Modeling the after-treatment system of Diesel and S.I. internal combustion engines by means of OpenFOAM

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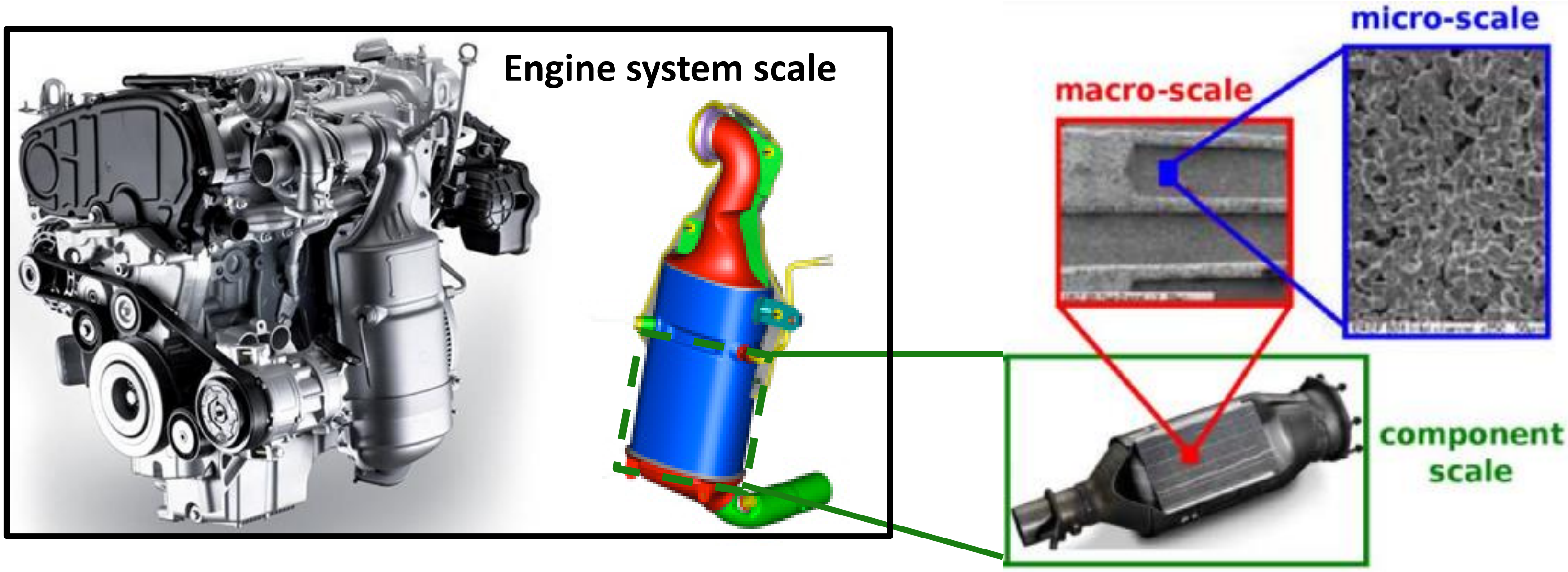
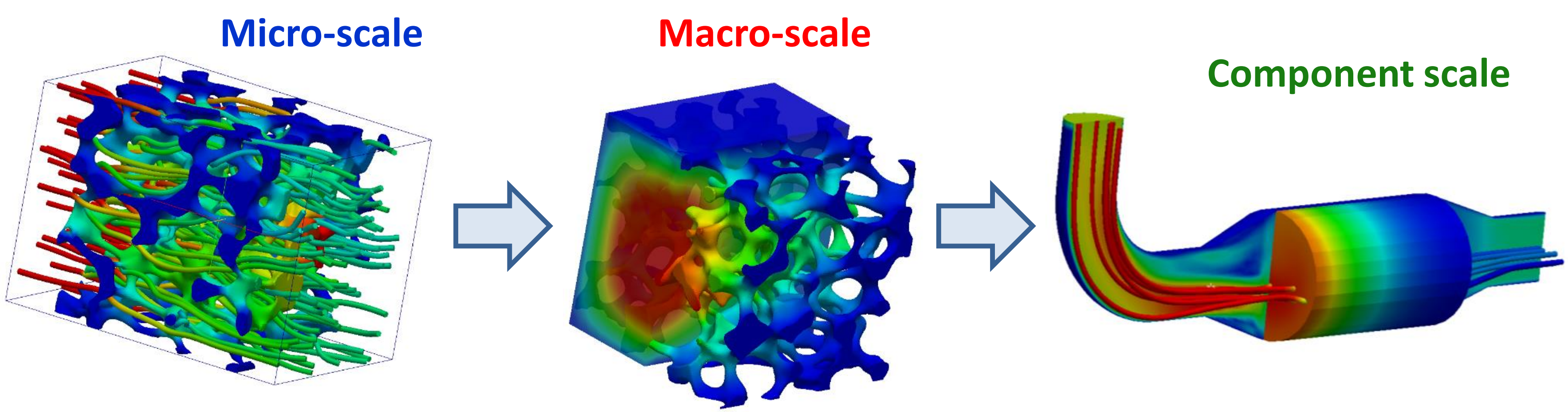
Outline

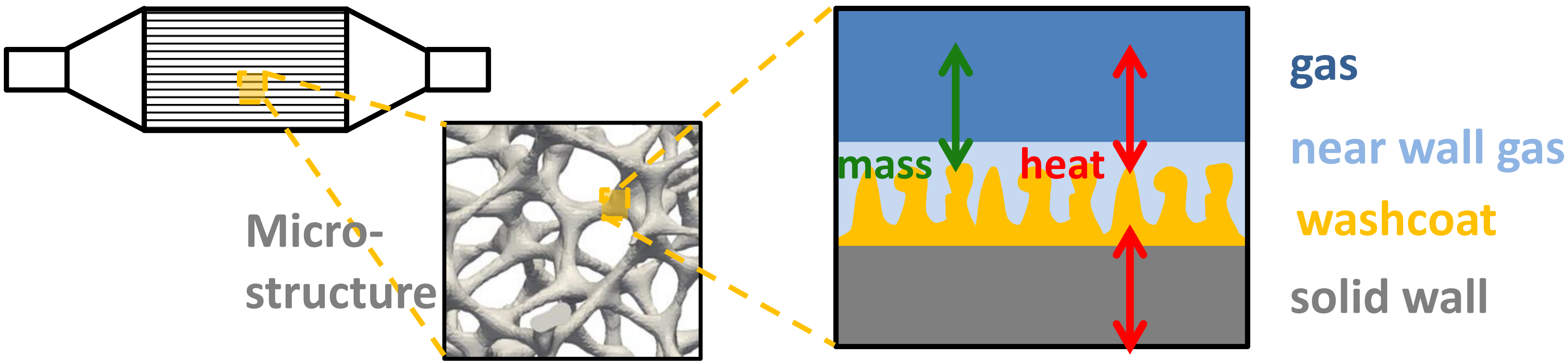
- Introduction
- Etherogeneous reaction modeling
  - microstructure (surface reaction)
  - macroscale
- Spray-wall interaction for DEF injection
  - Spray impingment: kinetic and thermal models
  - Wall film formation
- Optimization framework
- Industrial cases
- Work in progress

