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

A.Nappi, G. Montenegro, A. Della Torre, A. Onorati

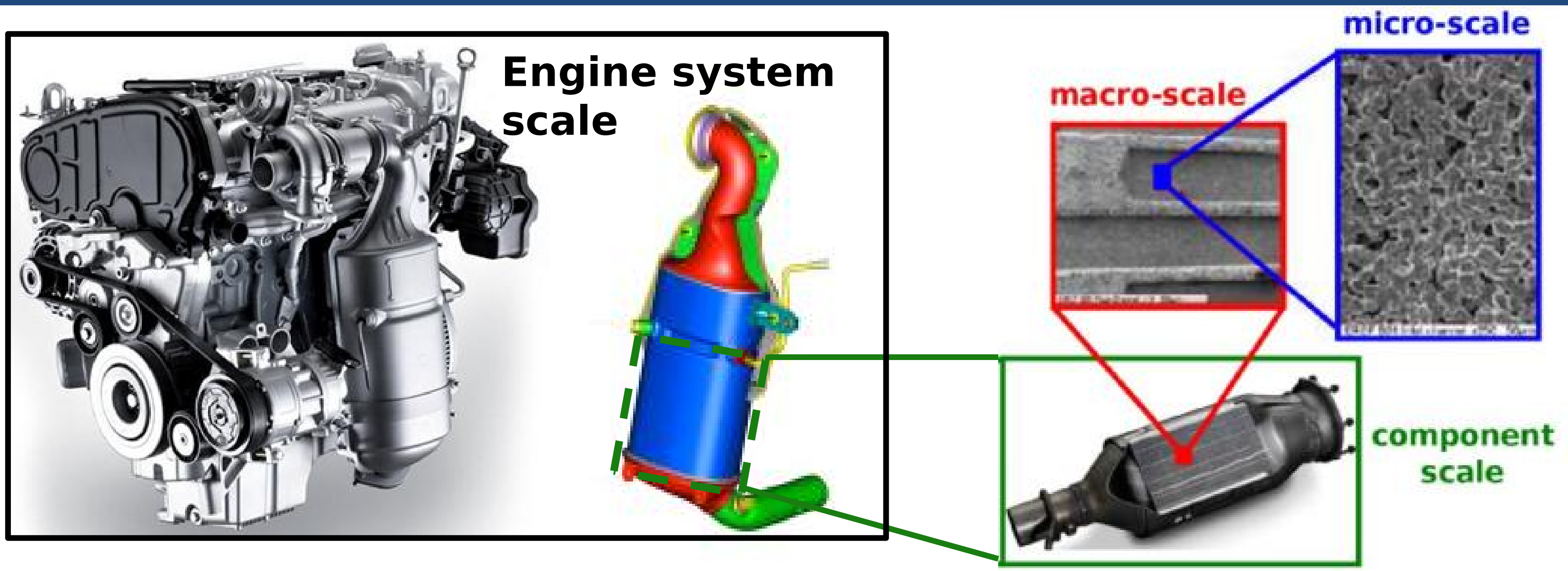
Internal Combustion Engine Group

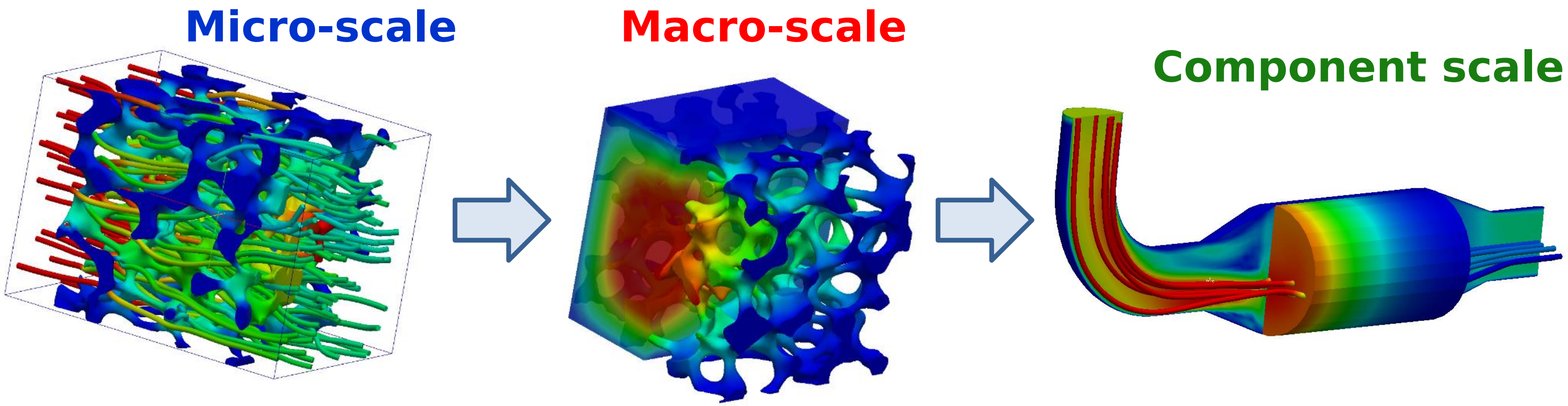
Department of Energy, Politecnico di Milano

Outline

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

Main concept applied to ICE





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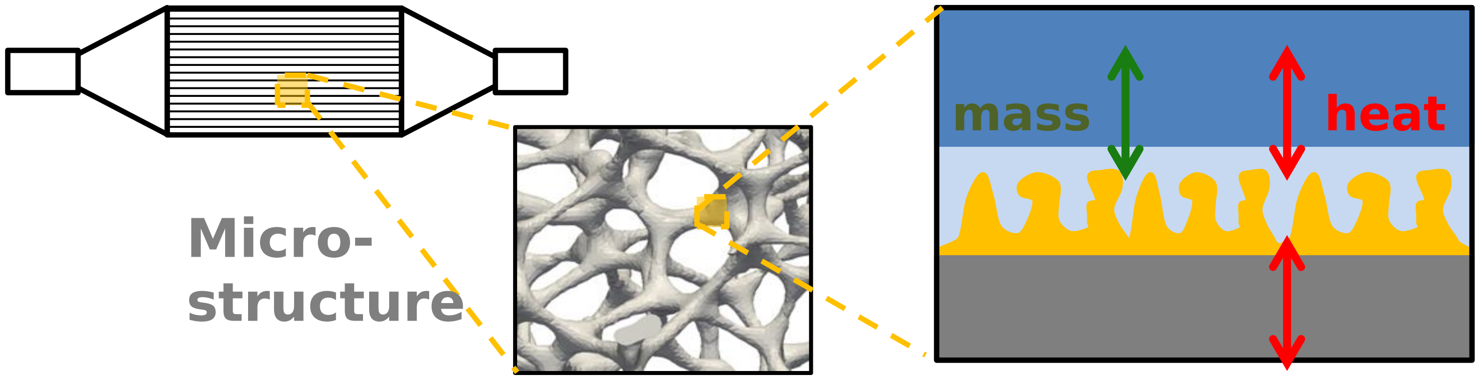
Previous work: micro-scale modelling

