POLITECNICO DI MILANO

Modeling Diesel after-treament systems: De-NOx with injection of urea/water solution and DPF

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Outline

Some considerations

- ICE are limited by emission regulation (US, Europe, Japan)
- Is CFD of any use in this field?
- Driving test cycles (FTP, NEDC ...) last for several seconds, 0.5 hours sometimes
- 1D for driving cycles and CFD for specific investigations and shape optimization

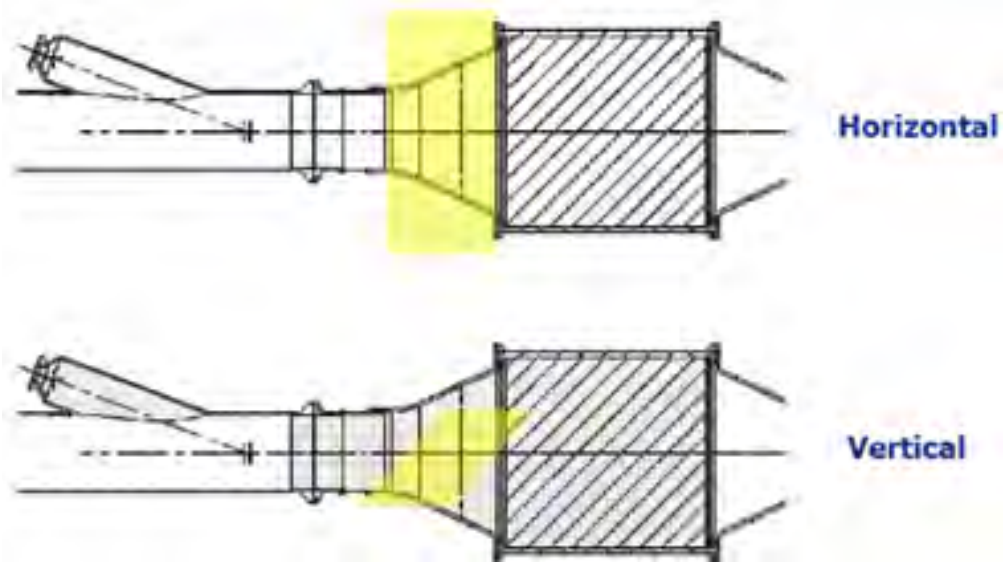
What shall we see?

- Modeling SCR systems
  - Water/Urea solution injection
  - DeNO$_x$ system
- Modeling the DPF

Analysis of mixing process

- Improve the mixer: pressure drop and mixing efficiency
- Review the literature, see what others have done in other fields and come up with some ideas...
- .... and simplify the problem
  - No spray injection
  - No wall film model
  - No chemical reactions
- An example of a typical system

Test rig



- Mist is injected inside the flow stream
- A light beam highlights the distribution of mist downstream of the mixer onto two different planes
- The best configuration can be judged on the basis of observation
- Observation is also supported by engine test bench data

Solver and assumptions

- Steady state solver for compressible flows: rhoSimpleFoam
- Added the possibility of tracking passive scalars (gaseous species such as H_2O, Urea, NH_3 and so on)
- Constant value (in time) boundary condition to reproduce fixed engine operating conditions
- The meshed geometry reproduces the mixer, the injection section, the SCR catalyst canning (without porous media) and part of the exhaust line with pipe bends

What is this all for?

- Evaluation of the pressure drop
- Estimation of the mixing efficiency

The calculation are compared to experimental results

Post processing regions

- Two sections oriented along the axis to evaluate and visualize the ”urea” distribution

- The distribution of urea is evaluated by the Uniformity Index

$$\mathbf{UI} = 1 - \frac{\sum \left(\bar{\mathbf{Y}} - \mathbf{Y}_i \right) A_i}{2 \bar{\mathbf{Y}} A}$$

- `faceZone` defined during mesh generation and run time plotting of UI
- Run time selection of UI according to different definitions available in the literature

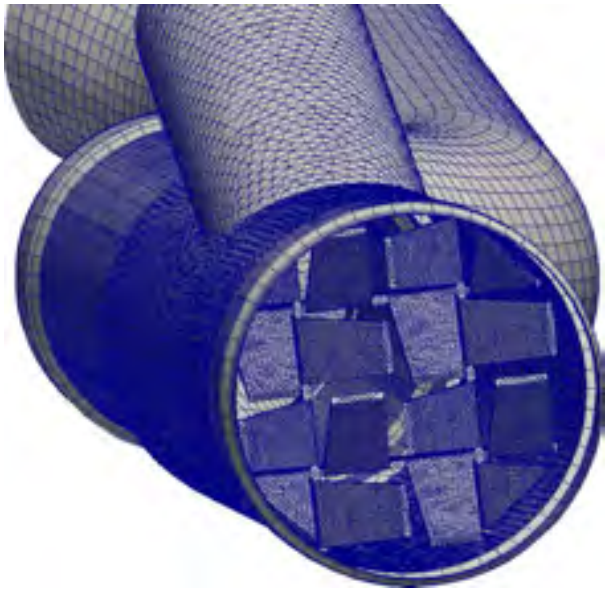
How to optimize?

- First of all we invent something (light bulb or see what is on the planet and get the best out of it)
- Prepare the mesh
- Run the simulations
- Have a look at the results

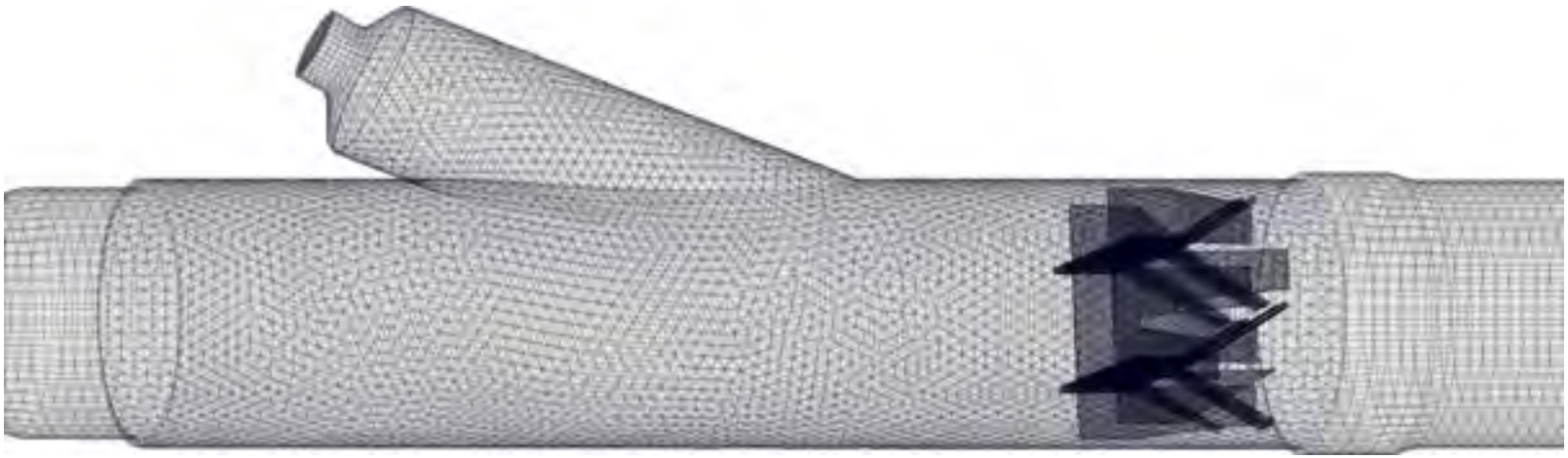
Are the results satisfying?

YES	NO
Then the configuration is promising Let's try to optimize it RBF optimization may become handy	Then it's good for the trash bin