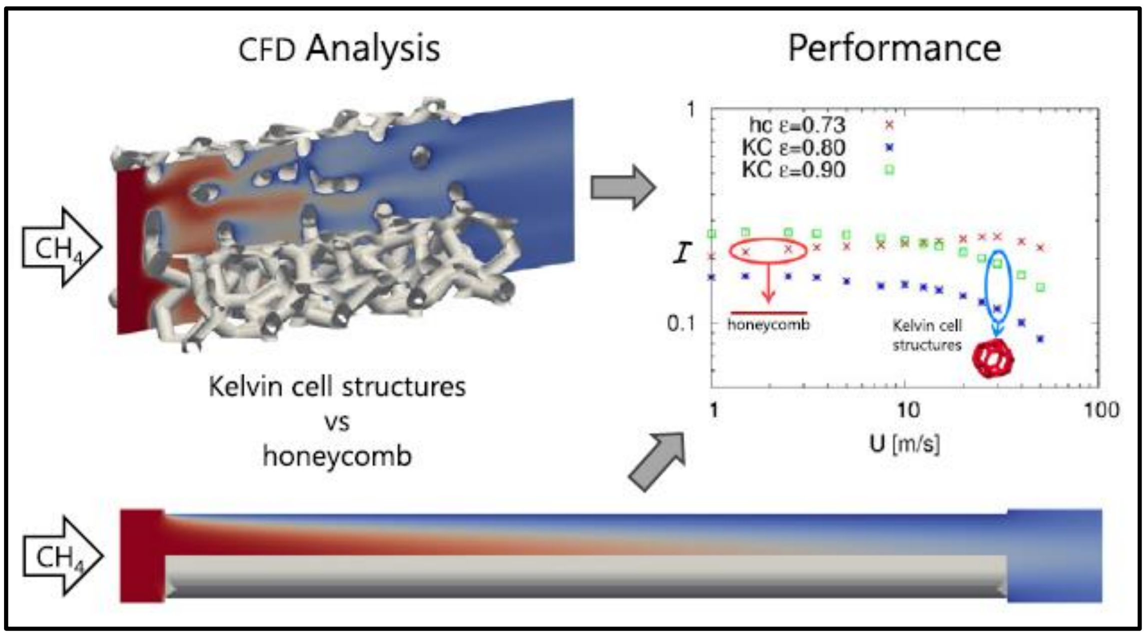
Main concept: applied to ICE

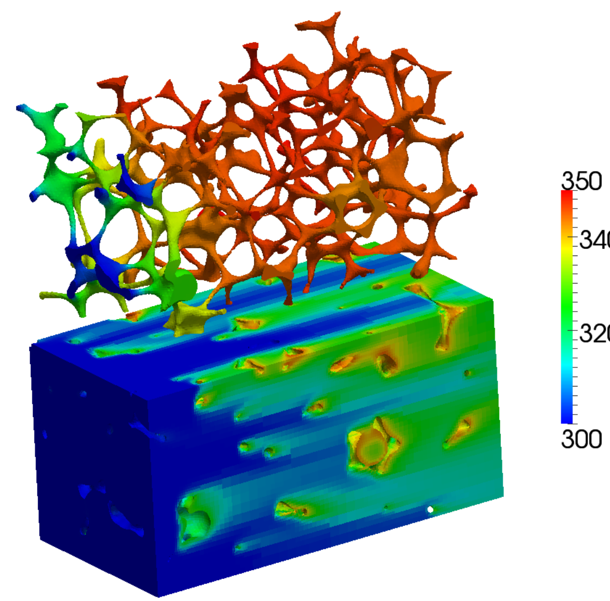




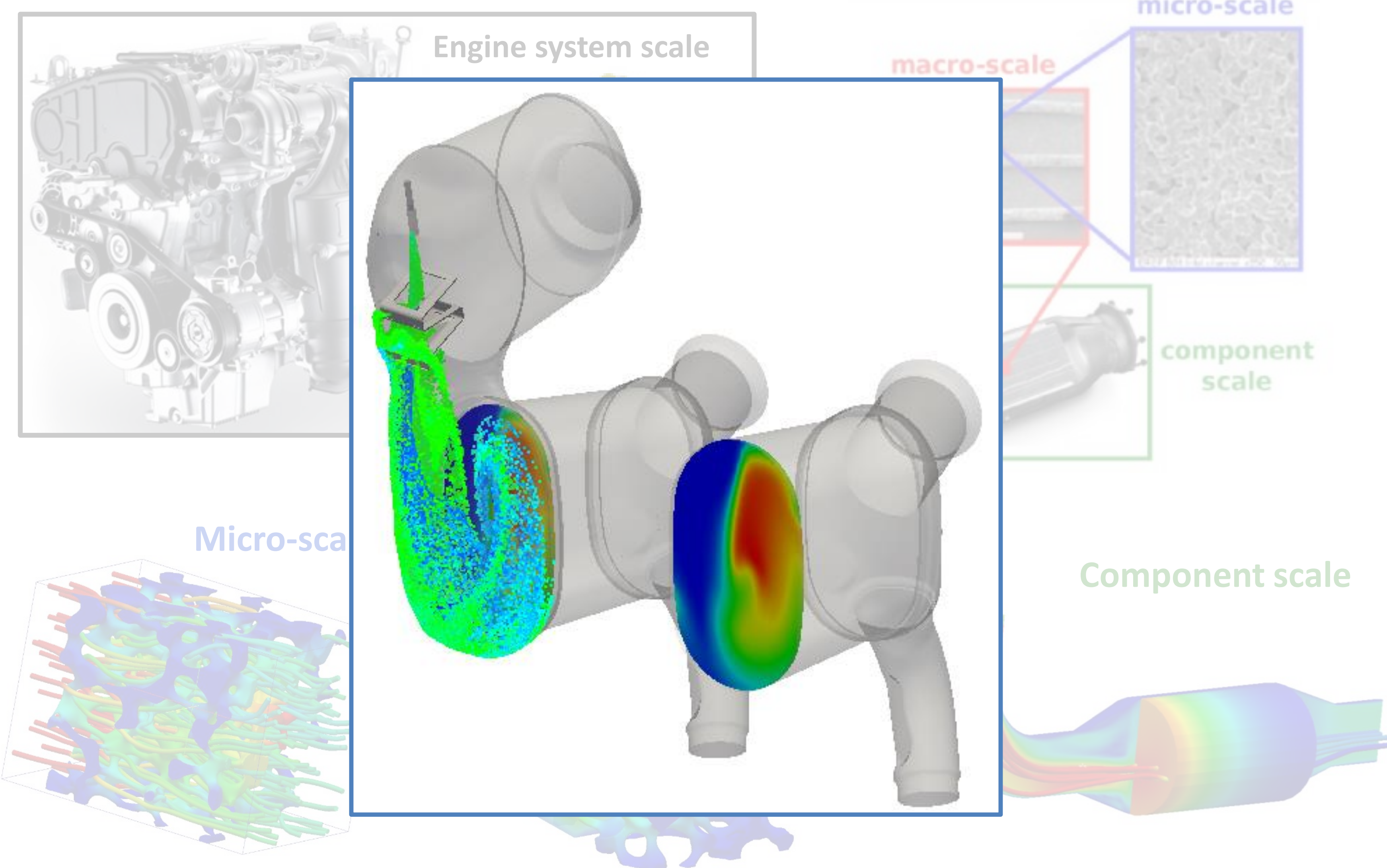
Previous work: micro-scale modelling







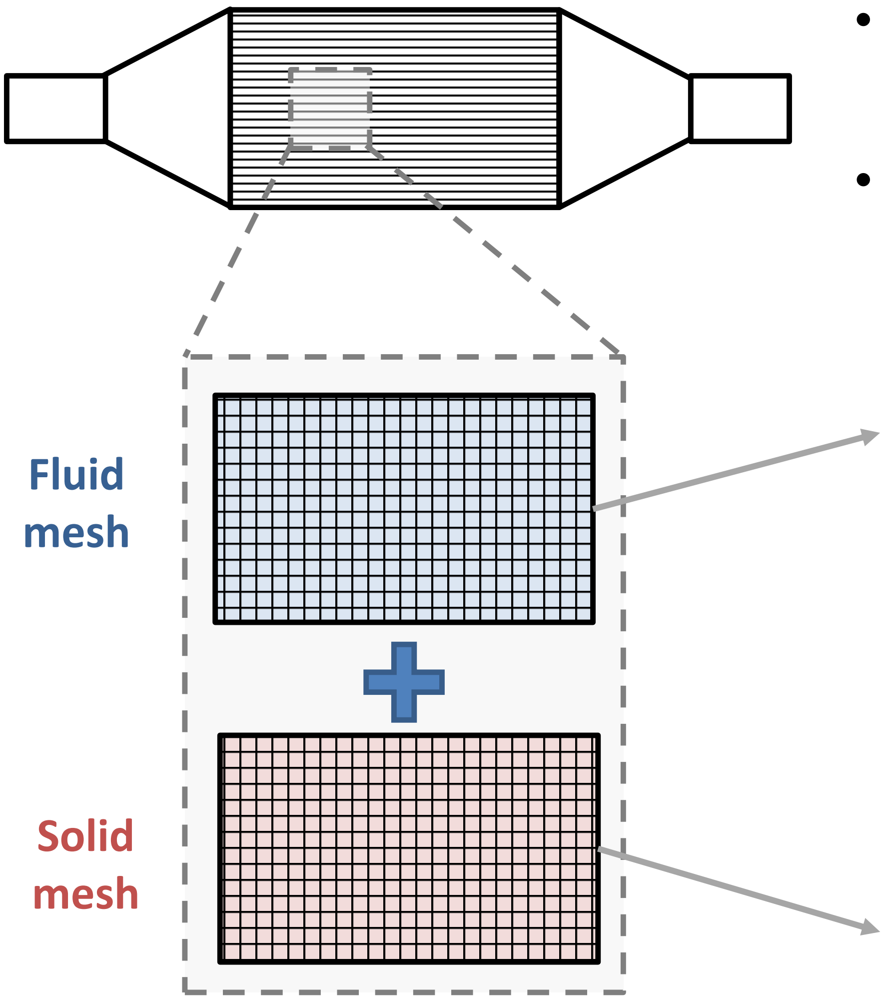
Full scale modeling

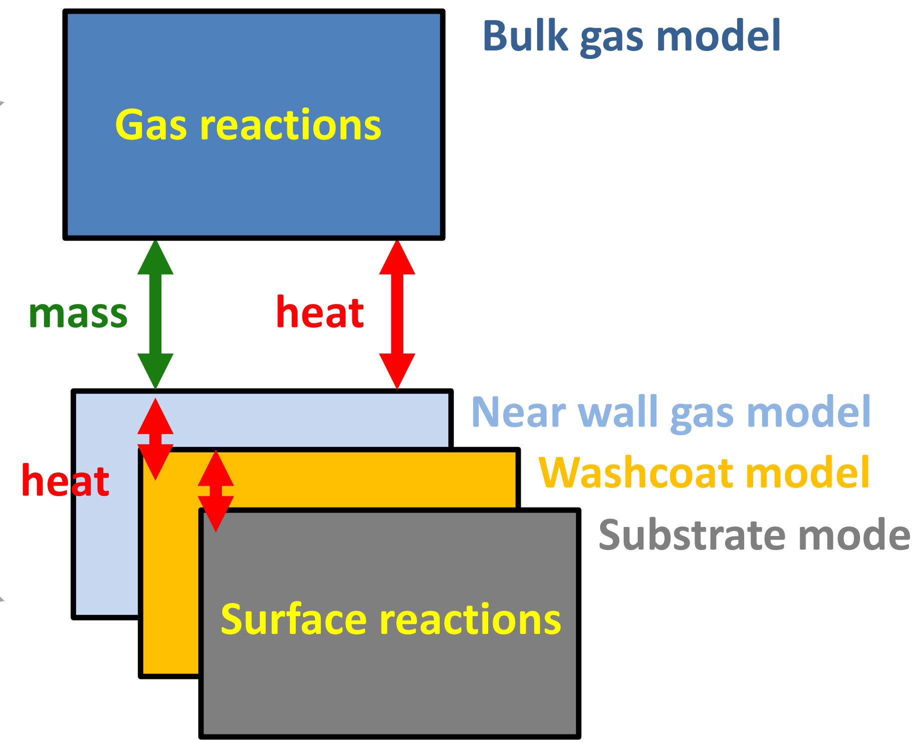


FULL SCALE MODELING

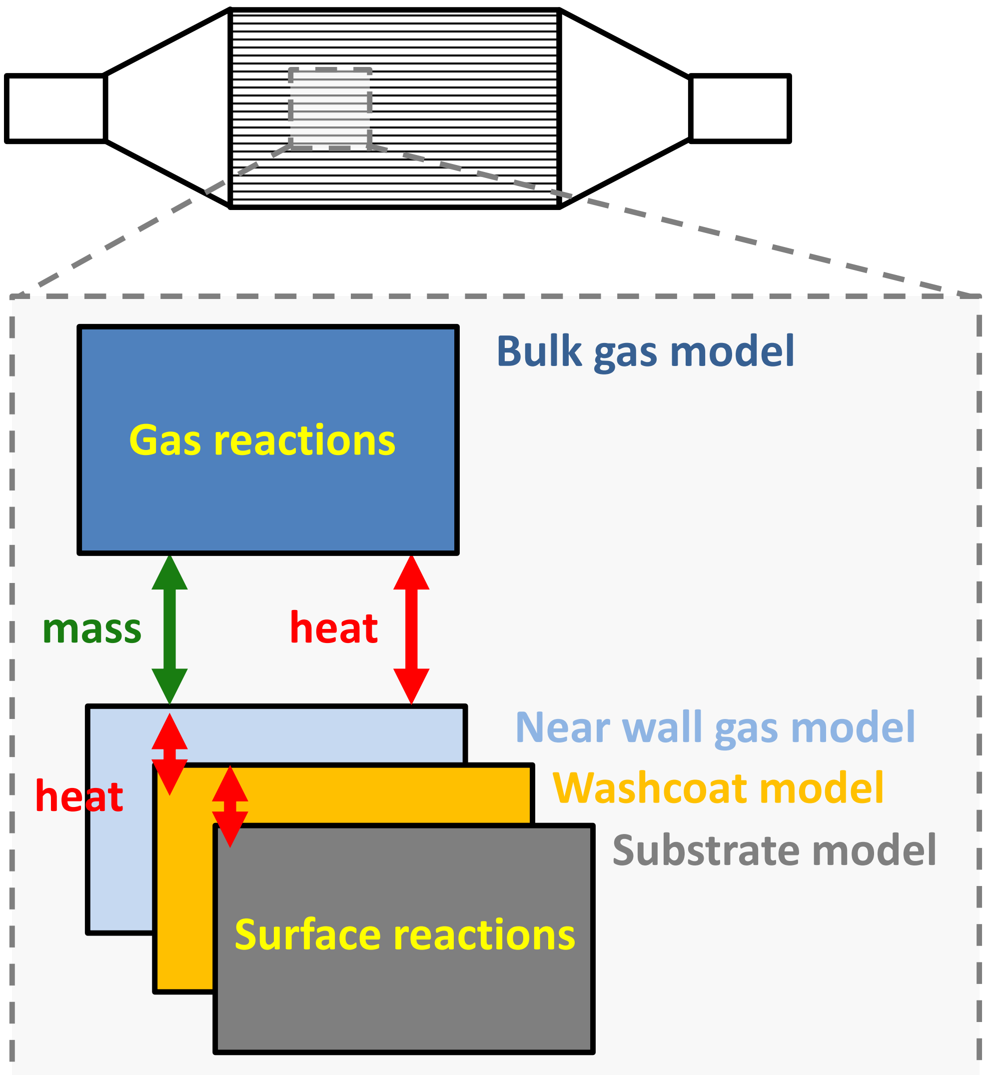
CFD macro-scale model for ATS simulations

- Macro-scale model is defined on two overlapping fluid and solid FV meshes
- Solid mesh support the modelling of different zones (gas, washcoat, solid)





Submodel for ATS simulations



Macro-scale model:

- *multi-region framework*
- *coupling between zones on different fluid or solid meshes*

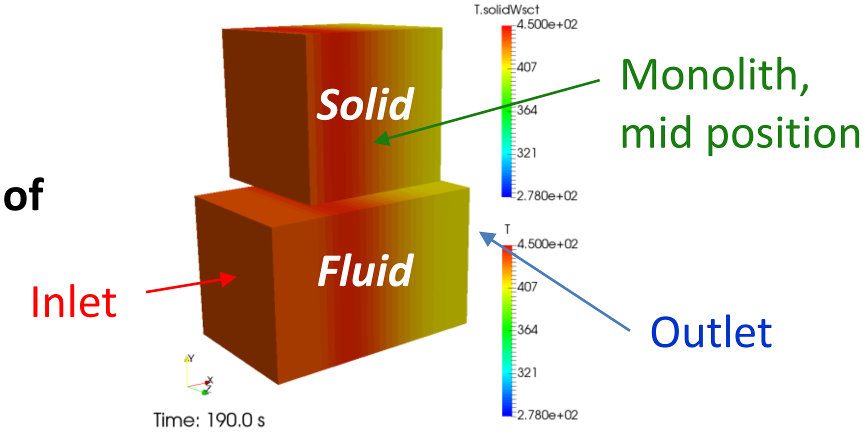
Coupling between fluid and solid regions requires specific models:

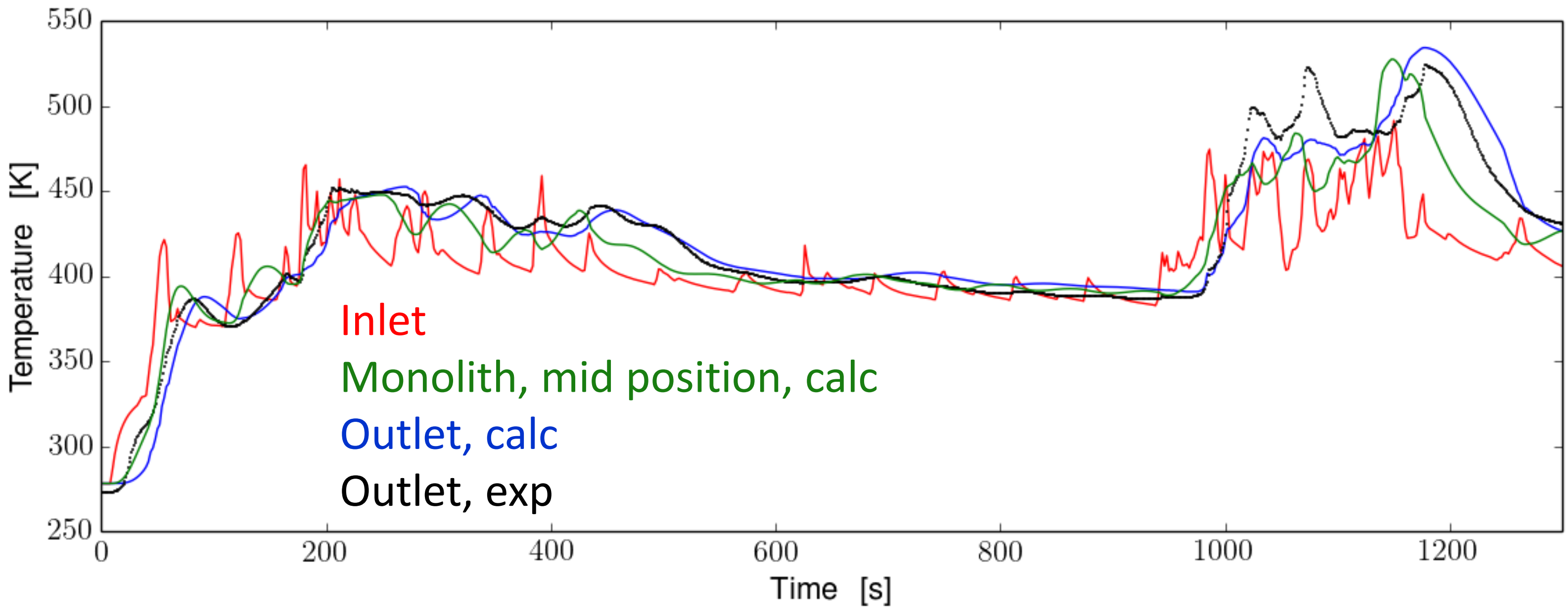
- *Geometry model*
- *Permeability model*
- *Heat transfer models (conduction, convection)*
- *Mass transfer model*
- *Reaction models*