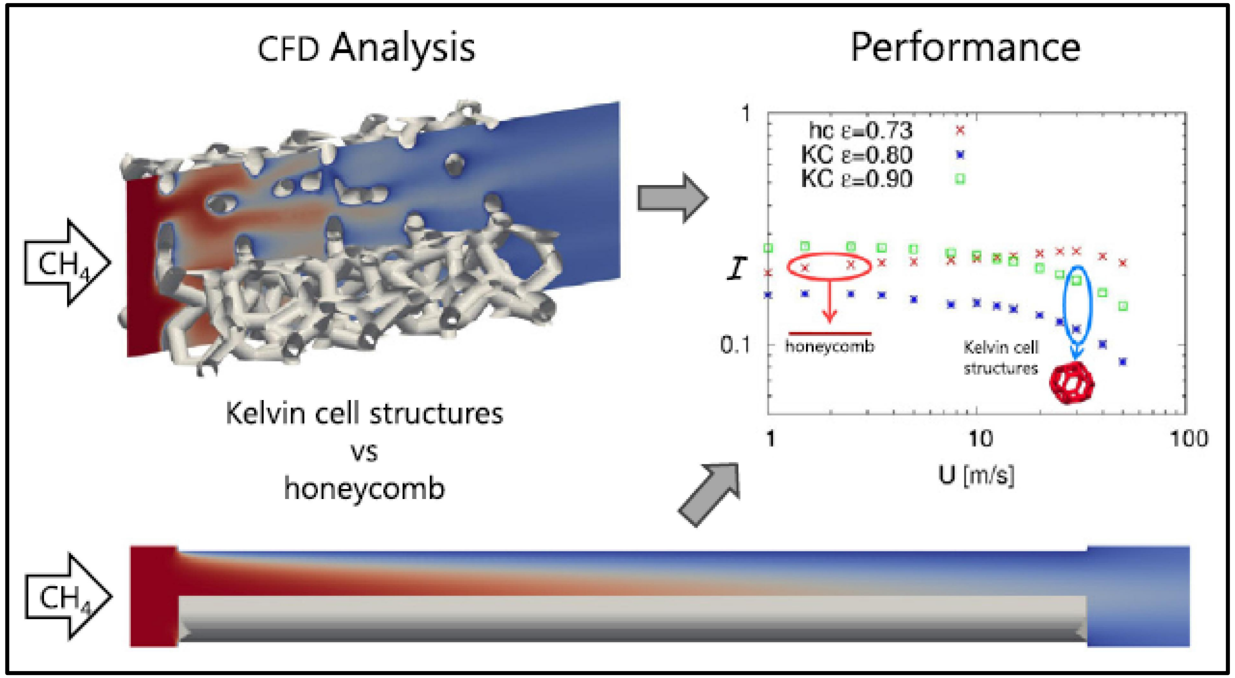


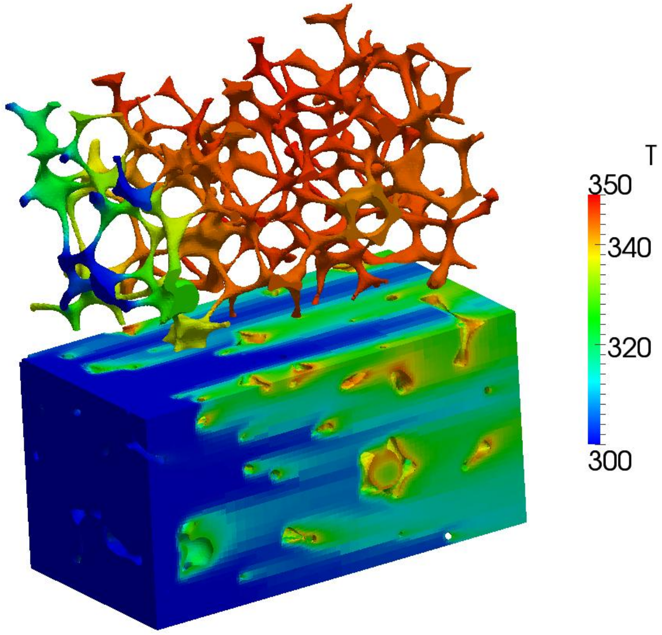
gas

near wall gas

washcoat

solid wall

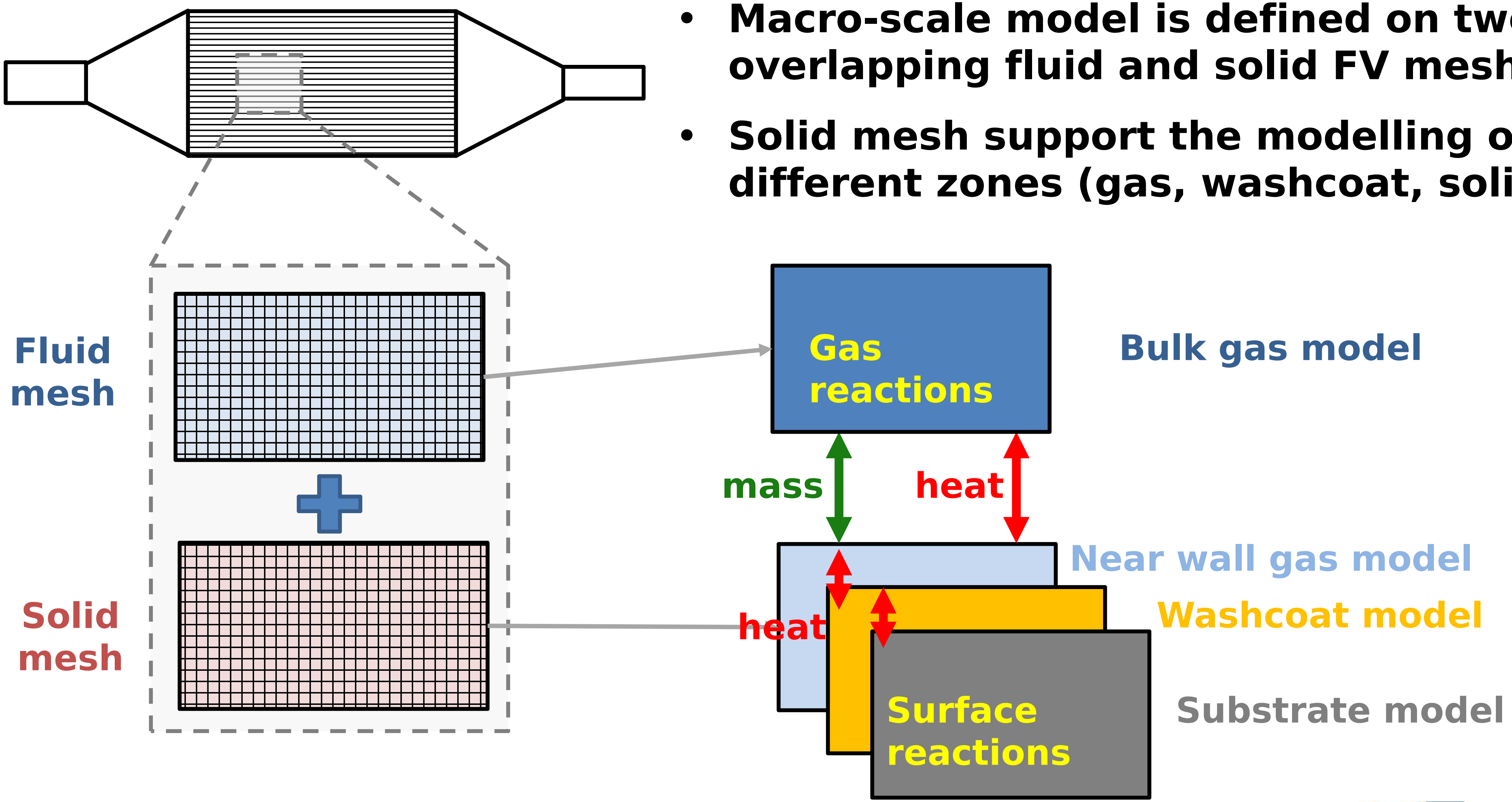




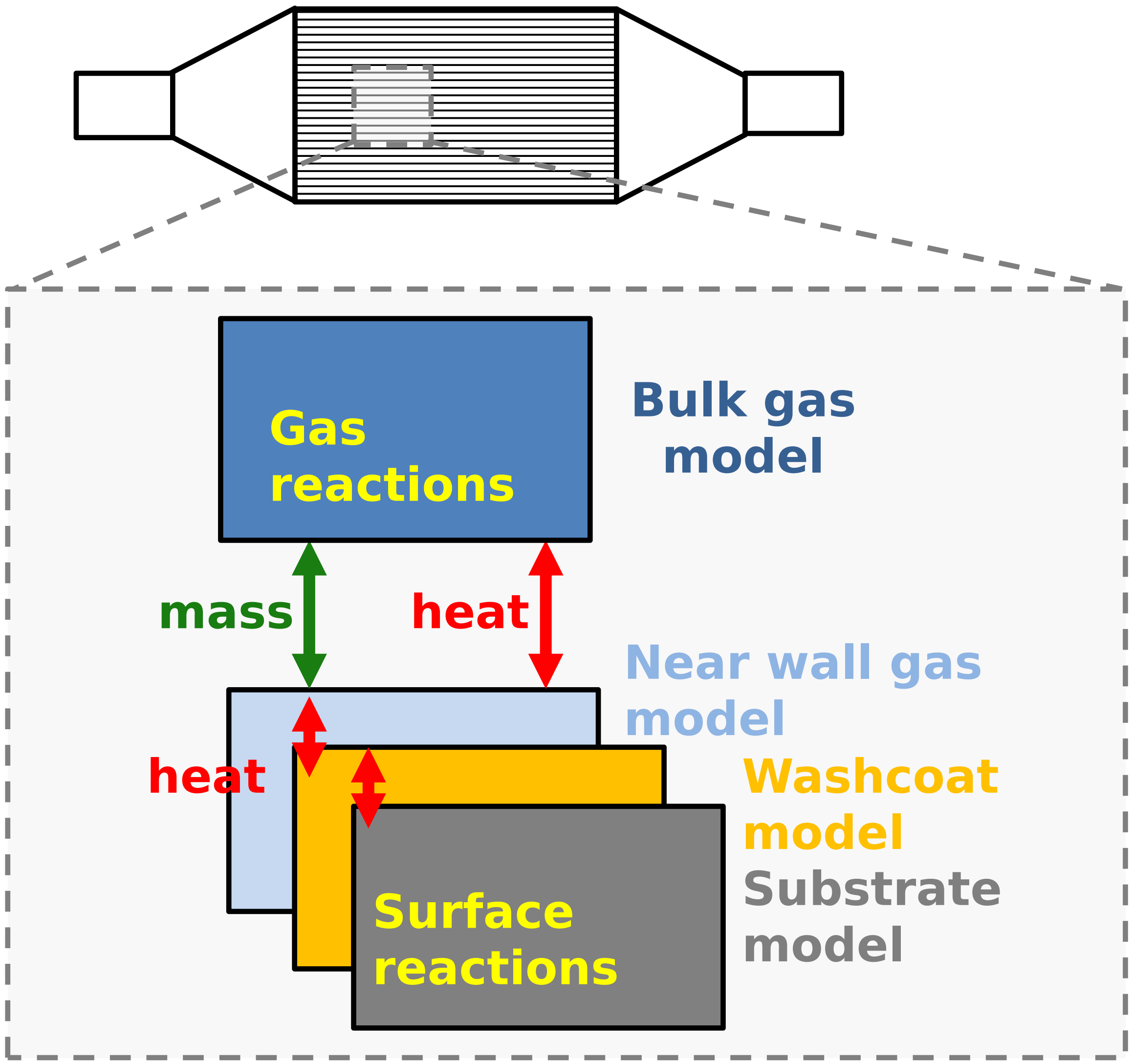
Implementation

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*

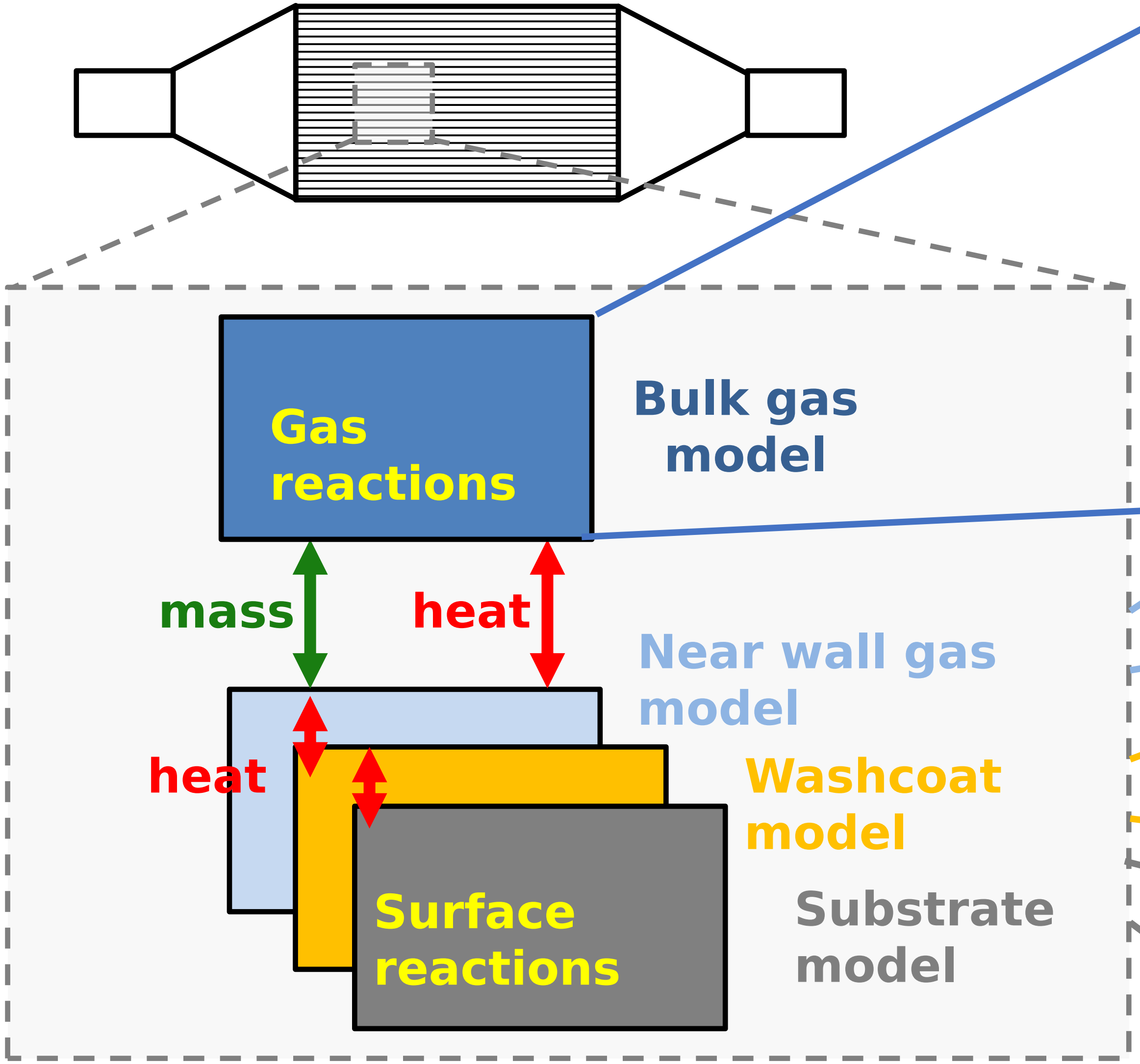
Coupling between fluid and solid regions requires specific models:

- *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.

Implementation

Submodel for ATS simulations



Bulk gas model

$$\frac{\partial \rho_g}{\partial t} + \nabla \cdot (\rho_g \mathbf{U_g}) = 0\,;$$

$$\frac{\partial \rho_g \mathbf{U_g}}{\partial t} + \nabla \cdot (\rho_g \mathbf{U_g} \mathbf{U_g}) = \rho_g \mathbf{g} - \nabla \cdot (\sigma_g) + \mathcal{R};$$

$$\frac{\partial \rho_g e_g}{\partial t} + \nabla \cdot (\rho_g e_g \mathbf{U_g}) = \rho_g \mathbf{g} \mathbf{U_g} - \nabla \cdot (\sigma_g \mathbf{U_g}) + \nabla \cdot (\lambda_g \nabla T_g) + \rho_g Q_g + \rho_g Q_g^R + Q^{w \to g}$$

$$\frac{\partial \rho_g Y_{g,i}}{\partial t} + \nabla \cdot (\rho_g Y_{g,i} \mathbf{U_g}) = \nabla \cdot (\rho_g \mathfrak{D}_{g,i} \nabla Y_{g,i}) + \rho_g R_{g,i} + \mathcal{J}_i^{wg \to g}$$

Near wall gas model

$$\frac{\partial \beta_{wg} \rho_{wg} Y_{wg,i}}{\partial t} = \beta_{wg} \rho_{wg} R_{wg,i} - \mathcal{J}_i^{wg \to g} \quad + \quad T_{wg} = T_w$$

Washcoat model

$$\frac{\partial \beta_w \rho_w c_w T_w}{\partial t} = \beta_w \rho_w Q_w^R - Q^{w \to wg} - Q^{w \to g} - Q^{w \to s}$$

