Visit to University of Bremen
Research group: MIMENIMA

Towards the application of open-cell foams as novel substrates for compact and efficient catalytic reactors

08/07/2019

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Politecnico di Milano - Dipartimento di Energia
Internal Combustion Engines Group

ICE GROUP
POLITECNICO DI MILANO

Outline

1. ***Few word about ICE Group at Politecnico di Milano***
2. ***Introduction***
3. ***Methodology:***
   - Fluid-dynamics and heat transfer at the micro-scale
   - Reaction simulations at the micro-scale
   - Geometrical modeling: on the adoption of Kelvin cells
4. ***Open-cells foams as catalytic substrates:***
   - Kelvin cells vs honeycombs
   - Design and optimization of open-cell foams catalyst
   - Full-scale simulation of ATS equipped with open-cell foams
5. ***Towards future solutions:***
   - Additive layering manufacturing of structured substrates
6. ***Conclusions***

Politecnico di Milano



- **Politecnico di Milano** is a public university.
- About **40.000** students (**25.000** students in the Engineering Faculties, 4.000 students in the Design Faculty, 11.000 students in the Architecture Faculty).
- **350** new PhD students per year.

Politecnico di Milano



- Politecnico has **1.140** academics (400 full professors, 390 associate professors and 350 lecturers) and **870** administrative and technical employes.
- Graduated in engineering at Politecnico represent about **12,7%** of all the graduated in engineering of Italy.

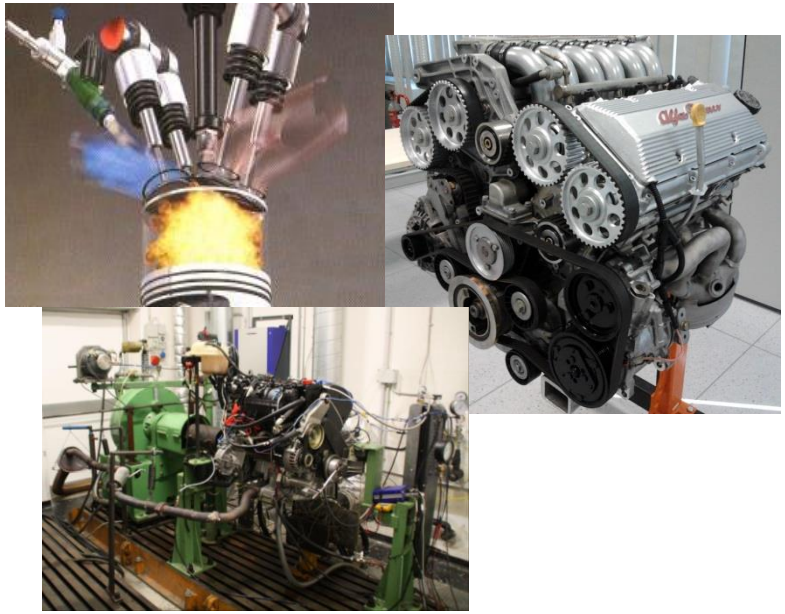
Department of Energy

Currently involves **110** academics and **100** young researchers: overall **210** people working in the energy field.

Research and teaching on the following topics:

- **Internal combustion engines**
- Powerplants and energy systems
- Combustion
- Turbo-machinery
- Fuel cells
- Thermodynamics
- After-treatment systems
- Acoustics
- Nuclear energy

The Internal Combustion Engine Group



The Academic Staff

Angelo Onorati, Full Professor
Gianluca D'Errico, Full Professor
Gianluca Montenegro, Associate Professor
Tommaso Lucchini, Associate Professor
Tarcisio Cerri, Assistant Professor
Augusto Della Torre, Assistant Professor

Research Grant

Lorenzo Sforza, PhD
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Andrea Marinoni, MSc
Cristian Ierardi, MSc

Ph.D students

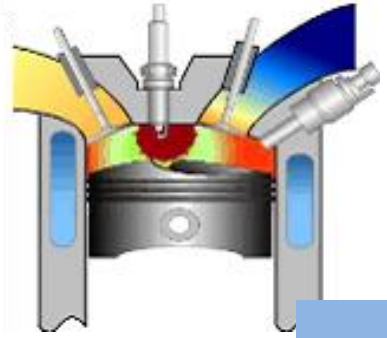
Davide Paredi, MSc
Giovanni Gianetti, MSc
Antonello Nappi, MSc
Matteo Tamborski, MSc

