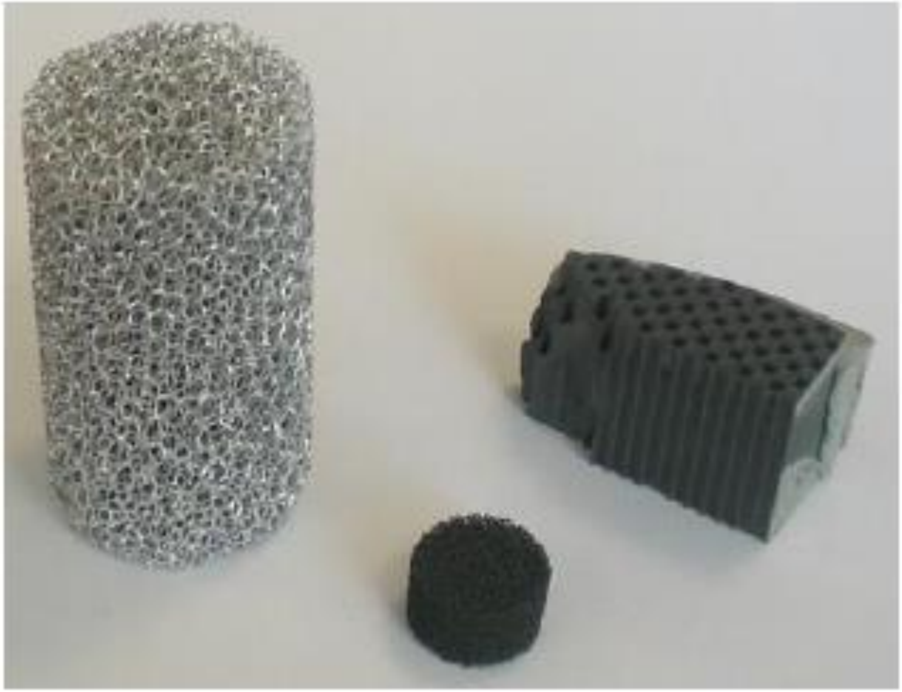


Film temperature



After-treatment: open-cell foams

CFD simulation of open-cell foams

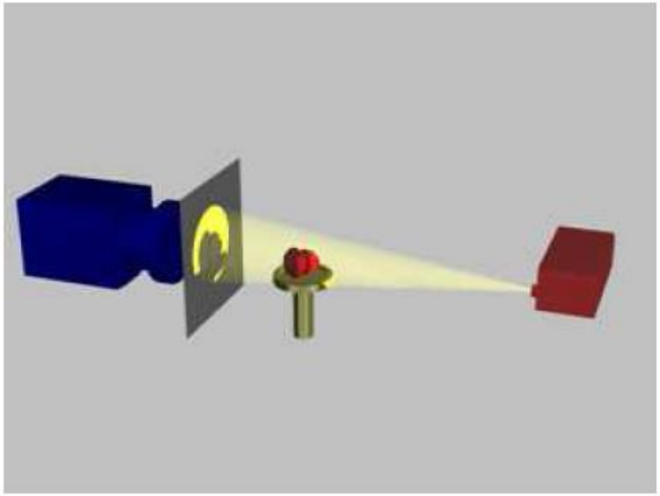


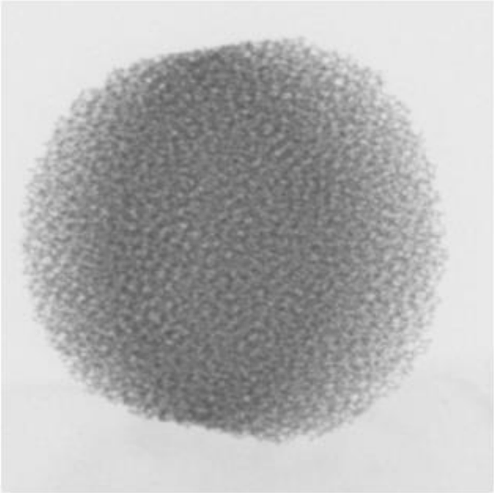
Foam samples

(in collaboration with **EMPA**, Dr. P. Dimopoulos)

Micro-CT scans (at University of Exeter)

- Micro-CT scanner applied for the reconstruction of foam micro-structure
- X-ray cone beam passes through a rotating sample
- A detector collects 2D projection images of the sample at different angles
- 3D voxel dataset is reconstructed from the 2D slices