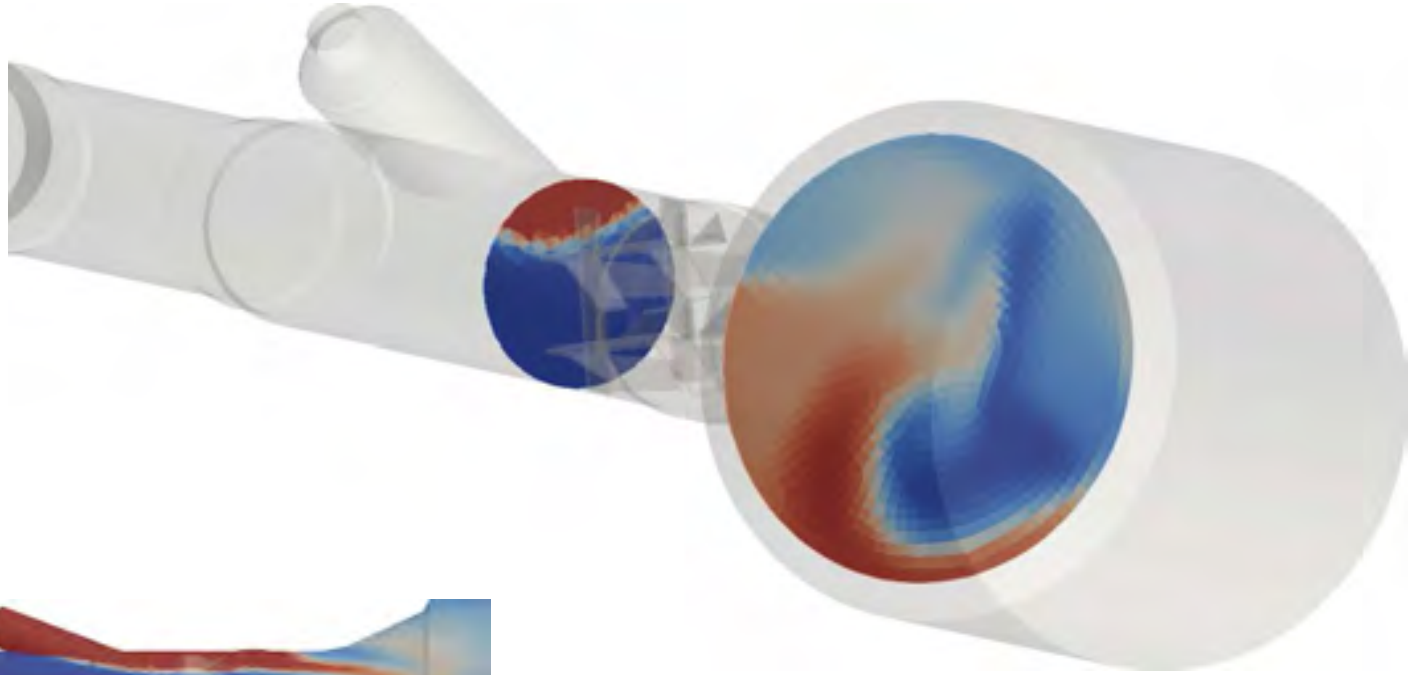
Example of mixer configuration

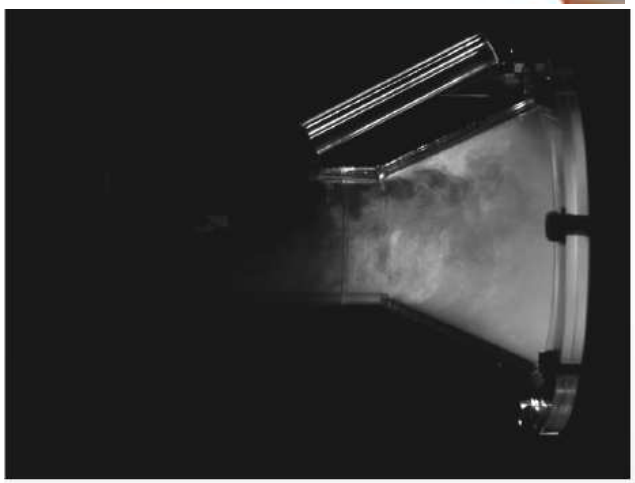


- Benchmark for the best compromise between pressure drop and mixing efficiency
- Currently mounted on exhaust systems



Example of mixer configuration

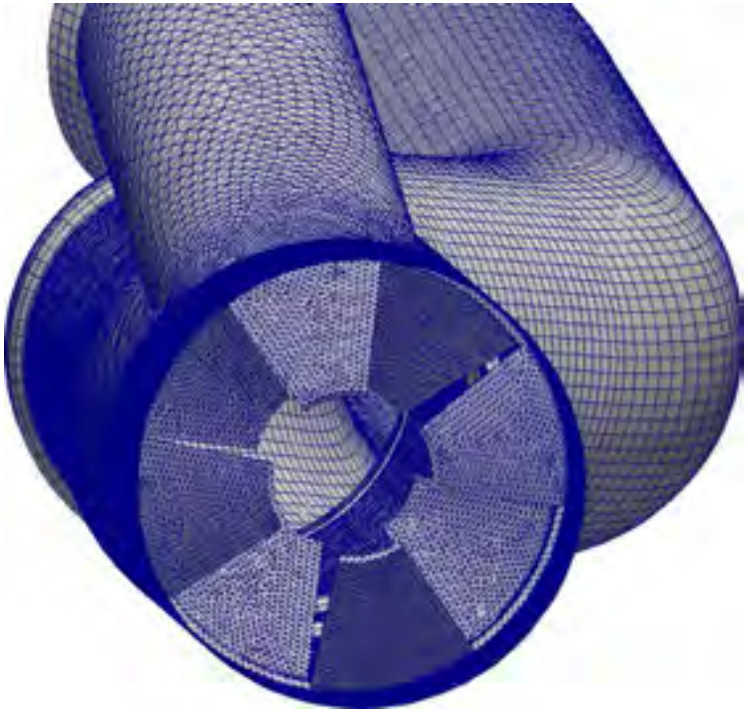




Considerations

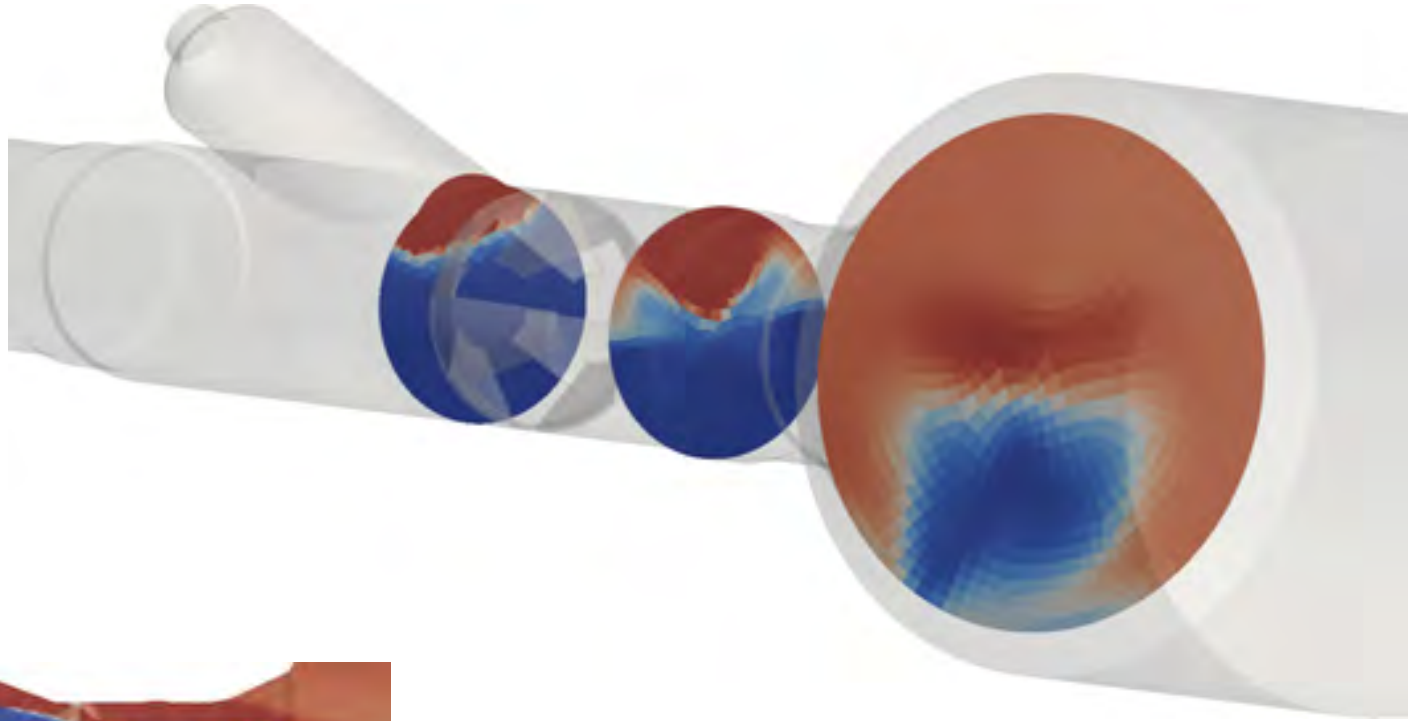
- The mixing efficiency can be regarded as good
- However there is a region where ”Urea” is not present

Example of mixer configuration



- This configuration shows a limited pressure drop and average mixing properties
- Hybrid mesh: tets + hex

Example of mixer configuration

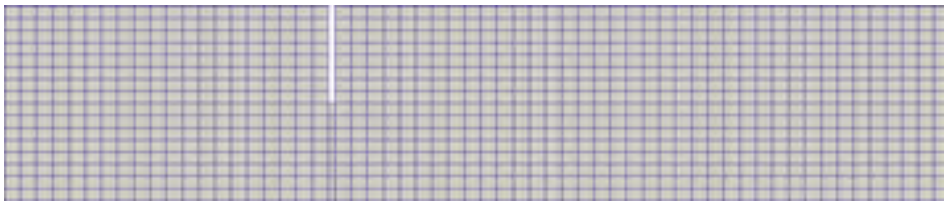


Considerations

- The distribution of Urea at the catalyst inlet can be considered good, with the exception of a small portion
- Similar effect can be noted at the experimental rig

