MICRO-SCALE AND FULL-SCALE CFD SIMULATION OF AFTER-TREATMENT DEVICES FOR INTERNAL COMBUSTION ENGINES

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

Department of Energy - Politecnico di Milano

ICE GROUP
POLITECNICO DI MILANO

Outline

- Characterization of the flow regimes occurring inside real open cell foams
  - Micro-CT scans
  - Surface reconstruction and mesh creation
  - Equivalent artificial and repeatable structures (cubic cells, Kelvin cells …)
  - Detailed simulation and flow analysis

- Developments of up-scaling and surface reactions with conjugate heat transfer in OpenFOAM^R

- Performances foam-type structures (Kelvin cell) vs honeycombs
  - Pressure drop
  - Mass transfer
  - Global performance

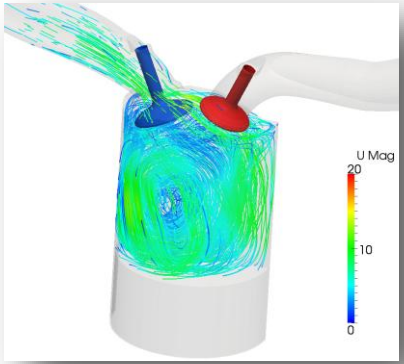
- Full scale simulation and comparison with honeycomb performance during a driving cycle

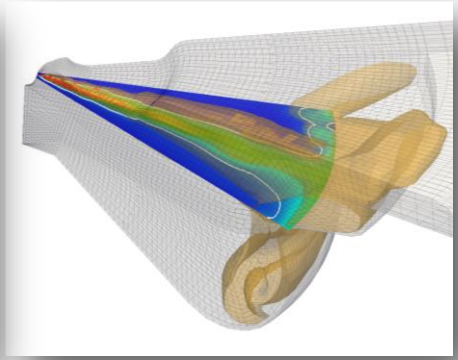
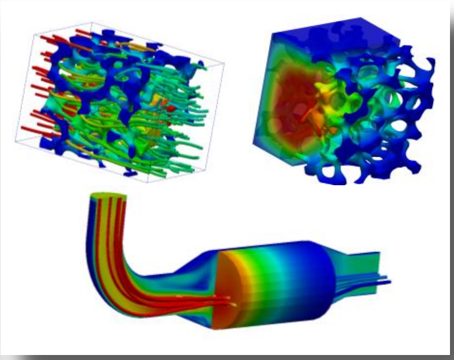
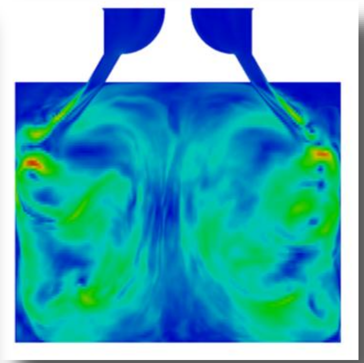
ICE GROUP
POLITECNICO DI MILANO

LibICE for OpenFOAM

INTERNAL COMBUSTION ENGINES

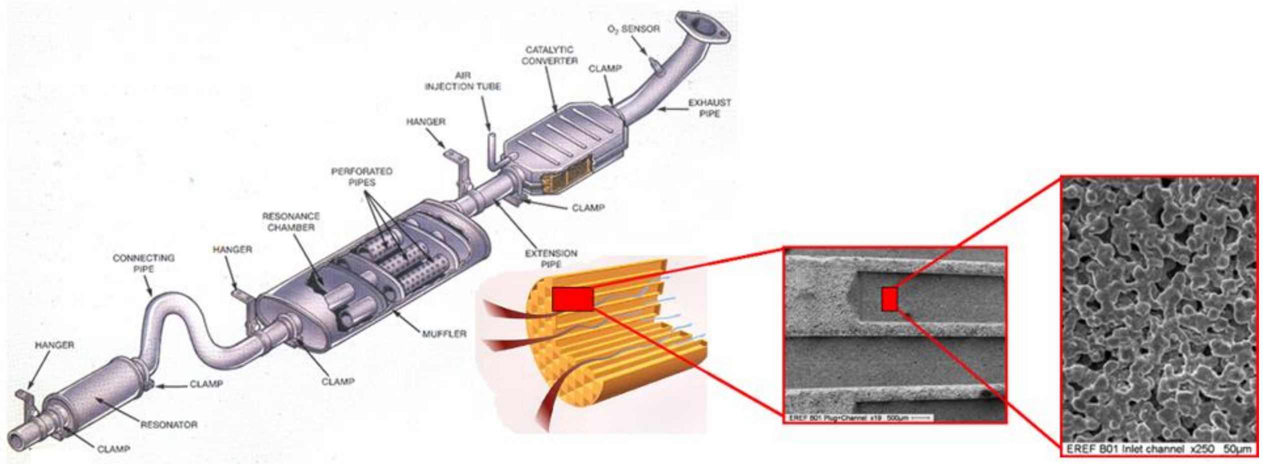
- GDI and Diesel spray modelling: atomization, cavitation, spray-wall interaction
- combustion models with complex chemistry for Diesel, SI and HCCI engines
- unsteady flows in intake and exhaust systems: plenums, silencers, 1D-3D coupling
- reacting flows in after-treatment devices: DPF, SCR, catalytic converter
- Large Eddy Simulation of engine-like geometries and injector internal nozzle flows
- 1D thermo-fluid dynamic models of the turbocharged engines