Micro-CT: image processing

Al foam

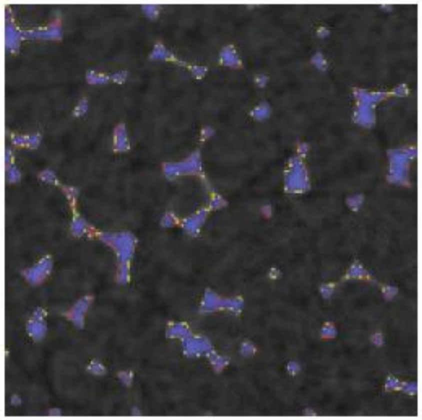
porosity: 95-97%

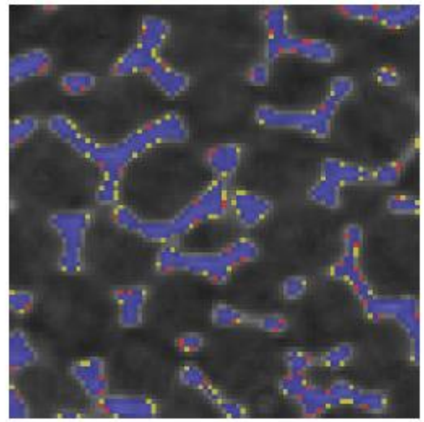
SiC foam

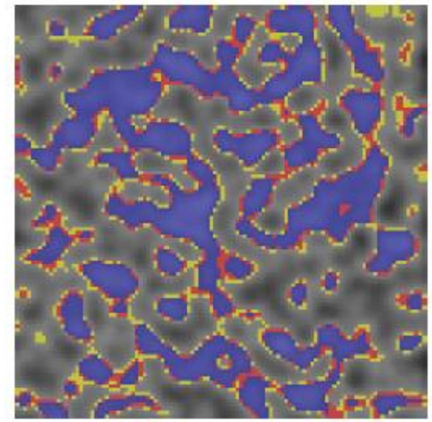
porosity: 85-90%

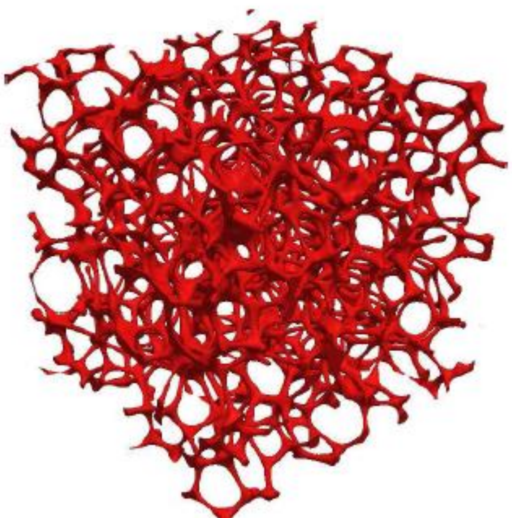
Cordierite

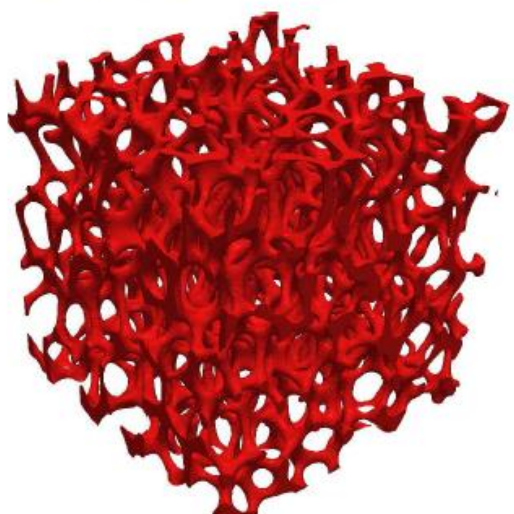
porosity: 45-55%





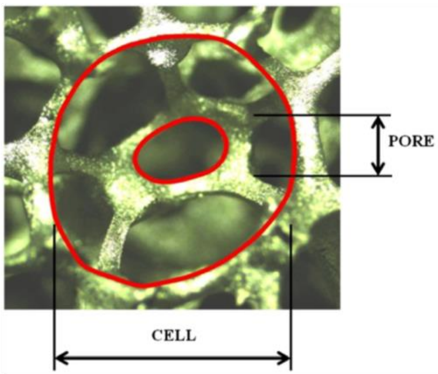


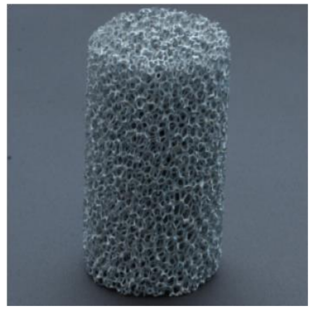




Open-cell foams for after-treatment systems

Open-cell foam



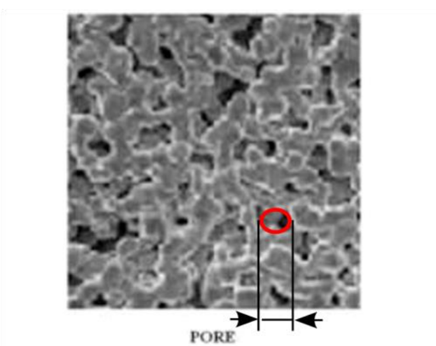


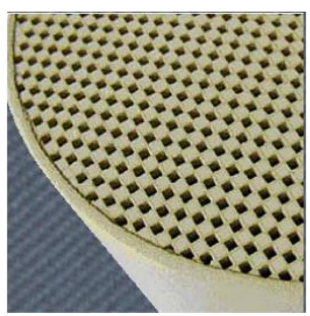
Al alloy
95% porosity
40 ppi

SiC
86% porosity
80 ppi

Applications:
Catalytic substrates for after-treatment devices (as an alternative to traditional honeycomb)