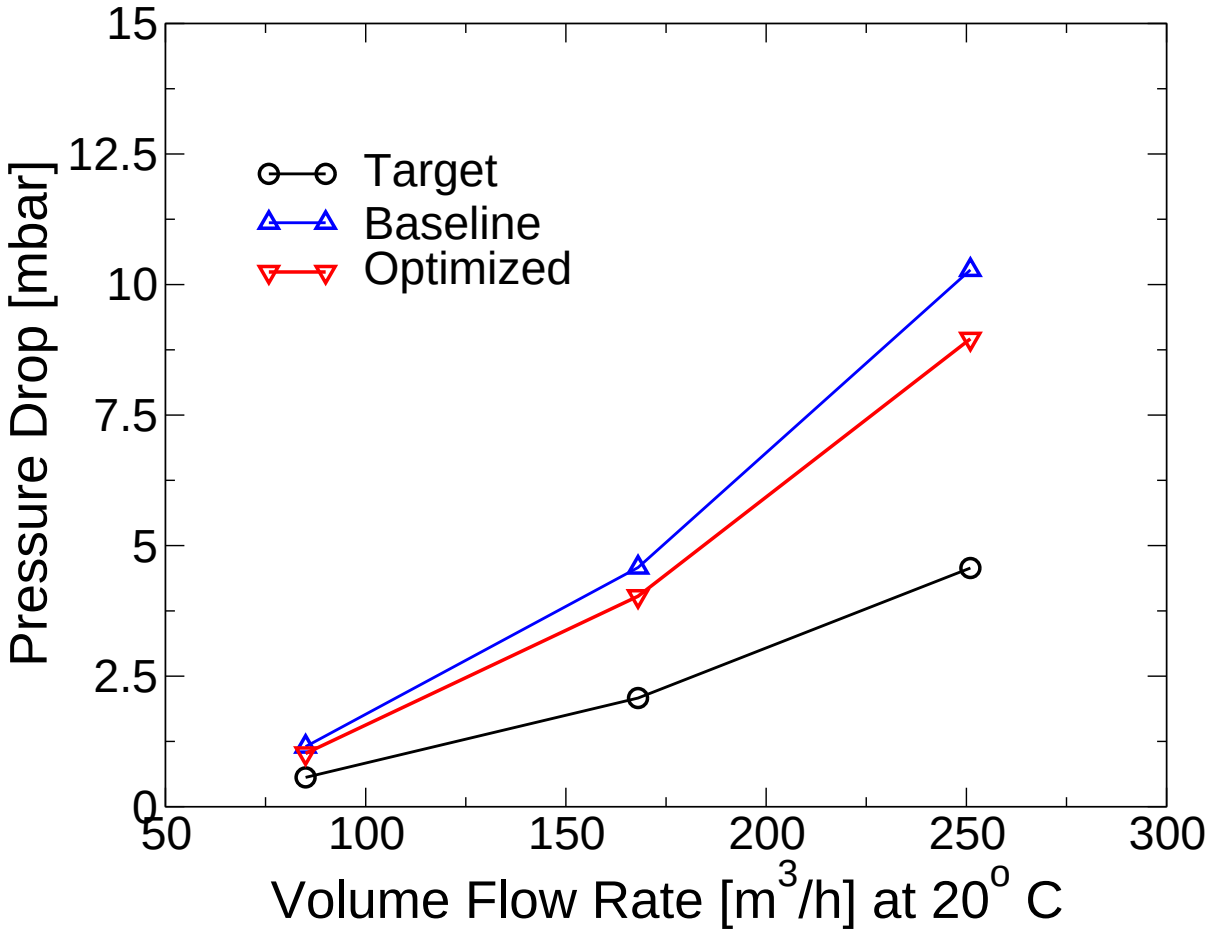
RBF shape optimization

- Radial basis function are used for the interpolation scheme adopted to deform the mesh
- The mesh is then deformed according to the definition of control points (like pinching and stretching a net)
- Simplex optimization algorithm with one parameter is used



- 3D geometry example

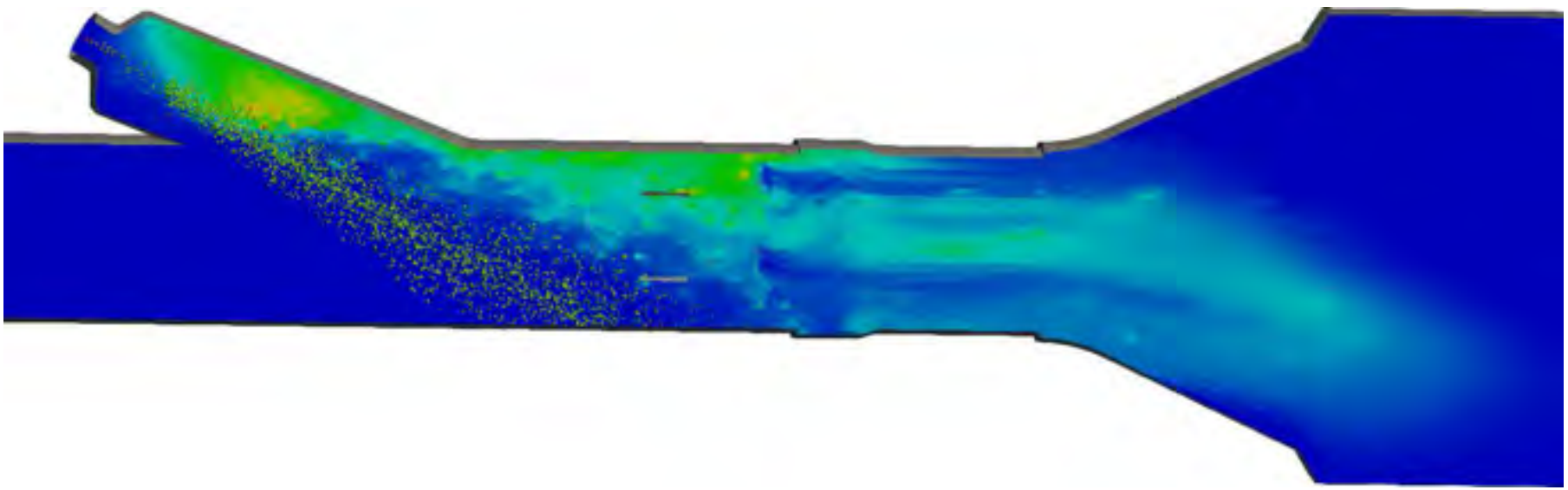
Optimized configuration



- Comparison between pressure loss of baseline and optimized configurations

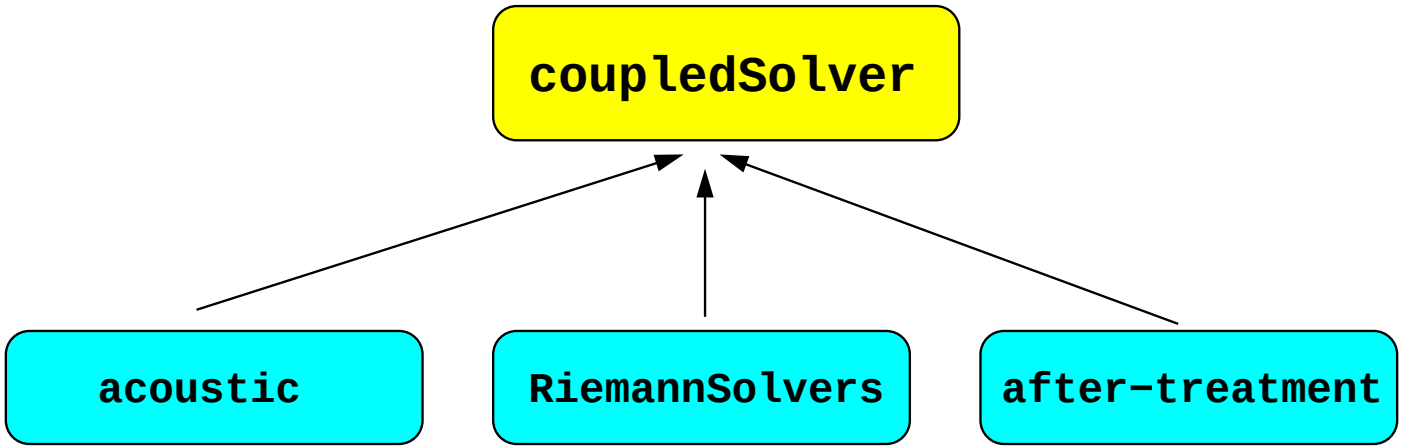
Getting close to real operating conditions

- The mixer configuration is tested with urea solution injection
- Wall film formation is not considered to speed up the calculation.
- The droplet impacting the wall is supposed to instantly evaporate. However only a fraction of the droplet will evaporate, the remaining liquid mass is deleted. This will reproduce a steady state liquid film.



... a little closer

Generalized external solver interface (class `coupledSolver`)



- Analysis of the mixing efficiency under real operating condition resorting to 1D-3D coupling:
  - Pulsating flow
  - Eventual backflows (possible for 4 cylinder engines)
  - Temperature discontinuities
- Wall film of multicomponent liquid mixtures with the functionality of predicting the formation of solid deposits
- Specific boundary condition to simulate the wall cooling effect due to the impact of the liquid jet on the pipe walls

SCR systems modeling

The chemical and physical processes taken into account are:

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

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

Numerical models

- The solver (`scrFoam`) implemented is an unsteady flow solver which considers Lagrangian transport of particles and accounts for the advection of information about the gas chemical composition

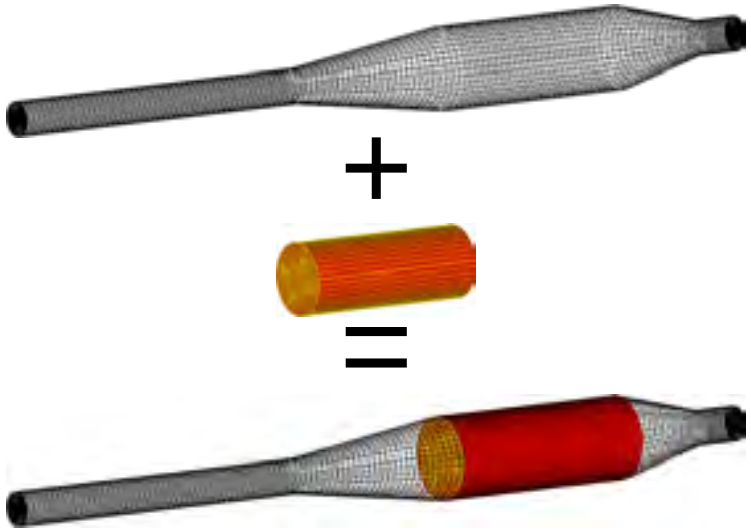
$$\frac{\partial (\rho \mathbf{Y}_i)}{\partial t} + \nabla \cdot (\rho \mathbf{U} \mathbf{Y}_i) + \dot{\omega}_i + \dot{Sp}_i = 0$$

- The source term $\dot{\omega}_i$ accounts for the chemical reactions contribution while $\dot{Sp}_i$ accounts for the mass coming from the spray evaporation

- Chemistry integration is operated recurring to an ODE solver based on to the SIBS method

$$\dot{\omega}_i = \frac{1}{\Delta t} \int_t^{t+\Delta t} \dot{\mathbf{Y}}_i (\mathbf{Y}_i, T, p)\, dt = \frac{\mathbf{Y}_i^{t+\Delta t} - \mathbf{Y}_i^t}{\Delta t}$$