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

Validation of the full model: 1D case DOC

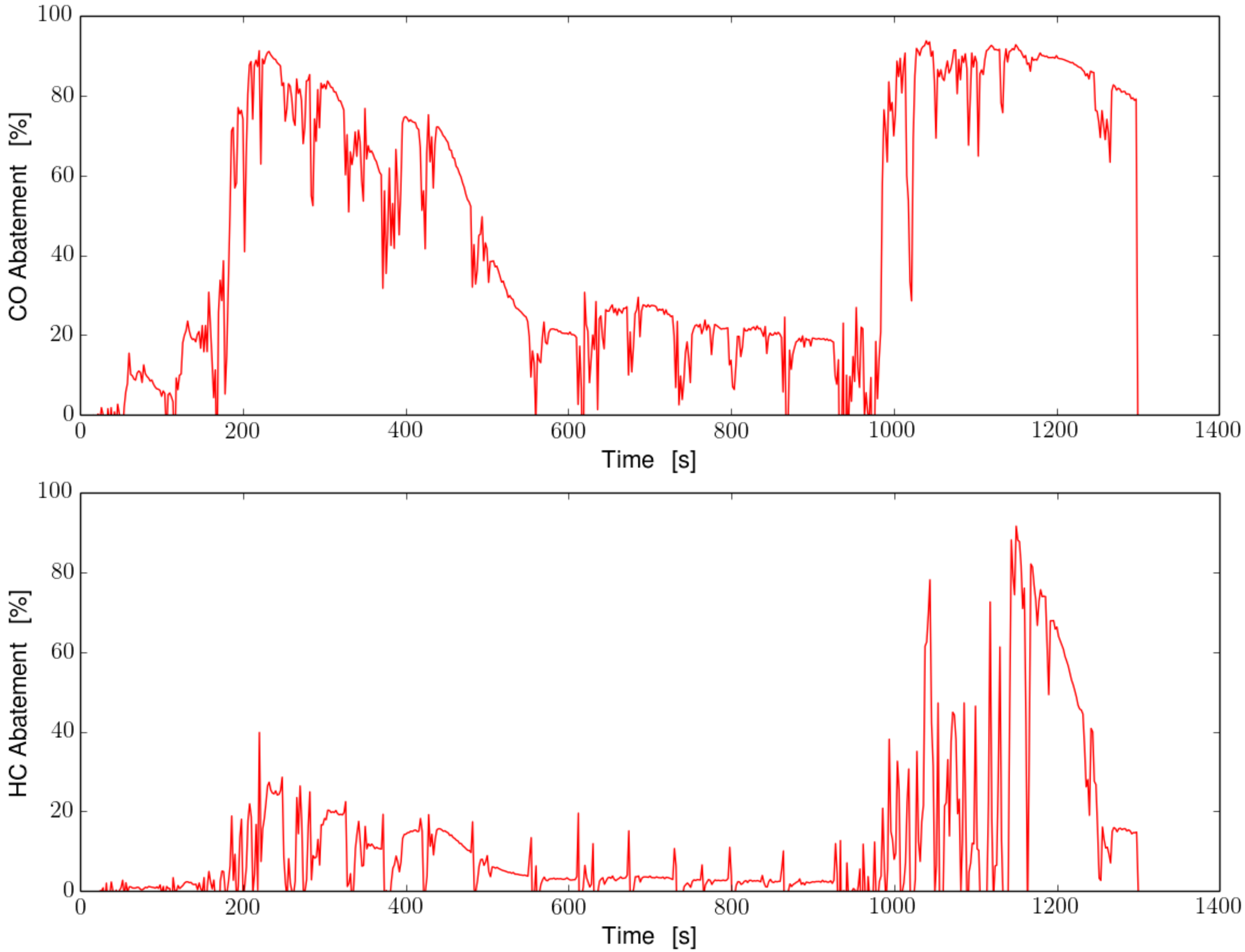
Comparison between simulated and measured temperature at the outlet of the catalyst





Validation of the full model: 1D case DOC

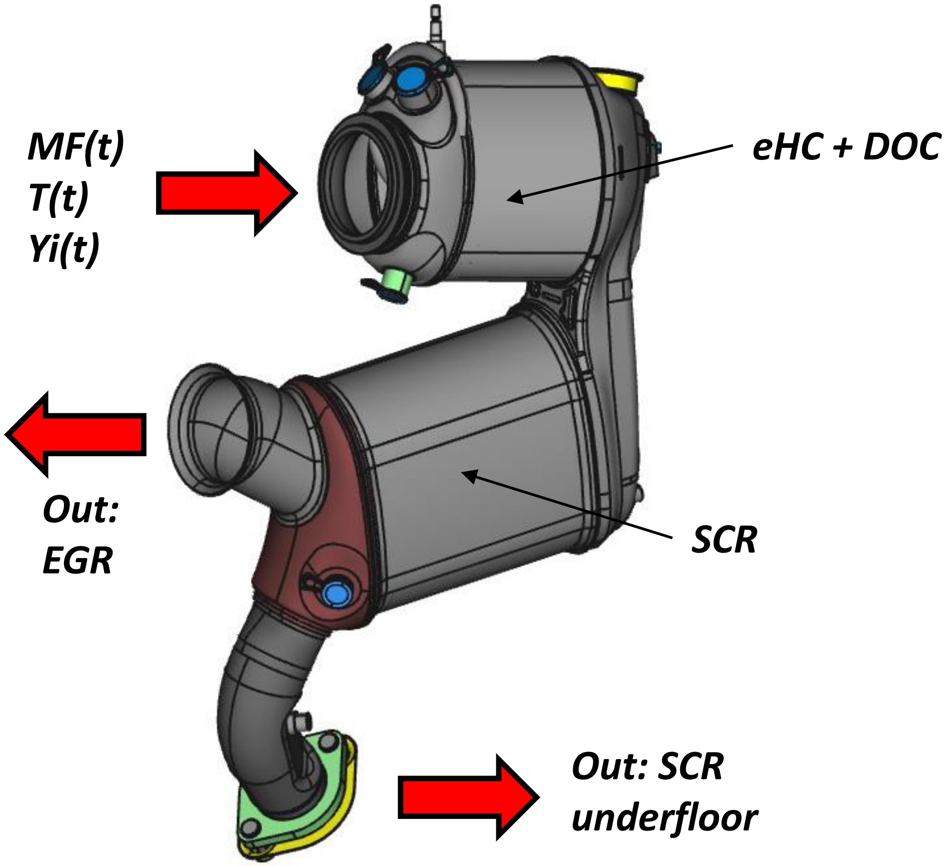
Calculated CO and HC abatement

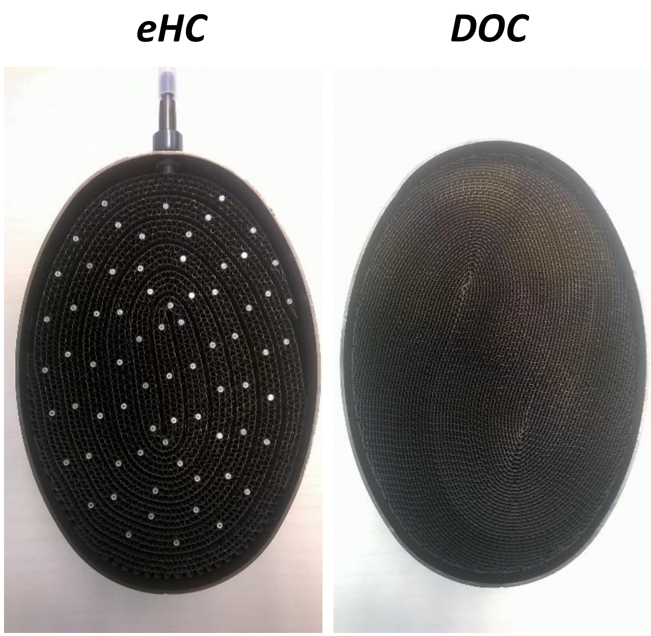


Application to the simulation of a real ATS system

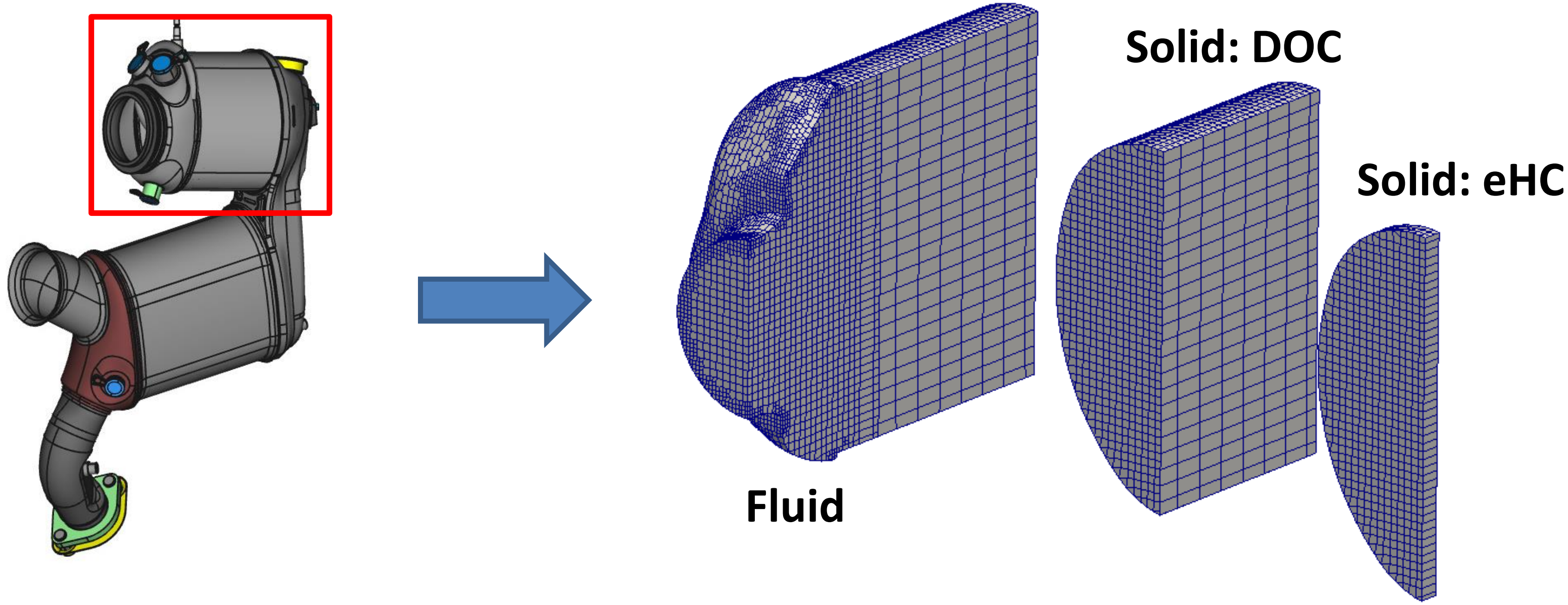
Full-scale 3D case including DOC monolith and electrical heating

a. Simulation of uniform electrical heating
b. Simulation of non-uniform electrical heating





Application to the simulation of a real ATS system



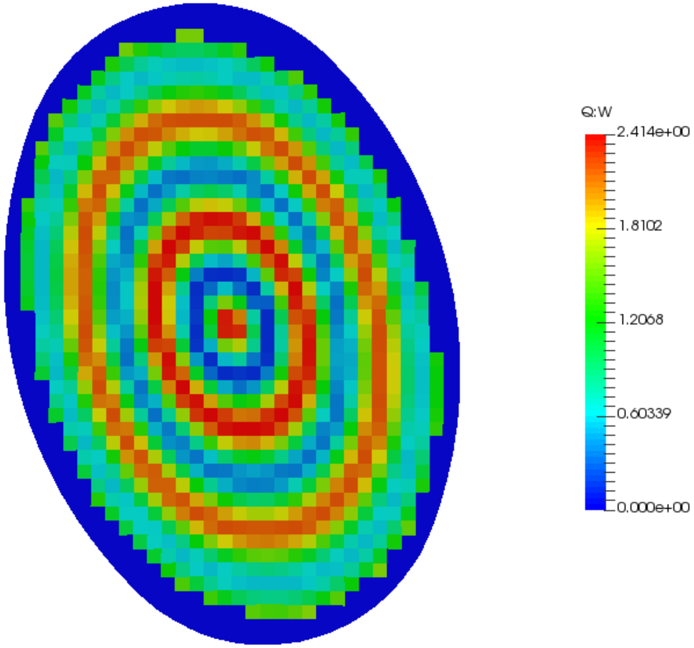
Application to the simulation of a real ATS system

A specific model has been implemented to take into account the non uniform distribution of the heat generated in the metallic eHC

Phenomenological model:

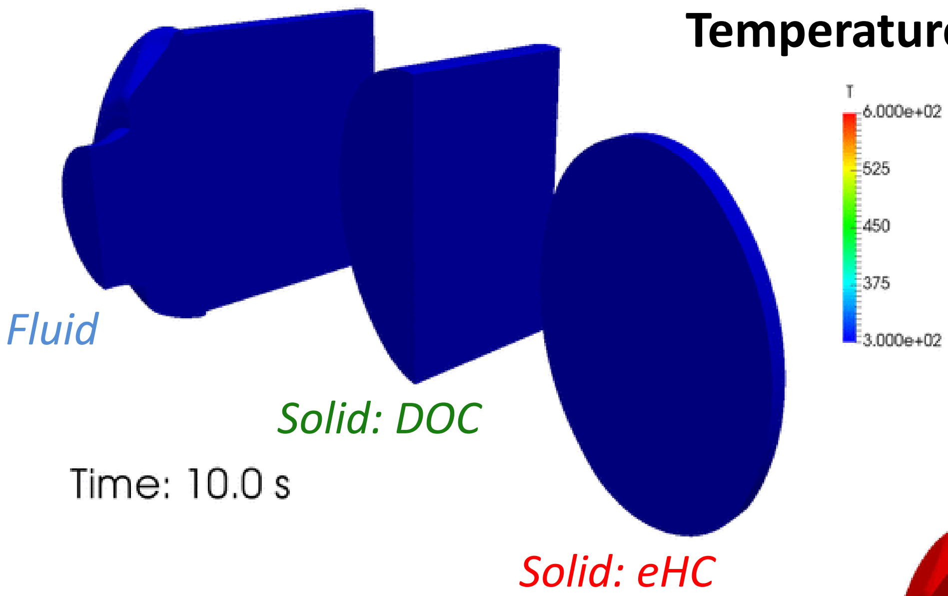
- Each spiral has a high T side and a low T side
- Non-uniformity decreases from center to boundary
- No heating at the boundary (short circuit)