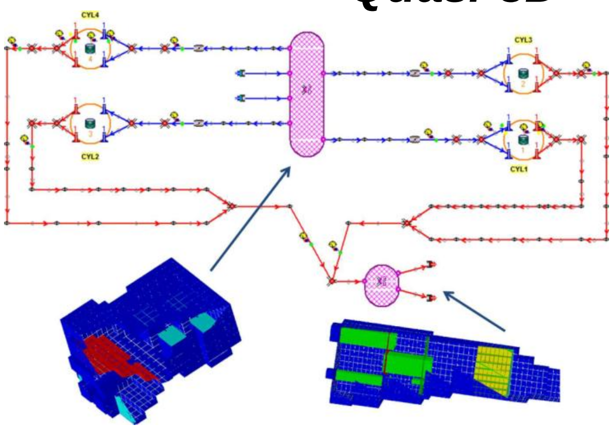




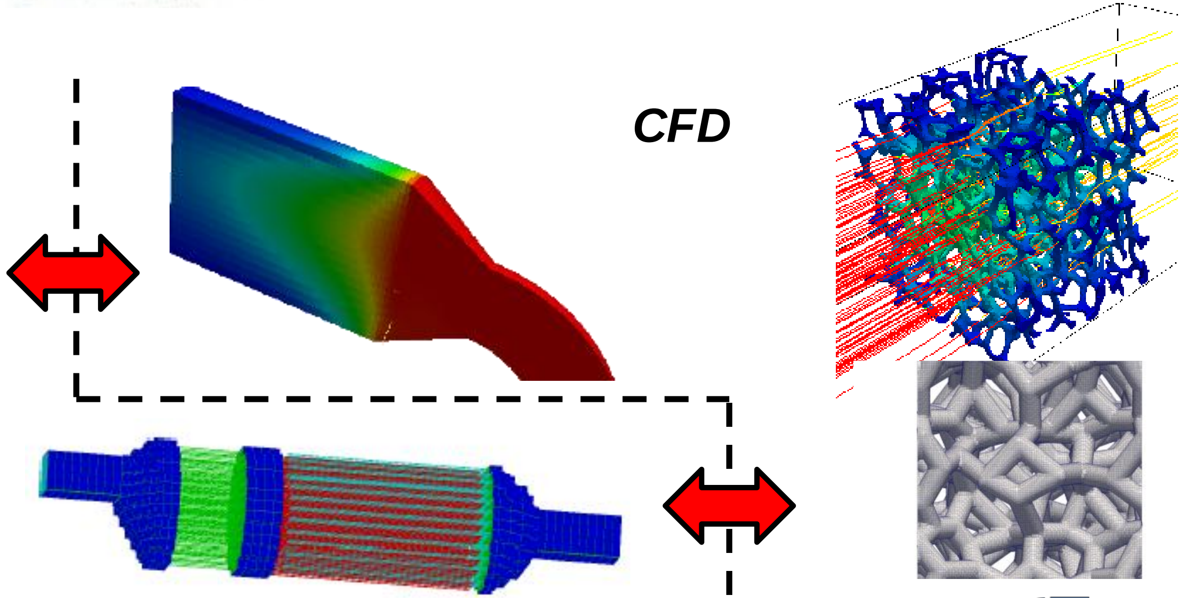
Main concept: applied to ICE

Engine scale ***Component scale*** ***Micro-structure scale***



Quasi-3D ***CFD***

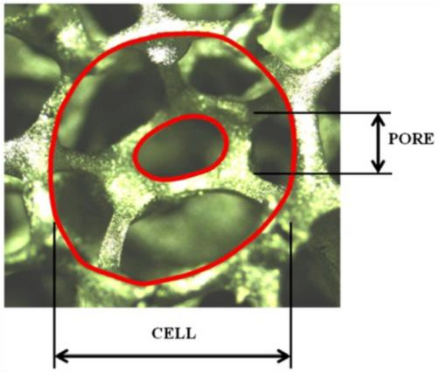


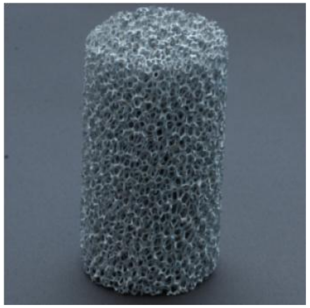


ICE GROUP
POLITECNICO DI MILANO

The substrates

Open-cell foam



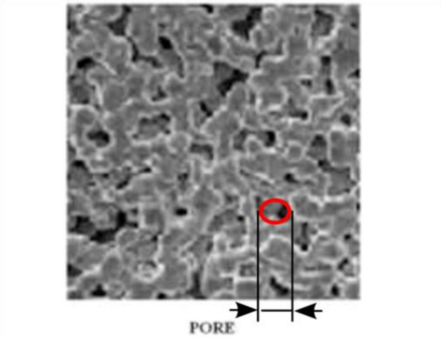


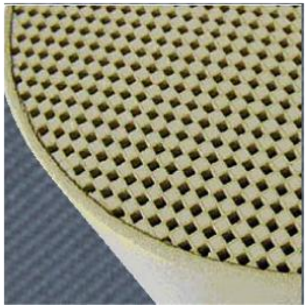
Al alloy
95% porosity
40 ppi

SiC
86% porosity
80 ppi

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

Filtering media





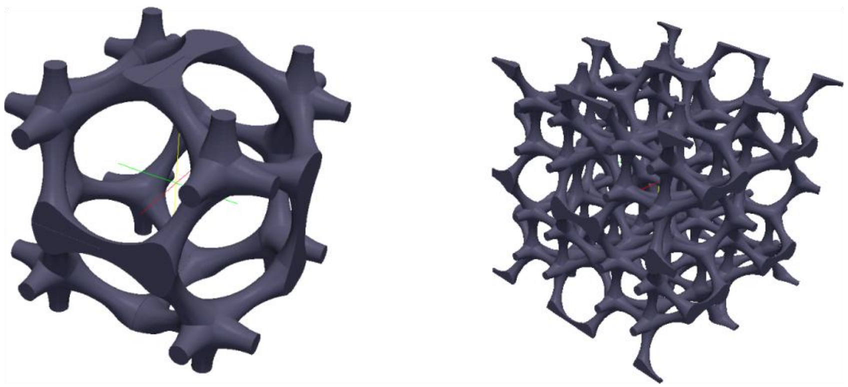
Cordierite
50% porosity
16 µm pore

Applications:
Removal of particulate matter from exhaust gas

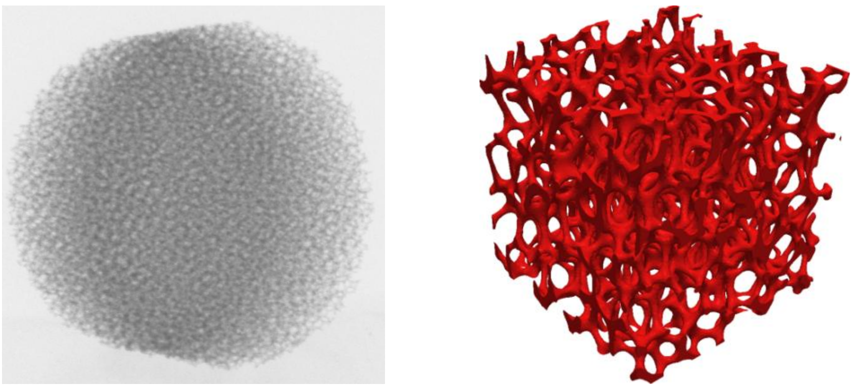
From the sample to the CFD model

Geometry reconstruction → **Mesh generation**

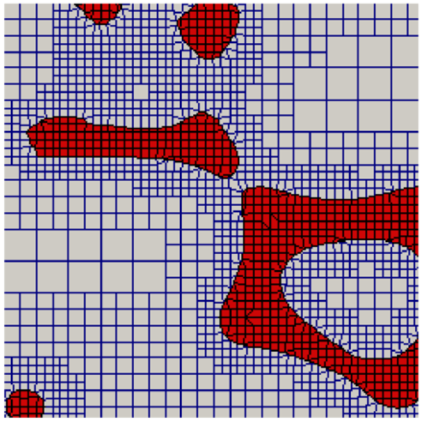
Geometry idealization



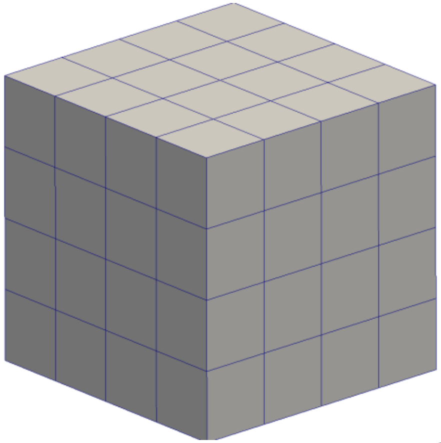
Micro-CT geometry reconstruction



snappyHexMesh



imageHexMesh

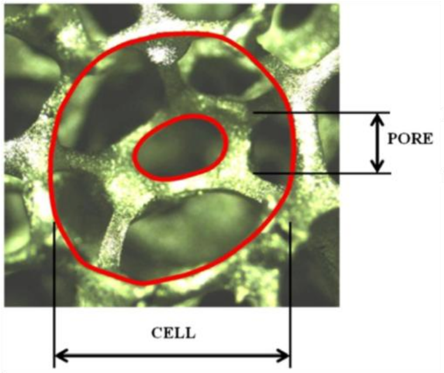


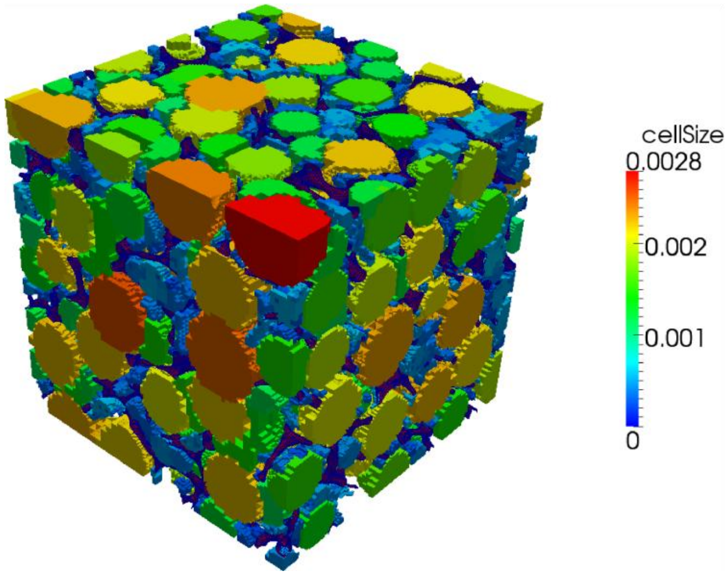
ICE GROUP
POLITECNICO DI MILANO

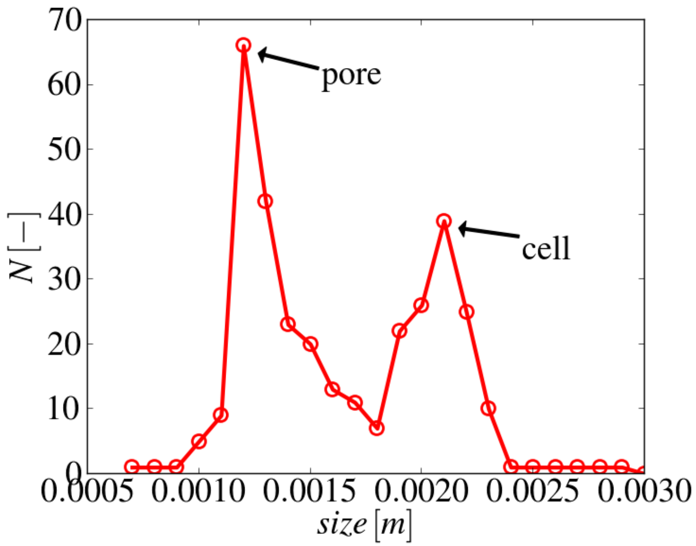
Geometry characterization

- Geometric parameters of the micro-structure computed on the CFD mesh
- Cell/pore size calculation: algorithm based on the opening size concept

	Al foam	Si-C foam	Cordierite
porosity [-]	0.96	0.87	0.50
spec. surf. $[m^2/m^2]$	664.6	4053.3	64833.6
cell size $[m]$	$2.1 \cdot 10^{-3}$	$5.0 \cdot 10^{-4}$	-
pore size $[m]$	$1.2 \cdot 10^{-3}$	$3.1 \cdot 10^{-4}$	$1.6 \cdot 10^{-5}$

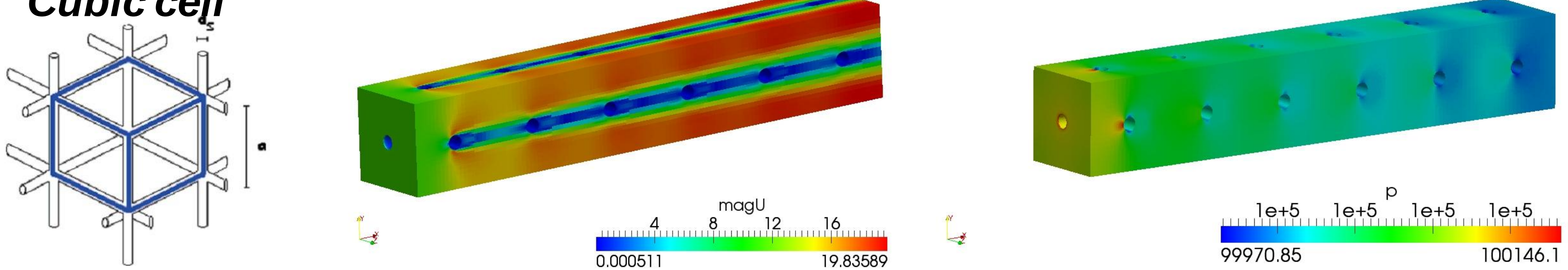




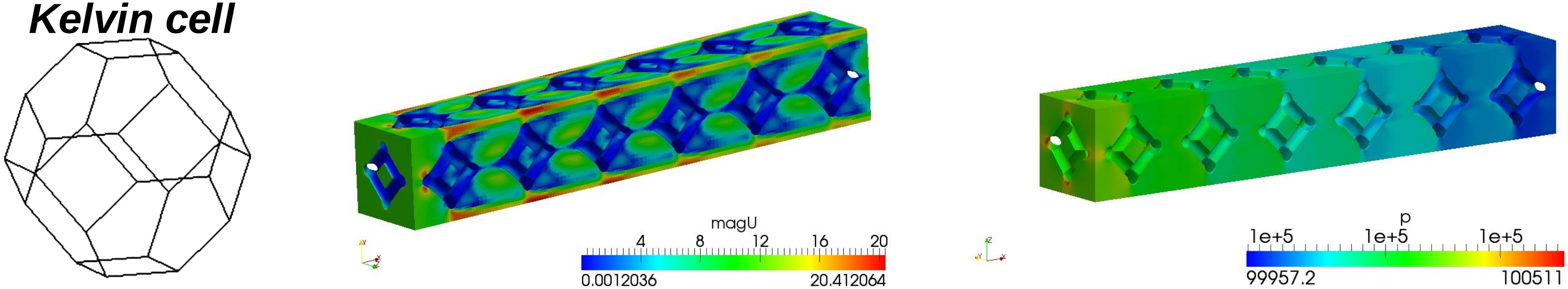


How can we approximate a real foam?