Reacting region



- A reacting region has been defined within the fluid region having specific properties in terms of:
  - flow resistance (flow through a porous media)
  - chemical reactions
  - substrate properties
- The reaction heat is included as a source term in the heat balance of the substrate mesh
- Heat transfer coefficient has been corrected to account for the heat exchange between the gas and the substrate

Reacting region

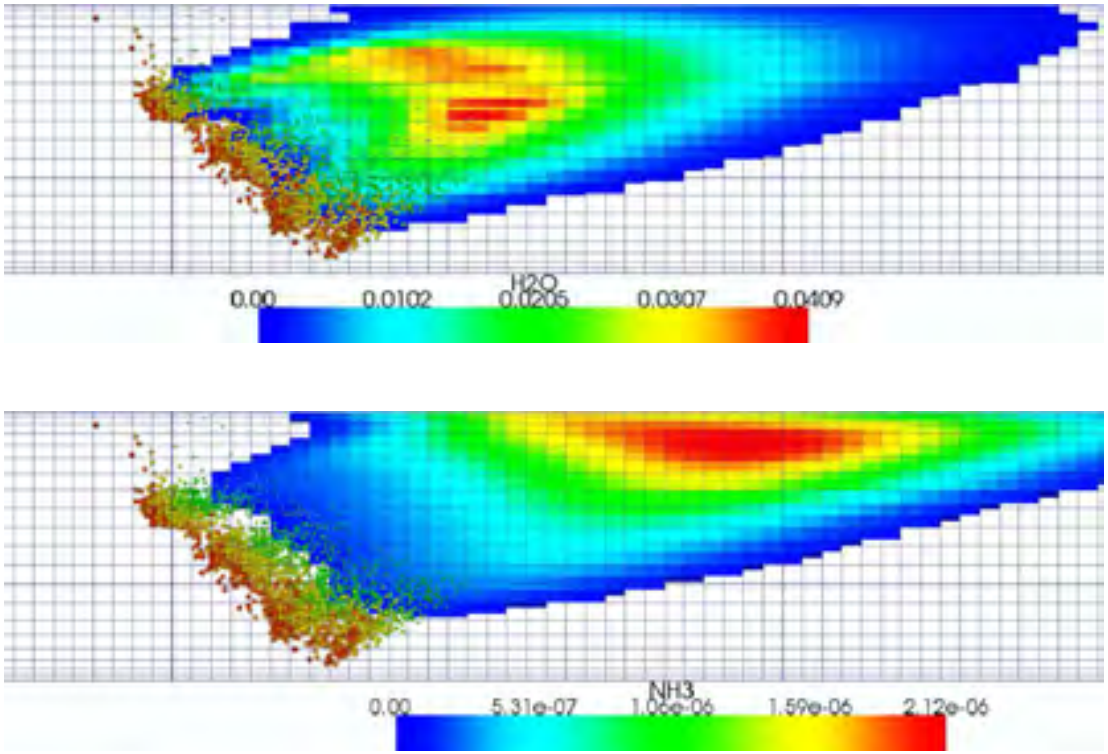
- Properties of each `reactingZone` are read from a dictionary file

```
monolithType    square;
cellDensity     62.0;
wallThickness   0.0000101;
voidFraction    0.1;
...             ...


adsorbedSpecies
2
(
    NH3
    O2
);
```

```
adsorptionModelNH3
{
    adsorptionCapacity 100;
    surfaceCoverageDepPar 0.5;
    k_ads  1.0;
    E_ads  2.0;
    k_des  3.0;
    E_des  4.0;
}

adsorptionModelO2
{...}
```

- Reactions for each zone are referenced by zone name and are defined using the `FOAMChemistryReader` format

Urea spray



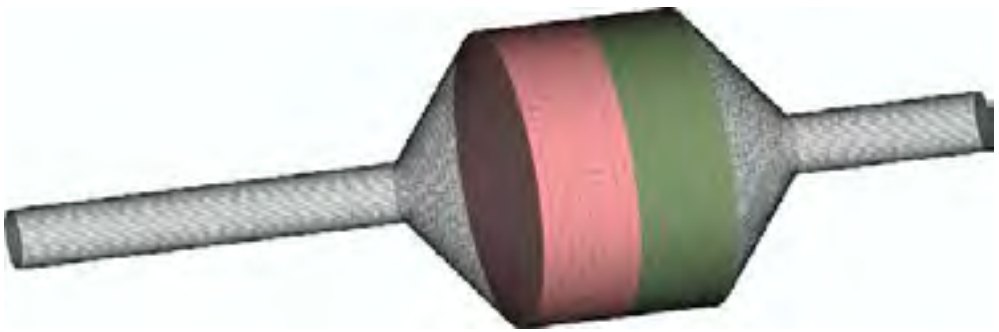
- Urea is modeled as a liquid fraction of the droplet and the properties of the liquid droplets are calculated accounting for the two different fractions
- Liquid urea properties have been added in oder to account for AdBlue or urea solutions injection with different mass fraction ratio
- Inclusion of chemistry to model the thermal decomposition of urea particles into HNCO and NH_3

Kinetic model: thermolysis and hydrolysis

- The hydrolysis and ammonia oxidation processes have been modeled on the basis of the work of Yim et al.

$A \xrightarrow{k_1} B + C$	Urea decomposition	$r_A = k_1 C_A$
$B + W \xrightarrow{k_2} C + D$	Hydrolysis	$r_B = k_2 C_B C_W$
$C \xrightarrow{k_3} N + E$	Ammonia oxidation	$r_C = k_3 C_C$

- Surface chemistry is solved only in region where reactions are supposed to occur: active sites
- S_{act} accounts or the properties of the substrate and washcoat loading as a cell property



$$k_i = A_i \exp\left[\frac{E}{RT}\right] S_{act}$$

Kinetic model: SCR

- Certain reactions depend on the surface coverage of certain reactants: NH_3 for example, in the case of SCR reactors, or O_2 in case of TWC.
- The reactants are usually adsorbed/stored and desorbed/released by and from the surface of the reactor according to specific reaction schemes.
- The global reaction will be affected by the degree of coverage of the surface with respect the highest adsorption/storage capacity of the reactor.

SOLID PHASE BALANCE

$$\Omega \frac{\delta \theta}{\delta t} = (r_{des} - r_{ads} - r_{ox} - r_{NO})$$

$$r_{ads} = k^0_{ads} C_{NH_3} (1 - \theta)$$

$$r_{des} = k^0_{des} \exp\left[-\frac{E^0_{des}}{RT}(1 - \alpha\theta)\right] \cdot \theta$$

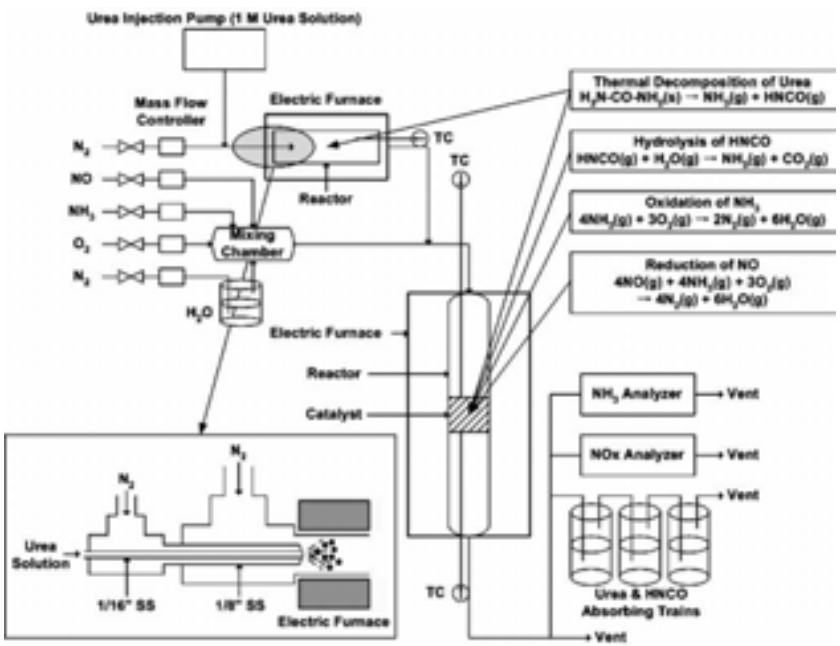
GAS PHASE BALANCE

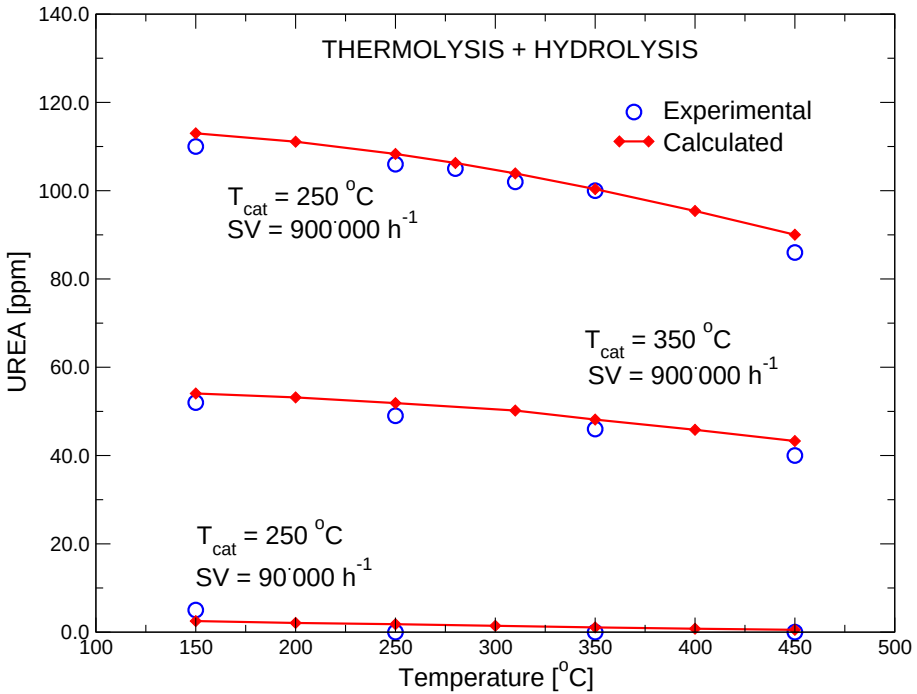
$$\dot{Y}_{NH_3} = (r_d - r_a), \qquad \dot{Y}_{NO} = \Omega r_{NO}$$