→ **Spatial distribution for the heat release**



DOC configuration with non-uniform heating

Temperature

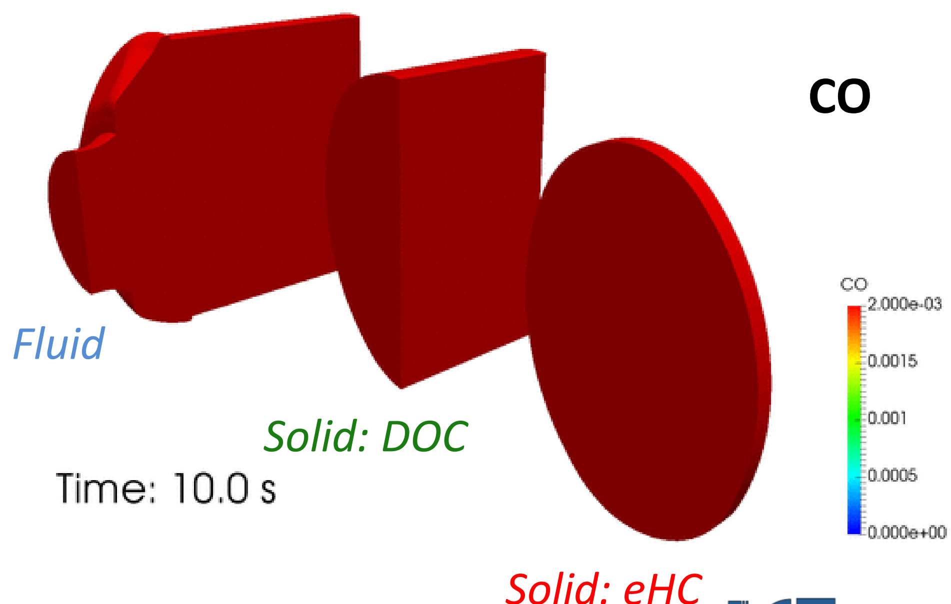


Non-uniform heating

P_{el} = 1 kW : 0-100 s

P_{el} = 0.5-0.2 kW : 100-300 s

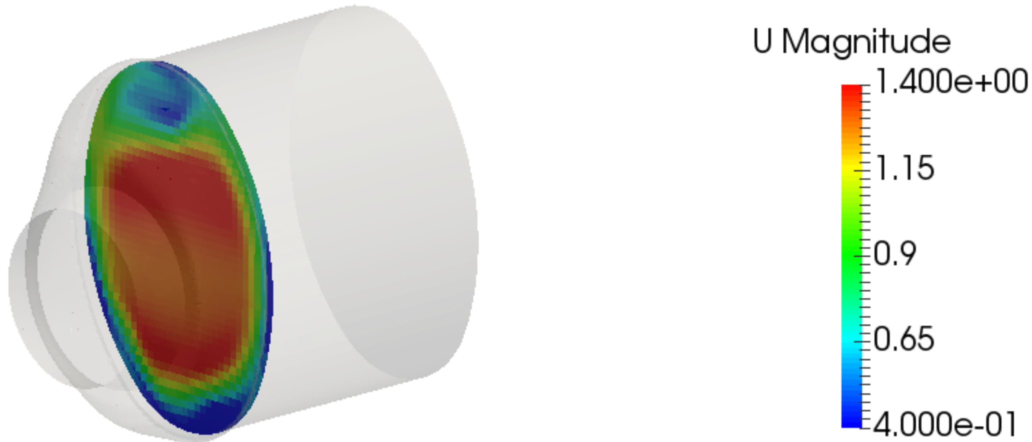
CO



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

Application to the simulation of a real ATS system

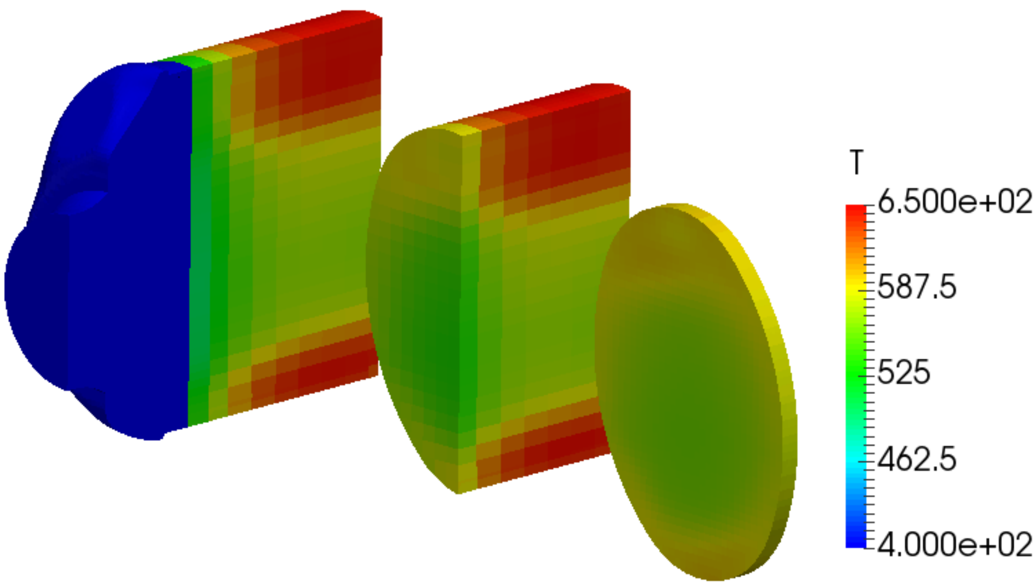
DOC configuration with uniform heating

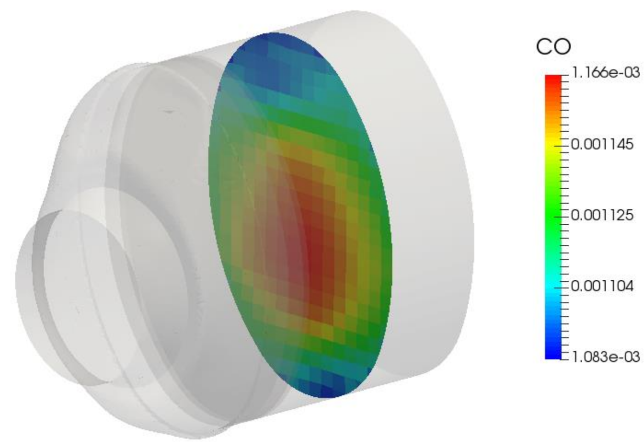


Time = 140 s

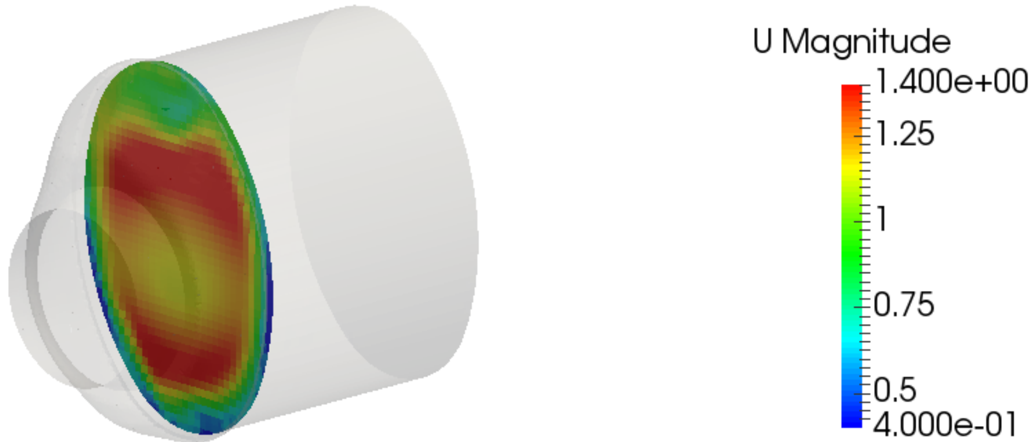
Uniform heating

P_{el} = 1 kW





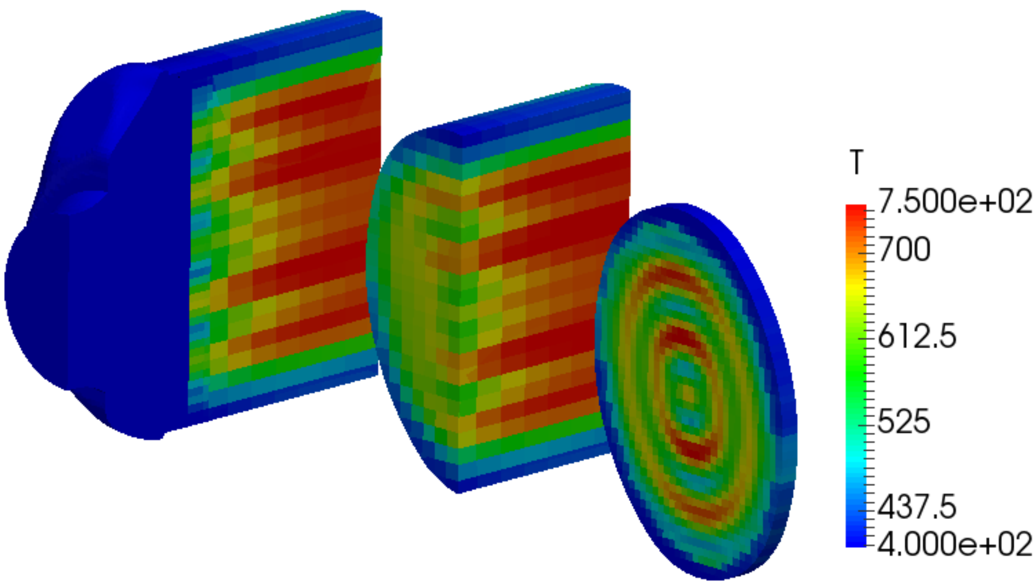
DOC configuration with non-uniform heating