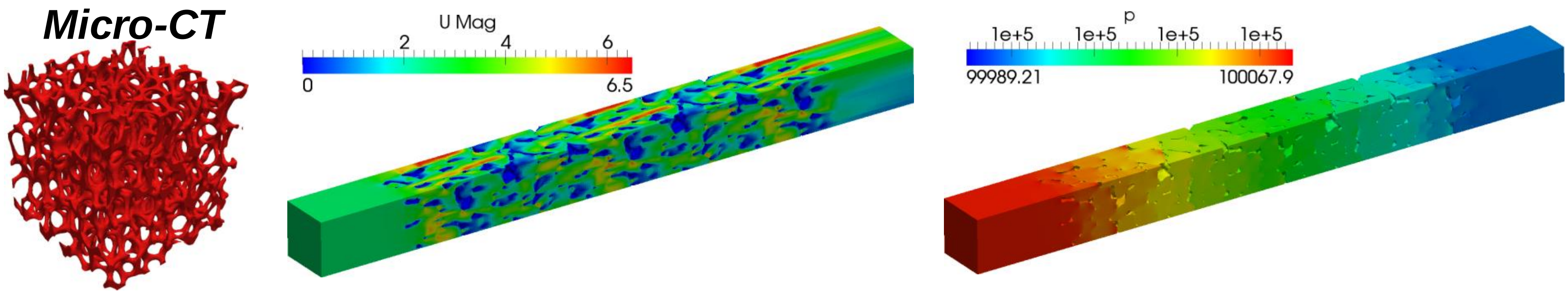
Cubic cell



Kelvin cell

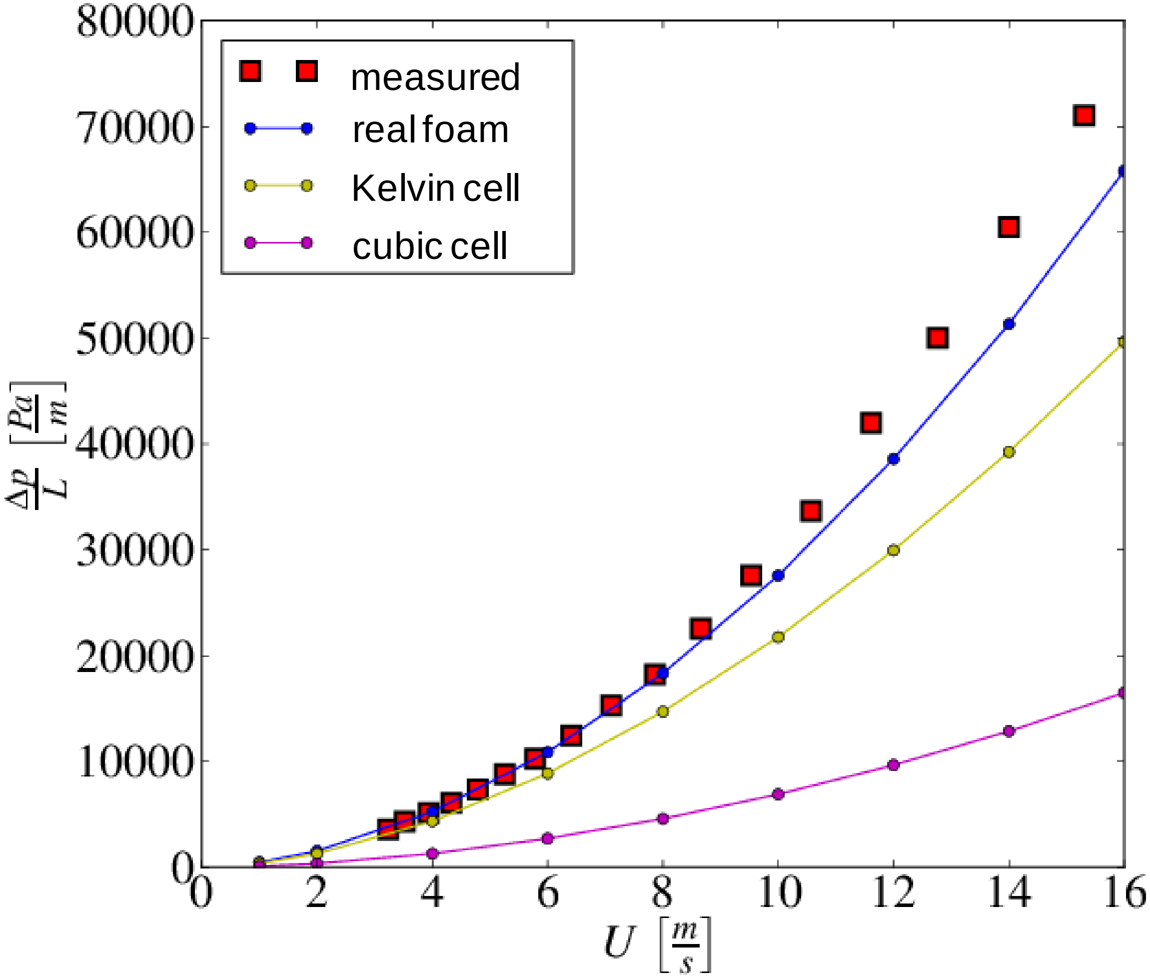


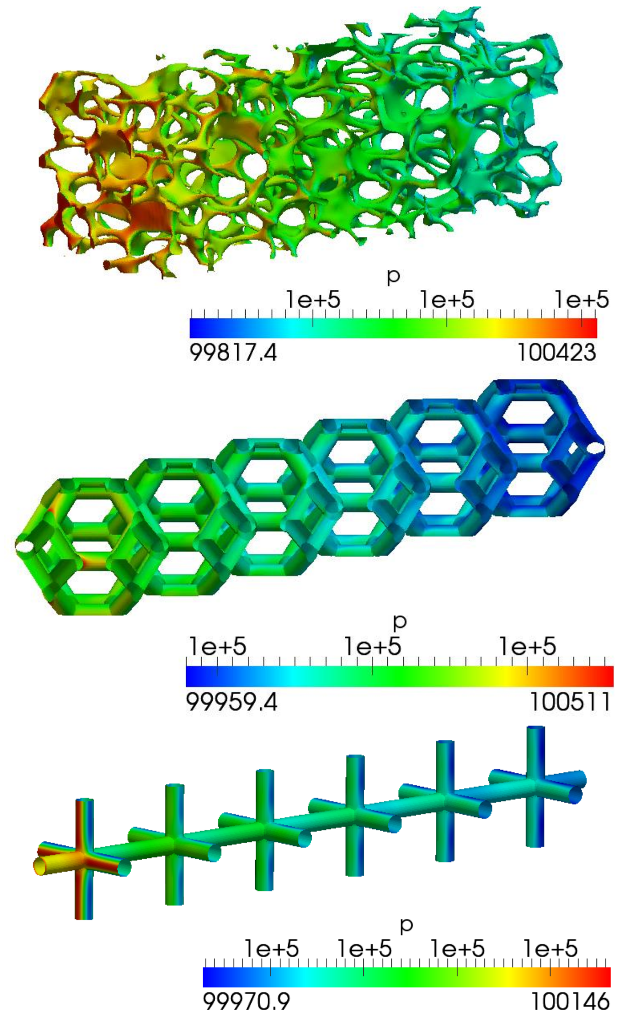
Micro-CT



Comparison of the pressure drop

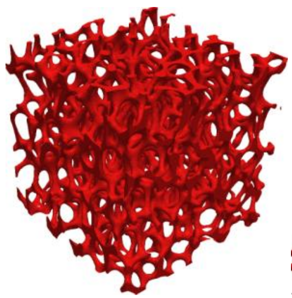
- Same porosity and cell size



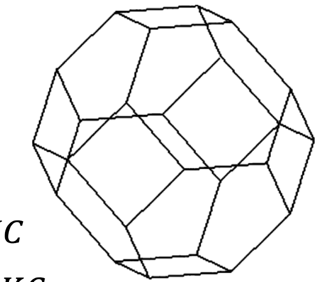


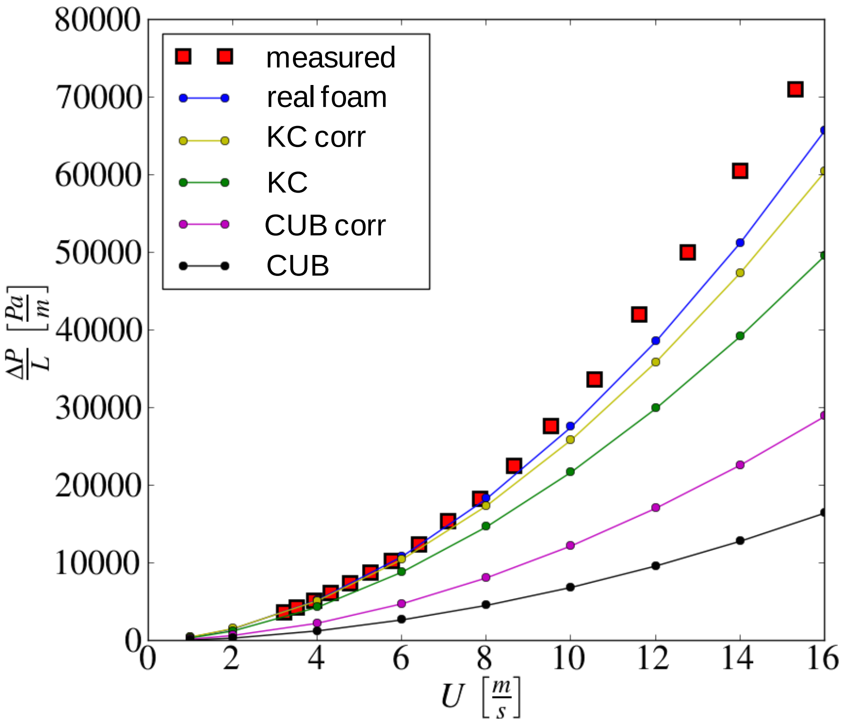
ICE GROUP
POLITECNICO DI MILANO

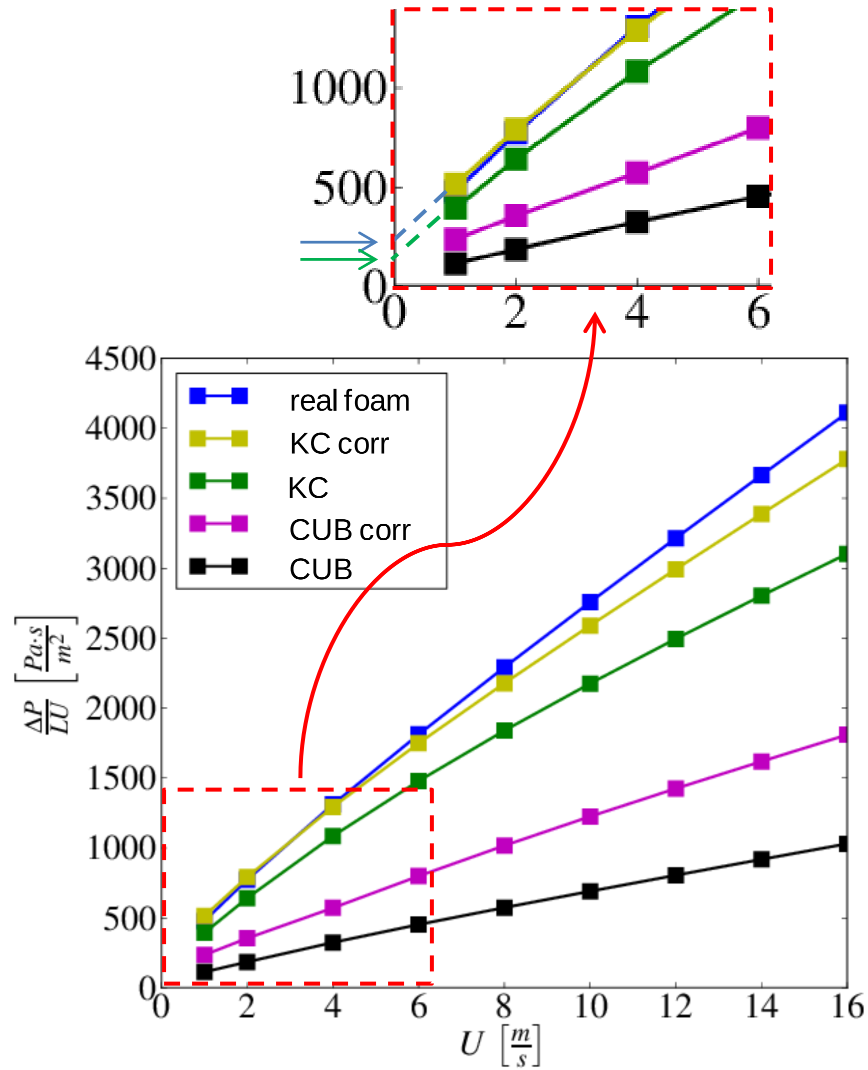
Correction of the KC model: pressure drop



$$\varphi_{real} = \varphi_{KC}$$
$$S_{V,real} = S_{V,KC}$$

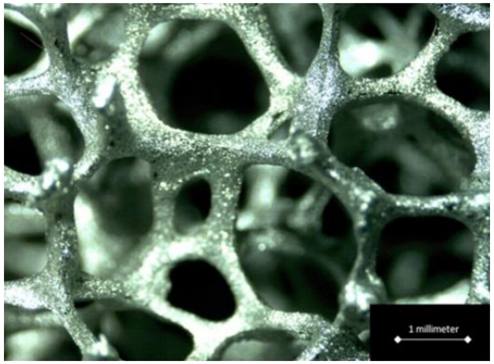




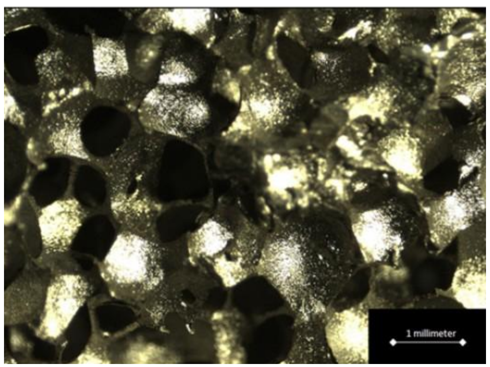


Comparison: pressure drop

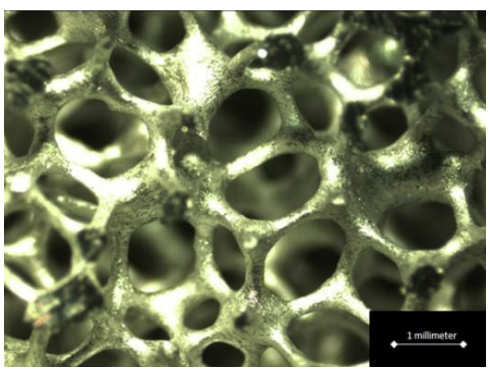
B



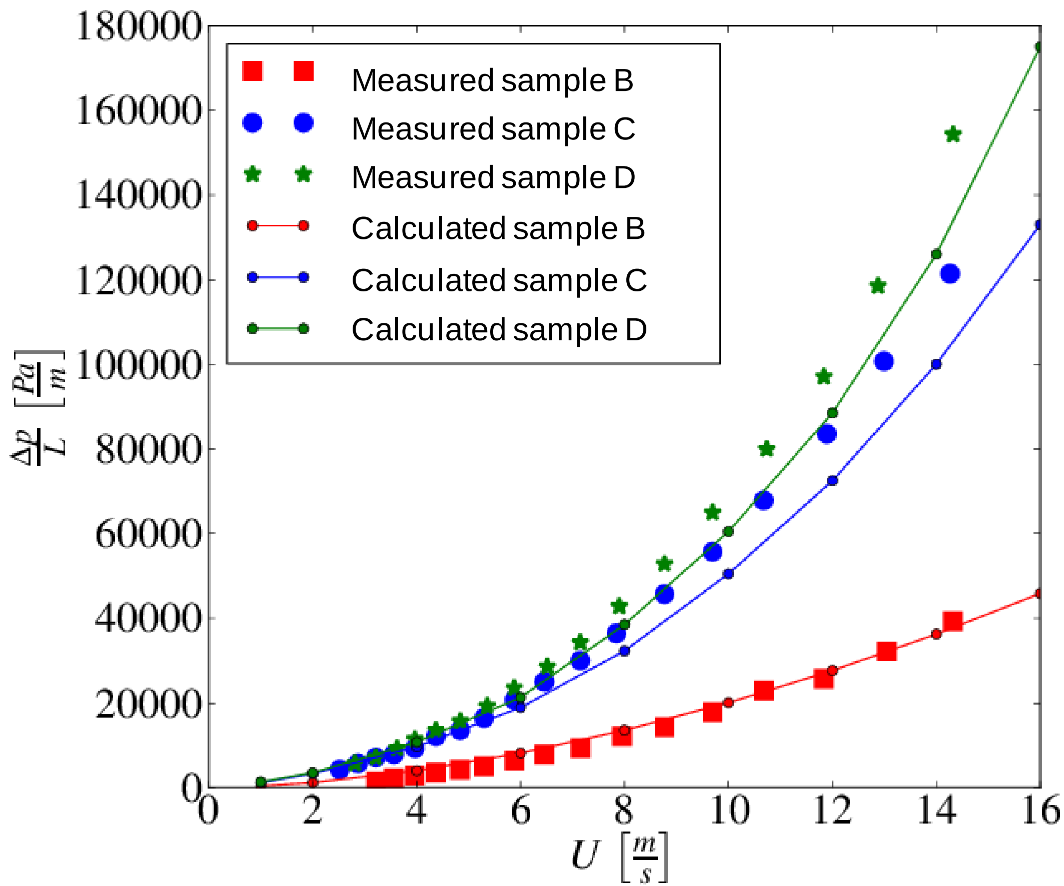
C



D



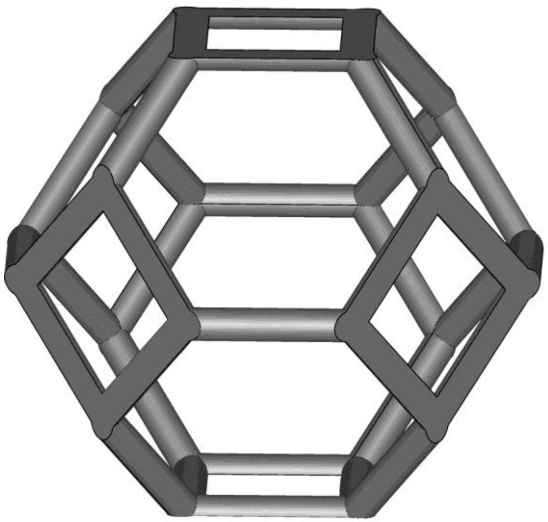
- Reconstruction of real sample by Kelvin cell type idealized foam



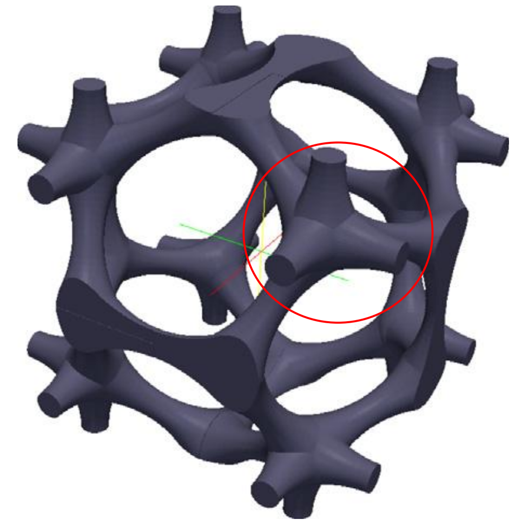
ICE GROUP
POLITECNICO DI MILANO

Further enhancement

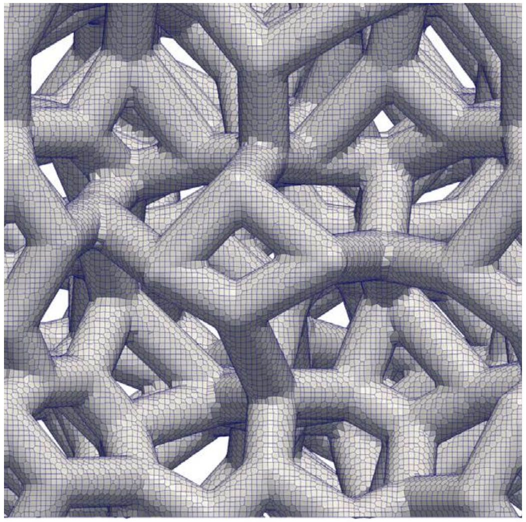
- Introduction of an additional degree of freedom



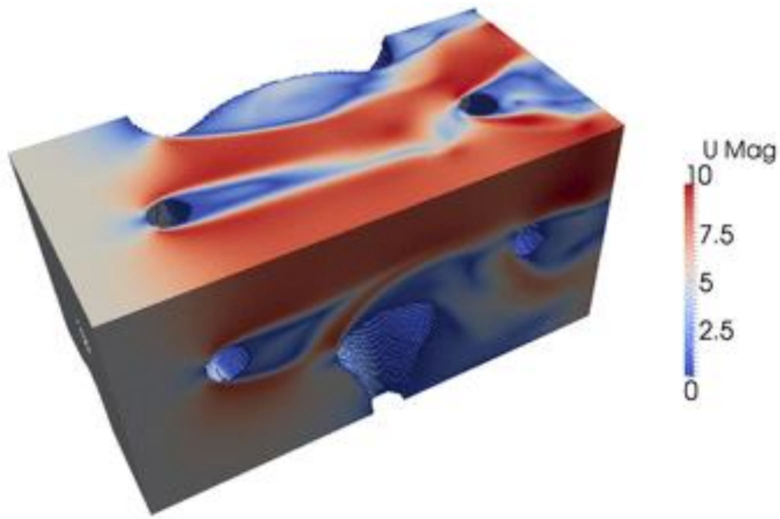
Material clustering at cell vertexes



Randomization (edge length)



Detailed simulation: cold flow

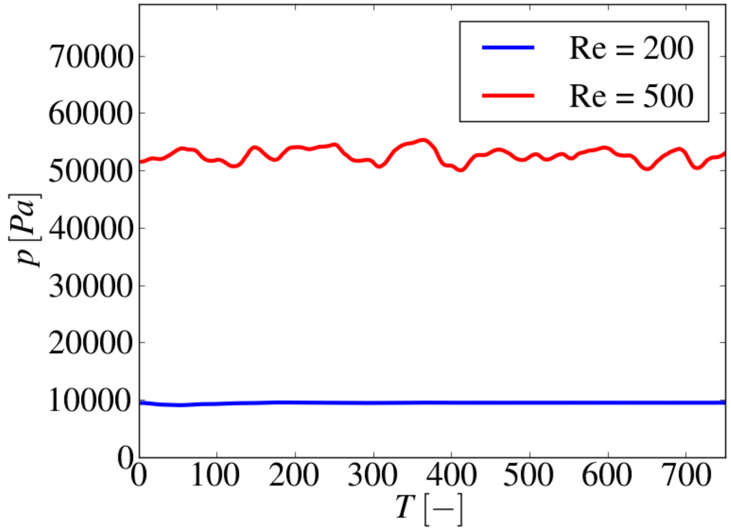


Numerical schemes accuracy:

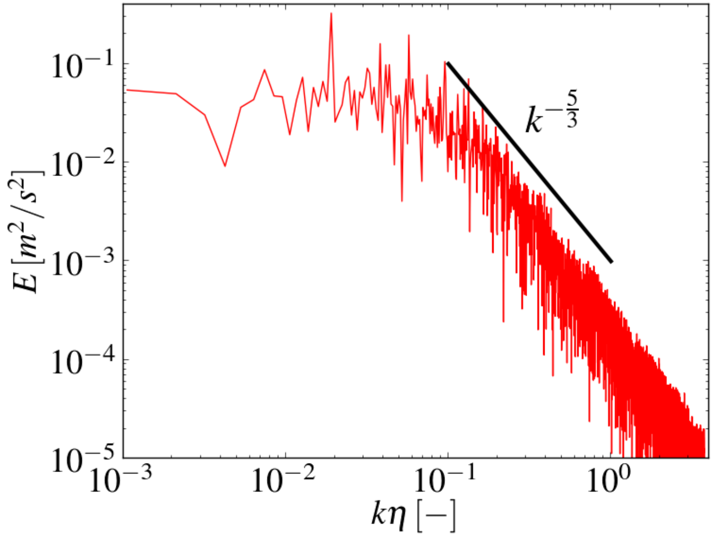
- ***Time:*** second order
- ***Space:*** third order

Re [-]	200	500
η [m]	$1.8 \cdot 10^{-5}$	$9.4 \cdot 10^{-6}$
τ_η [s]	$9.0 \cdot 10^{-6}$	$1.8 \cdot 10^{-6}$
$\Delta x/\eta$ [-]	1.1	2.1

Pressure



TKE spectrum



ICE GROUP
POLITECNICO DI MILANO

From Micro-scale to Macro-scale

Upscaling of the micro-scale governing equations:

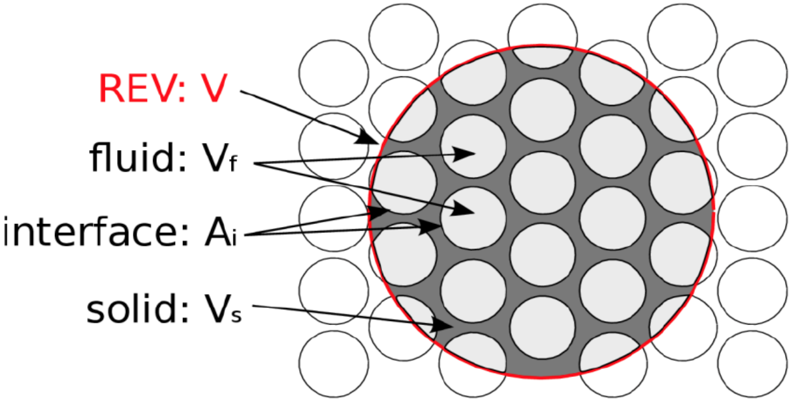
- Local volume average operator:

$$\langle \varphi \rangle^V = \frac{1}{V}\int_V \varphi \, dV, \qquad \varphi = \langle \varphi \rangle^i + {}^i\varphi$$

- Time average operator:

$$\bar{\varphi} = \frac{1}{\Delta t}\int_{\Delta t} \varphi \, dt, \qquad \varphi = \bar{\varphi} + \varphi'$$

- Double decomposition concept



Theorem of local volumetric average

$$\langle \nabla\varphi \rangle^V = \nabla\left(\Phi\langle \varphi \rangle^i\right) + \frac{1}{V}\int_{S_i} \mathbf{n}\, \varphi \, dS$$

$$\langle \nabla\cdot\varphi \rangle^V = \nabla\cdot\left(\Phi\langle \varphi \rangle^i\right) + \frac{1}{V}\int_{S_i} \mathbf{n} \cdot \varphi \, dS$$

$$\left\langle \frac{\partial\varphi}{\partial t} \right\rangle^V = \frac{\partial}{\partial t}\left(\Phi\langle \varphi \rangle^i\right) + \frac{1}{V}\int_{S_i} \mathbf{n} \cdot (\mathbf{U}_\mathbf{i}\varphi)\, dS$$

Application of volumetric average operators on the micro-scale governing equations

⬇

Appearance of **extra source terms**

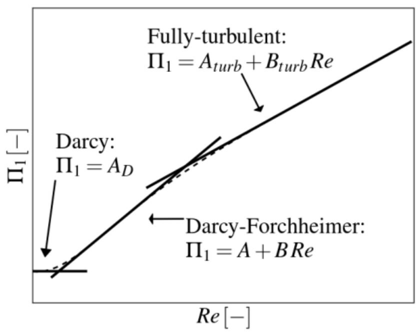
Extracting information for upscaling

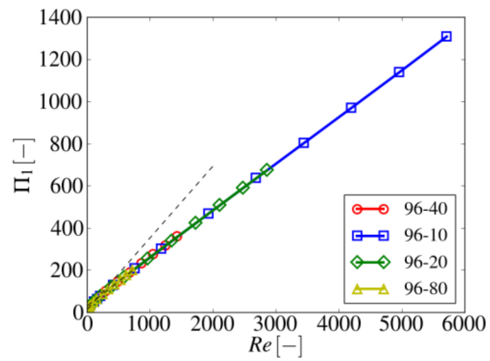
Non-dimensional relationships evaluated on the basis of **micro-scale simulations**

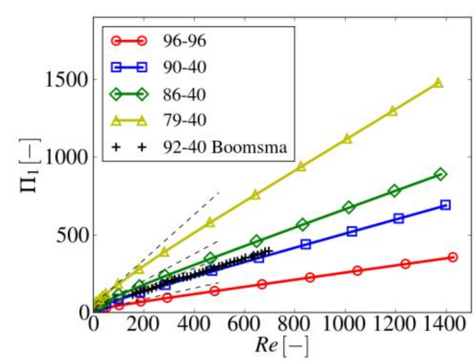
$$\mathbf{\Pi_1} = \frac{\mathfrak{R}\, d_c^2}{\hat{\mathbf{U}}\,\hat{\mu}} = \mathcal{F}_{\Pi_1}\left(\mathbf{Re} = \frac{\rho\,\hat{\mathbf{U}}\,d_c}{\hat{\mu}}\right) \qquad \mathbf{\Pi_2} = \frac{\mathfrak{R}\, d_c}{\hat{\rho}\,\hat{U}^2} = \mathcal{F}_{\Pi_2}\left(\frac{1}{\mathbf{Re}} = \frac{\hat{\mu}}{\hat{\rho}\,\hat{\mathbf{U}}\,d_c}\right)$$

Variable pore density | *Variable porosity*

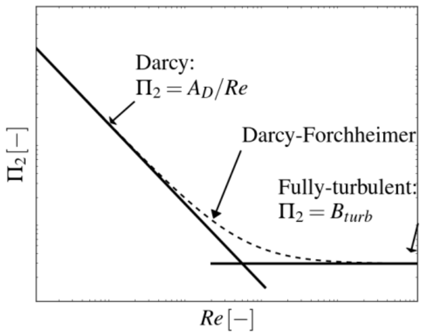
$\Pi_1(Re)$

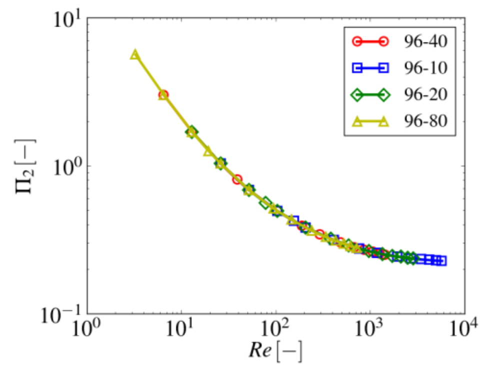


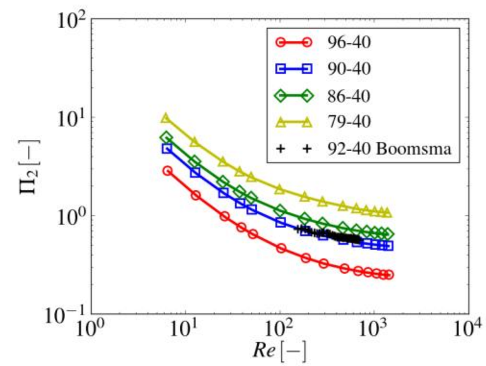




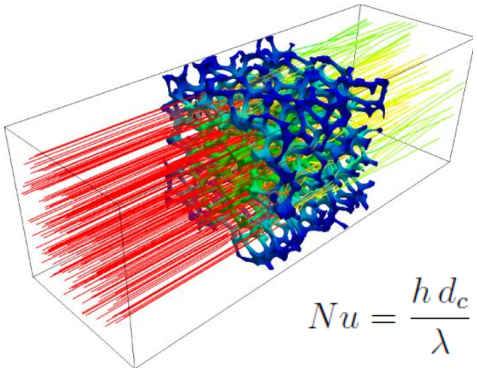
$\Pi_2(Re)$







Modelling the heat transfer source term



Non-dimensional relationship evaluated on the basis of **micro-scale simulations**

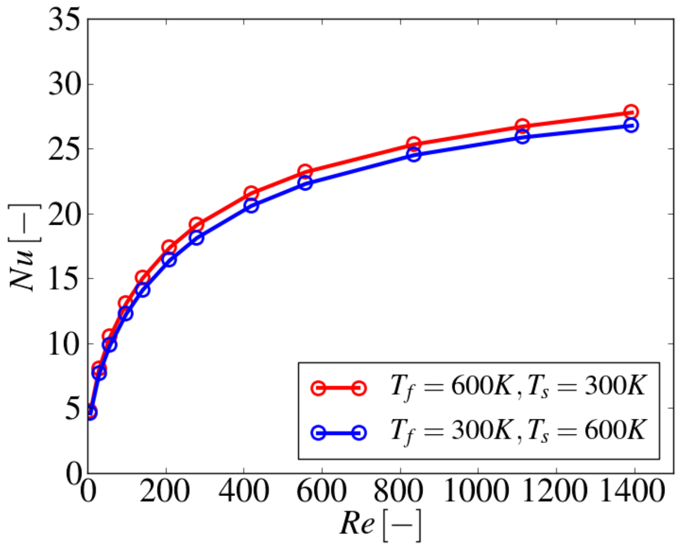
$$Nu = \frac{h\, d_c}{\lambda} = \mathcal{F}_{Nu}\left(Re = \frac{\hat{\rho}\, \|\hat{\mathbf{U}}\|\, d_c}{\hat{\mu}},\ Pr = \frac{\hat{\mu}\, \hat{c}_{p,f}}{\hat{\lambda}_f} \right)$$

Inter-phase **heat transfer source term** in macro-scale energy equation

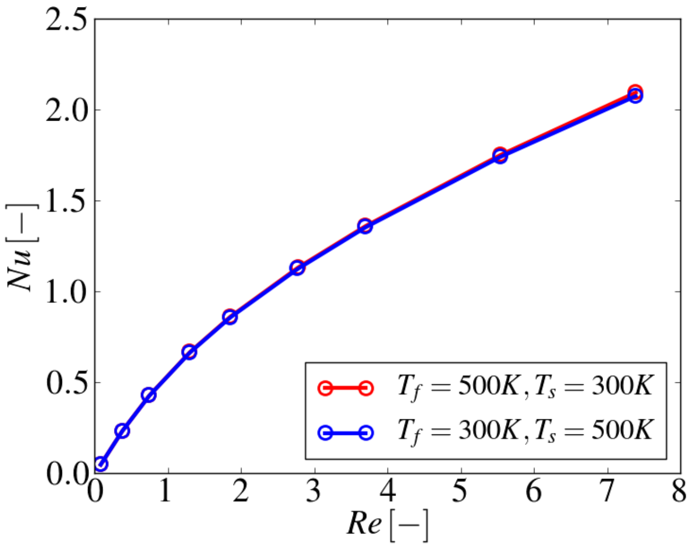
$$Q^{f \to s} = Nu\, \frac{\lambda_f}{d_c}\, \sigma\, V \left(\hat{T}_s - \hat{T}_f \right)$$

Nu(Re)

Al foam



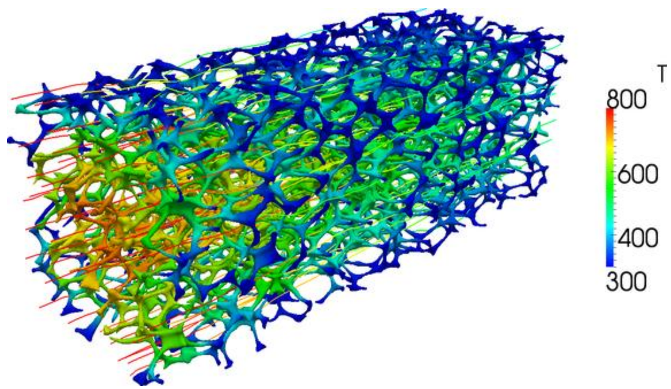
SiC foam



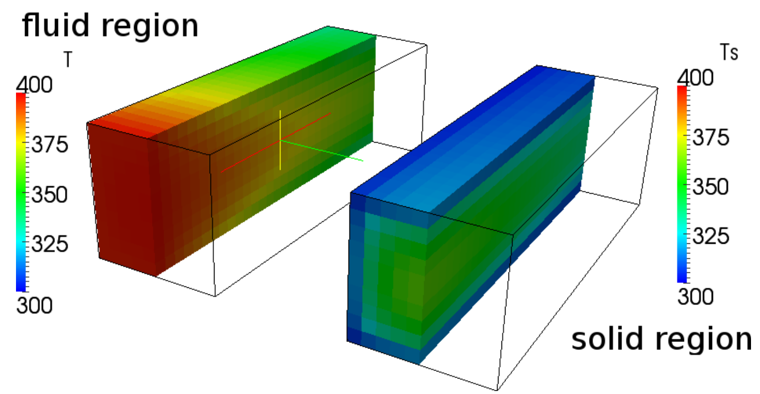
Examples of application

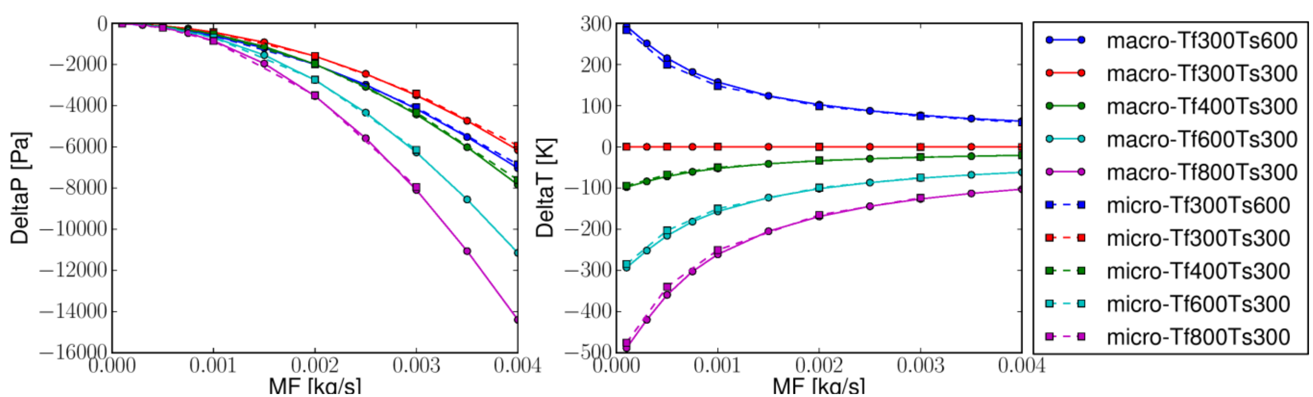
- Macro-scale approach is based on a multi-regions framework, in which fluid and solid phases are simulated on different (partially or totally) overlapping mesh.
- Models are introduced for the coupling between the solid and fluid phases.