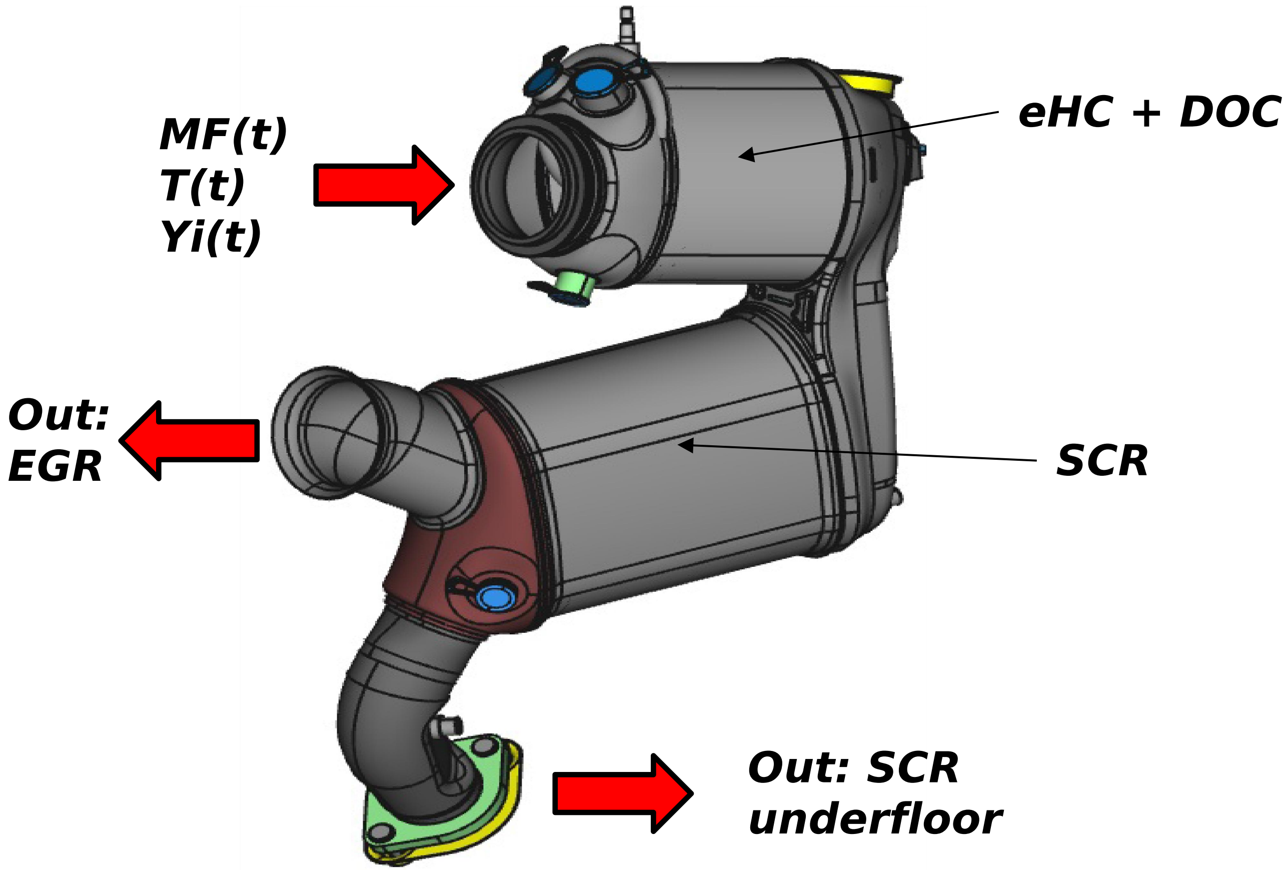
Substrate model

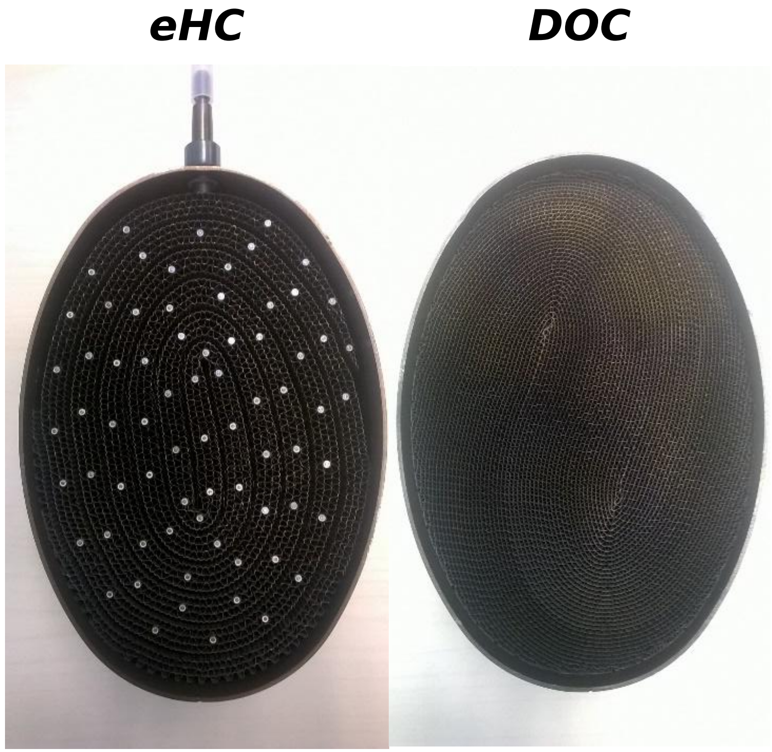
$$\frac{\partial \beta_s \rho_s c_s T_s}{\partial t} = \beta_s \rho_s Q_s + \nabla \cdot (\boldsymbol{\lambda}_s \nabla T_s) + Q^{w \to s}$$

Application to the simulation of a real ATS system

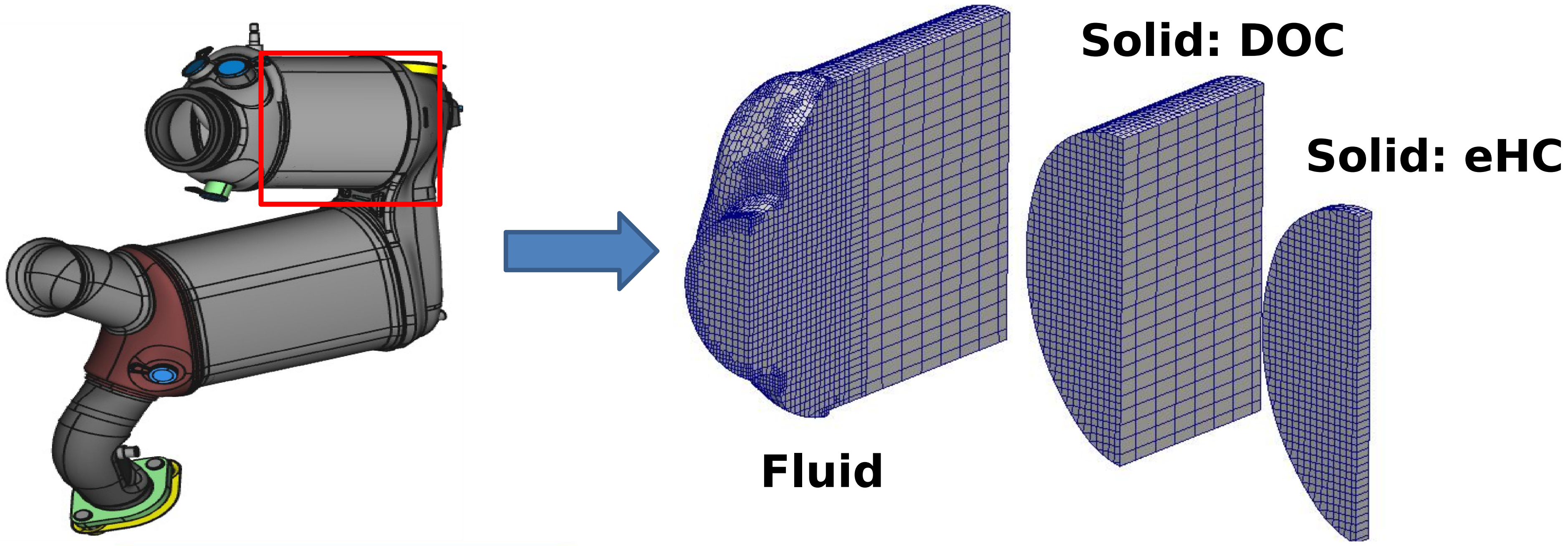
Full-scale 3D case including DOC monolith and electrical heating

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





Application to the simulation of a real ATS system



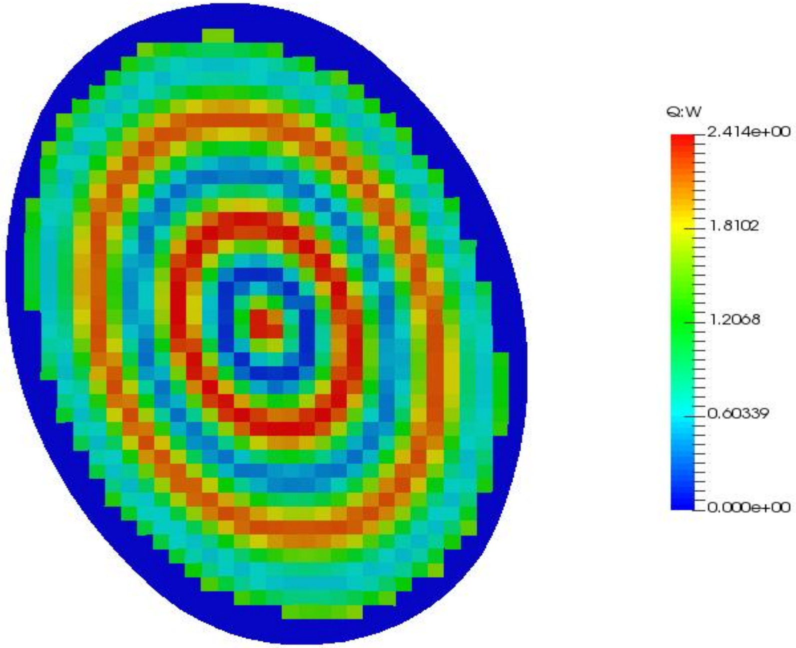
Application to the simulation of a real ATS system

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

Phenomenological model:

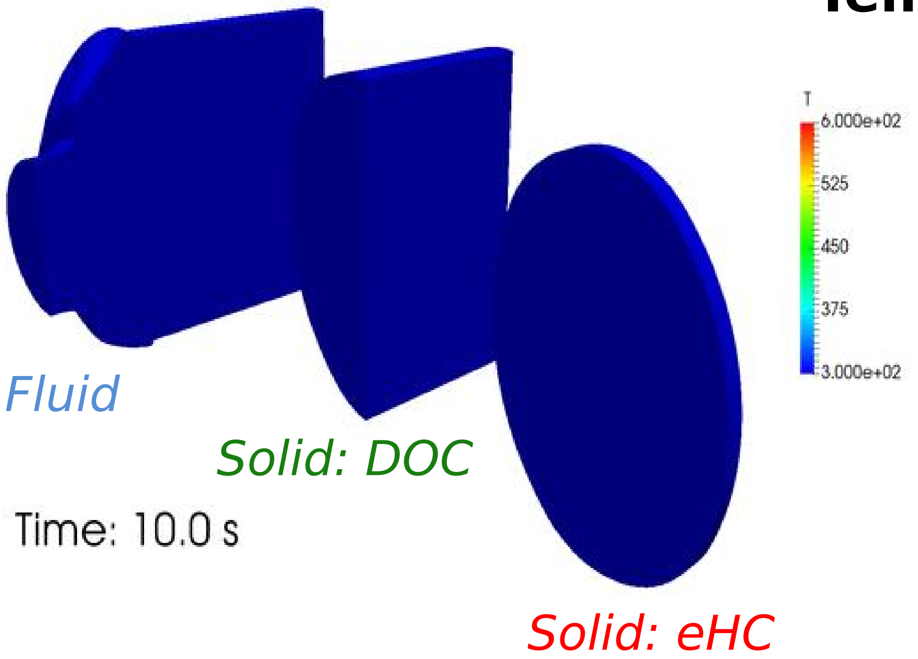
- Each spiral has a high T side and a low T side
- Non-uniformity decreases from center to boundary
- No heating at the boundary (short circuit)

Spatial distribution for the heat release



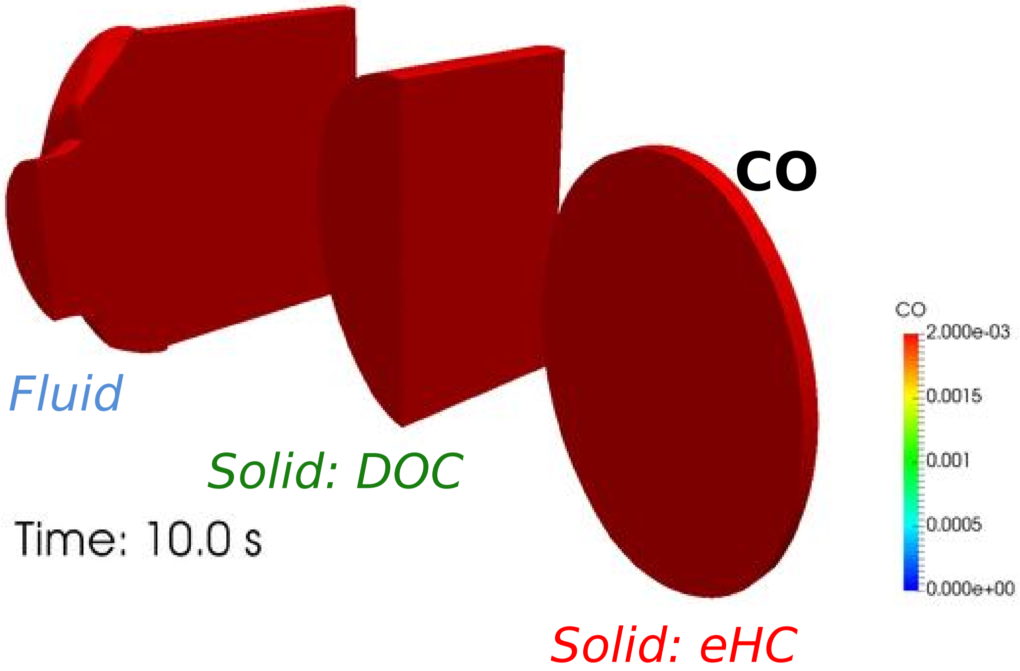
DOC configuration with non-uniform heating