Filtering media





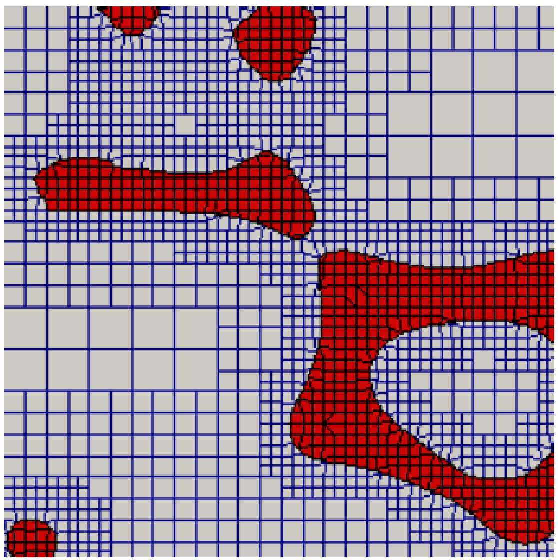
Cordierite
50% porosity
16 µm pore

Applications:
Removal of particulate matter from exhaust gas

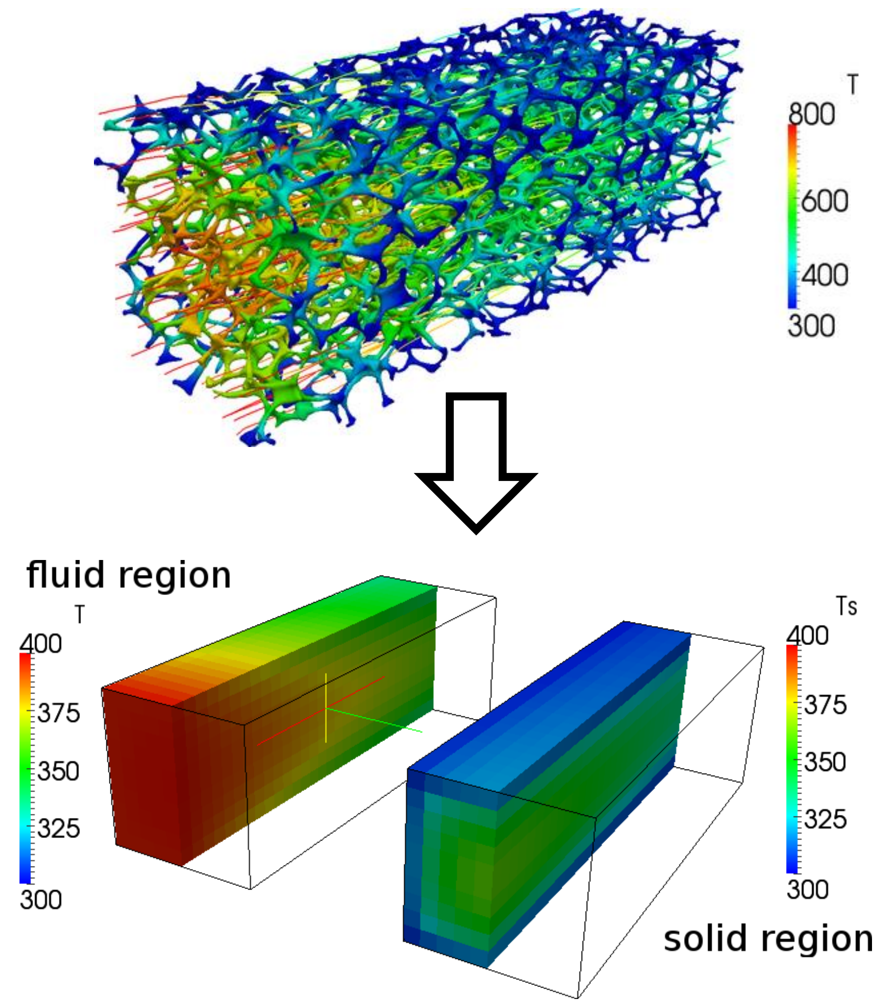
Open-cell foams for after-treatment systems