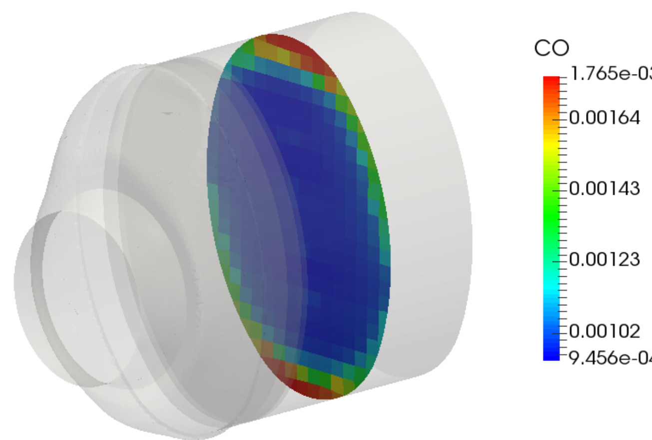


Time = 140 s

Non-uniform heating

P_{el} = 1 kW

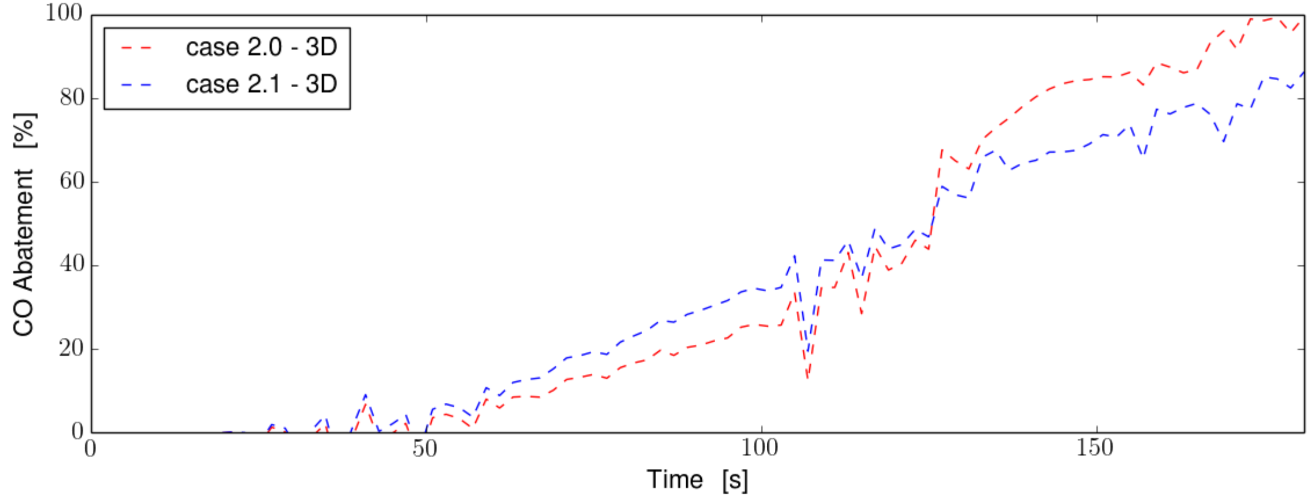




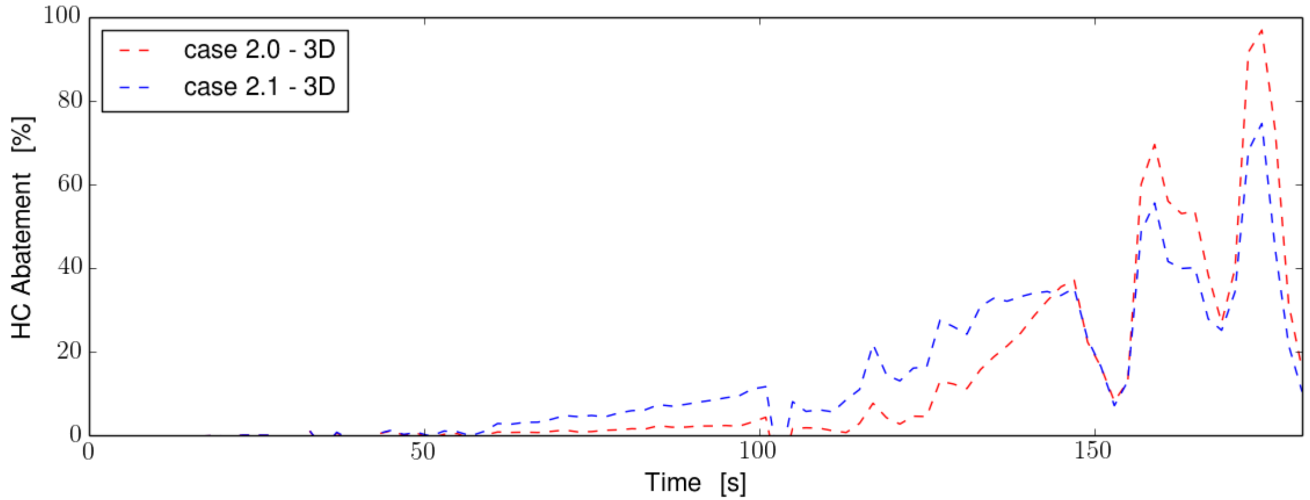
3D model

DOC: comparison uniform vs non-uniform heating

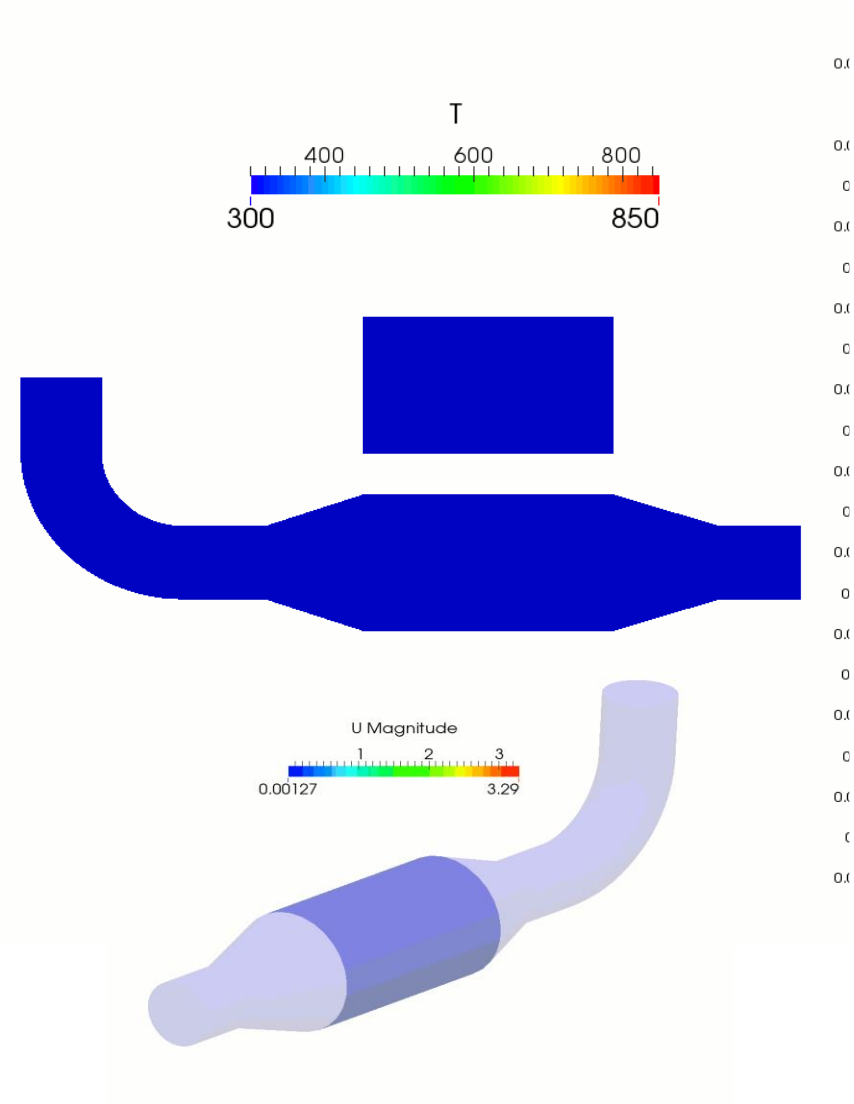
CO



HC



TWC: implementation of Koltsakis model



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

$CO + H_2O \rightarrow CO_2 + H_2$

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

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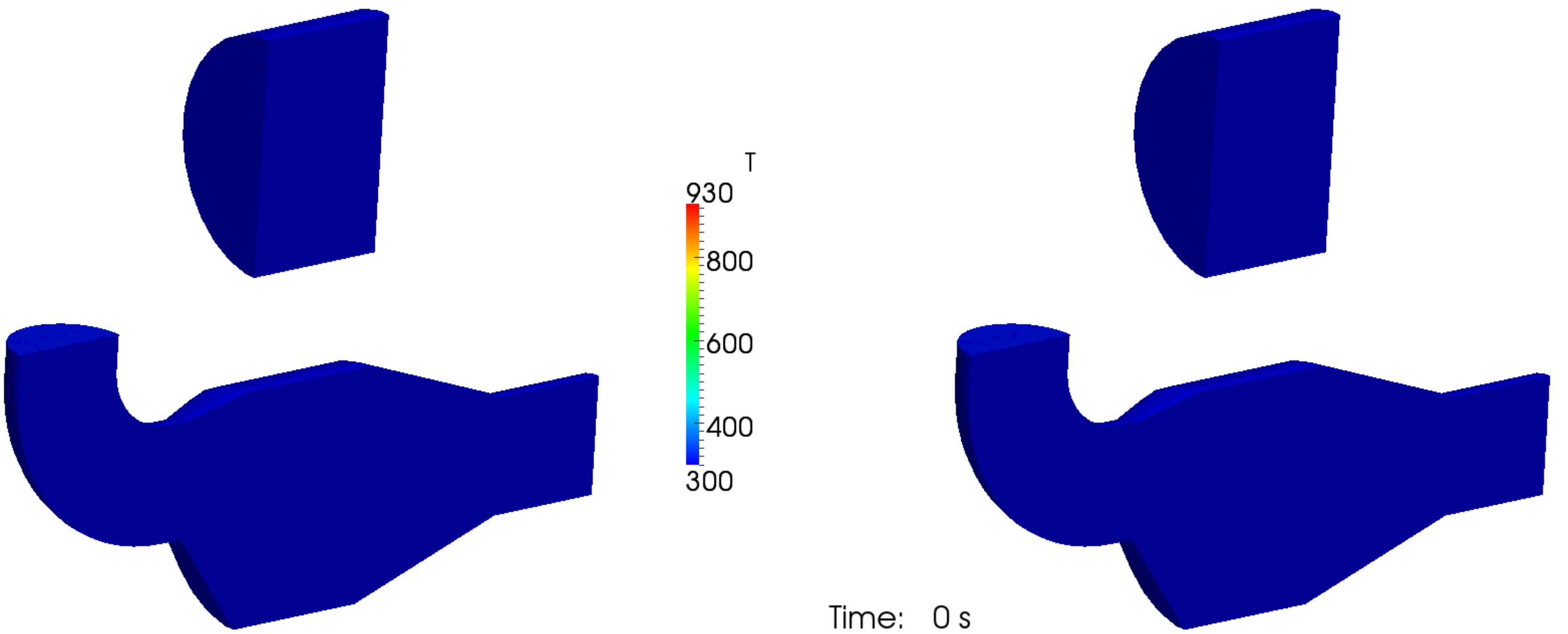
TWC: comparison of different substrate types

- NEDC cycle of a 2.0 L engine, 4 Cyl, naturally aspirated
- Measured exhaust gas T and mass flow and the engine flange as BC.
- Open cell foam properties from micro scale simulations



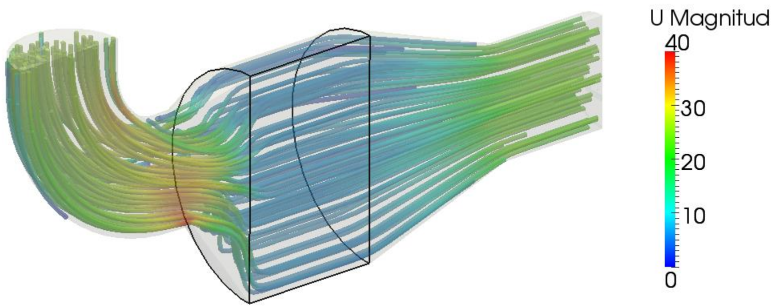
HONEYCOMB

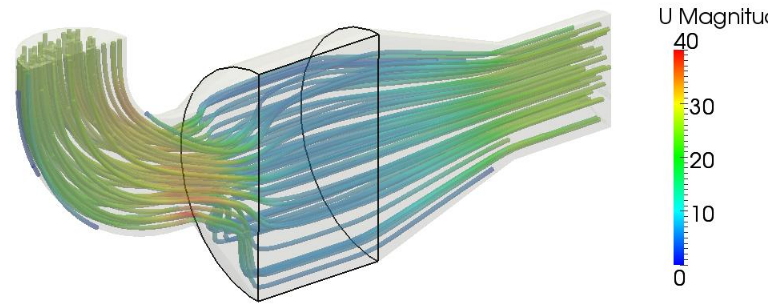
OPEN CELL FOAM

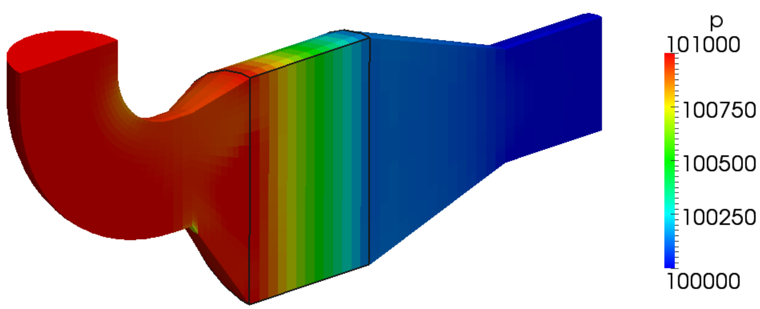
TWC: comparison of different substrate types

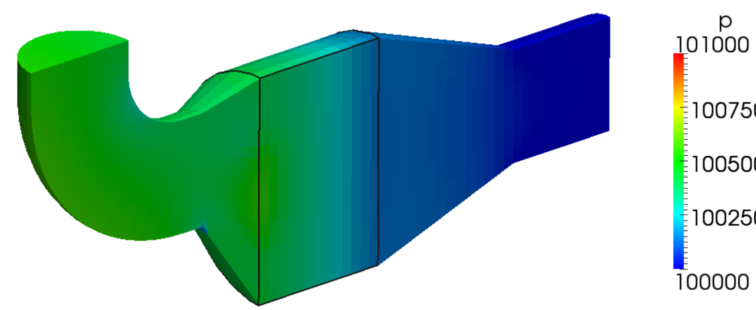
HONEYCOMB

OPEN CELL FOAM



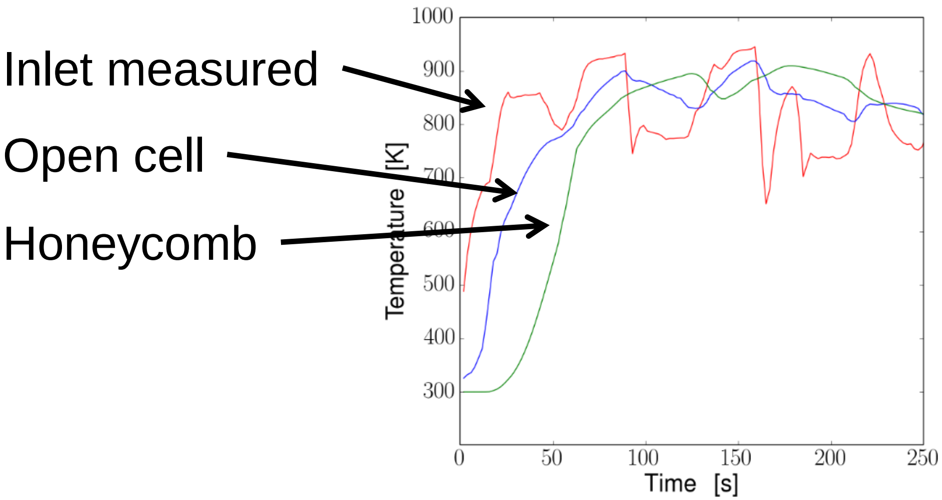


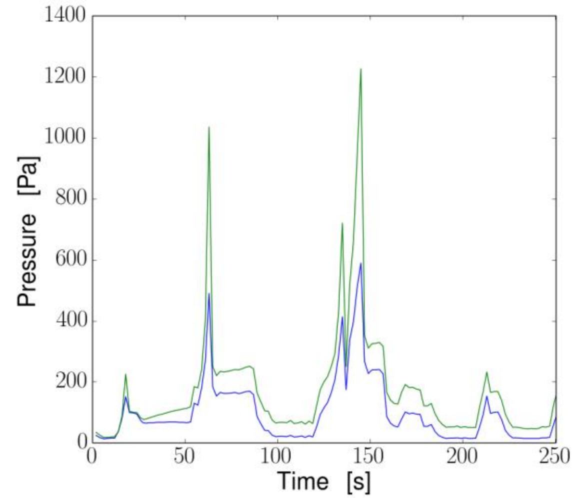


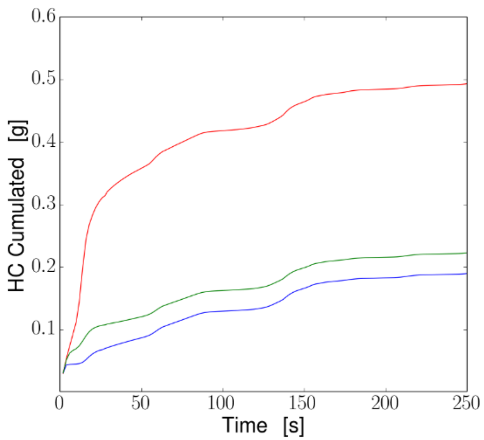


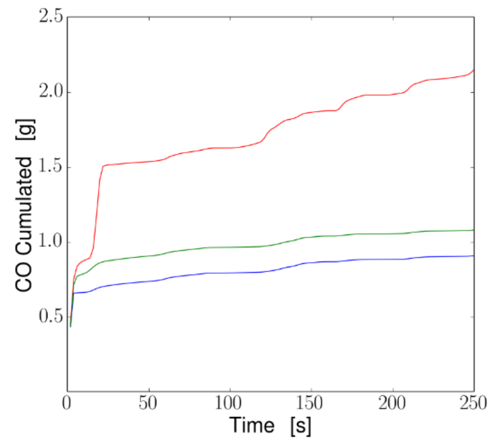
TWC: comparison of different substrate types