Temperature



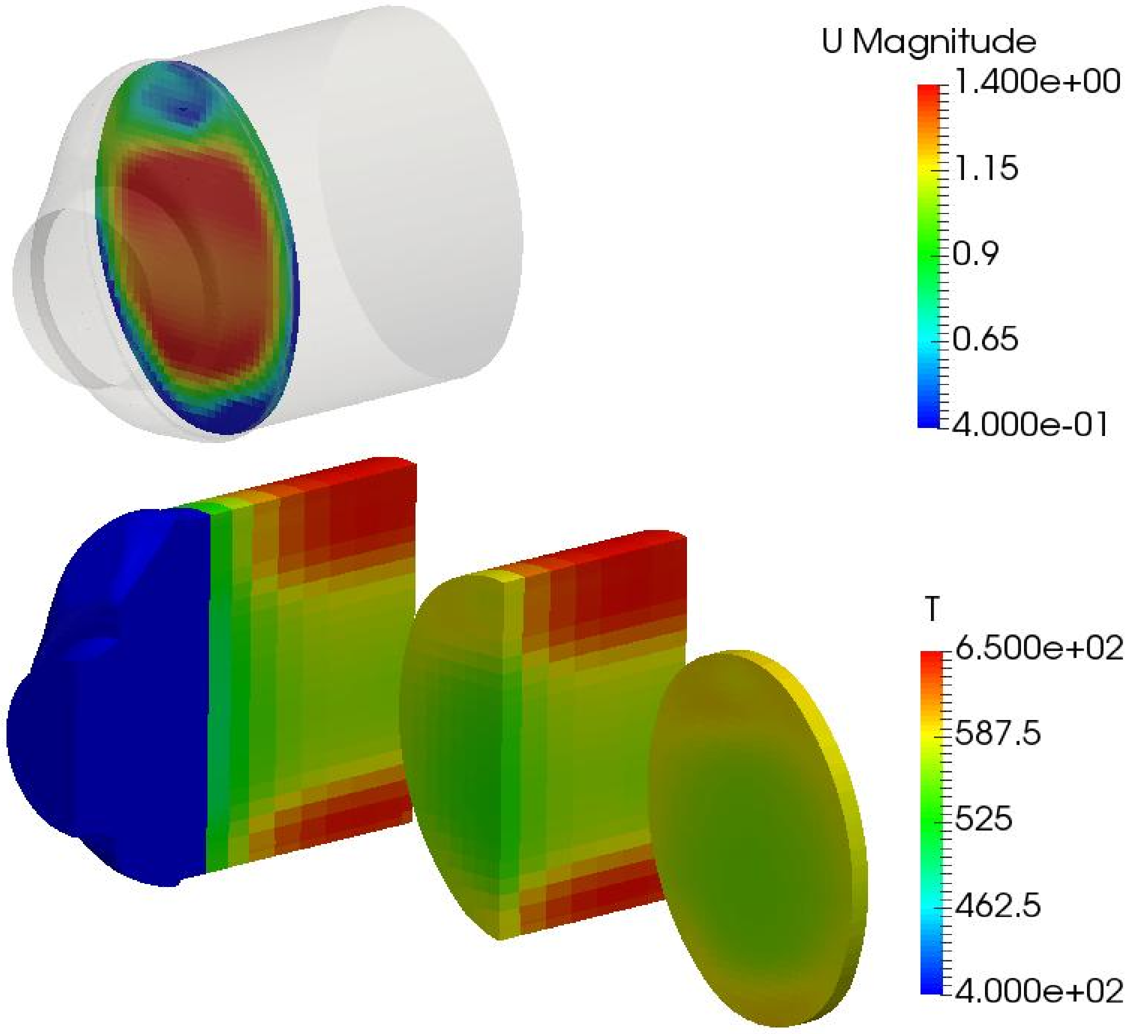
Non-uniform heating
P_{el} = 1 kW : 0-100 s
P_{el} = 0.5-0.2 kW : 100-300 s

CO



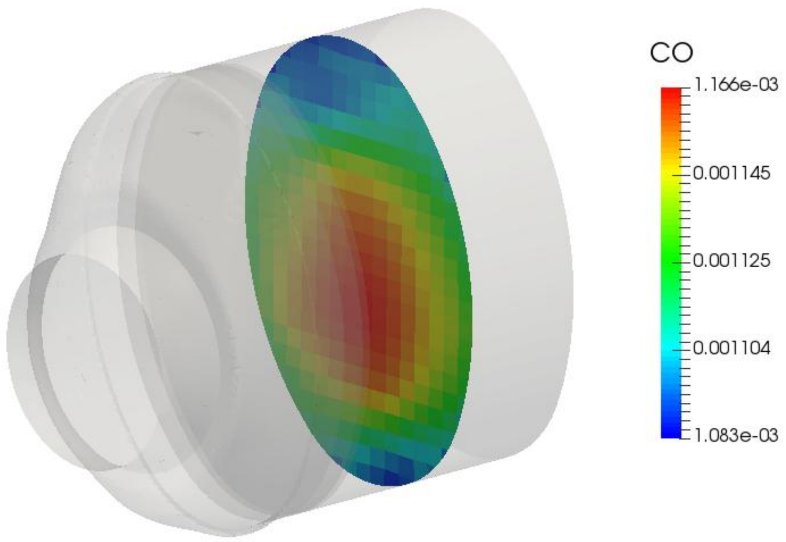
Non-uniformity of the heating generates hot spots ➡ **earlier light-off**

DOC configuration with uniform heating

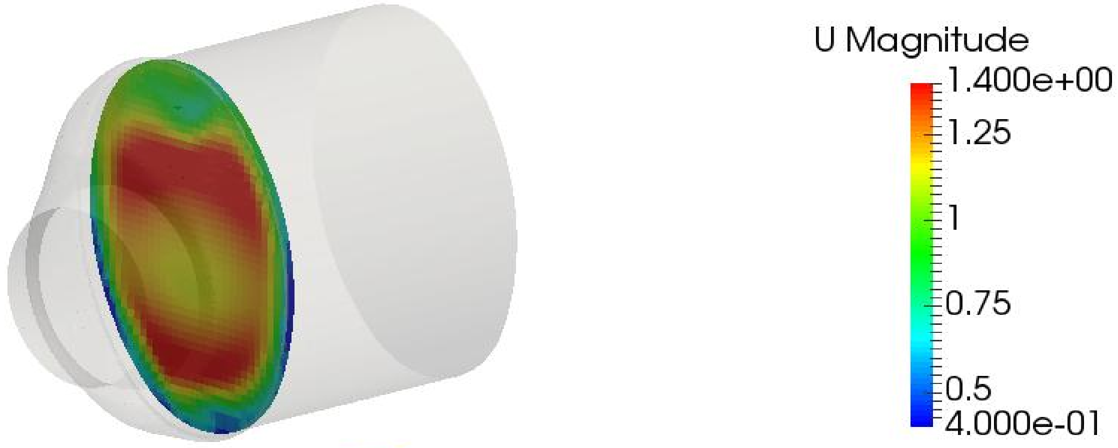


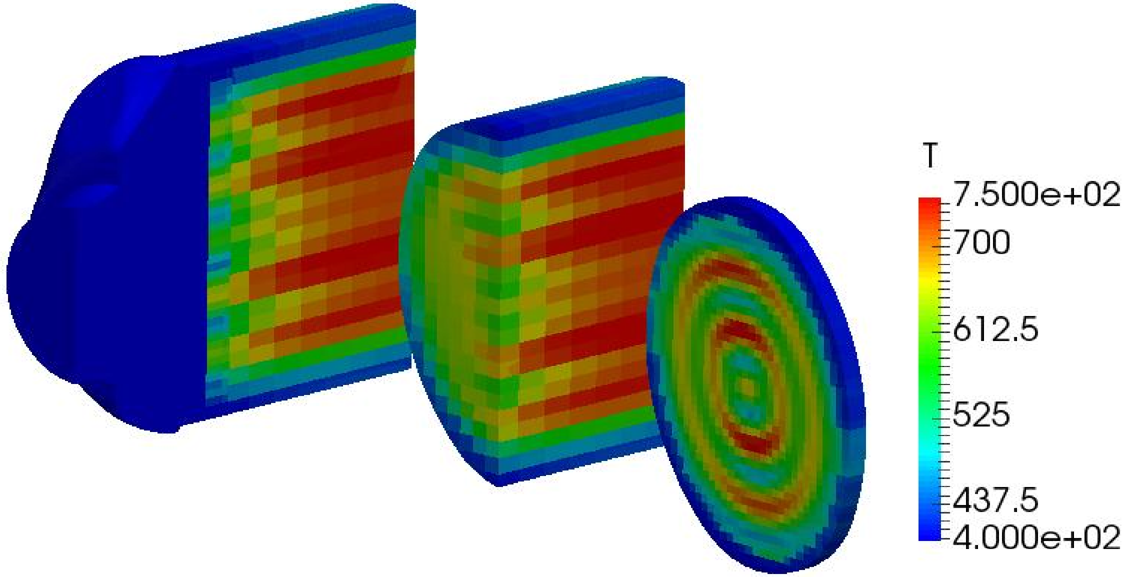
Time = 140 s

Uniform heating
P_{el} = 1 kW



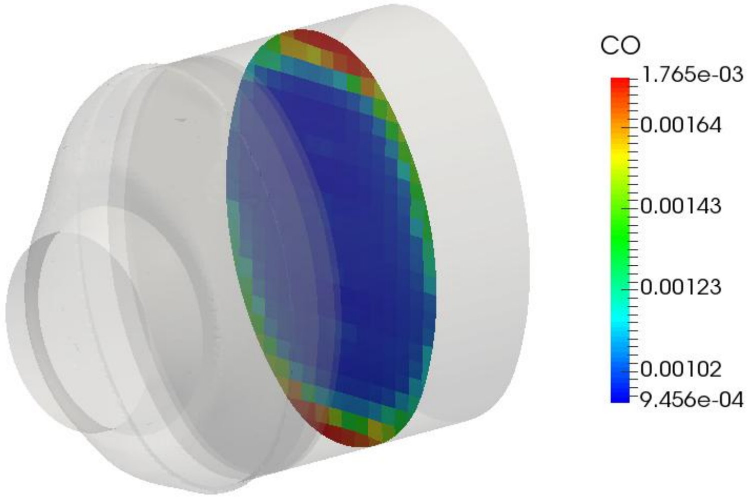
Application to the simulation of a real ATS system
DOC configuration with non-uniform heating