$$r_{NO} = k_{NO} \exp\left[-\frac{E^0_{NO}}{RT}\right] C_{NO} C^{\beta}_{O_2} \theta$$

$$r_{ox} = k_{ox} \exp\left[-\frac{E_{ox}}{RT}\right] \theta$$

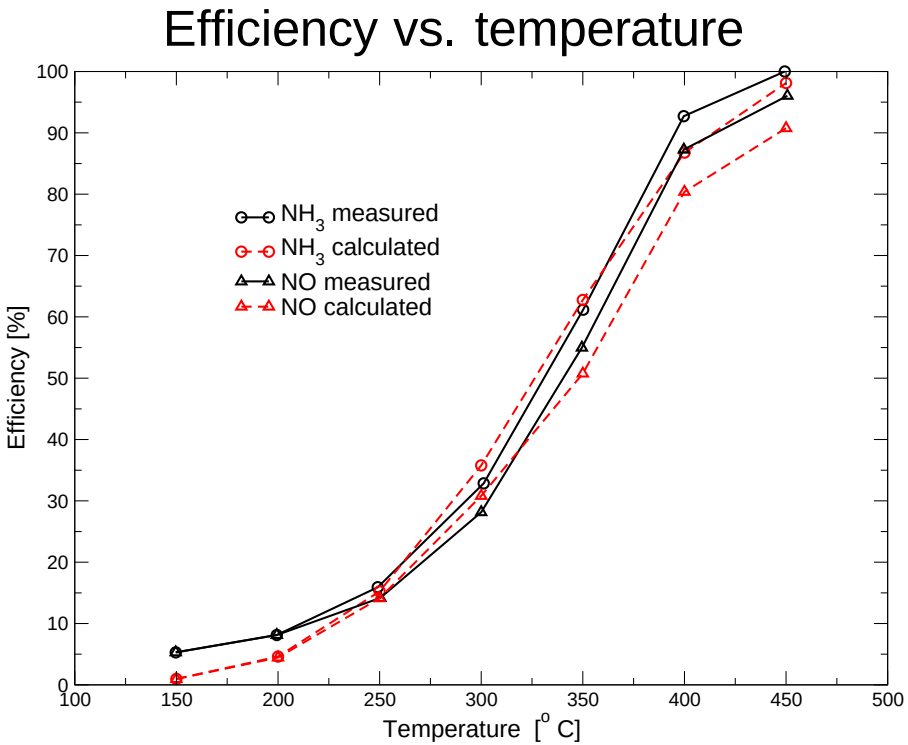
Validation: hydrolysis and thermolysis

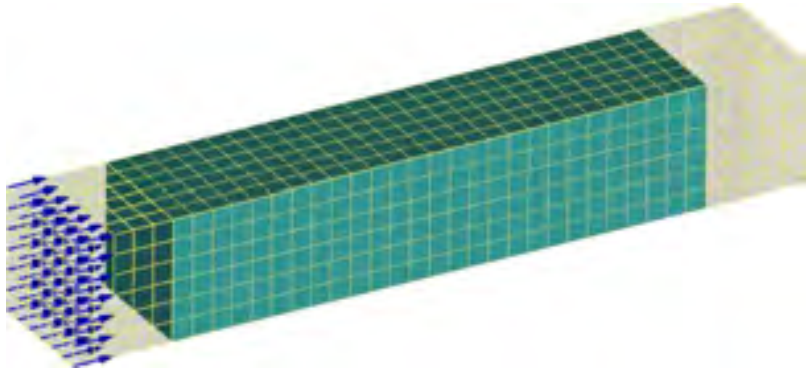


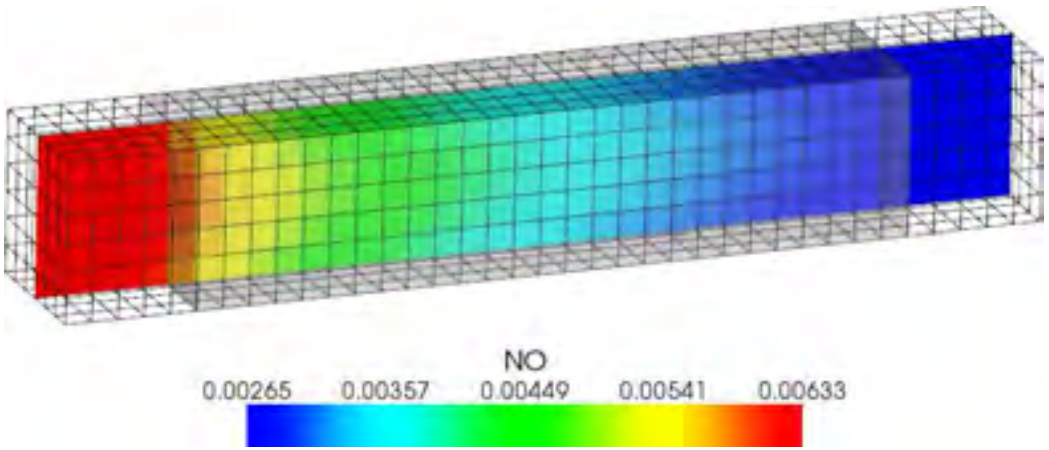


- The model has been validated resorting to measurements published in the literature on Fe-Zeolite catalysts
- The simulations have been carried out fixing the catalyst temperature on the basis of experimental data