Micro-scale approach



Macro-scale approach

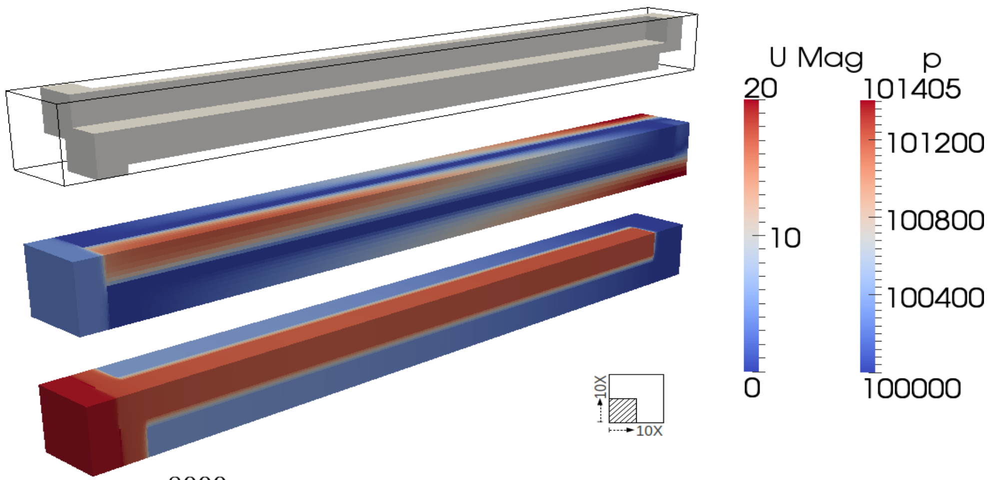


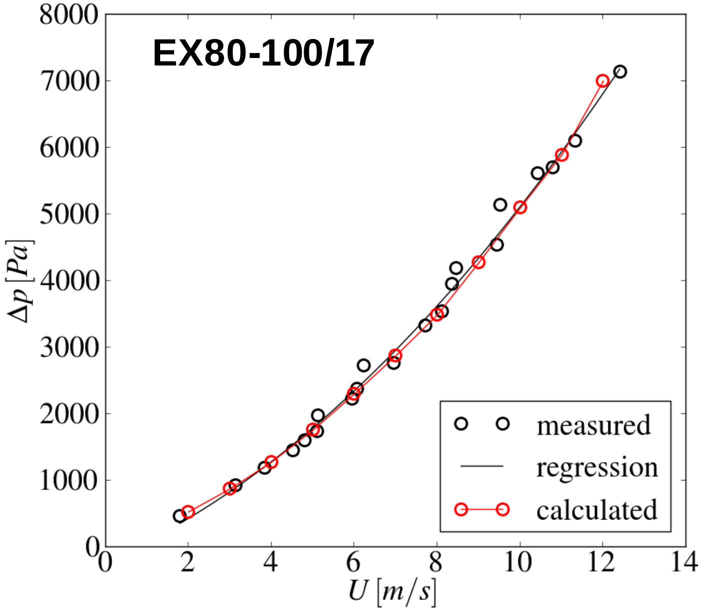


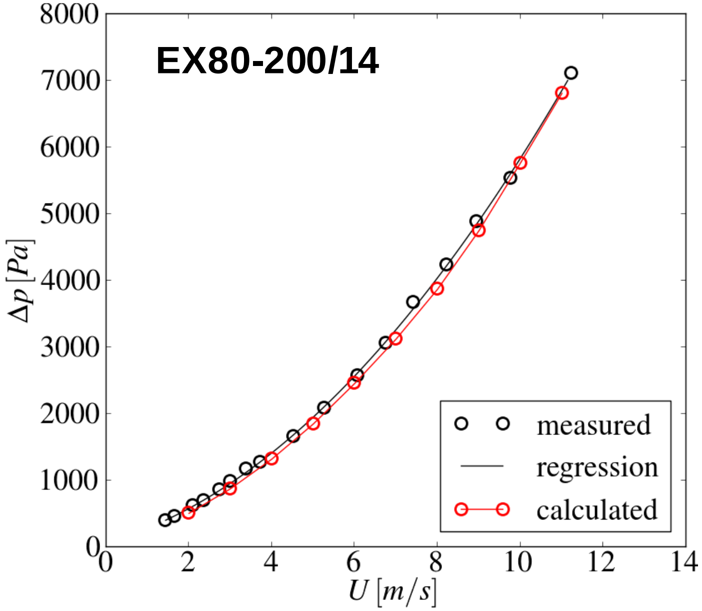
Check on consistency between macro- and micro-scale approaches

Examples of application

Simulation of flow trhrough a couple of DPF channels



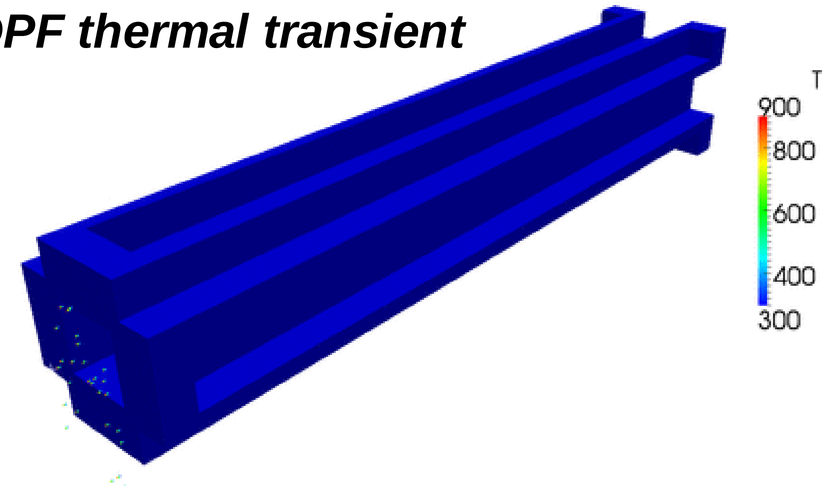


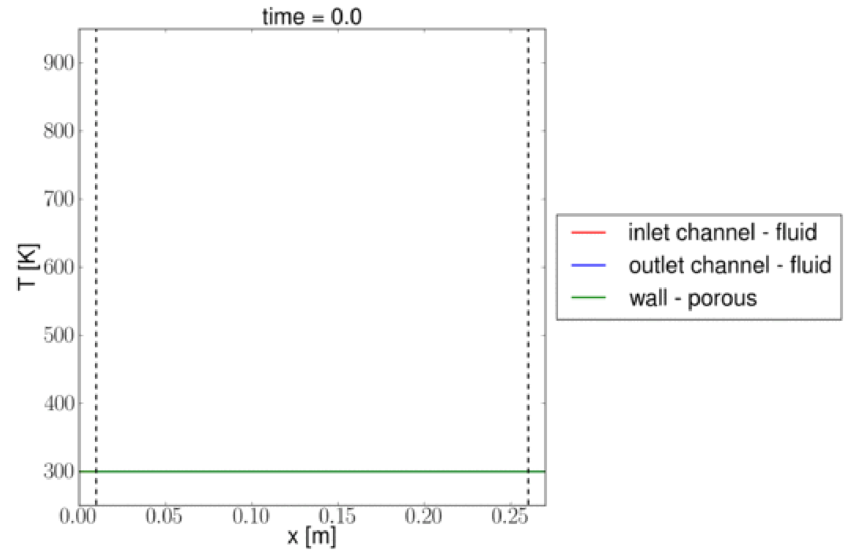


ICE GROUP
POLITECNICO DI MILANO

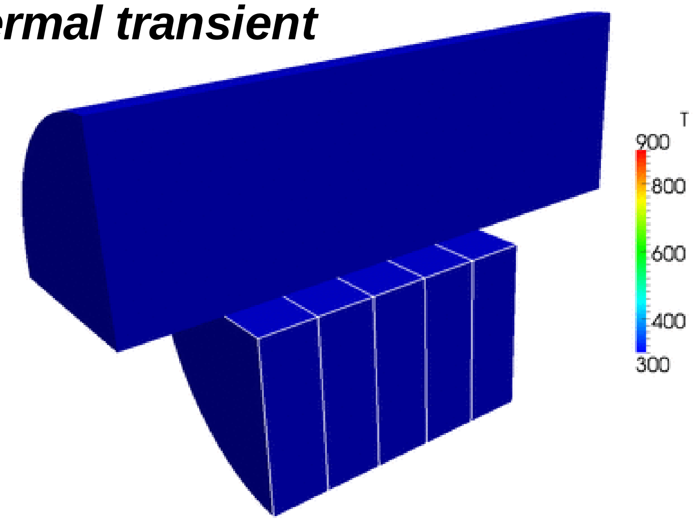
Examples of application

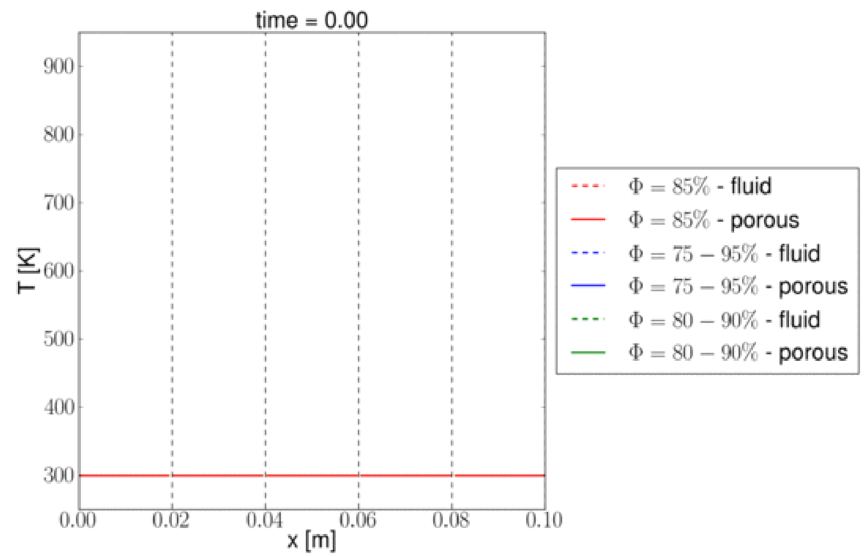
DPF thermal transient





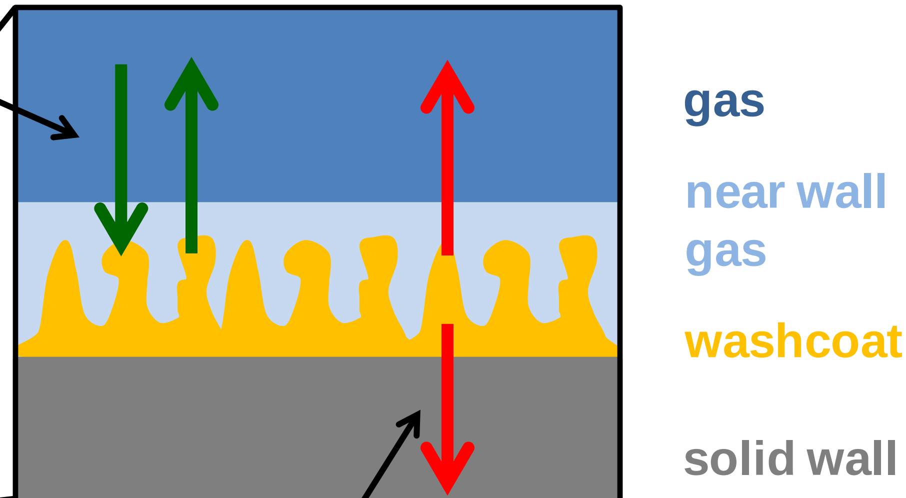
Multi-layer foam catalyst thermal transient

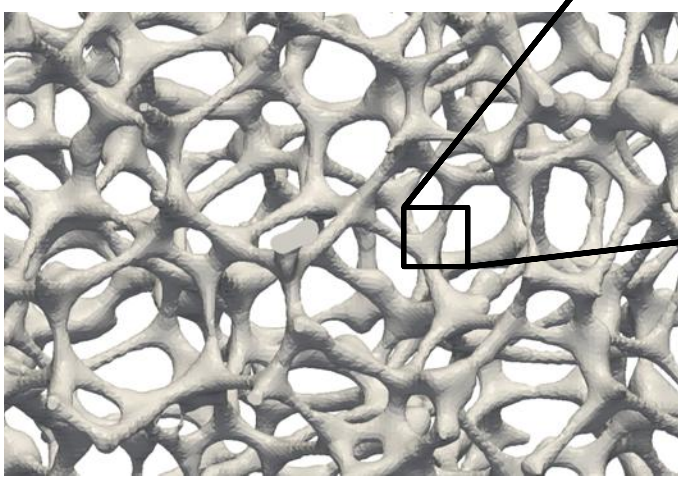




Modelling catalytic reactions

Mass transfer between gas phase and catalytic surface inside the washcoat





Reaction heat is released and transferred to fluid and solid phase

Definition of the washcoatZone

Definition of the **washcoatZone**, which contains the geometric information and supports CHT simulations in a multi-region framework

```
class washcoatZone
{
    // Private data
        //- Name of this zone, or a regular expression
        keyType key_;

        //- Dictionary containing the parameters
        dictionary dict_;

        //- Reference to the fluid finite volume mesh
        const fvMesh& mesh_;

        //- List of fluid faces belonging to the zone
        labelList faces_;

        //- List of fluid cells owner of the zone faces
        labelList cells_;

        //- Reference to the solid finite volume mesh (for cht)
        const fvMesh& sMesh_;

        //- Name of the solid face zone (for cht)

        ...
```

Reference to the fluid mesh and definition of the connectivity

Reference to the solid mesh and definition of the connectivity

The reactingWashcoatZone

The generic **washcoatZone** is extended to **reactingWashcoatZone** in order to model surface reactions:

```
class reactingWashcoatZone
:
    public washcoatZone
{
    // Private data

        //- Disallow default bitwise copy construct
        reactingWashcoatZone(const reactingWashcoatZone&);

        //- Disallow default bitwise assignment
        void operator=(const reactingWashcoatZone&);

        //- Washcoat solver
        autoPtr<Foam::washcoat::washcoatSolver> wsctSolver_;

        ...
```