Time = 140 s

Non-uniform heating
P_{el} = 1 kW



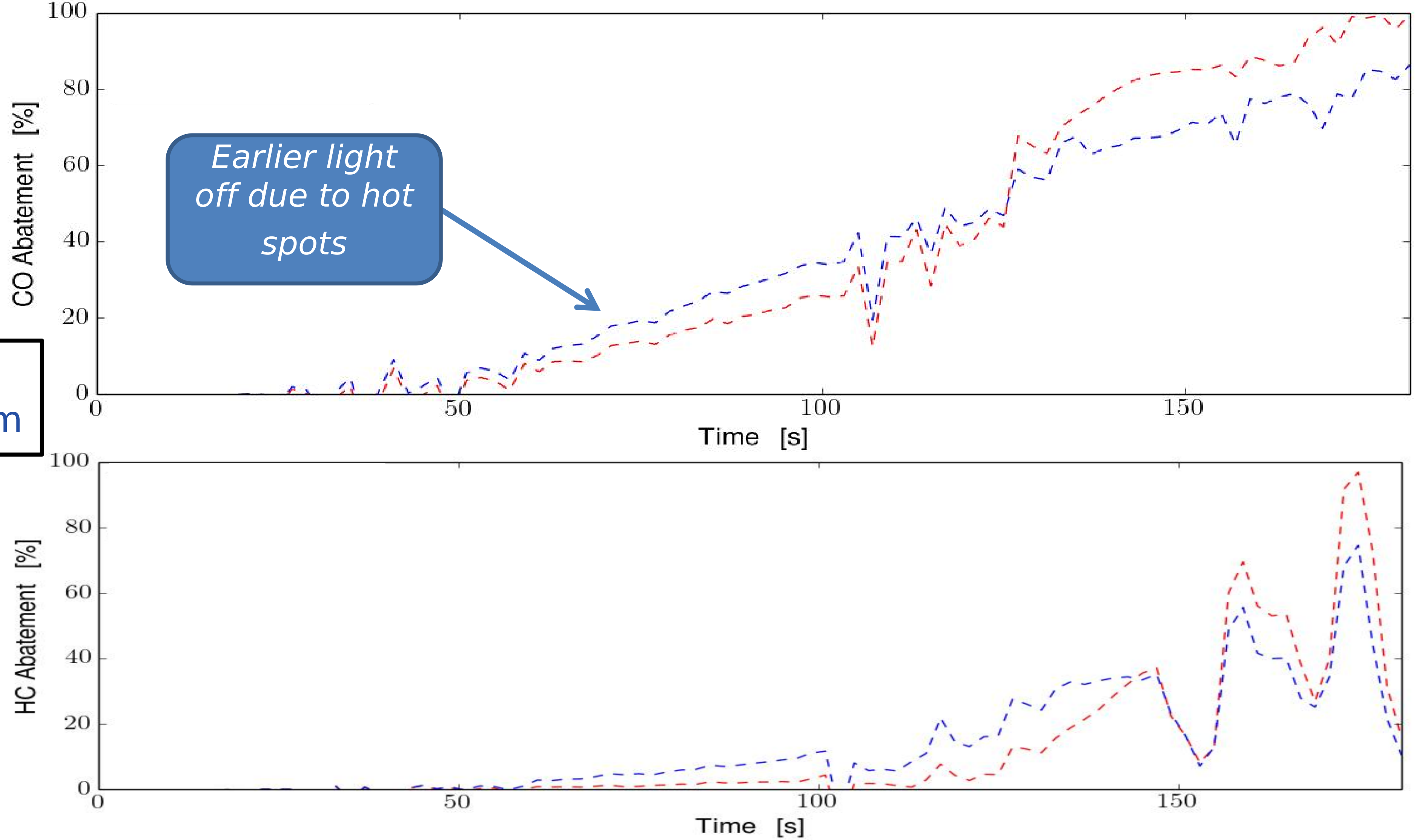
3D model

DOC: comparison uniform vs non-uniform heating

CO

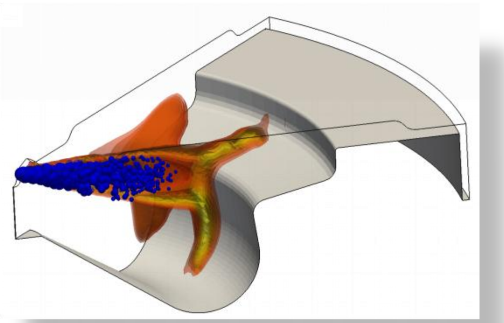
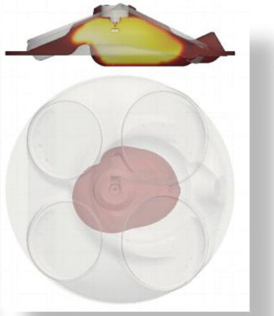
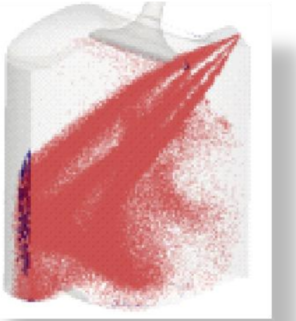
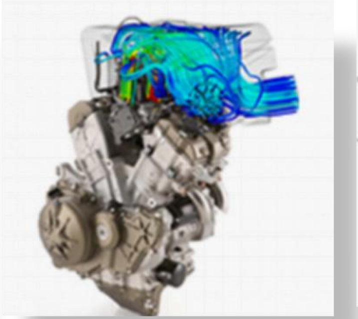
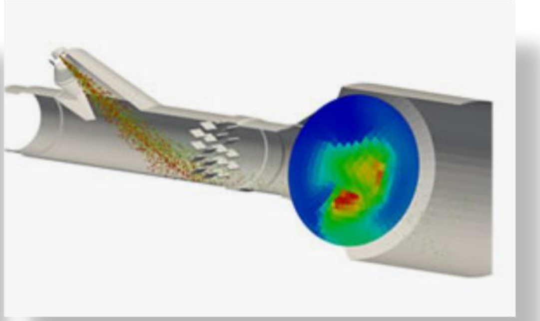
HC

Uniform
Non uniform



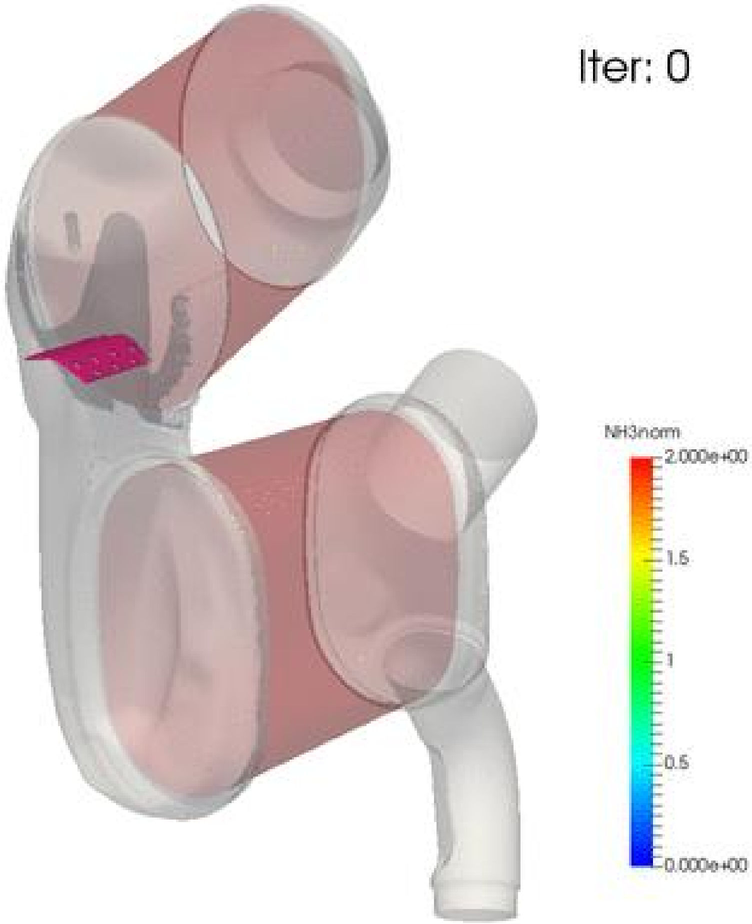
Lib-ICE: I.C.E. modeling using the OpenFOAM® technology

- Mesh motion for complex geometries
- Combustion
- Lagrangian sprays + liquid film
- Unsteady flows in intake and exhaust systems: plenums, silencers, 1D-3D coupling.
- Reacting flows in after-treatment devices: DPF, catalyst, SCR.

OPTIMIZATION FRAMEWORK

Optimization procedure



CAD: definition of the parametric geometry

CFD: calculation of the «simulated» responses (50 + N samples)

Surrogate model

GA: calculation of the «approximated» responses (1000 samples)

Optimum at the N^{th} iteration

Err < toll

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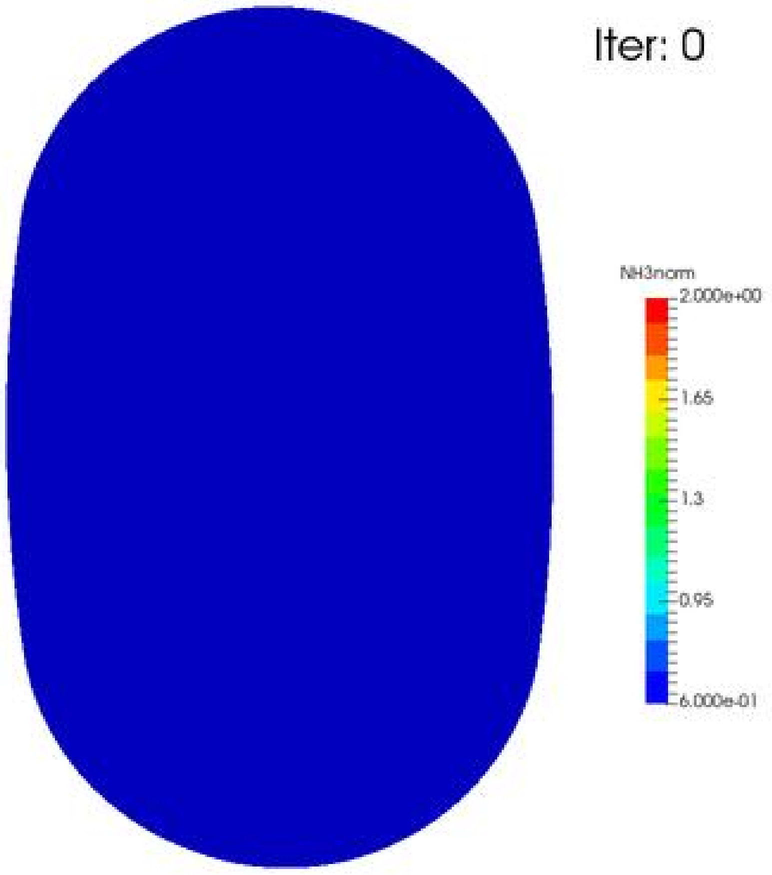
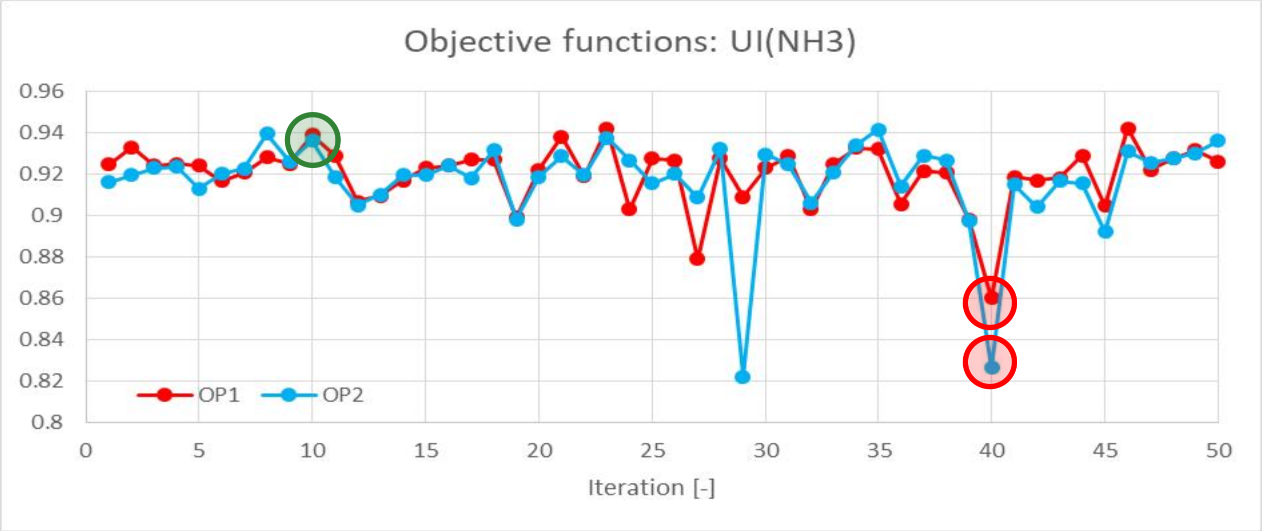
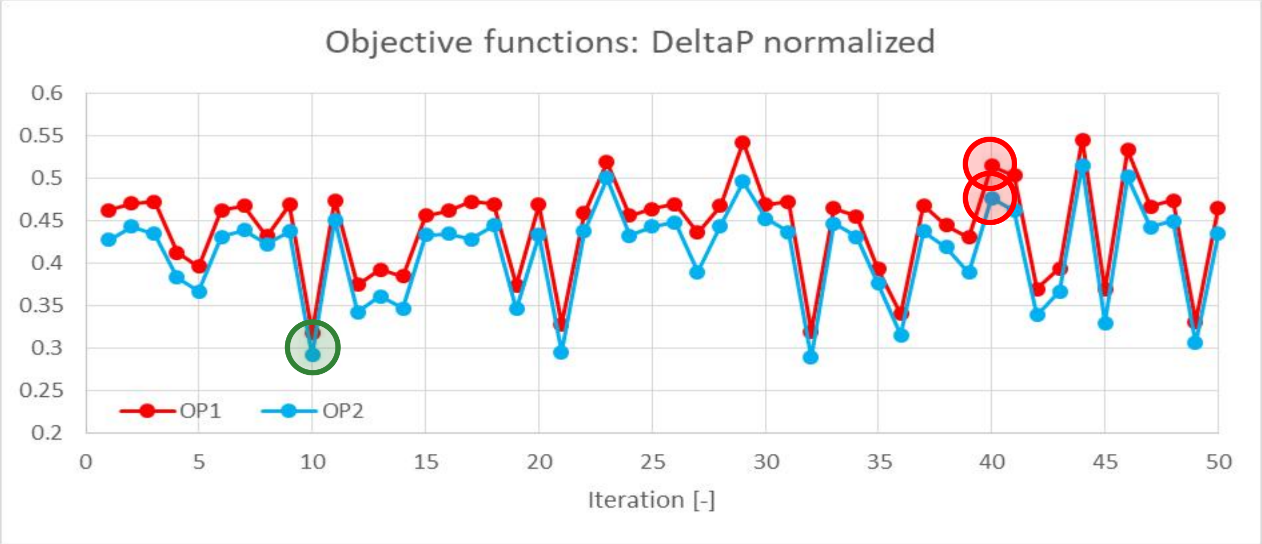
Optimization: DOE