From micro-scale to full scale simulation of after-treatment systems:

snappyHexMesh

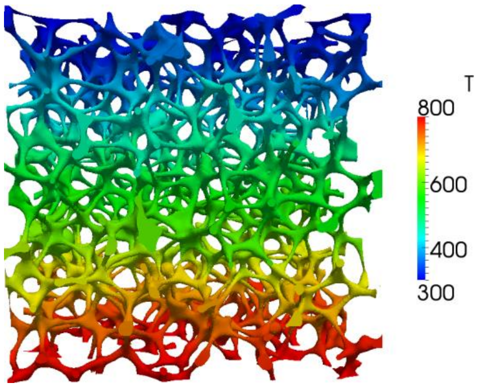


2.1 mln cells
93% hex - 7% pol

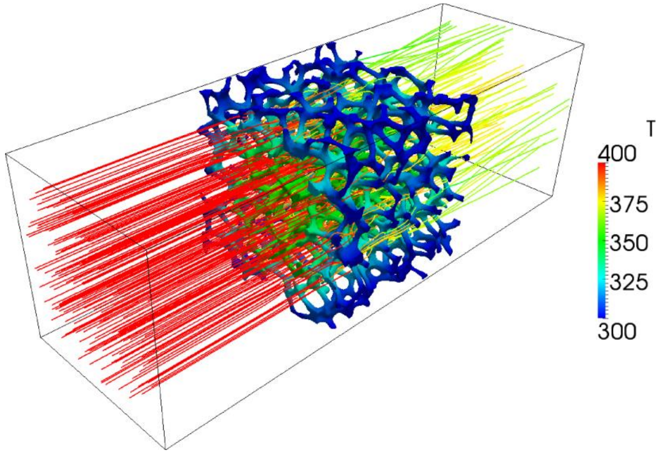


Micro-scale: heat-transfer simulations

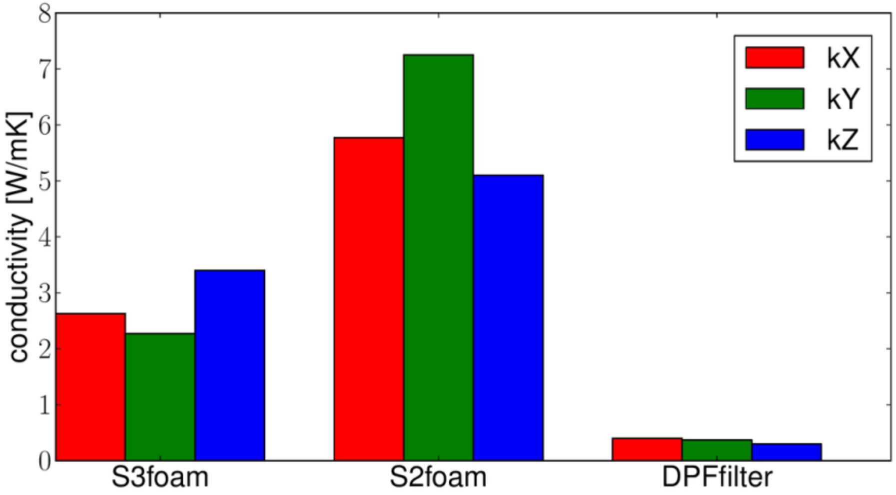
Solid conduction simulations