Washcoat solver is run-time selectable

Washcoat solver is based on 3 run-time selectable sub-models:

- Diffusion
- Reactions
- Heat transfer

Specialization of the `washcoatSolver`

- On the basis of the **`washcoatSolver`** class, different solvers can be implemented and chosen at runtime. For example:

```
template<class MassMdl, class ReacMdl, class HeatMdl>
class BaruahWashcoatSolver
:
    public washcoatSolver,
    public MassMdl,
    public ReacMdl,
    public HeatMdl
{
    ...
```

The solver is derived from **`washcoatSolver`** and templated submodels for the diffusion, reaction and heat-transfer

`BaruahWashcoatSolver` is derived from templated submodels which are run-time selectable:

- **`MassMdl`** : generic model for the diffusion between the fluid and the substrate
- **`ReacMdl`** : generic model for the surface reactions
- **`HeatMdl`** : generic model for the heat release and heat transfer

```
washcoatSolver BaruahWashcoatSolver<constantWsctMassDiffusionModel,
                                    infinitelyFastWsctChemistryModel,
                                    laminarWsctHeatTransferModel>;
```

```
washcoatSolver singleStepWashcoatSolver<constantWsctMassDiffusionModel,
                                        infinitelyFastWsctChemistryModel,
                                        laminarWsctHeatTransferModel>;
```

The washcoat dictionary

```
/*--------------------------------*- C++ -*----------------------------------*\
| =========                 |                                                 |
| \\      /  F ield         | OpenFOAM: The Open Source CFD Toolbox           |
|  \\    /   O peration     | Version:  2.1.x                                 |
|   \\  /    A nd           | Web:      www.OpenFOAM.org                      |
|    \\/     M anipulation  |                                                 |
\*---------------------------------------------------------------------------*/
FoamFile
{
    version     2.0;
    format      ascii;
    class       dictionary;
    location    "constant";
    object      washcoats;
}
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

2
(
    washcoat0
    {
        washcoatSolver BaruahWashcoatSolver<detailedWsctMassDiffusionModel,
                                            infinitelyFastWsctChemistryModel,
                                            laminarWsctHeatTransferModel>;
```

Number of washcoat zones

Washcoat solver

The `washcoat` dictionary

```
2
(
    washcoat0
    {
        ...

        wsctProperties
        {
            loading loading [ 1 -2 0 0 0 0 0 ] 0.16;
            specificSurface specificSurface [ 0 0 0 0 0 0 0 ] 1;
            thickness thickness [ 0 1 0 0 0 0 0 ] 1.0e-6;
            porosity porosity [ 0 0 0 0 0 0 0 ] 0.5;
            rho rho [1 -3  0  0 0 0 0] 2800;
            Cp  Cp  [0  2 -2 -1 0 0 0] 897;
            K   K   [1  1 -3 -1 0 0 0] 150;
        }

        thermoType
        {
            type                heWsctThermo;
            mixture             wsctSingleStepReactingMixture;
            transport           constIso;
            thermo              hConst;
            energy              sensibleEnthalpy;
            equationOfState     rhoConst;
            specie              specie;
        }
        ...
```

Washcoat properties

Termodynamic model

The `washcoat` dictionary

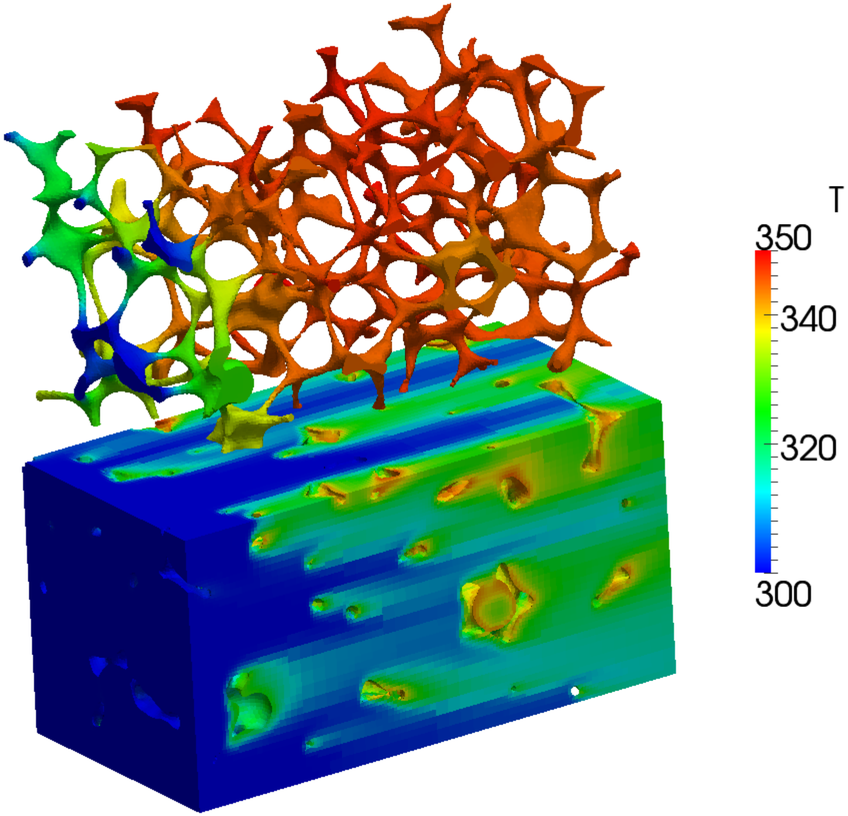
```
2
(
    washcoat0
    {
        ...
        species
        (
            O2
            H2O
            CH4
            CO2
            N2
        );
        inertSpecie N2;
        fuel CH4;

        wsctChemistryReader wsctFoamChemistryReader;
        foamChemistryFile "$FOAM_CASE/constant/wsctReactions.wall1";
        foamChemistryThermoFile "$FOAM_CASE/constant/thermo.wsct";

        ...
```

Species involved in the surface reactions

ICE GROUP POLITECNICO DI MILANO

Reacting flow simulation

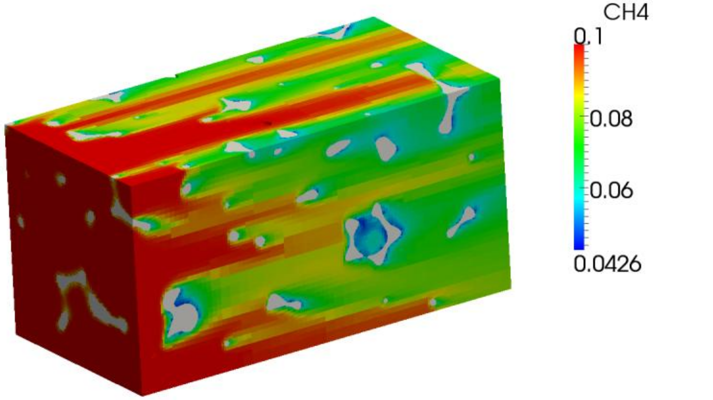
Al foam 95% porosity – 40 ppi / Micro-CT reconstruction

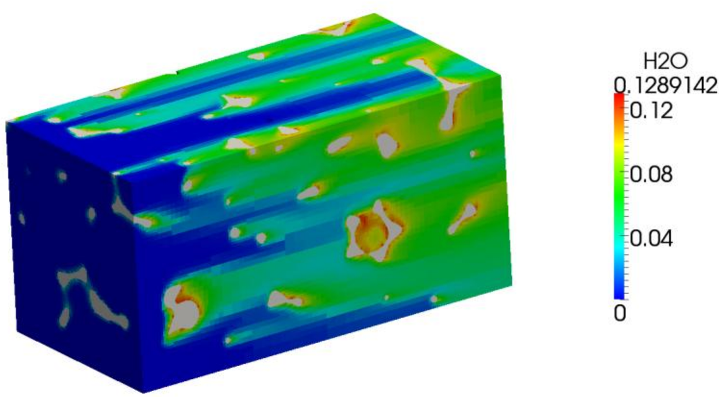


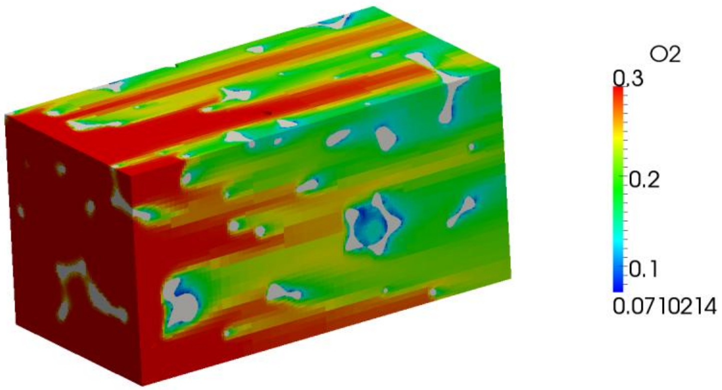
- Surface reaction on washcoat region
- Baruah-like solver
- Infinitely fast reaction model
- Conjugate heat transfer
- Fluid: inlet T=300K
- Solid: fixed T=300K on the inlet side, adiabatic elsewhere