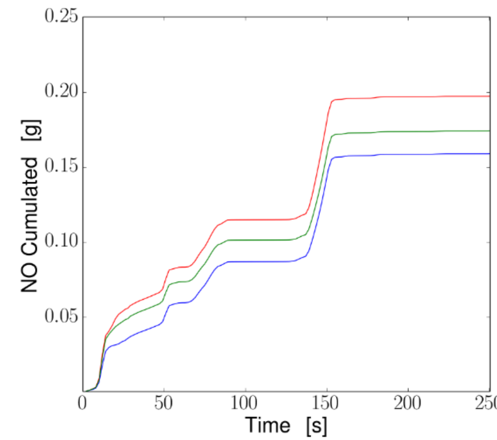
- NEDC cycle (first 300 seconds) with two different technologies









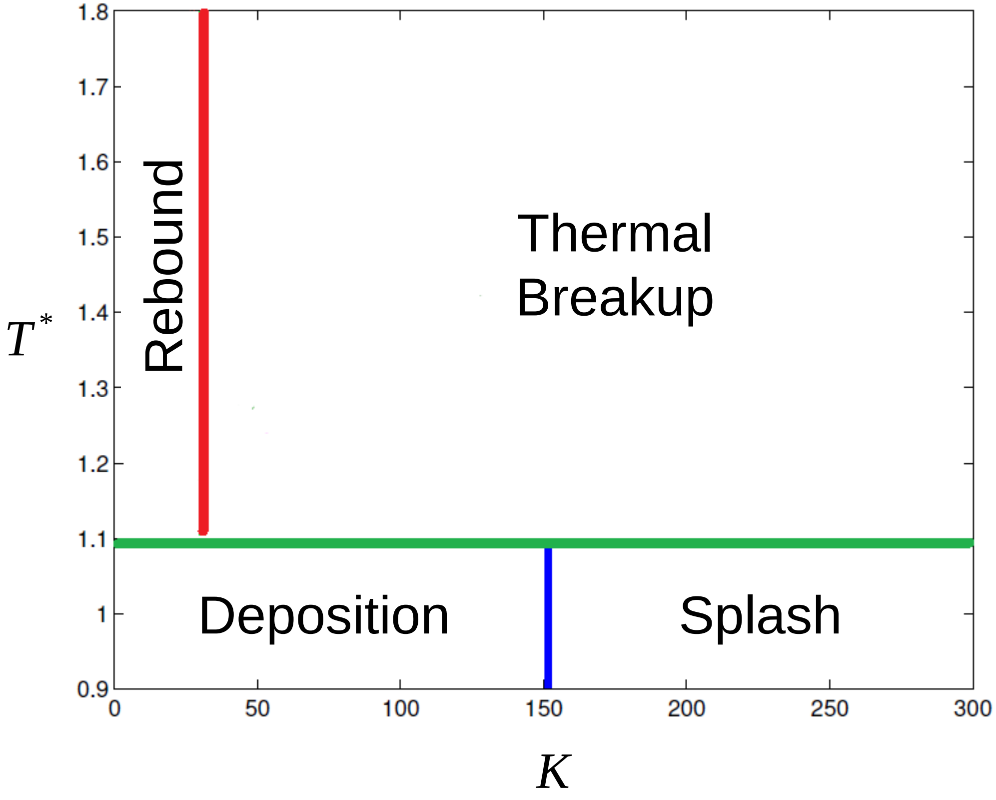


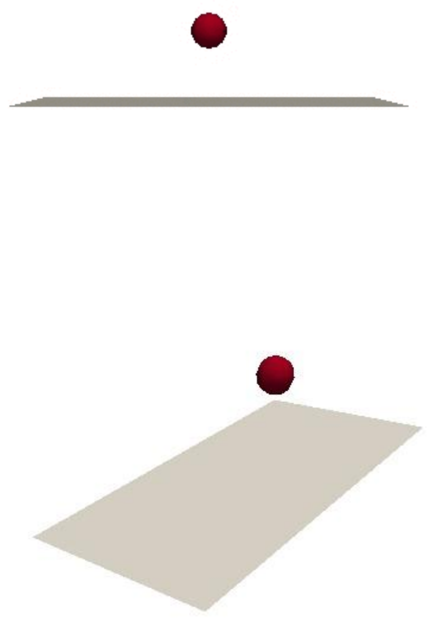
SPRAY & WALL FILM MODELING

Thermal aspects of spray-wall interaction

Extension of standard impingement regimes

a. Review of rebound models
b. Thermal aspect taken into account



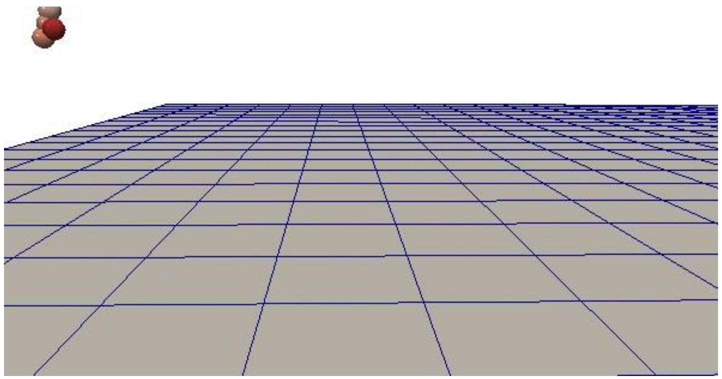


Thermal aspects of spray-wall interaction

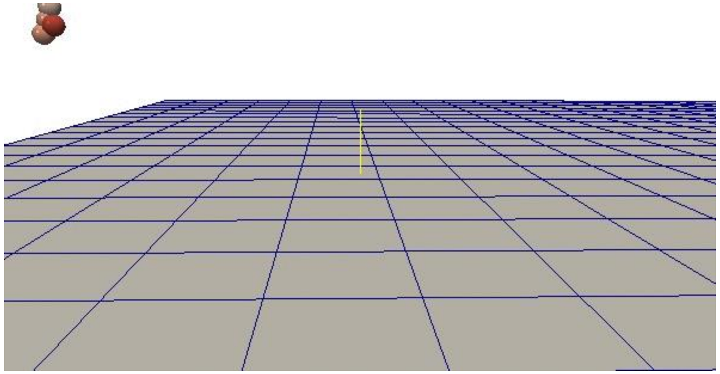
Splashing threshold shift

Absolute We = 264
Normal We = 137

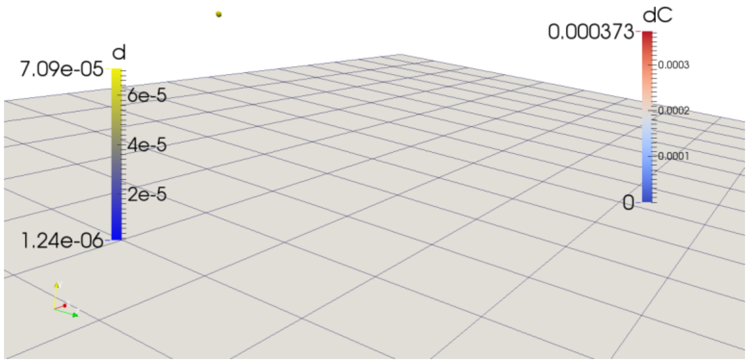
T* = 0.8



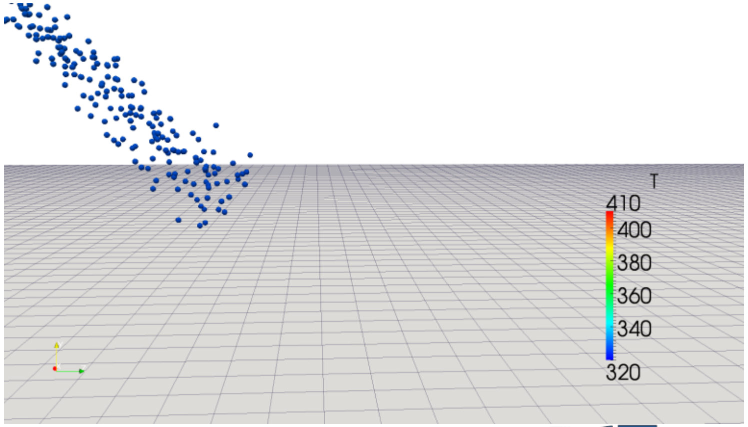
T* = 1.2



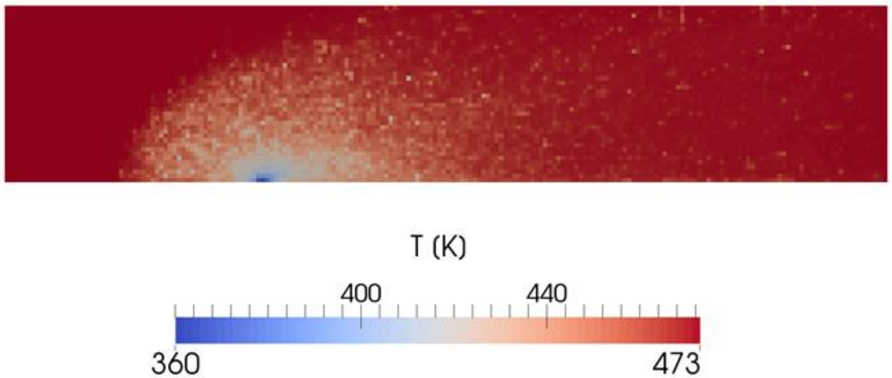
Non-zero contact time

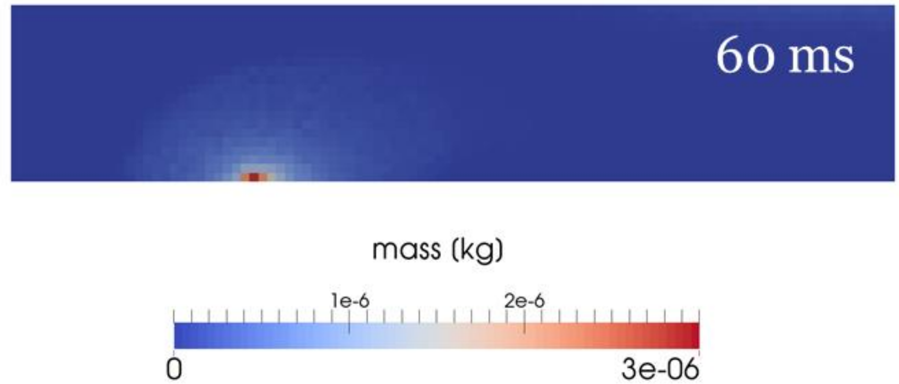


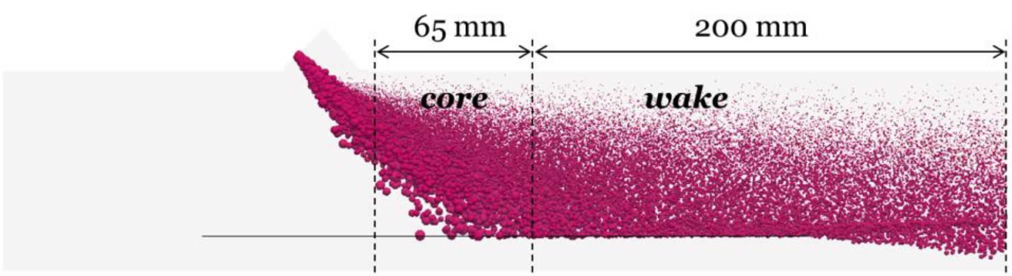
Conjugate Heat Transfer

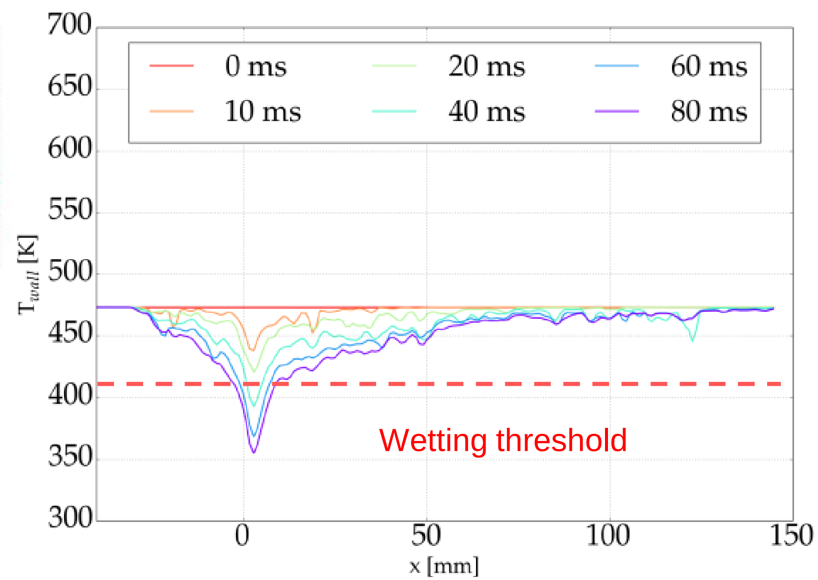


Thermal aspects of spray-wall interaction



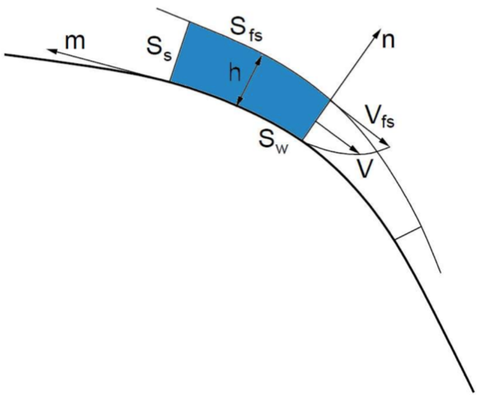






- CHT on dry wall
- The temperature drop before the wetting condition is predicted