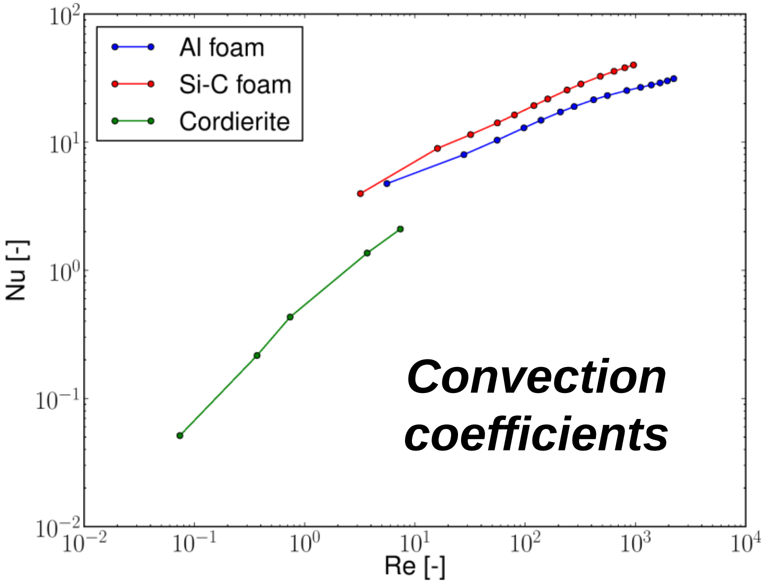


Conjugate heat-transfer simulations



Conduction coefficients

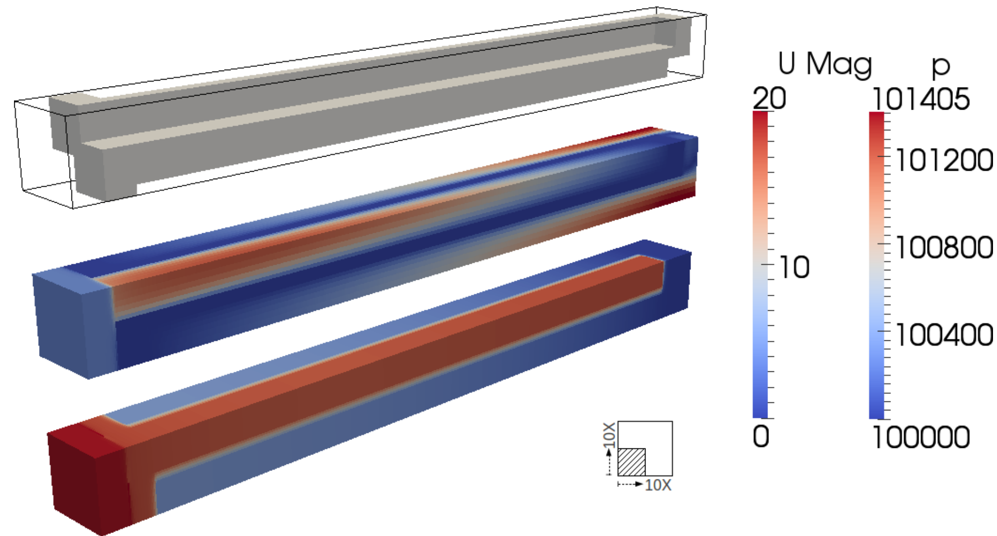


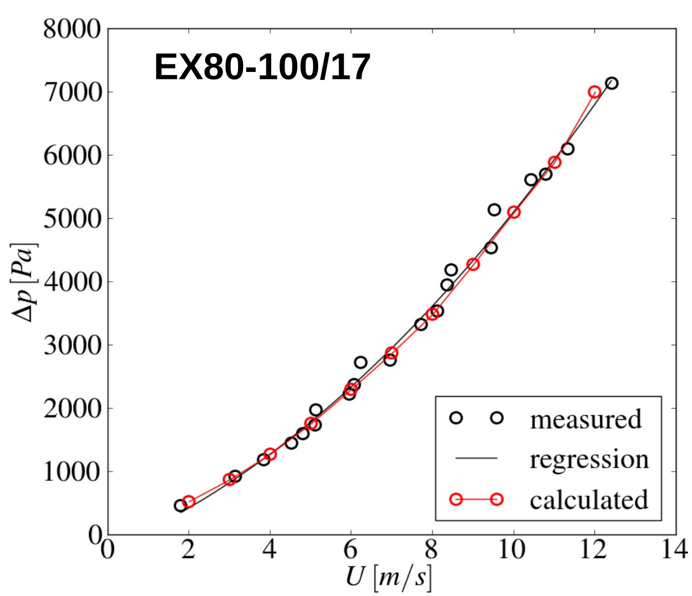


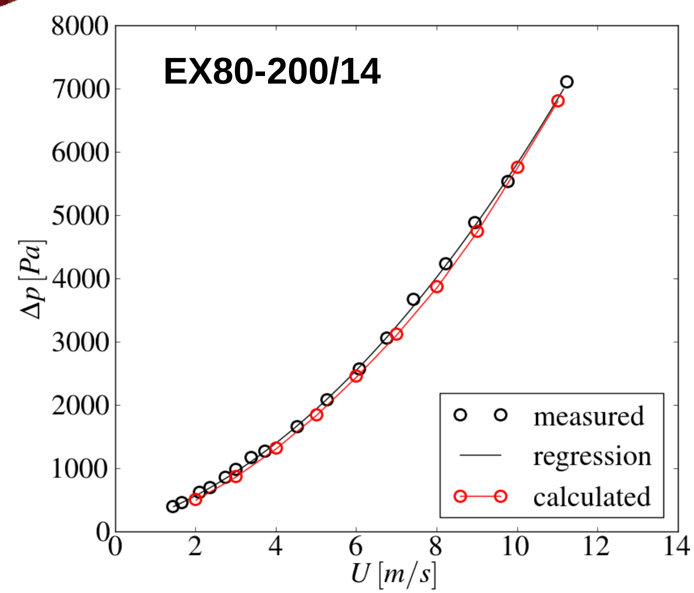
Convection coefficients

Validation: Diesel Particulate Filter