Validation: SCR

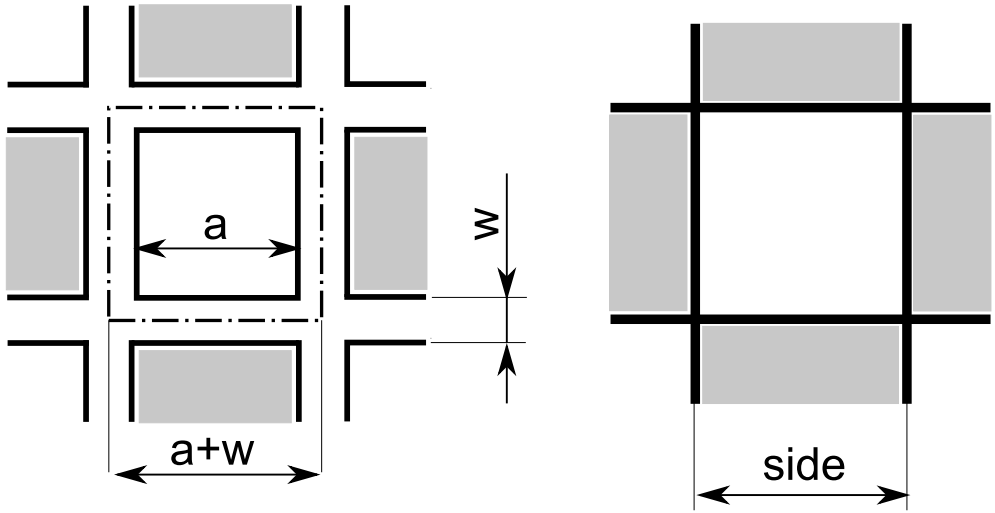




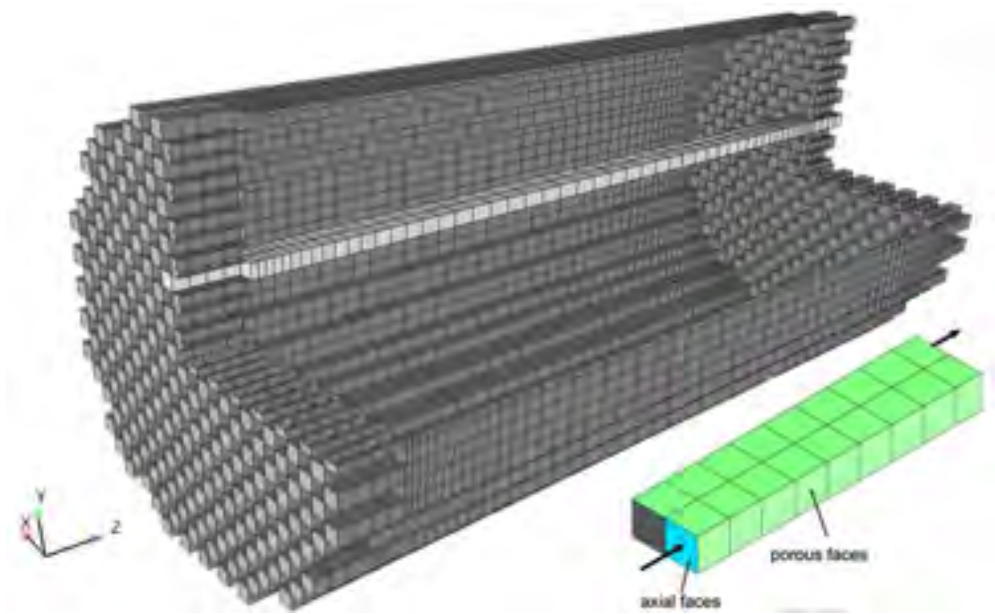


DPF Modeling by OpenFOAM® : porous face approach

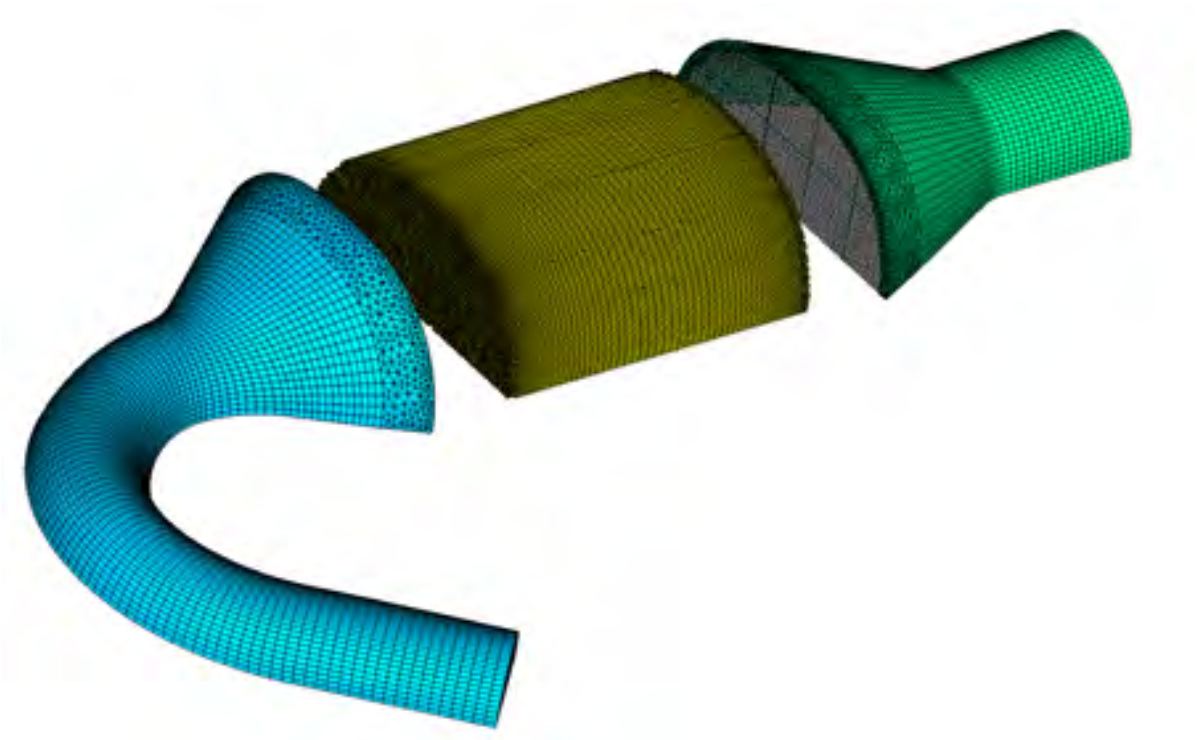
1. Porous wall characteristics defined as a cell-face property.



2. Flow field in channels is 1D: **transverse cell size = channel size**
   - **Straightforward mesh generation** of the filter, easier definition of the whole layout
   - **Faster simulations**, reduced number of computational cells to model

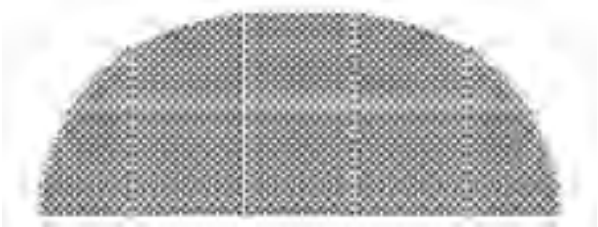


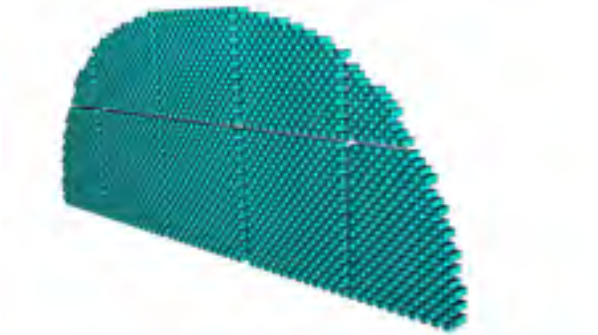
Case Setup and Automatic Mesh Handling

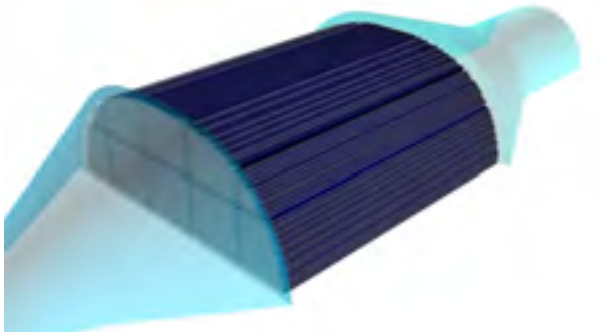


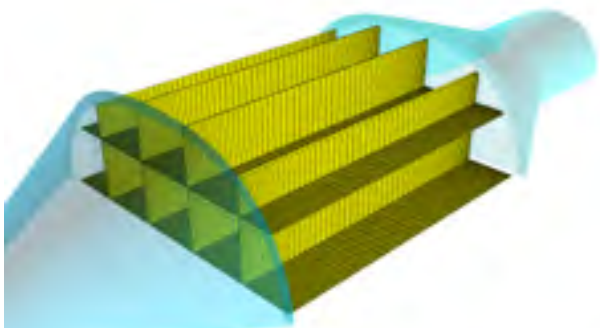
- Mesh blocks are **generated separately** by a grid generator.
- Plug-ends, filter channels and closed-ends are set up by automatically
- Blocks are merged into one block

Case Setup: Filter Monolith





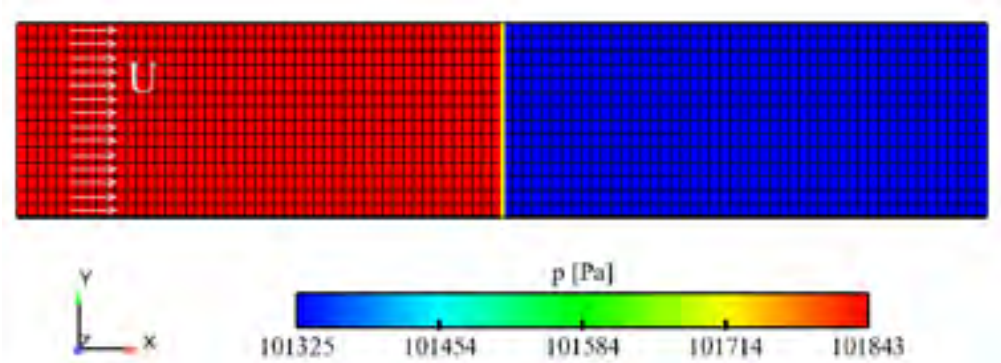




- monolith **inlet and outlet ends** show a typical open-closed “chessboard” arrangement;
- **plug ends** are automatically generated by extruding inlet and outlet ends of the monolith they have non-permeable walls and automatically grouped and set as ”walls”
- **porosity is modeled as a cell-face property**; porous walls dividing inlet and outlet channels of the monolith are grouped in a faceSet defined as ”porous”
- The **solid region** for the DPF material and the cement strips is used to **model the heat exchange to the surroundings**

New internal face condition: porous jump

- Development and validation of a new internal face condition (`porousJump`) to model **a steady-state propagation of a sudden finite change in flow properties** within the computational domain



- `porousJump` class has been used to model **thin membranes with known velocity/pressure-drop characteristics**, by the implementation of the Darcy law
- Flow equations are solved by means of **transient-SIMPLE algorithm**
- **Validation on the basis of experimental measurements** carried out on ICE simulations

Porous jump: mathematical model

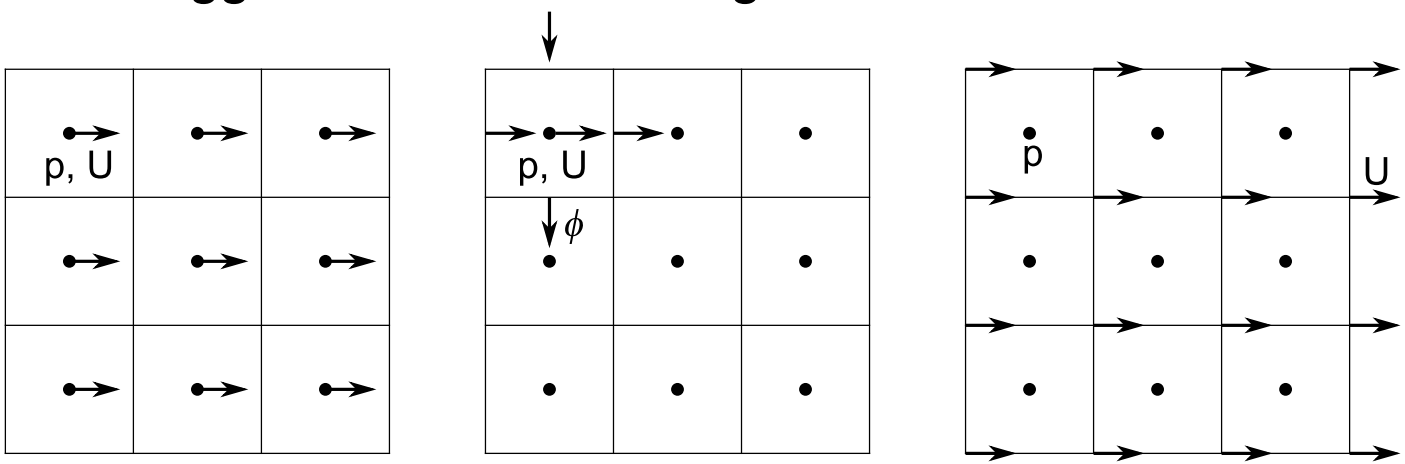
- Momentum equation for flows through porous media:

$$\int_\Omega \frac{\partial(\rho \mathbf{u})}{\partial t}\, d\Omega + \int_A \rho \mathbf{u}\mathbf{u}\cdot\mathbf{n}\, dA = -\int_\Omega \nabla p\, d\Omega + \int_\Omega \nabla\cdot\boldsymbol{\sigma}\, d\Omega + \int_\Omega \rho\mathbf{g}\, d\Omega + \mathbf{S}$$