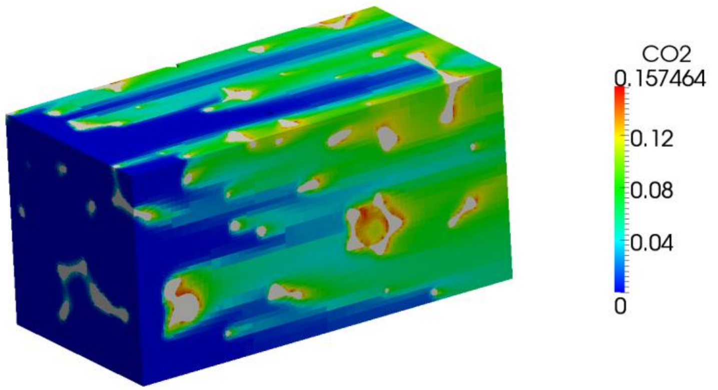
Reacting flow simulation

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

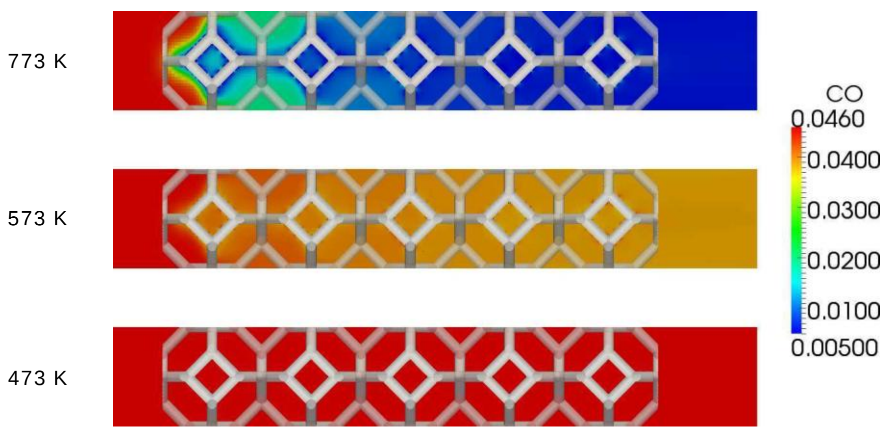


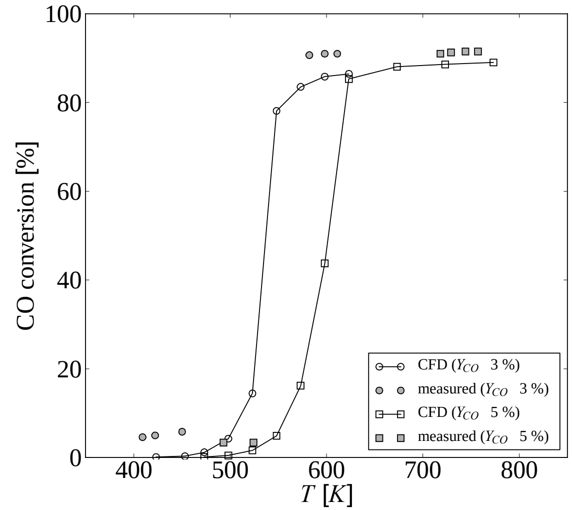


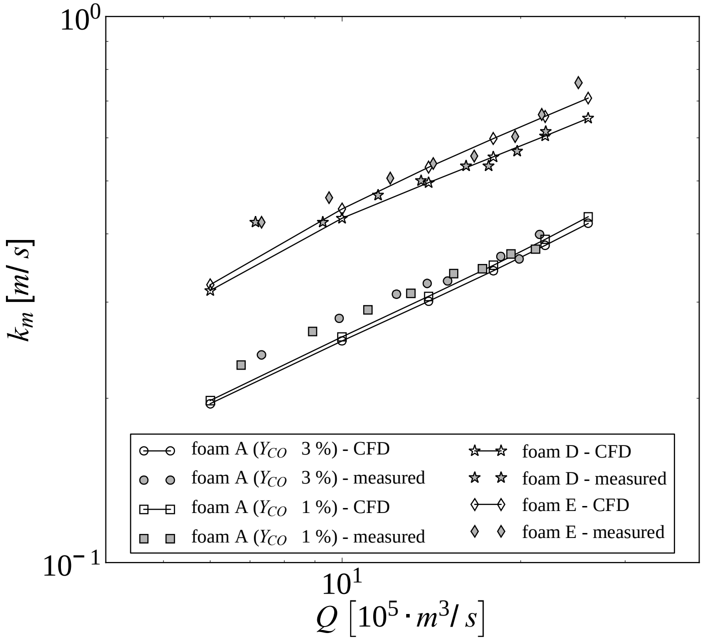


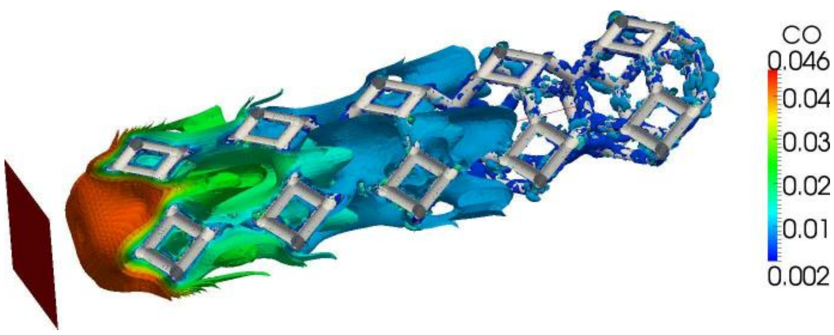


Diffusion limit validation

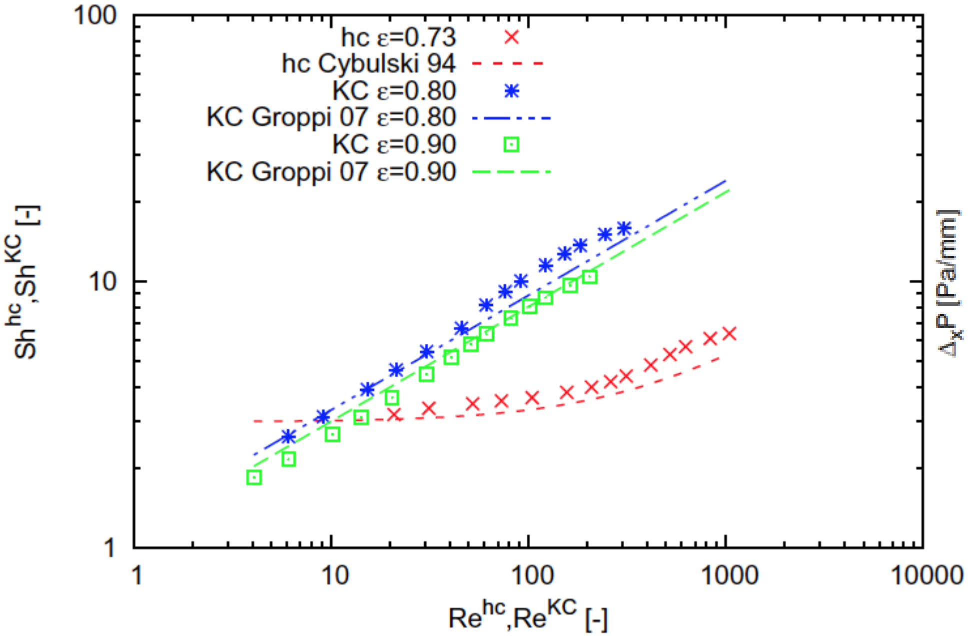


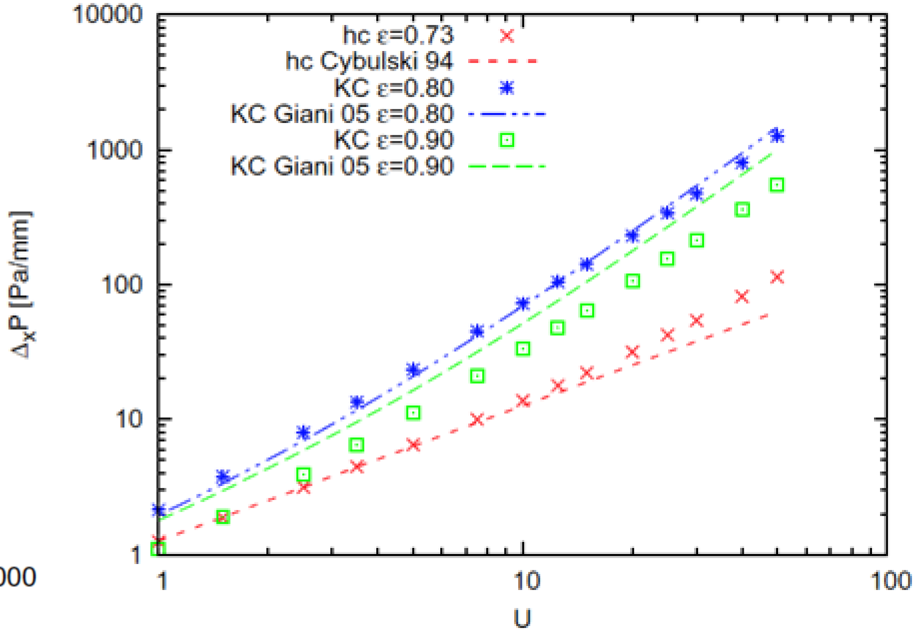


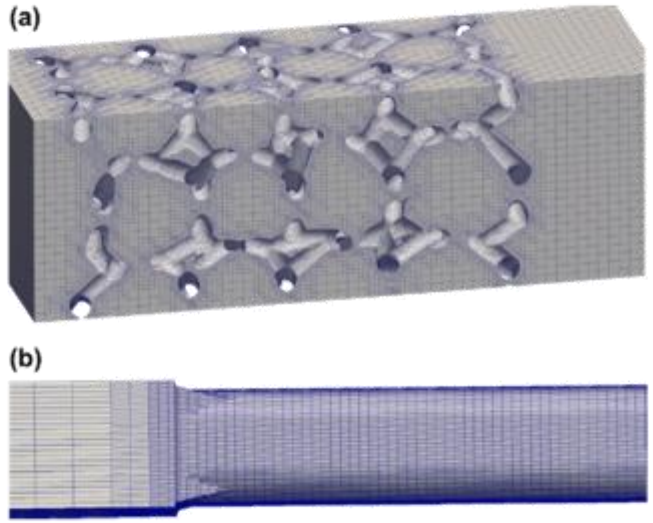




KC vs honeycomb





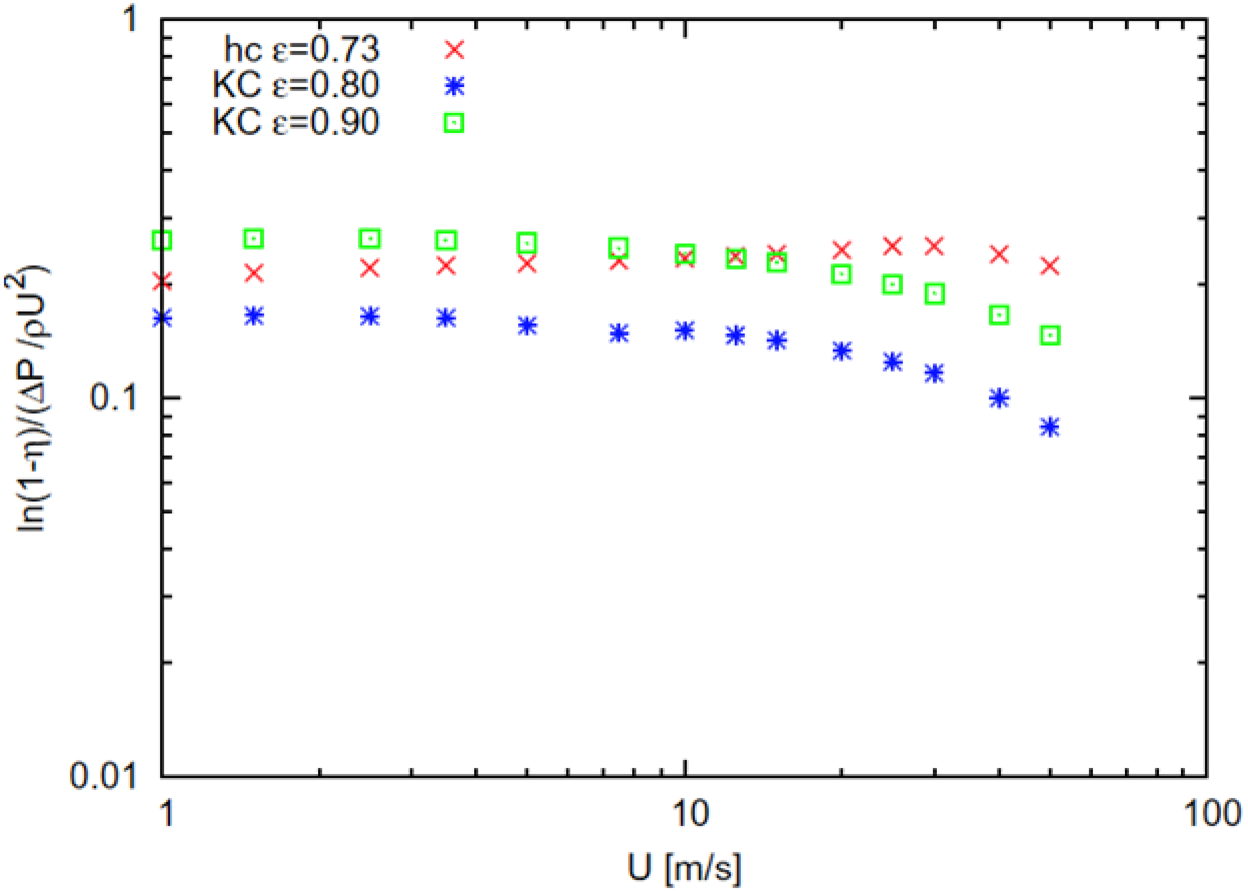


- The results of simulations compare fairly well with the correlations available in the literature

- There is still not agreement among authors in literature

ICE GROUP POLITECNICO DI MILANO

Performance Index: KC vs honeycomb

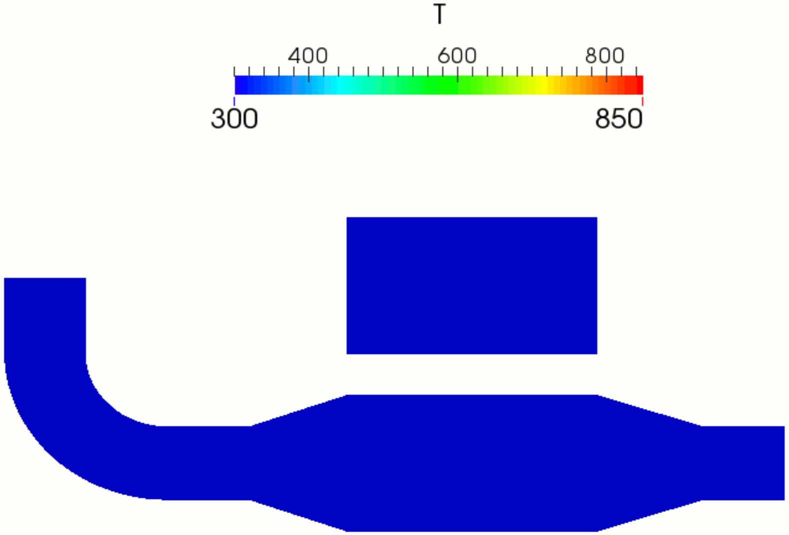


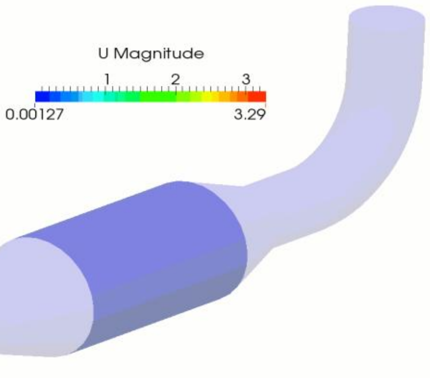
$$I = \frac{-\ln(1-\eta)}{\Delta P/(\rho u^2)}$$

- The open cell foam exhibit a better performance if:
  - porosity is high
  - velocity is low (Darcean velocity)

ICE GROUP
POLITECNICO DI MILANO

Application example: TWC





CO oxidation
$CO + 0.5O_2 \rightarrow CO_2$

H_2 oxidation
$H_2 + 0.5O_2 \rightarrow H_2O$

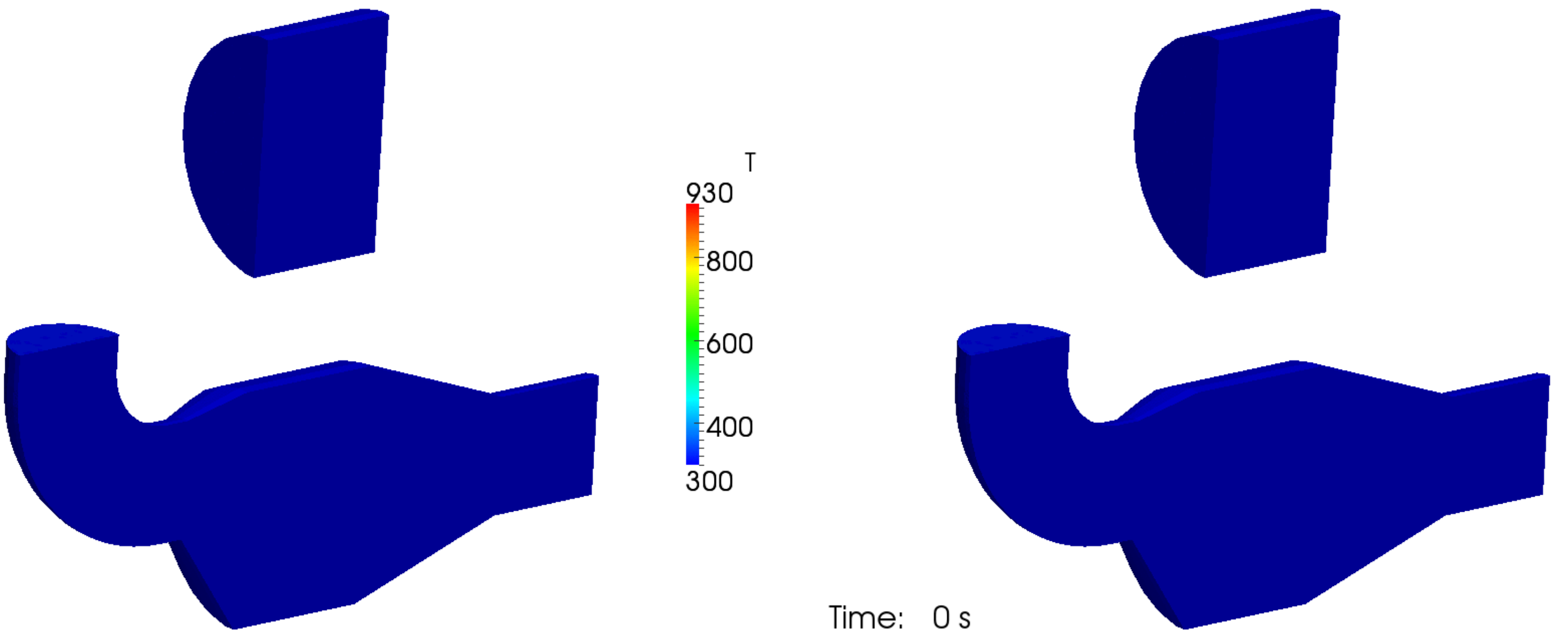
HC oxidation
$C_3H_6 + 3O_2 \rightarrow 3CO_2 + 6H_2O$

NO_x reduction
$CO + NO \rightarrow CO_2 + 0.5N_2$
$H_2 + NO \rightarrow H_2O + 0.5N_2$

Steam water reforming
$CO + H_2O \rightarrow CO_2 + H_2$
$C_3H_6 + 3H_2O \rightarrow 3CO_2 + 6H_2$

Full scale: honeycomb vs open cell foam

NEDC cycle of a 2.0 L engine (4 Cyl, naturally aspirated) simulated imposing the measured exhaust gas T and mass flow ad the engine flange.