Simulation of flow through a **couple** of **DPF channels**



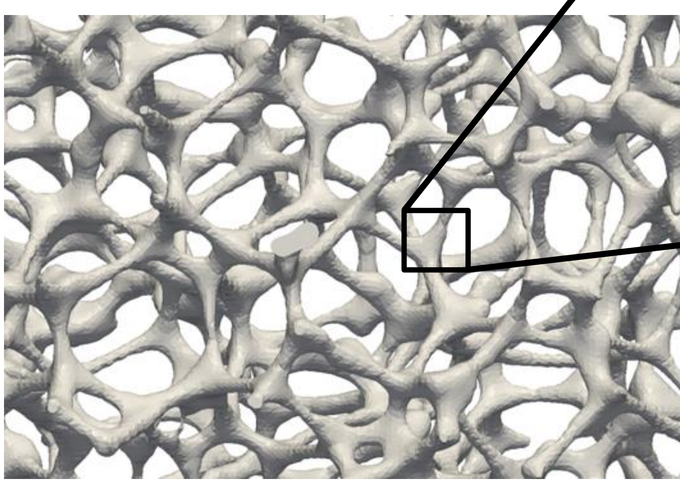


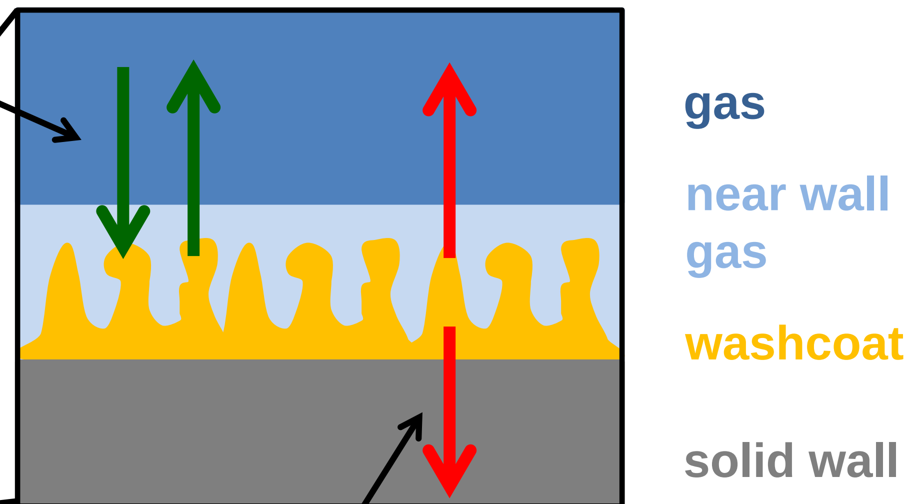


Modelling catalytic reactions

A library for the modelling of **surface reactions** has been implemented on the basis of the **OpenFOAM** code.