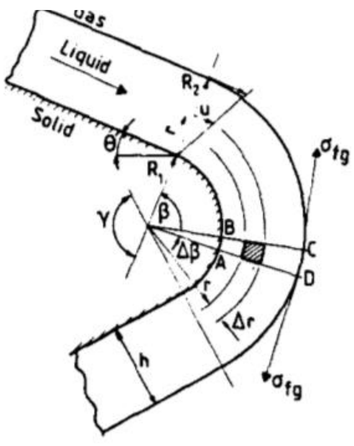
Solution of the liquid film



$$\frac{\partial h Y_{f,k}}{\partial t} + \nabla \cdot (h \vec{u}_f Y_{f,k}) = S_{M,k} + S_{V,k}$$

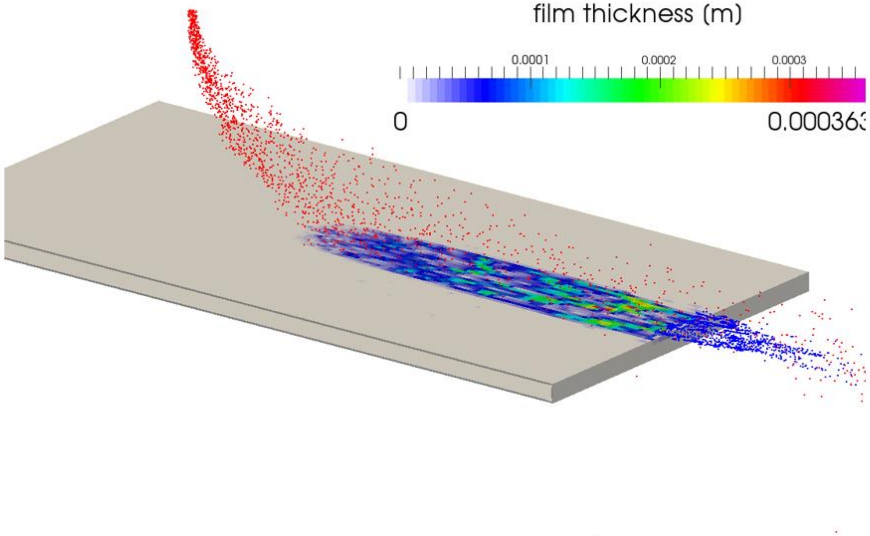
$$\frac{\partial h \vec{u}_f}{\partial t} + \nabla \cdot (h \vec{u}_f \vec{u}_f) = -\frac{1}{\rho_f} \nabla (h p_f) + \vec{\tau}_g - \vec{\tau}_w + h \vec{g} + \vec{S}_U$$

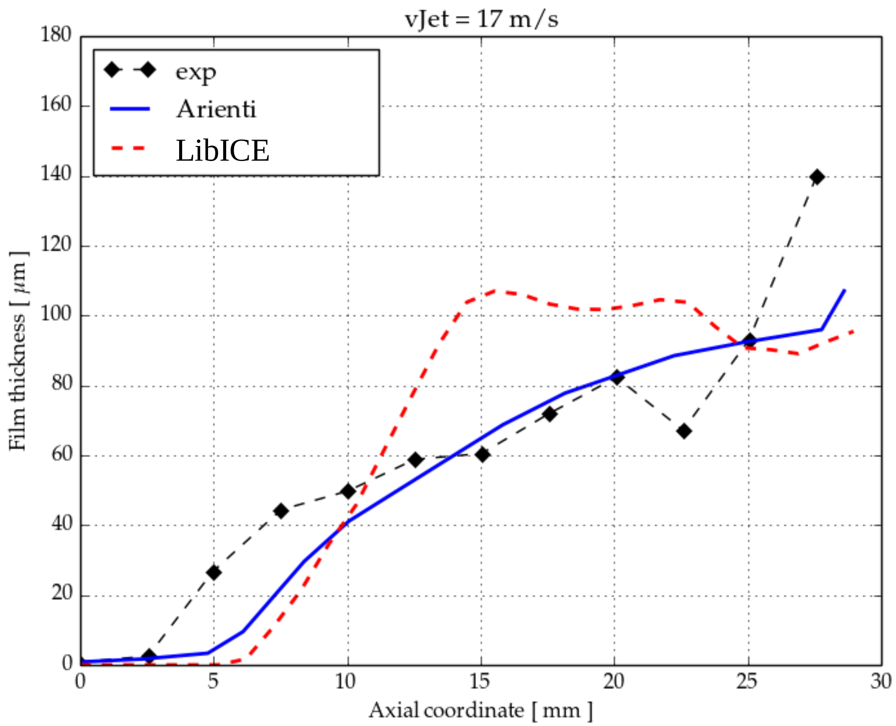
$$\frac{\partial h \hat{H}_{s,f}}{\partial t} + \nabla \cdot \left(h \vec{u}_f \hat{H}_{s,f} \right) = j_g - j_w + S_H$$



- Film stripping model triggered when the inertial forces exceed the surface tension ones.
- Gravitational acceleration is also taken into account.
- Minumum parcel mass and capability to store mass to guarantee mass continuity
- User selectable diameter distribution for stripped parcels

Solution of the liquid film

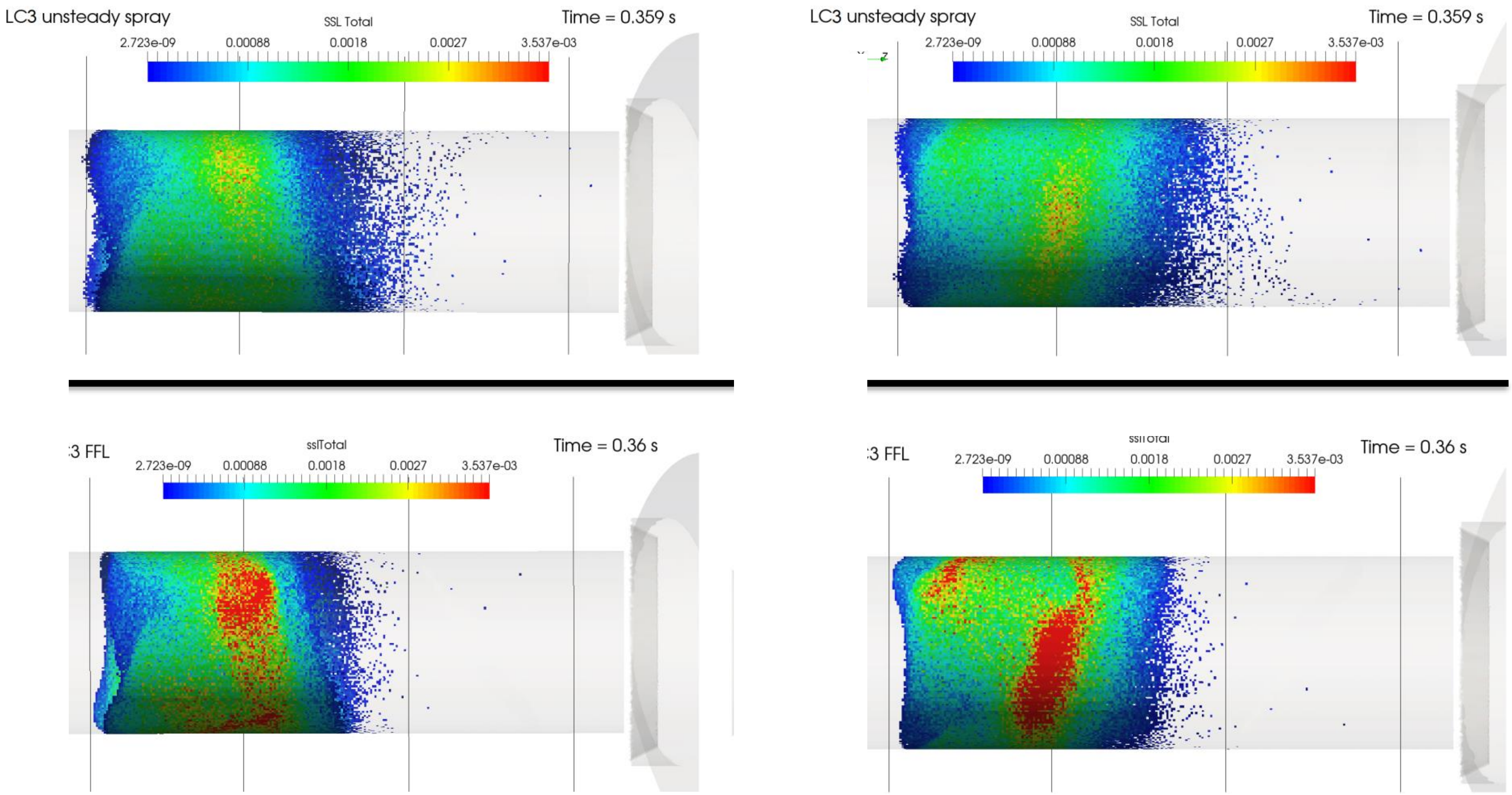




- Arienti test case for validation of film formation/dragging and film stripping
- Heat transfer between wall, film and surrounding gas.
- CHT has not been considered

Dynamic aspects of spray-wall interaction

Comparison between unsteady and frozen flow impingement reveals relevant differences due to flow fluctuations.



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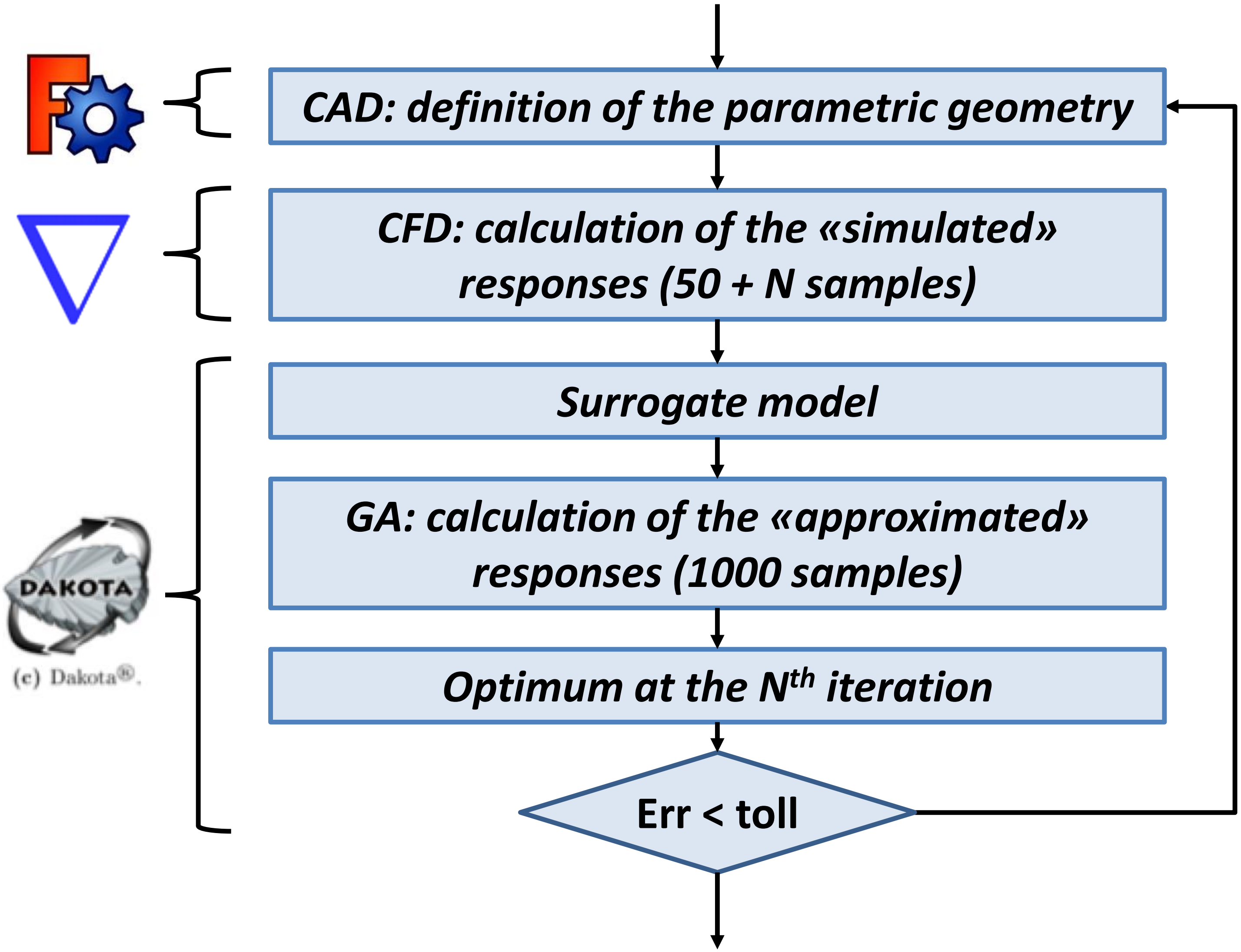
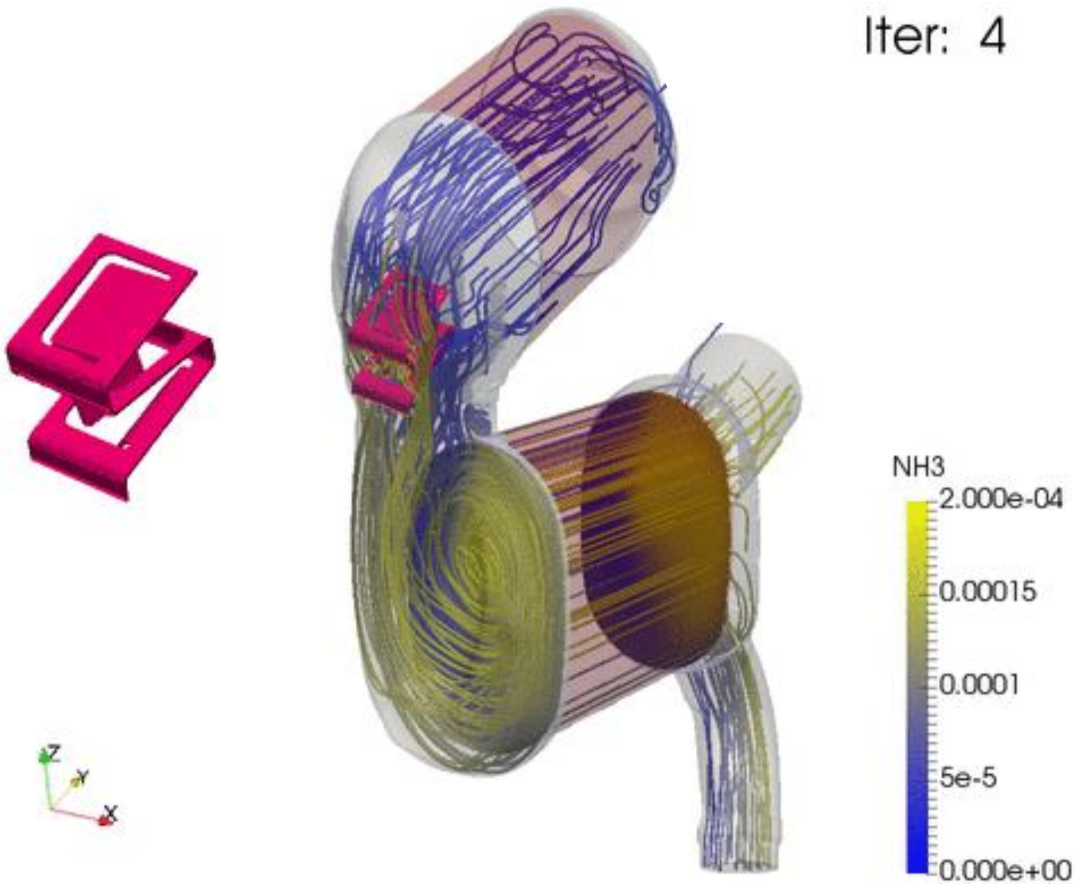
OPTIMIZATION FRAMEWORK