- **S** is the **porous sink term** (Darcy + Forchheimer):

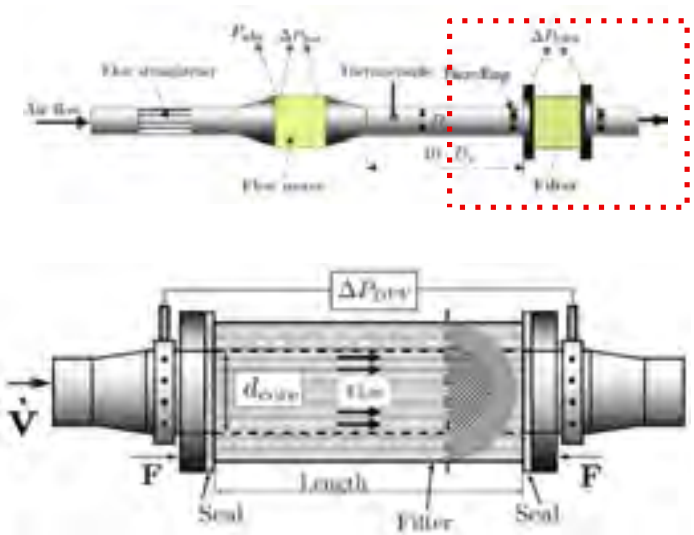
$$\mathbf{S} = \sum_{i=1}^{n_{por}} \left(\frac{\mu \cdot w_s}{k_p} \mathbf{u}_{f_i \perp} + \frac{1}{2}\beta\rho\mathbf{u}_{f_i\perp}^2 \right) A_{f_i}$$

- A surface sink term is insert it into Navier-Stokes continuous equations resorting to a **pseudo-staggered variables arrangement**

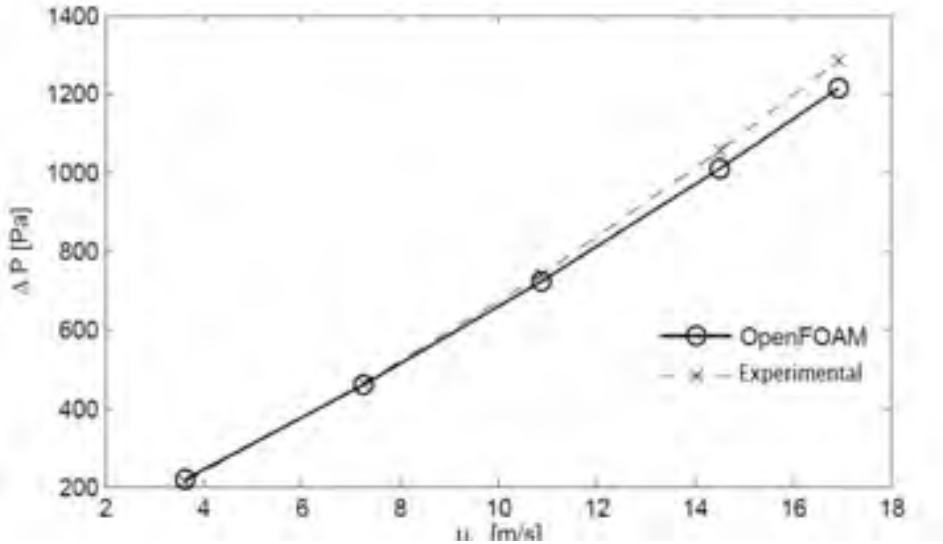


Code validation: hydrodynamics

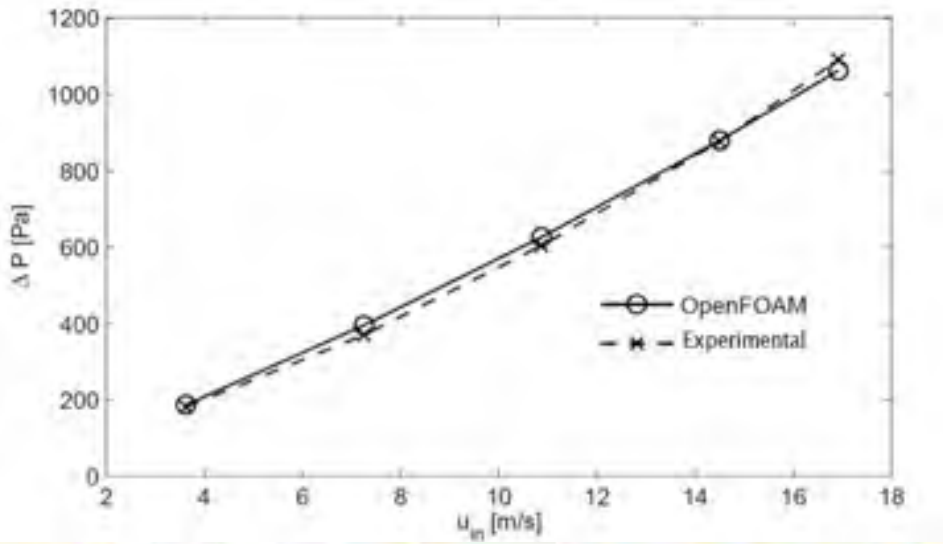
Experimental data from Masoudi et al.



monolith length: 114 mm



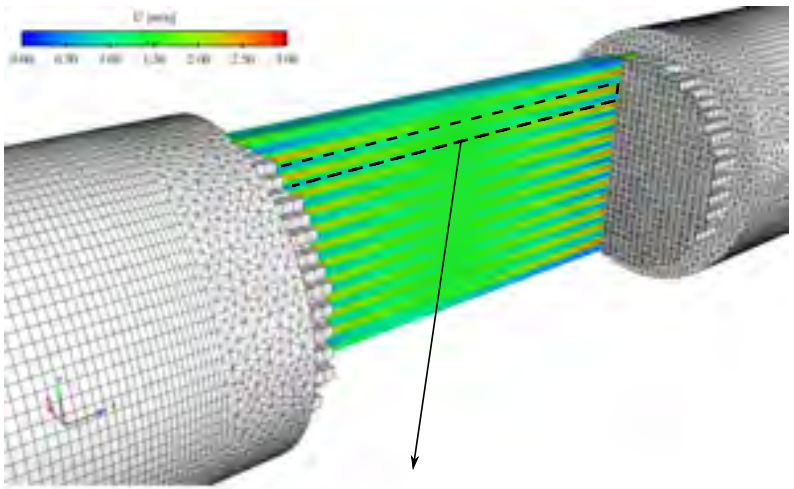
monolith lenght: 165 mm



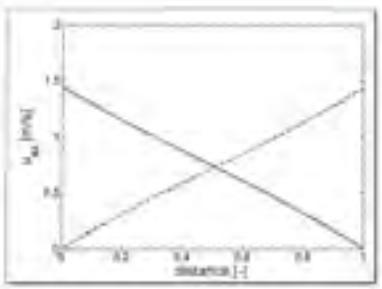
- **Flow conditions**: p_{out} = 101325 Pa, T = 300 K
- **Clean trap permeability** of the porous medium $k_p = 8.2 \cdot 10^{-13}\ m^2$,
- k_p **was kept constant** as the inlet flow rate was varied through the simulations