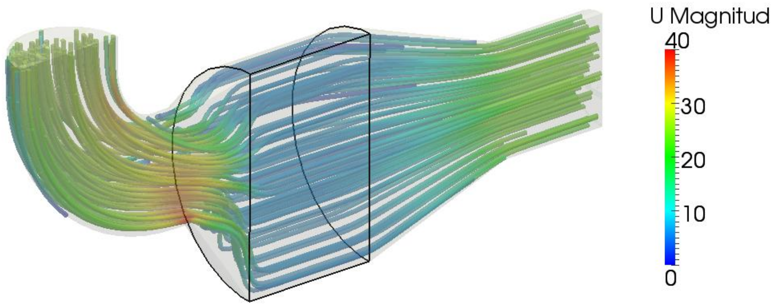
HONEYCOMB

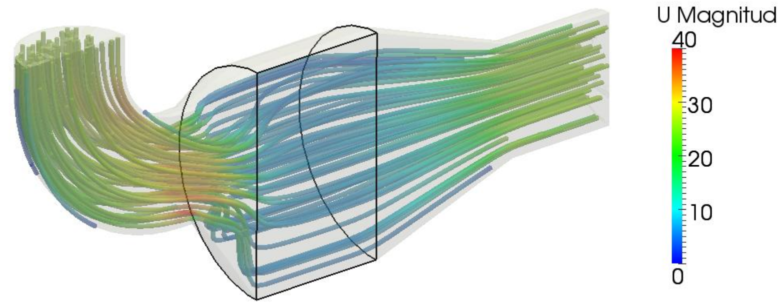
OPEN CELL FOAM

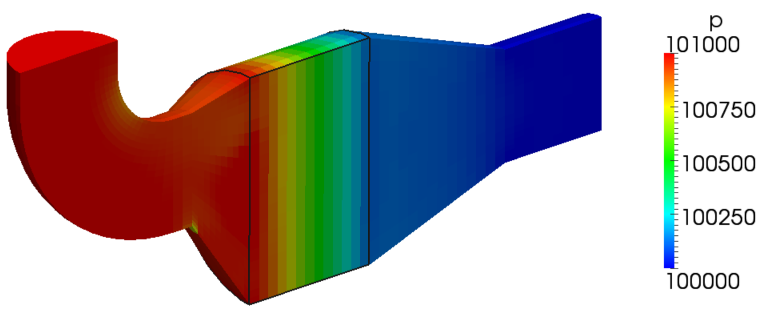
Full scale: honeycomb vs open cell foam

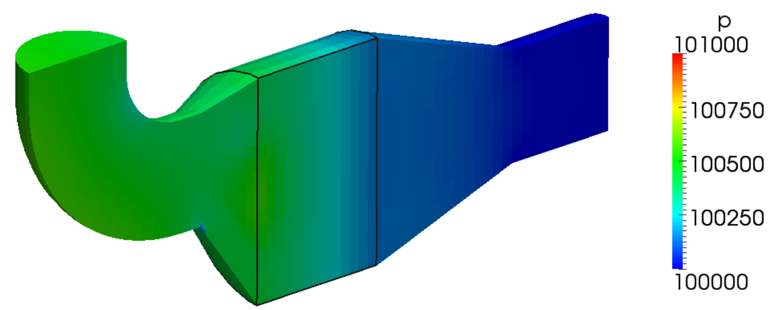
HONEYCOMB

OPEN CELL FOAM



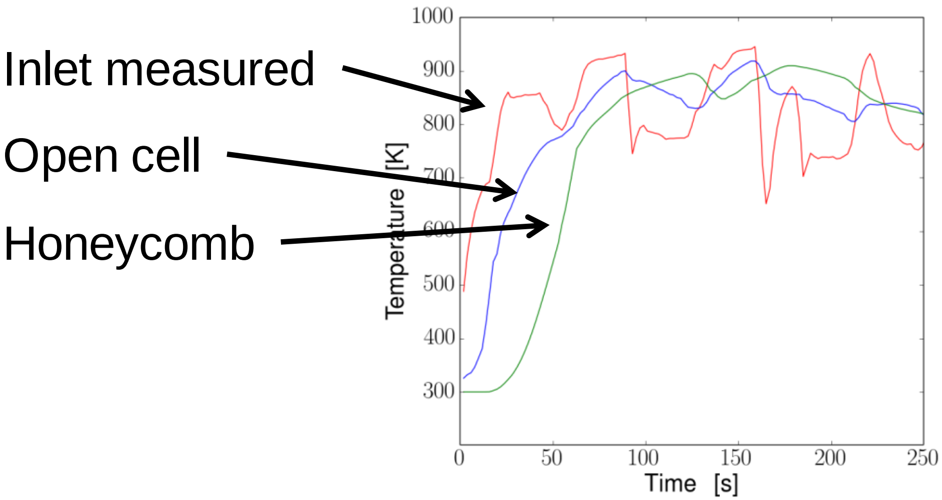


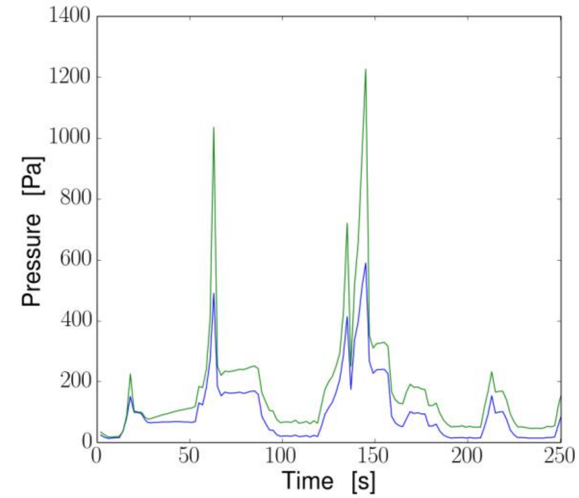


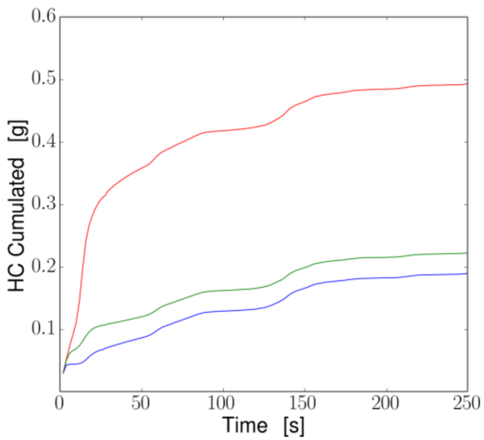


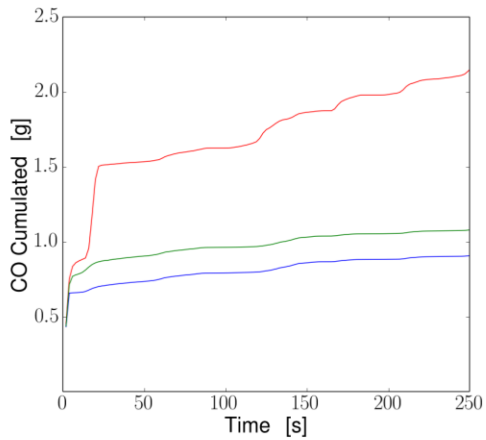
Full scale: honeycomb vs open cell foam

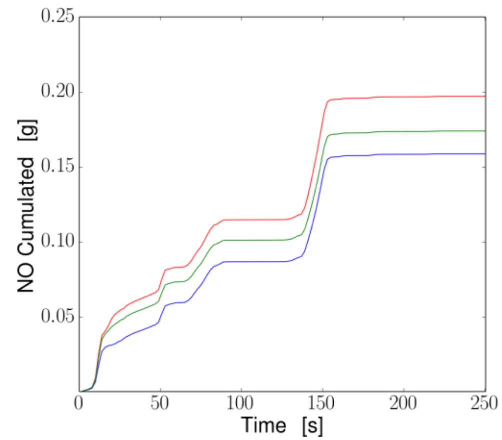
- NEDC cycle (first 300 seconds) with two different technologies











Conclusions and … work in progress

- Implementation of a fully coupled surface reacting model applicable to microstructure or channel scale simulations

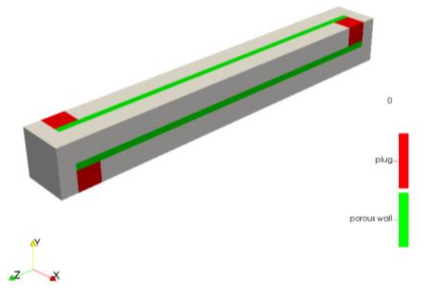
- Averaging techniques have made possible full scale simulations in a consistent way with the microscale approach

- Full scale simulation of open cell substrates are fundamental to better understand the effectiveness of a solution with respect to a consolidated technology

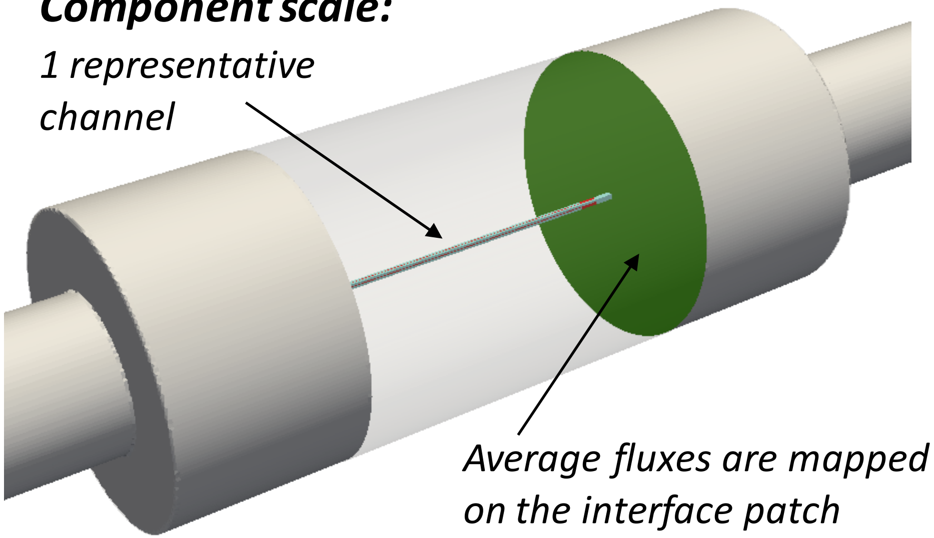
WIP: Channel scale DPF/GPF or CAT

- 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.

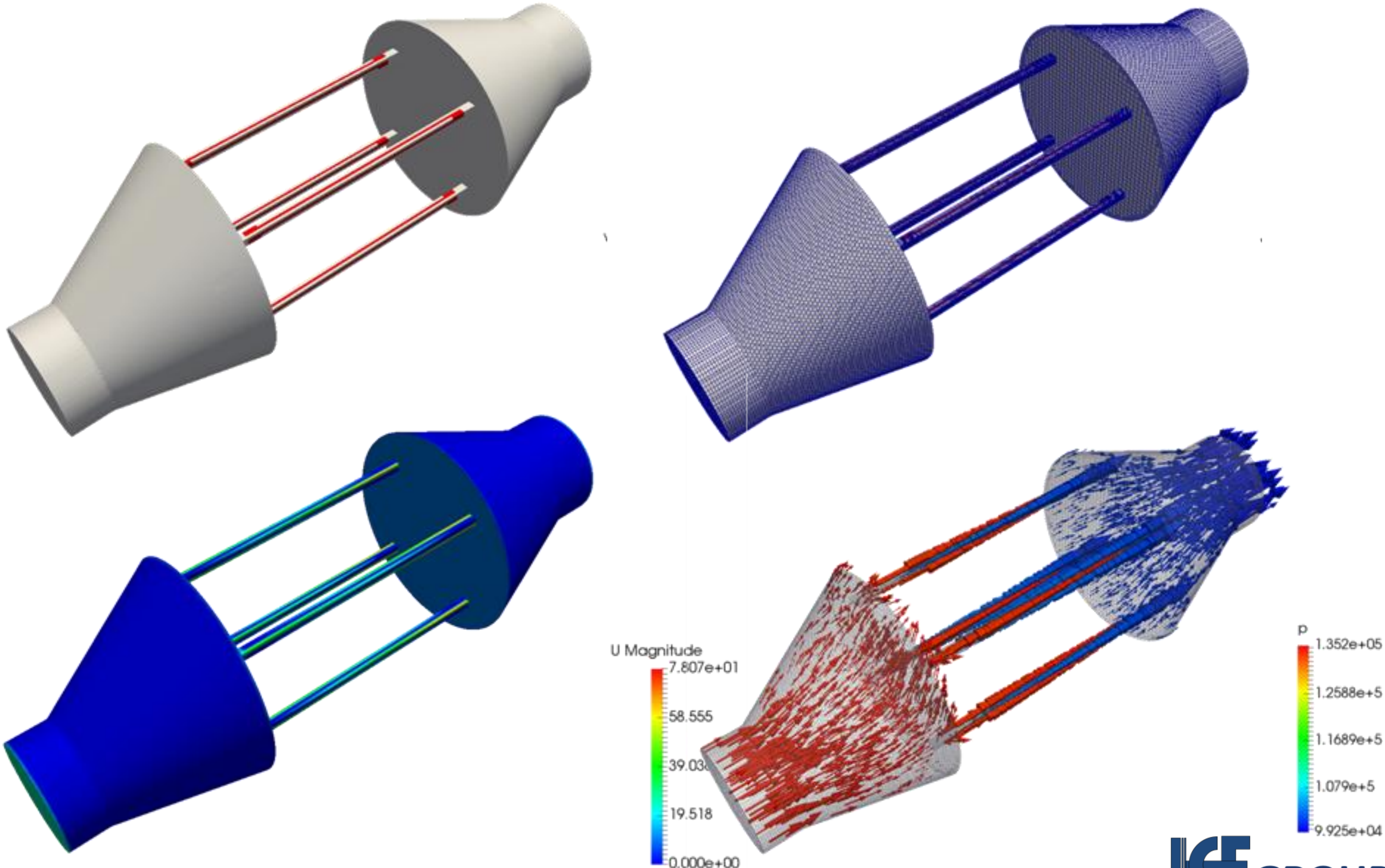
Channel scale:



Component scale:



WIP: Channel scale DPF/GPF or CAT



Acknowledgements

- Dr. Francesco Lucci

- Prof. Gavin Tabor

- The authors gratefully acknowledge financial support the Italian Ministry of Education, University and Research, Rome (MIUR, Progetti di Ricerca Scientifica di Rilevante Interesse Nazionale, prot. 2010XFT2BB), within the project IFOAMS: Intensification of Catalytic Processes for Clean Energy, Low-Emission Transport and Sustainable Chemistry using Open-Cell Foams as Novel Advanced Structured Materials.

ICE GROUP
POLITECNICO DI MILANO