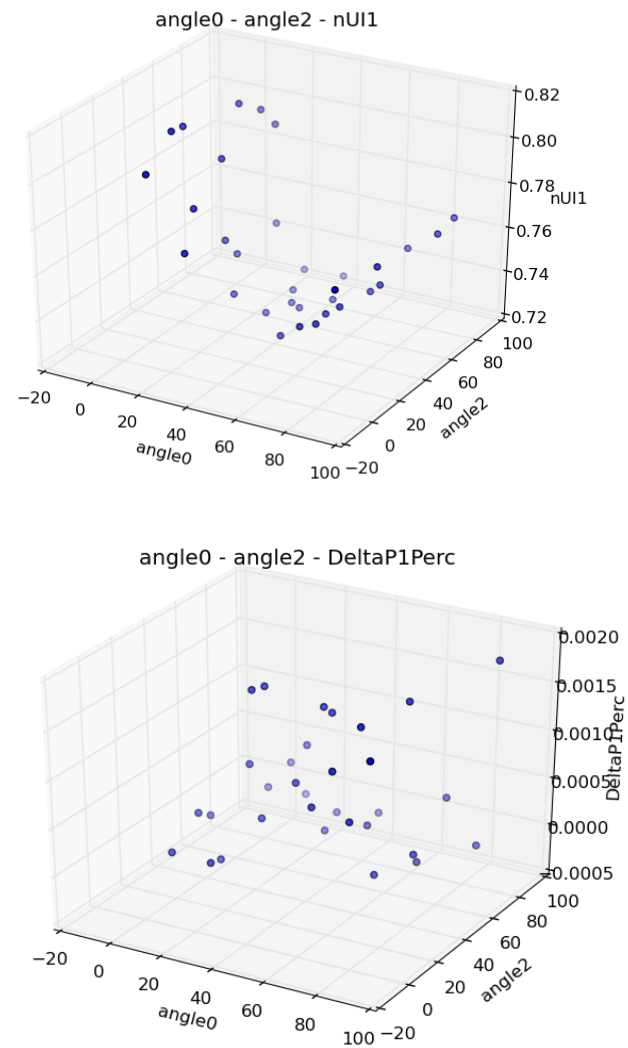
Optimization procedure



Geometrical optimization of the mixer

Optimization: DOE





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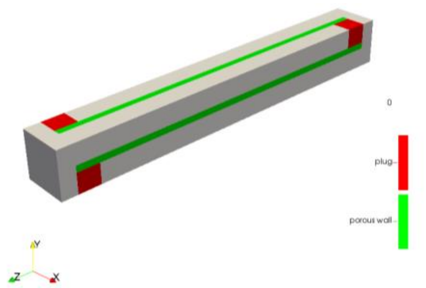
WORK IN PROGRESS

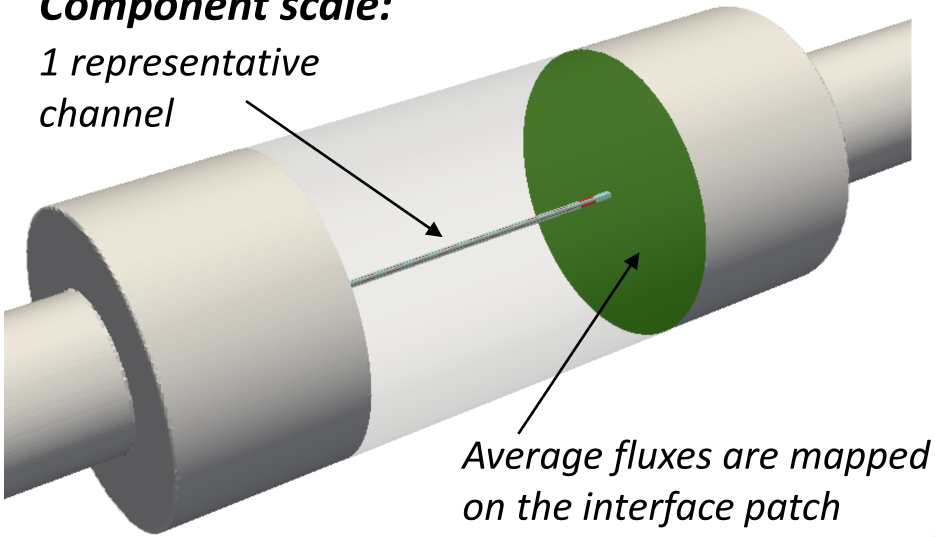
Channel scale DPF/GPF or CAT

- Channel representation is needed for fluid-dynaic and acoustic simulation
- The monolith is divided in sectors and where fluid-dynamic equations are solved on a single representative couple of channels.
- Fluxes are mapped on the remaining portion of the sector not connected to the representative channel.

Channel scale:

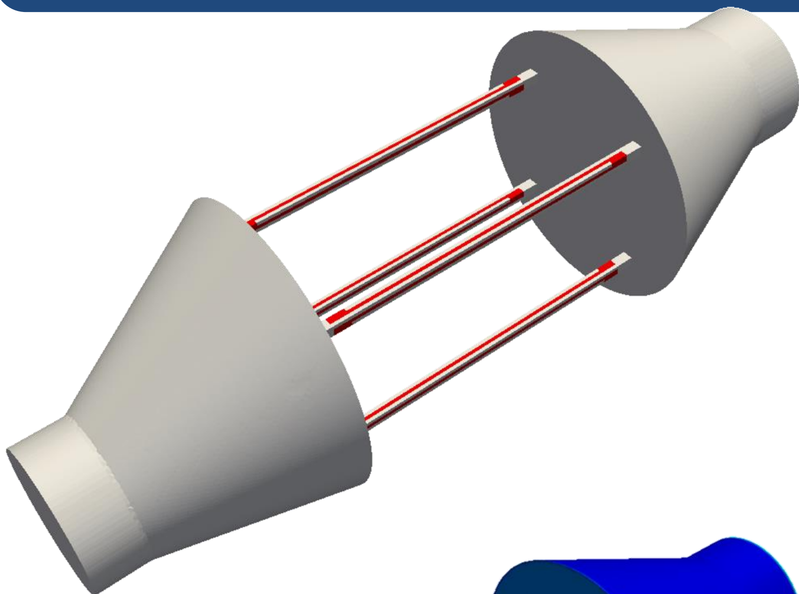


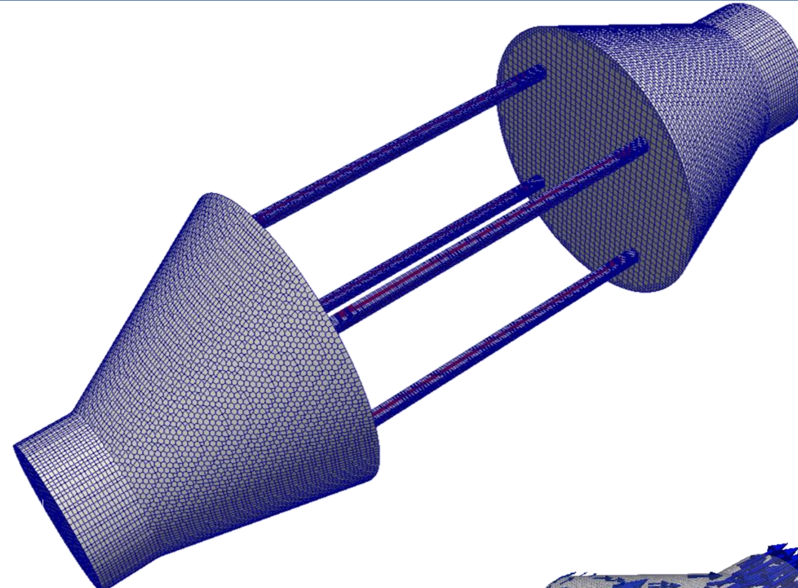
Component scale:

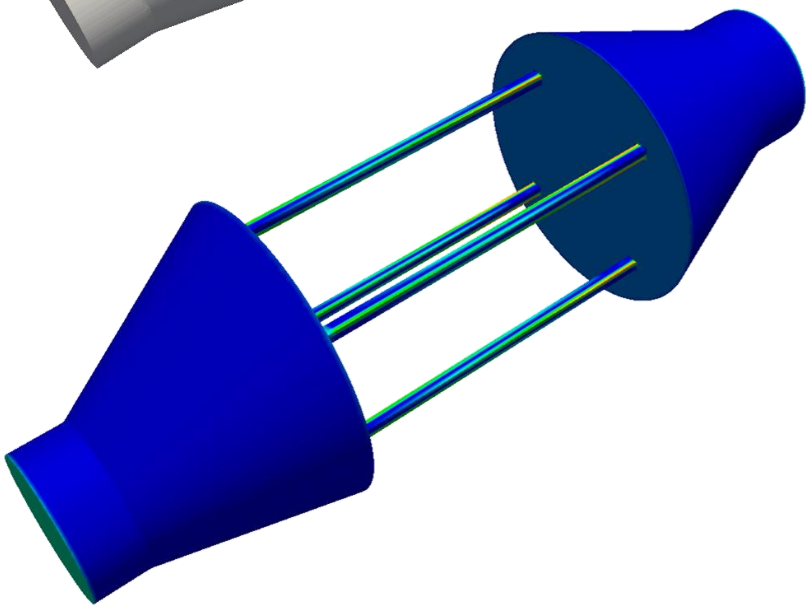


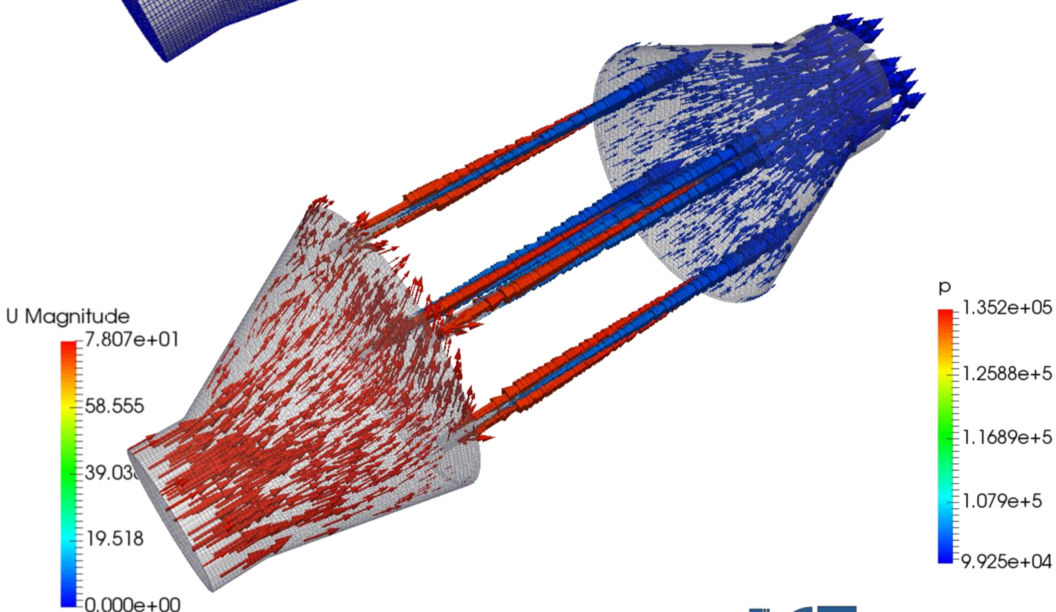
Work in progress

Channel scale DPF/GPF or CAT









Conclusions

- Models for **macro-scale and micro-scale simulation** of complex **after-treatment devices** have been implemented and are fully integrated.

- The macro scale model is based on a **multi-region framework** with overlapping fluid and solid meshes to describe the phenomena occurring in the catalytic substrates:
  - Heat transfer
  - Mass transfer
  - Catalytic reactions

- Integration with spray and wall film models for the simulation of complete ATS.

- Finally, the OpenFOAM model can be easily embedded in an **optimization procedure** to address geometry or parameter optiimization.

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