Mass transfer between gas phase and washcoat catalytic surface

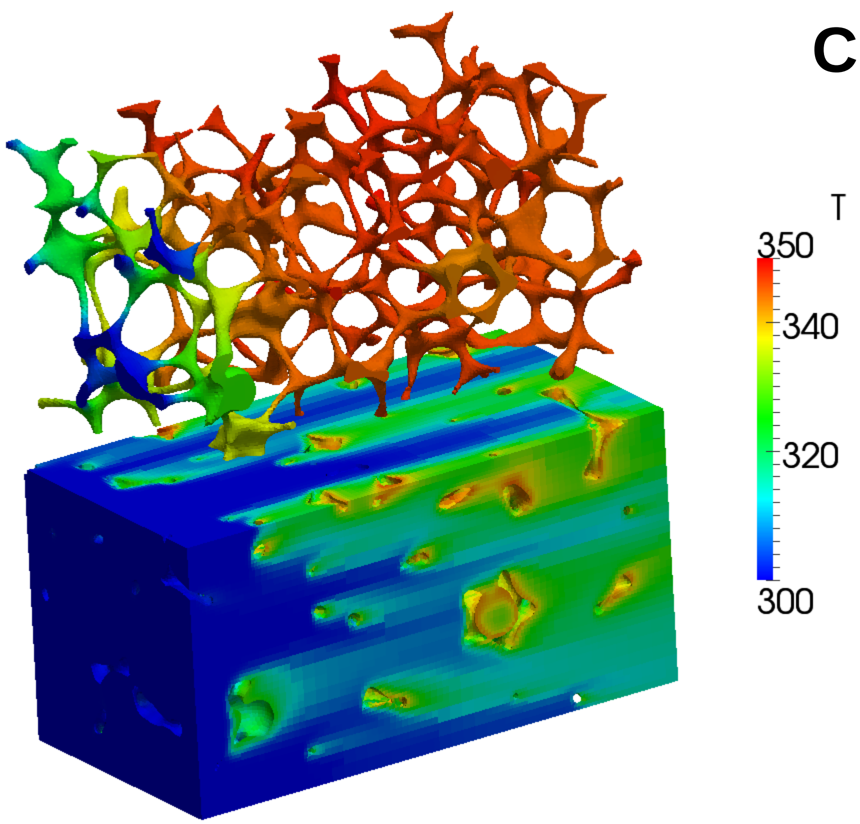




Reaction heat is released and transferred to fluid and solid phase

Reacting flow simulation

Al foam 95% porosity – 40 ppi / Micro-CT reconstruction

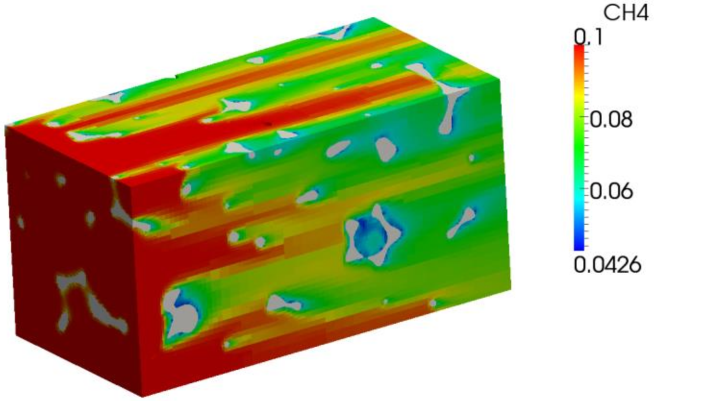


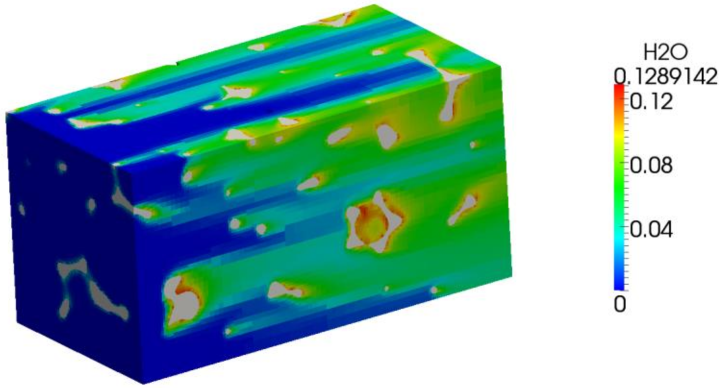
$$CH_4 + O_2 \rightarrow CO_2 + H_2O$$

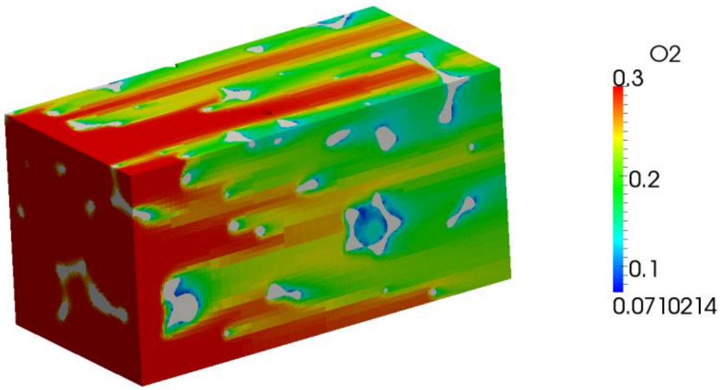
- Surface reaction on washcoat region
- Infinitely fast reaction model
- Conjugate heat transfer
- Fluid: inlet T=300K
- Solid: fixed T=300K on the inlet side, adiabatic elsewhere.