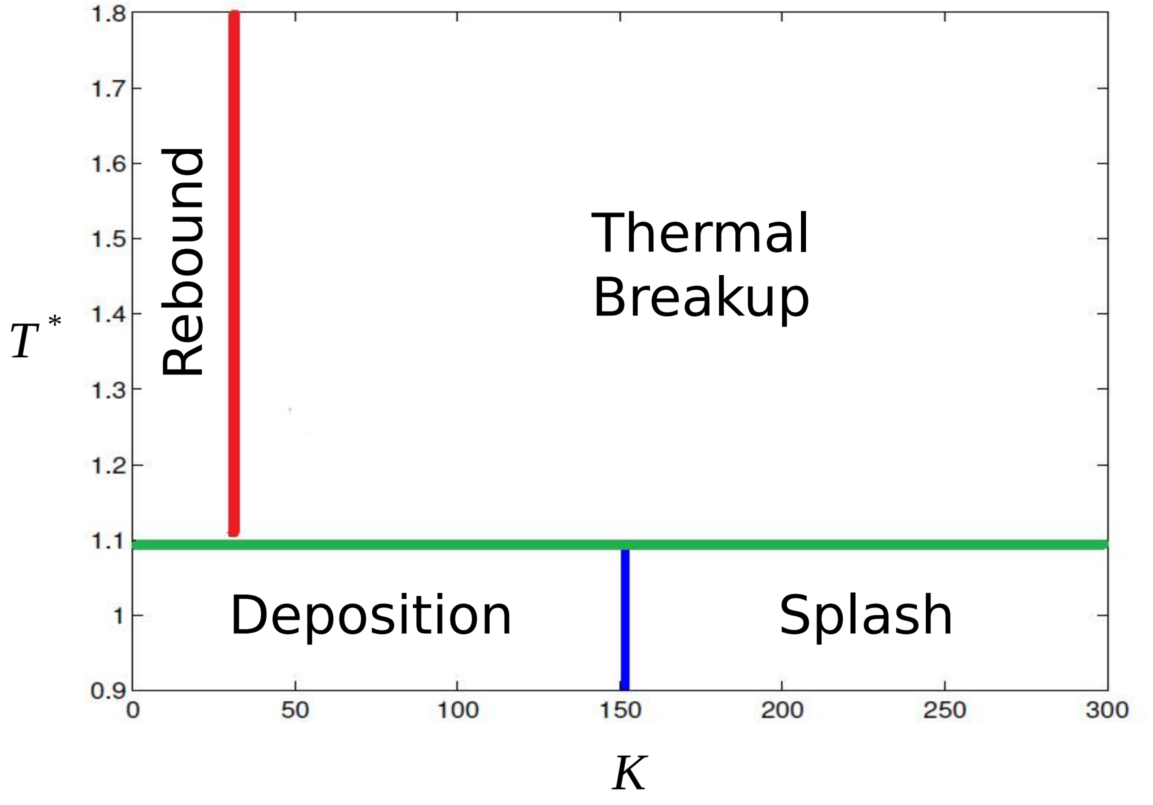


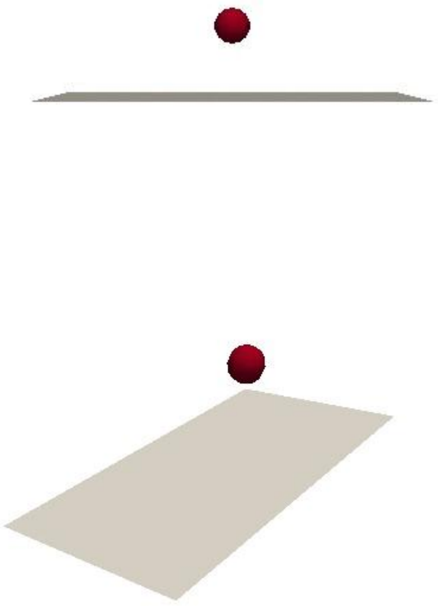
SPRAY & WALL FILM MODELING

Thermal aspects of spray-wall interaction

Extension of standard impingement regimes

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



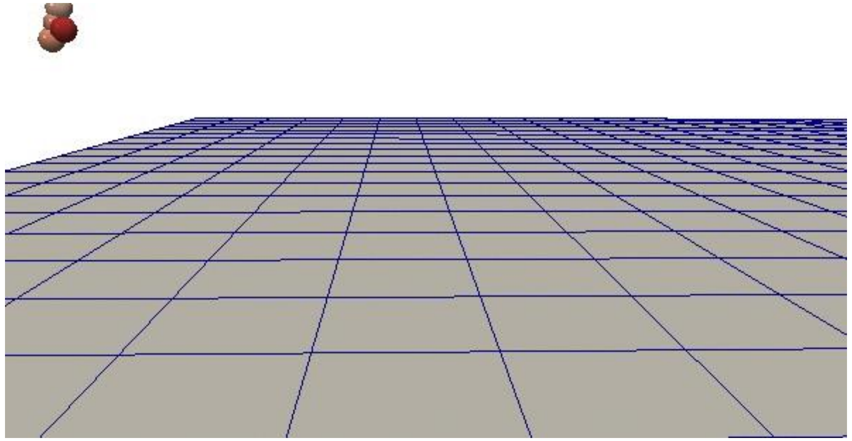


Thermal aspects of spray-wall interaction

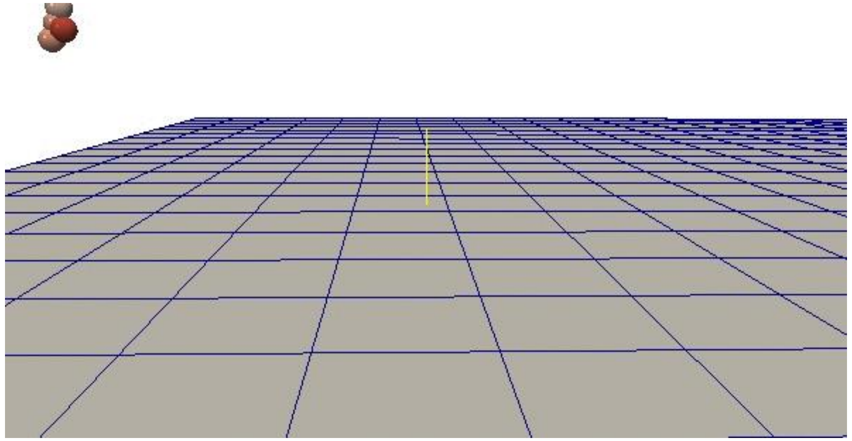
Splashing threshold shift

Absolute We = 264
Normal We = 137

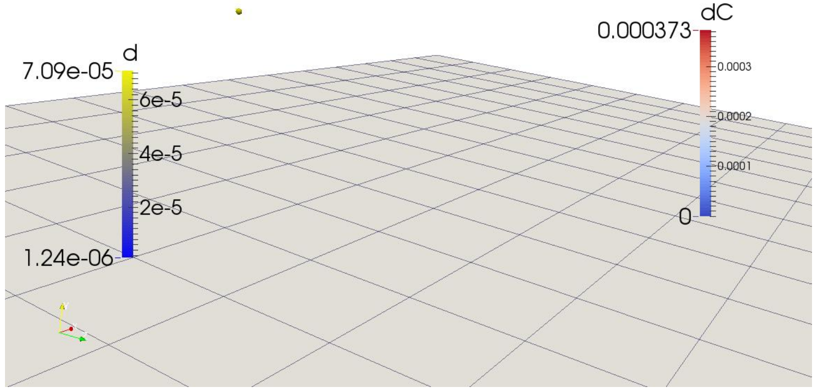
T* = 0.8



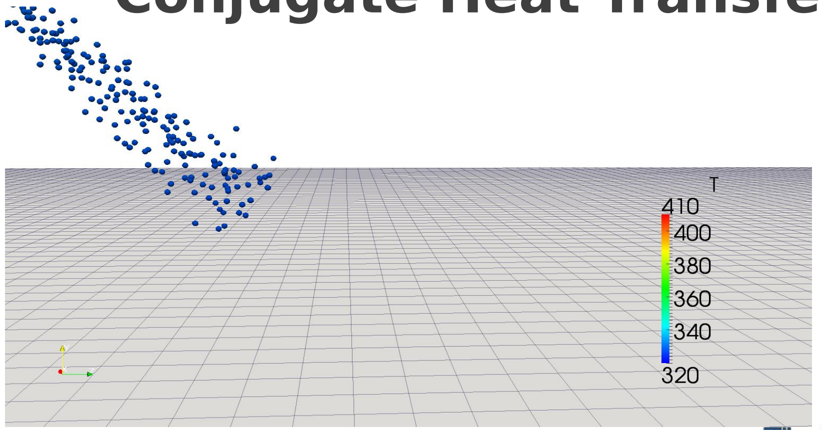
T* = 1.2



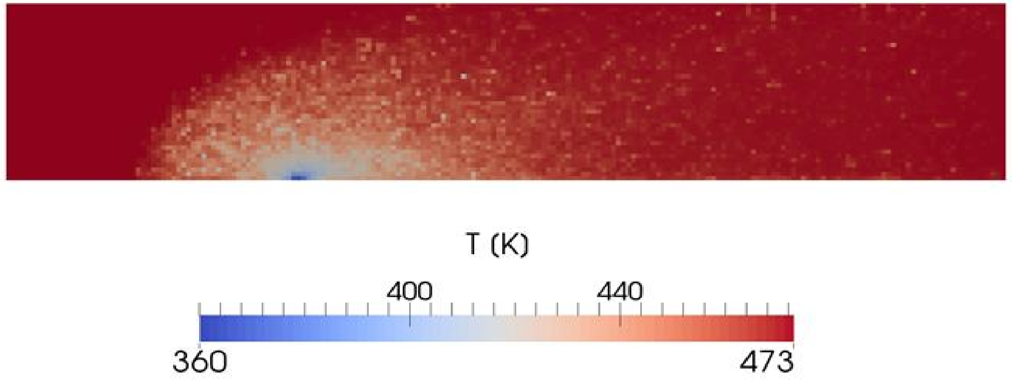
Non-zero contact time

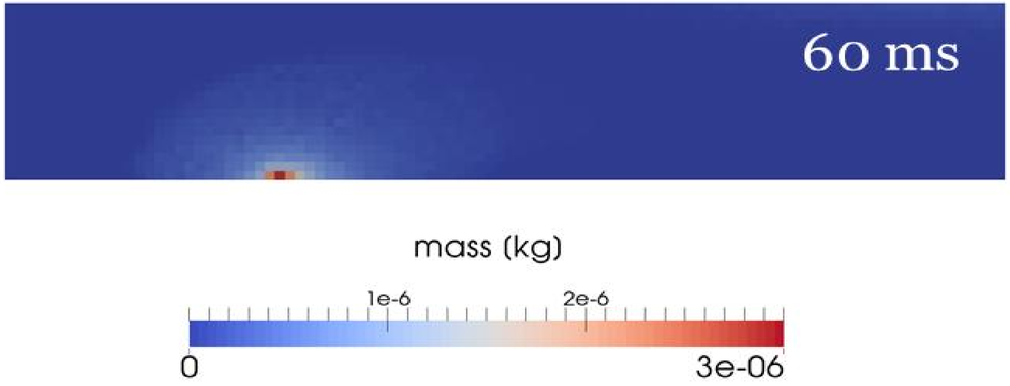


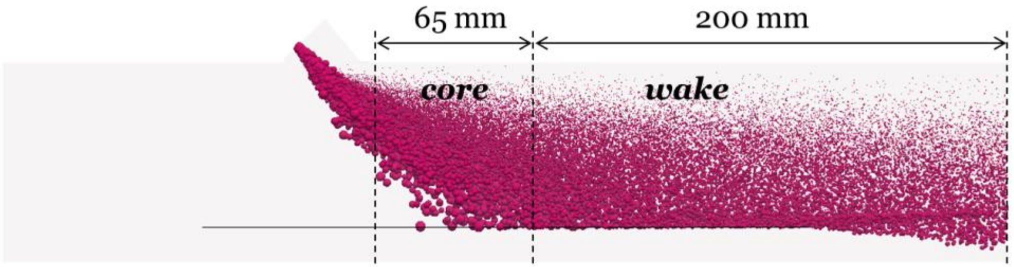
Conjugate Heat Transfer

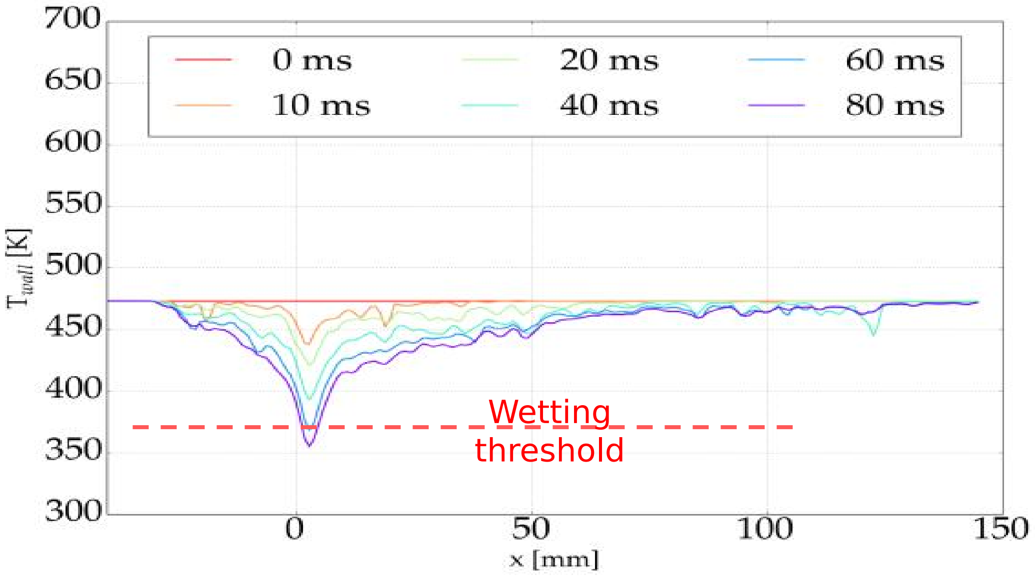


Thermal aspects of spray-wall interaction



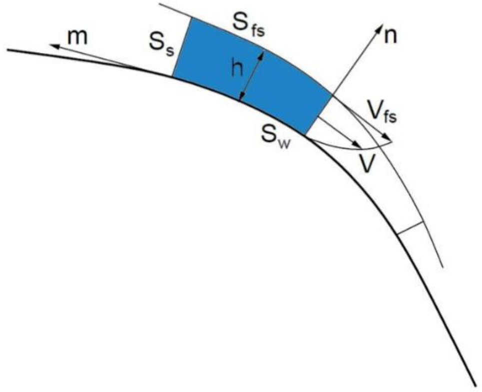






- CHT on dry wall
- The temperature drop before the wetting condition is predicted