Code validation: hydrodynamics

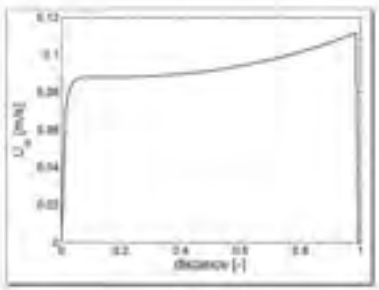
Velocity field



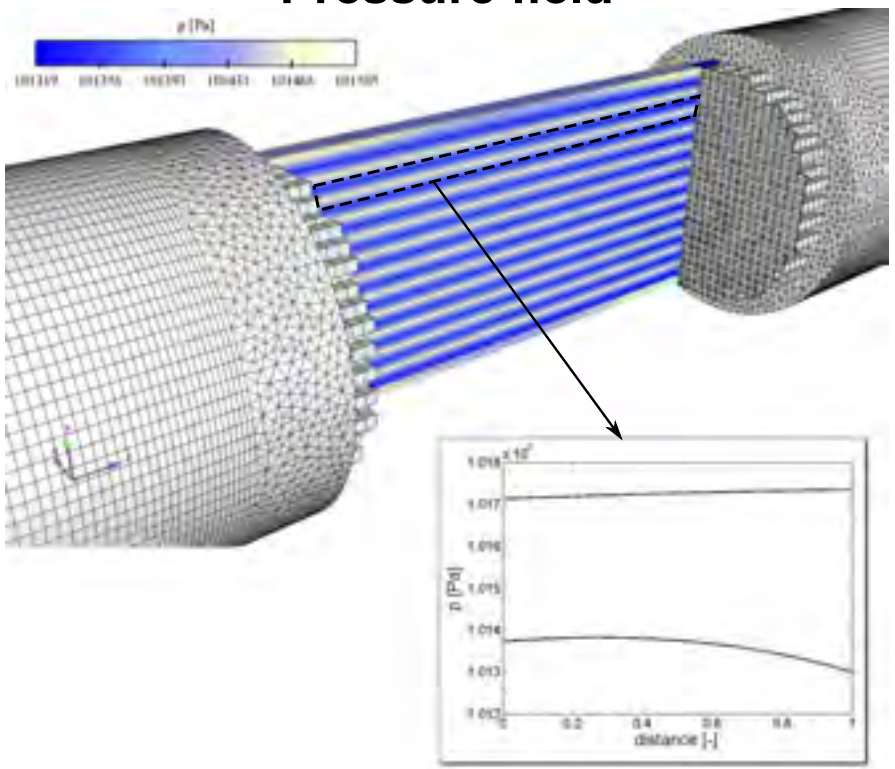
Axial Velocity



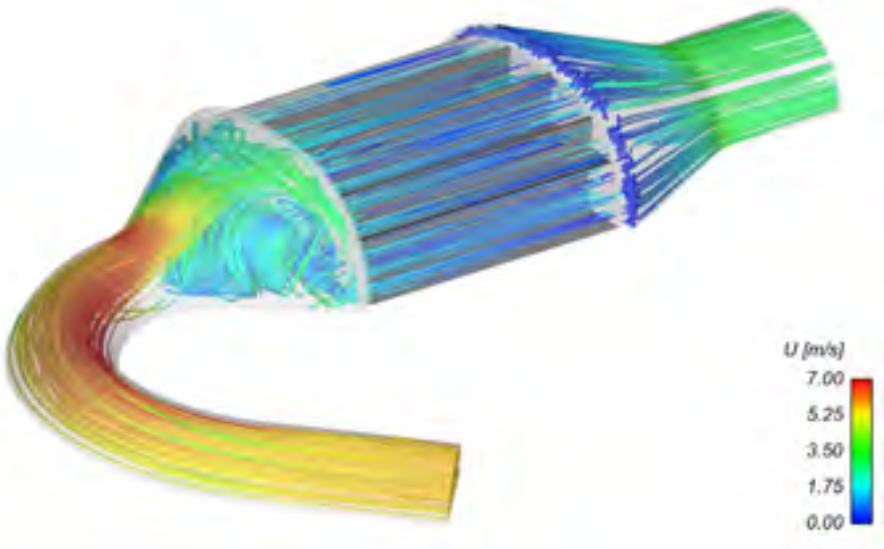
Wallflow Velocity

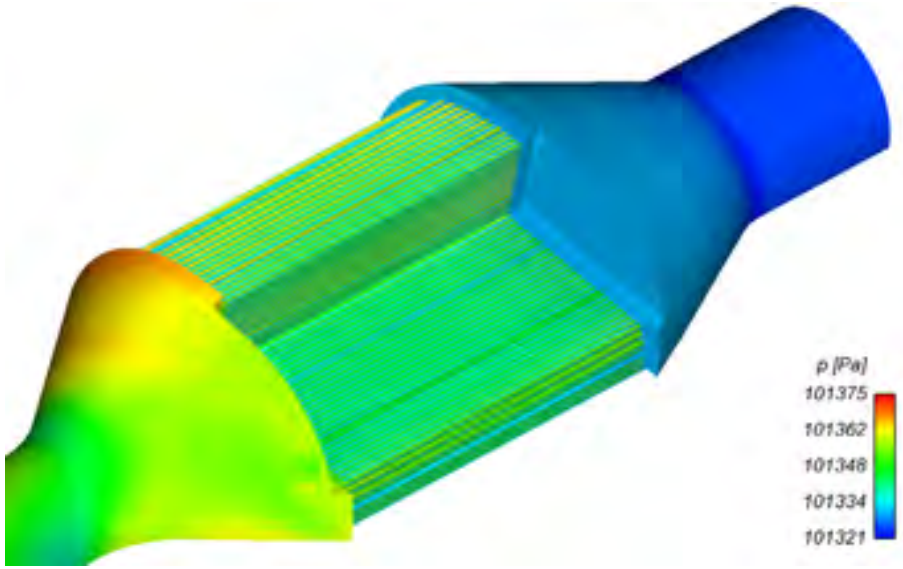


Pressure field

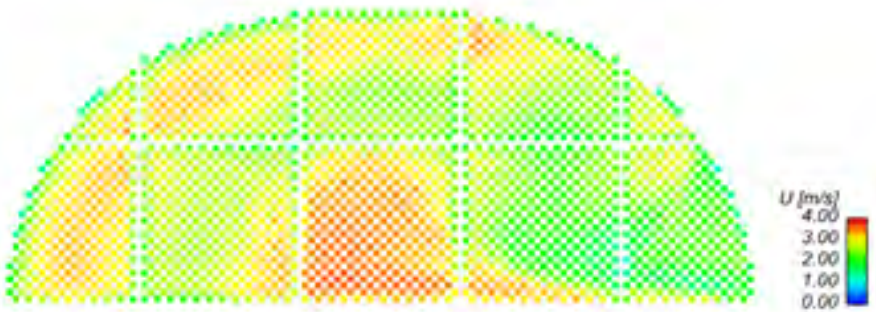


Non-uniform distribution of the flow at filter ends

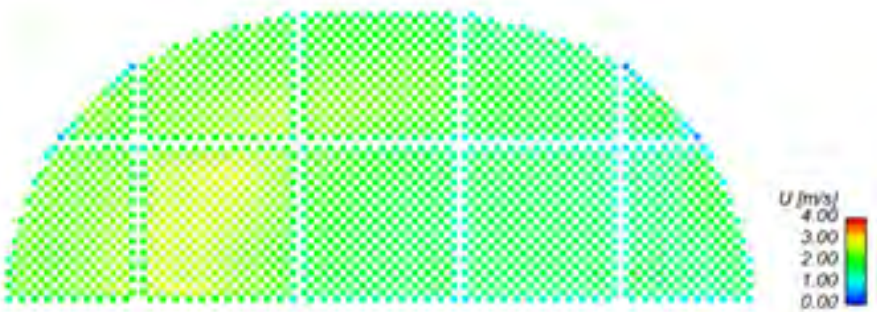




Velocity distribution on the filter inlet plane



Velocity distribution on the filter outlet plane



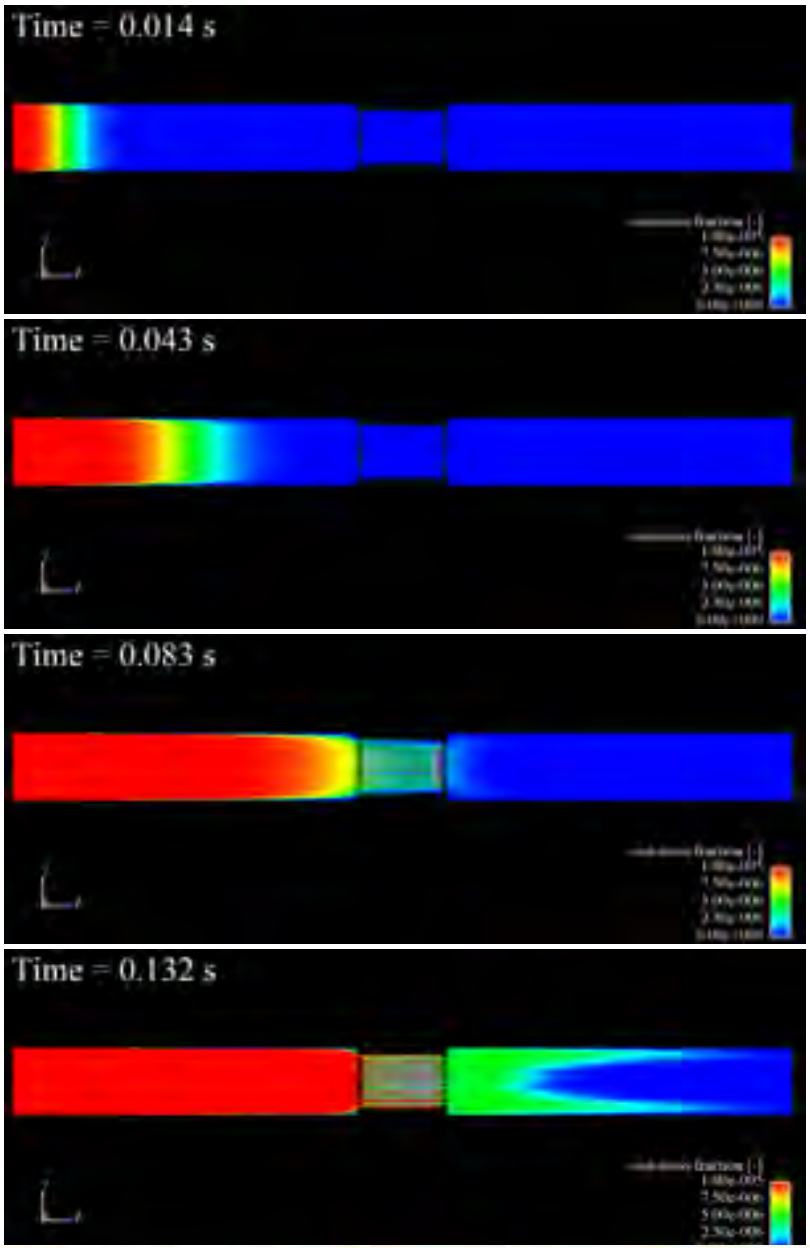
Soot transport and deposition

- Soot is transported as a passive scalar: Stokes number of soot particles in engine exhaust gas flow is very low ($\mathrm{St} < 10^{-4}$);

$$\frac{\partial(\rho \mathbf{Y})}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{u} \mathbf{Y}) + \mathbf{D} = 0$$

- Soot is removed by an implicit sink term **D** applied on porous faces ;

- The trapped soot particles change the collection efficiency and filter resistance



Conclusions

The latest development of the Lib-ICE library for aftertreatment simulation have been presented:

- **SCR simulation**
  - SCR modeled as a volume zone with specified properties
  - Lagrangian transport of water/urea droplets
  - ad-hoc kinetic chemistry model
- **Diesel Particulate Filter simulation**
  - Detailed study of full-scale complete 3D geometries
  - Soot deposition model to study filter loading
- The structure of the developed classes allows the parallel simulation resulting in good scaling factor and in a remarkable reduction of the simulation runtime

Thank you for your attention!

Internal Combustion Engine
Group

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