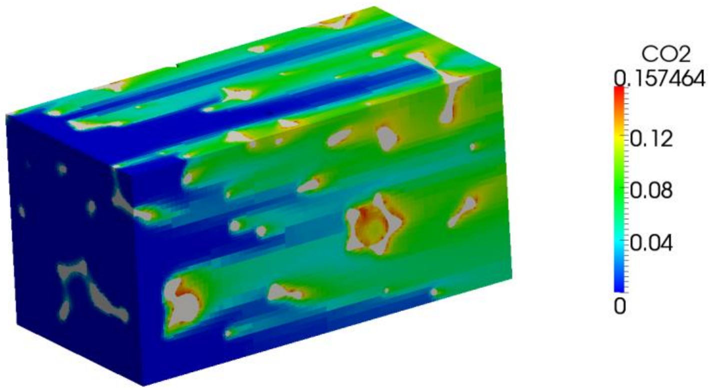
Reacting flow simulation

Al foam 95% porosity – 40 ppi / Micro-CT reconstruction

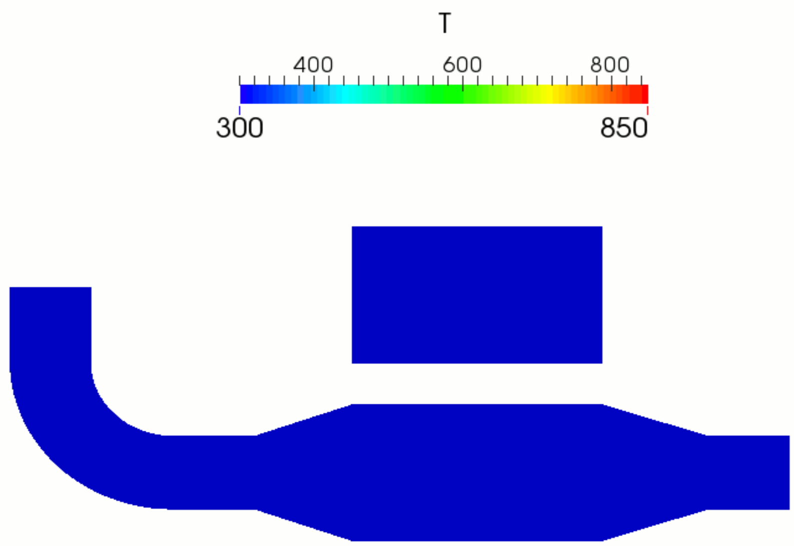


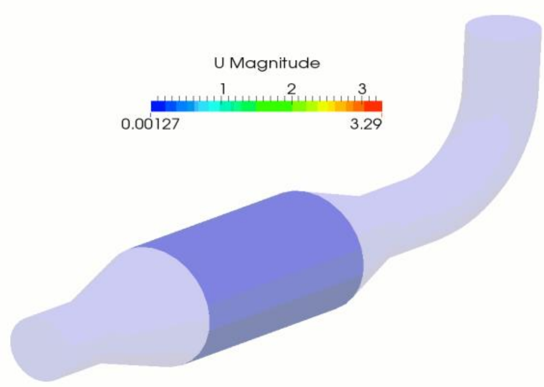






Application example: TWC





CO oxidation

$CO+0.5O_2 \rightarrow CO_2$

H_2 oxidation

$H_2+0.5O_2 \rightarrow H_2O$

HC oxidation

$C_3H_6 + 3O_2 \rightarrow 3CO_2 + 6H_2O$

NO_x reduction

$CO+NO \rightarrow CO_2+0.5N_2$

$H_2+NO \rightarrow H_2O + 0.5N_2$

Steam water reforming

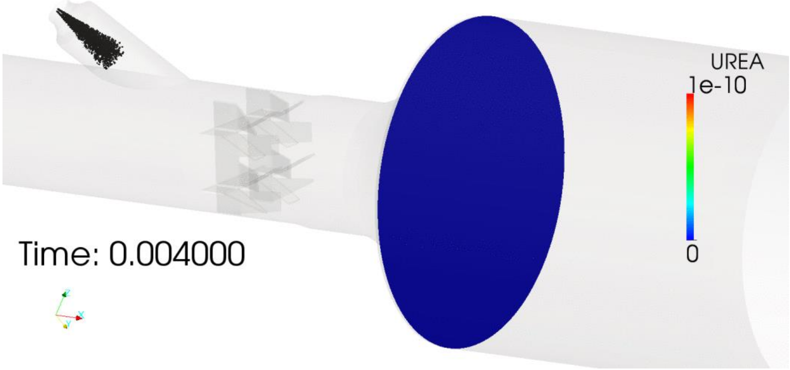
$CO+H_2O \rightarrow CO_2 + H_2$

$C_3H_6 + 3H_2O \rightarrow 3CO_2 + 6H_2$

Conclusions

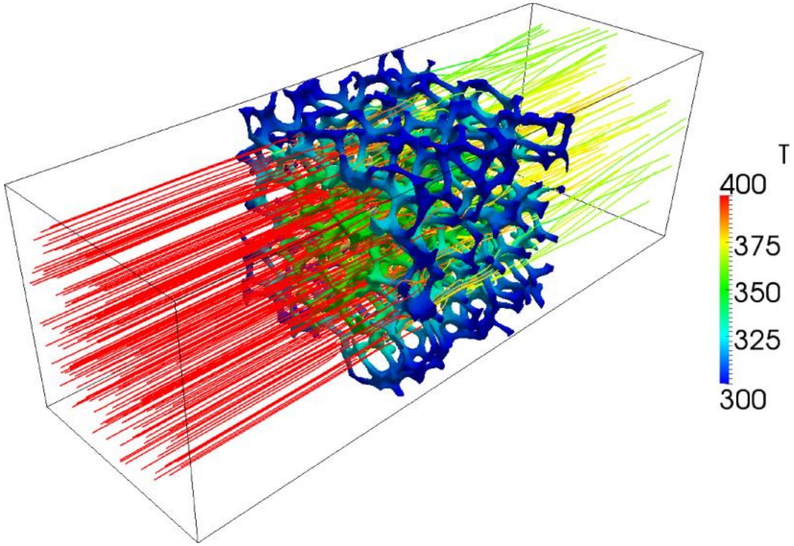
CFD models (both 1D and 3D) represent **robust tools** to investigate the behavior of after-treatment systems and help the design for maximum conversion efficiency.

Our experience is focused on self-developed libraries in **GASDYN** (1D) and **OpenFOAM** (LibICE).



Conclusions

New solutions for catalytic substrates, based on **open-cell foams**, will be studied, to achieve a general improvement of **performances** (pressure loss, warm-up, precious metal loading…).



Conclusions

Thanks for your attention!

Questions?