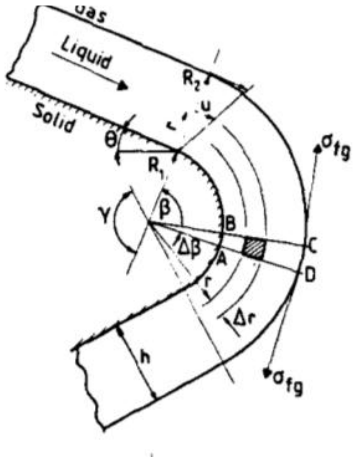
Solution of the liquid film



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

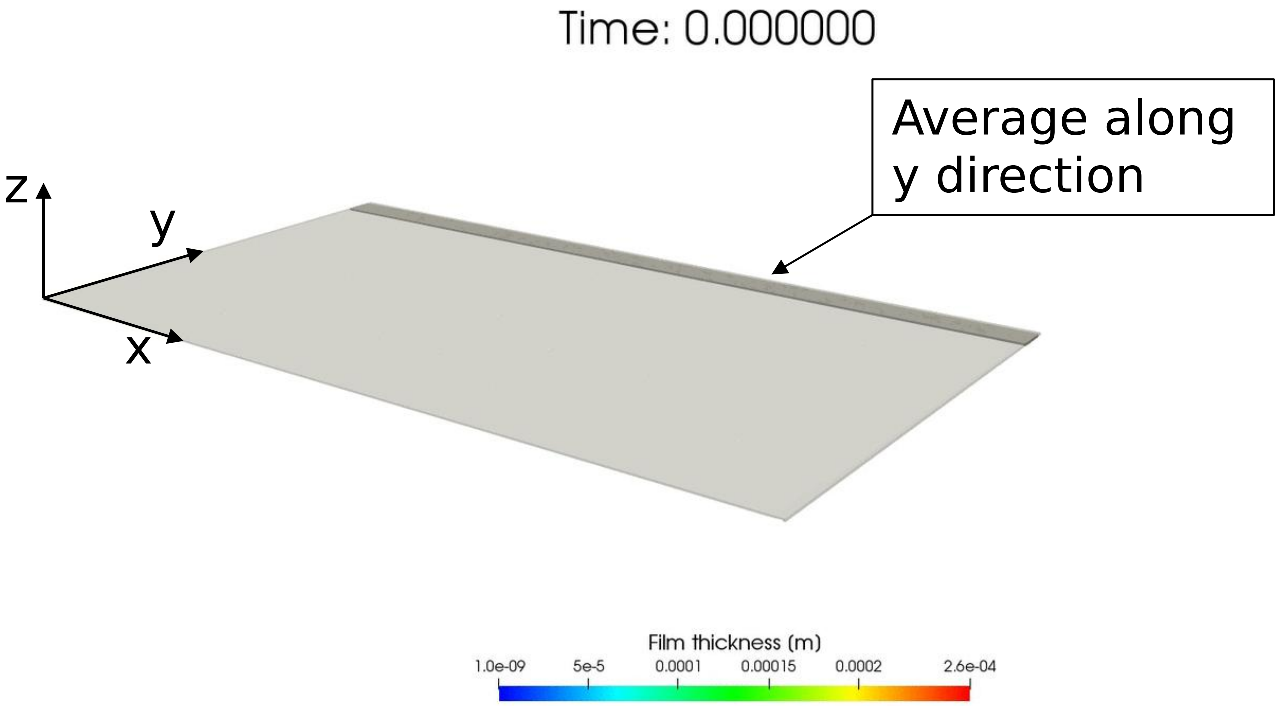
$$\frac{\partial h \vec{u}_f}{\partial t} + \nabla \cdot (h \vec{u}_f \vec{u}_f) = -\frac{1}{\rho_f} \nabla (h p_f) + \vec{\tau}_g - \vec{\tau}_w + h\vec{g} + \vec{S}_U$$

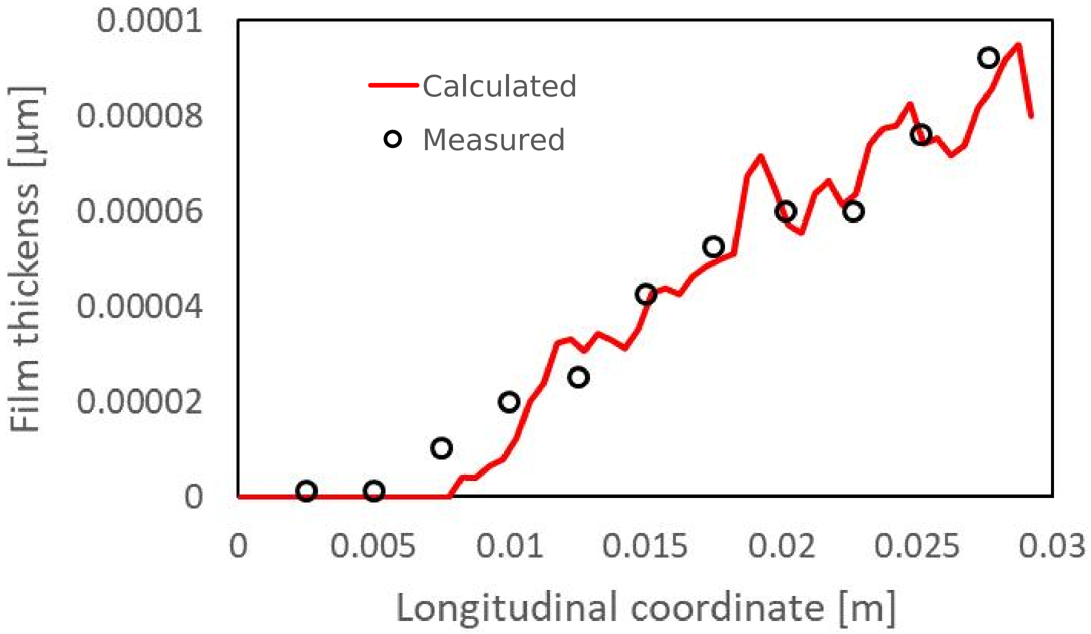
$$\frac{\partial h \hat{H}_{s,f}}{\partial t} + \nabla \cdot \left(h \vec{u}_f \hat{H}_{s,f} \right) = j_g - j_w + S_H$$

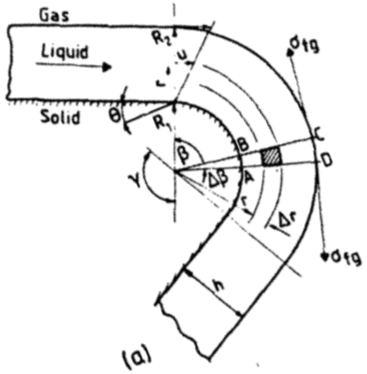


- Film stripping model triggered when the inertial forces exceed the surface tension ones.
- Gravitational acceleration is also taken into account.
- Minumum parcel mass and capability to store mass to guarantee mass continuity
- User selectable diameter distribution for stripped parcels

Validation case: high mass flow rate

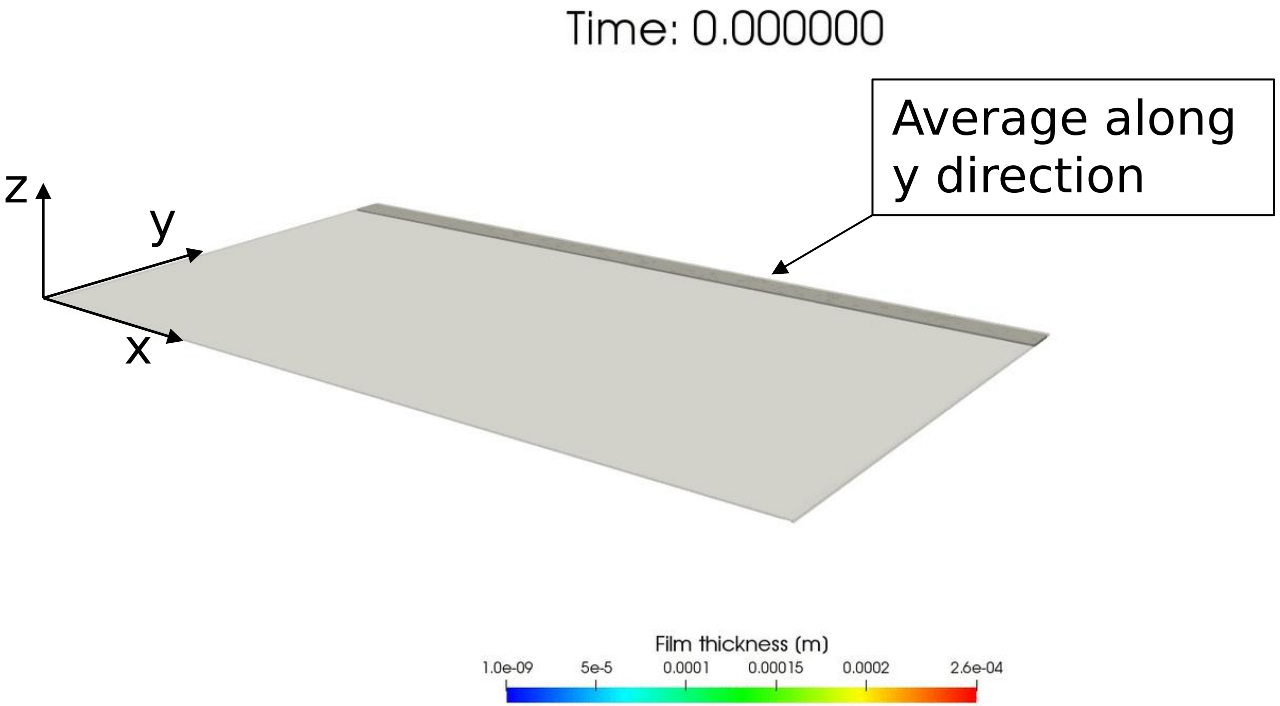


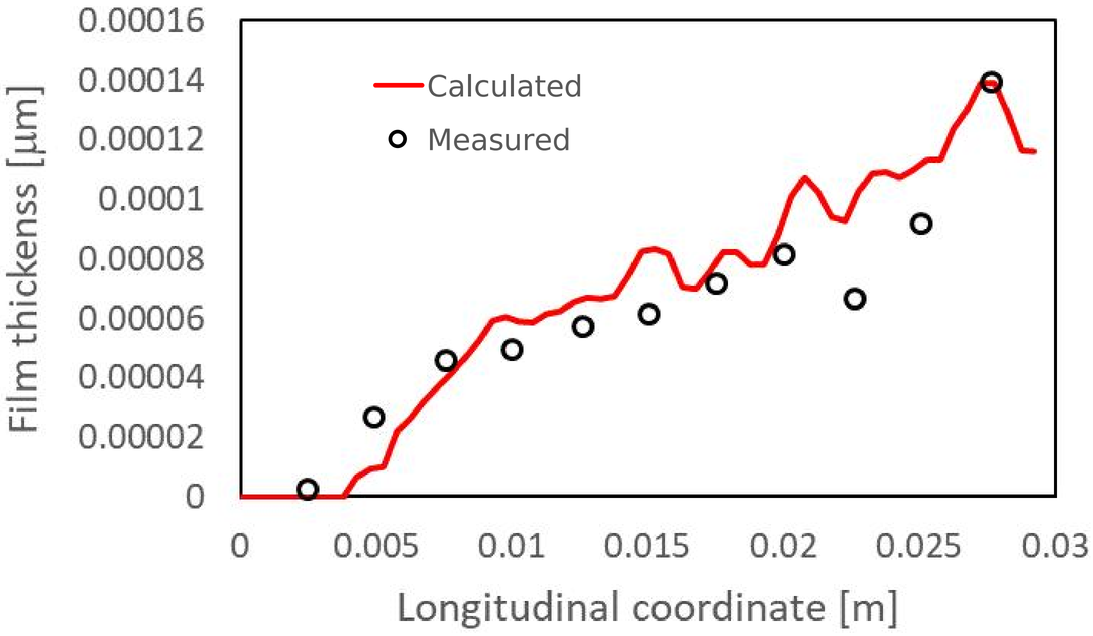




- Good prediction of film evolution
- Stripping of droplet at the edge of the plate

Validation case: low mass flow rate





- Decreasing the gas mass flow the impingement occurs at a different longitudinal position
- Accurate prediction at different mass flow regime

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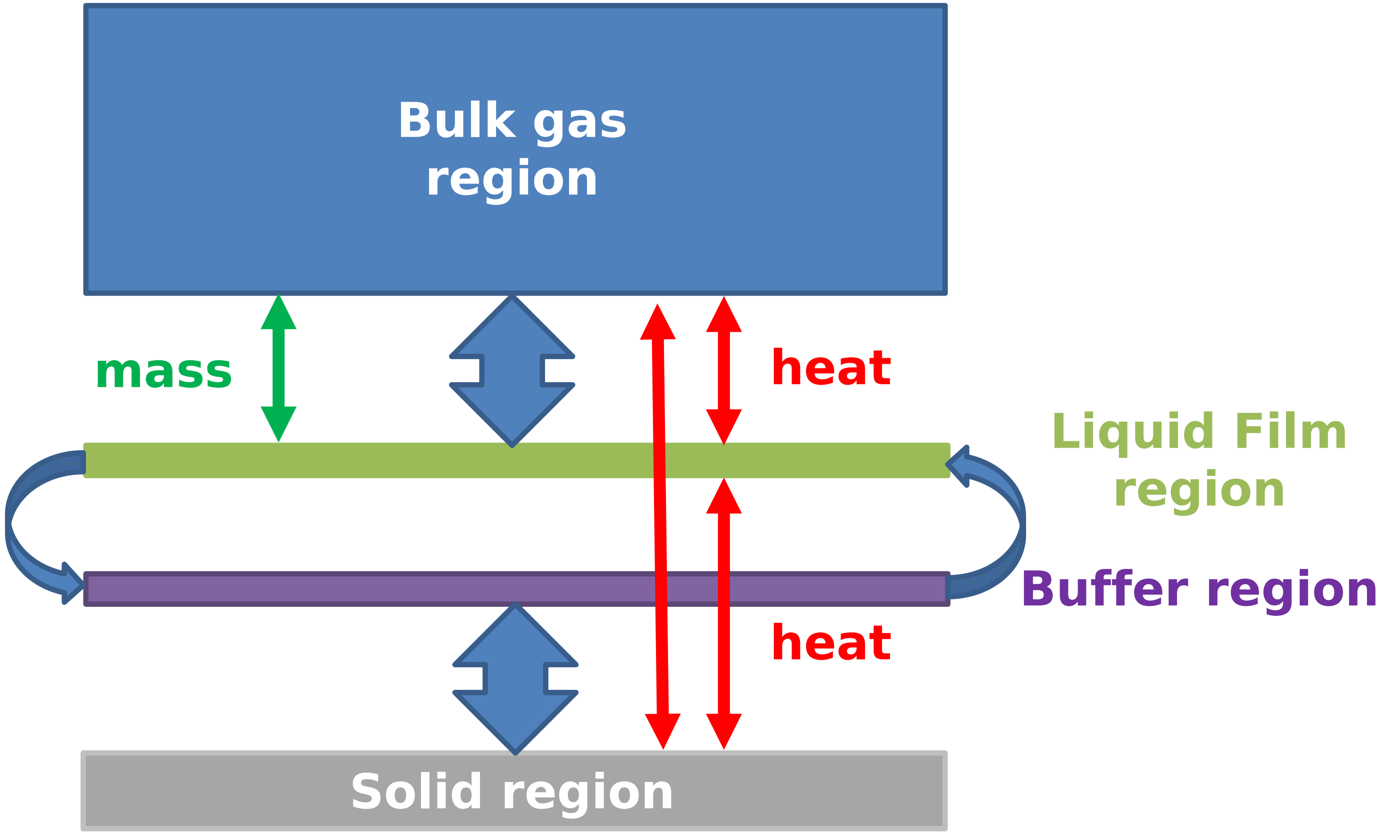
Thermal aspects of spray-wall interaction

To obtain coupling between solid region, liquid film and fluid a new approach was developed, based on the use of a buffer region.



Exchange of source terms due to:

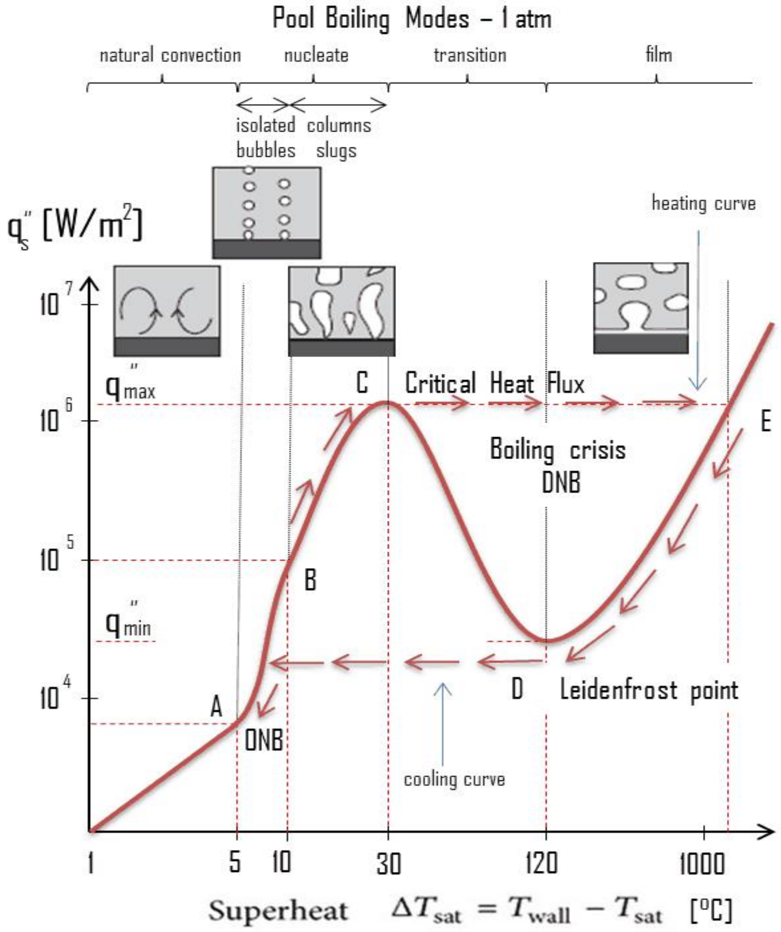
- Droplet impingement
- Solid/Fluid convective heat transfer
- Film/Solid conductive heat transfer

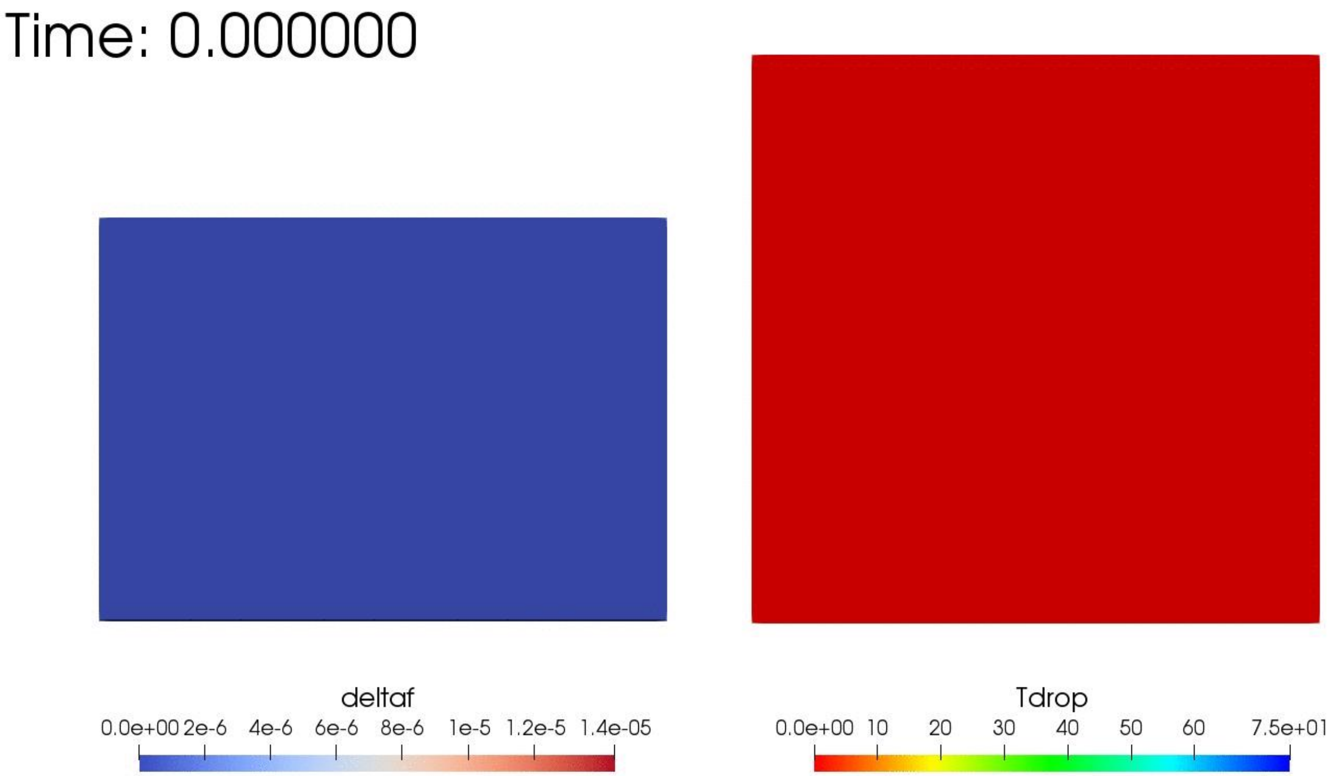
The buffer region can represent both film and gas depending on the presence/absence of film.

WORK IN PROGRESS

Work in progress: spray modeling
Thermal interaction in different temperature ranges

Current developments seek to validate the thermal heat transfer between spray and wall in different temperature ranges.

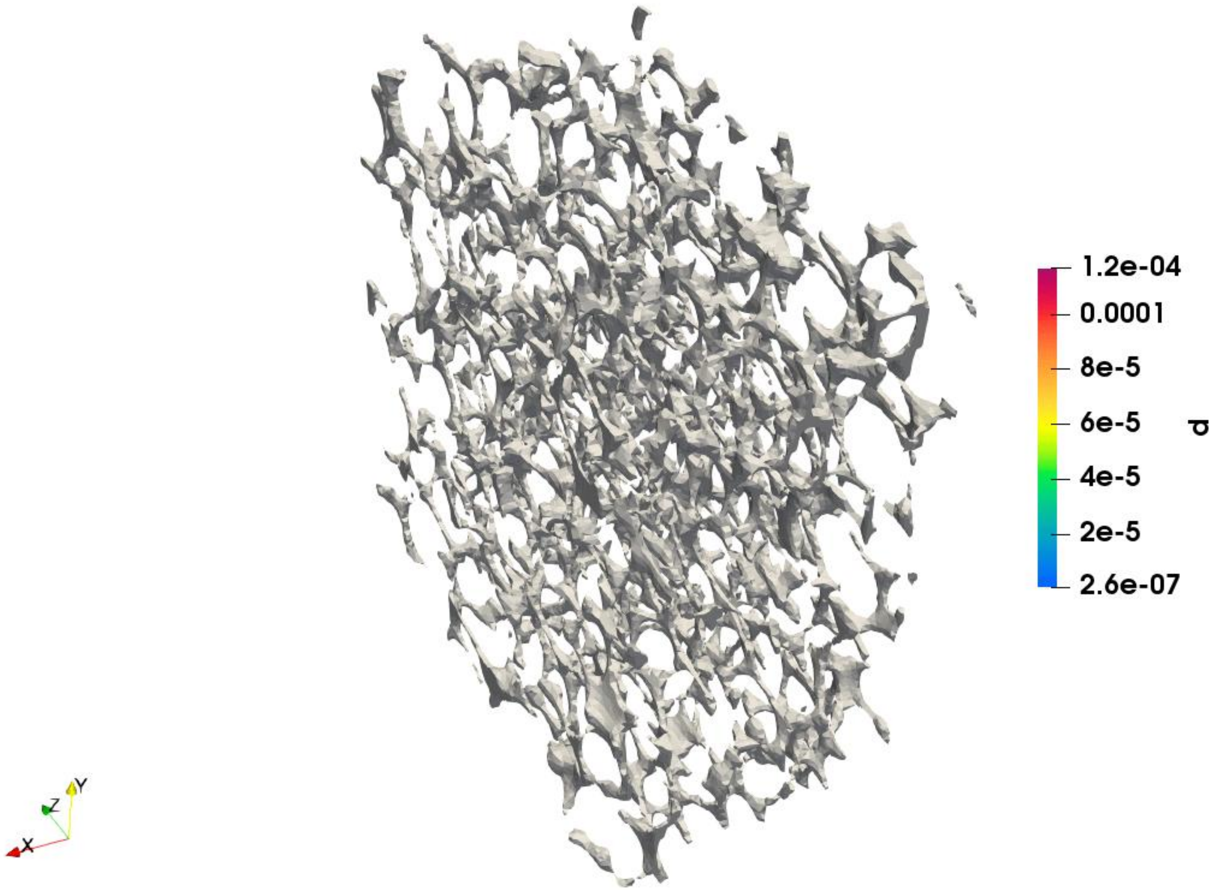




Application to advanced substrates

The models developed are currently being applied to foam structures.

Promising results in term of enhanced mass transfer



Conclusions

- Models for **macro-scale and micro-scale simulation** of complex **after-treatment devices** have been implemented: these models are based on a **multi-region framework** and describe the phenomena occuring in catalytic substrates:
  - Ø Heat transfer
  - Ø Mass transfer
  - Ø Catalytic reactions

- These models can be easily embedded in an **optimization procedure** to address geometry or parameter optimization.

- Complete modeling of the spray/wall interaction and film dynamics is possible, and can be applied to the simulation of the ATS.

Acknowledgment

- *G. Montenegro*
- *A. Della Torre*
- *A. Vespertini*

Thank you!