MSc students

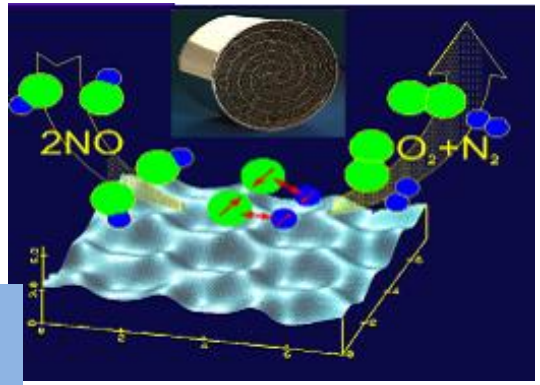
15-20 per year

Research interests

Combustion process

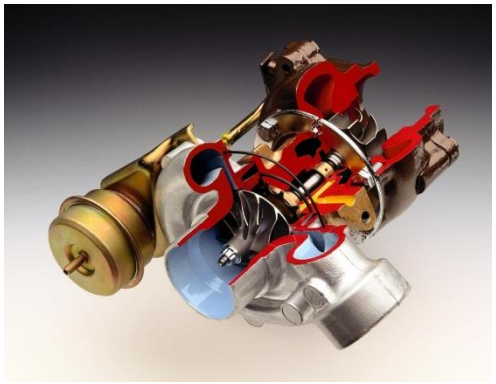


Emission control

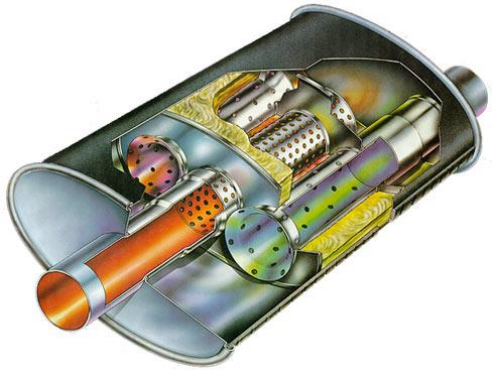


Focus on the Internal Combustion Engine

Turbocharging



Acoustics

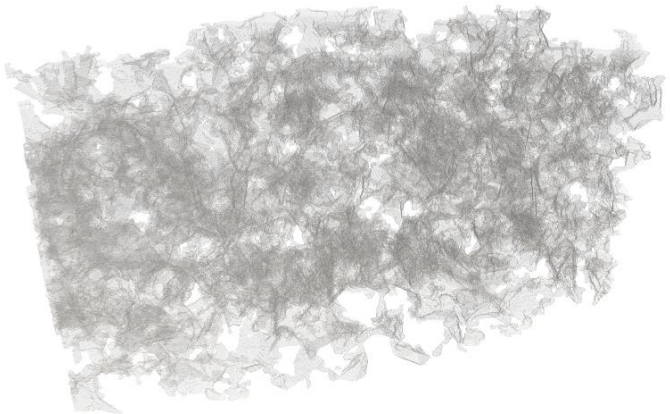


Alternative fuels

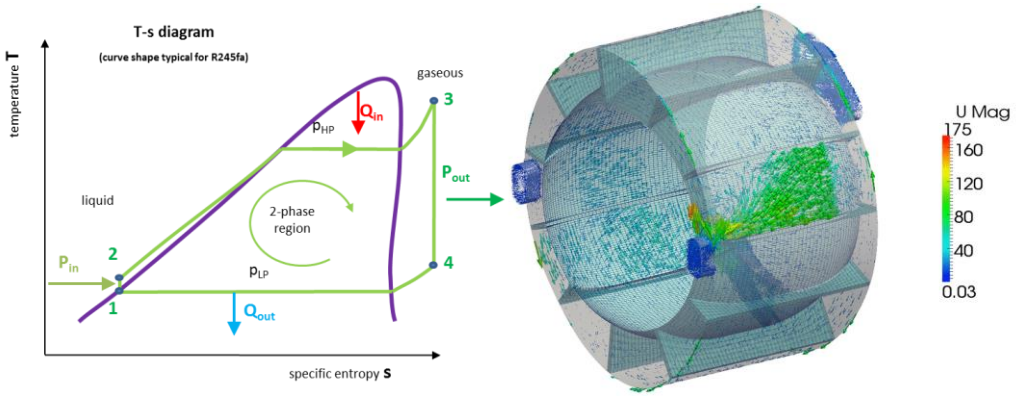
Research interests

…and some other research activities

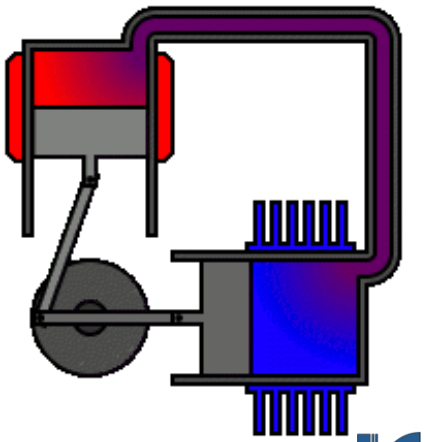
Oil&Gas:
Multiphase flow at the micro-scale



Waste heat recovery:
Organic rankine cycle

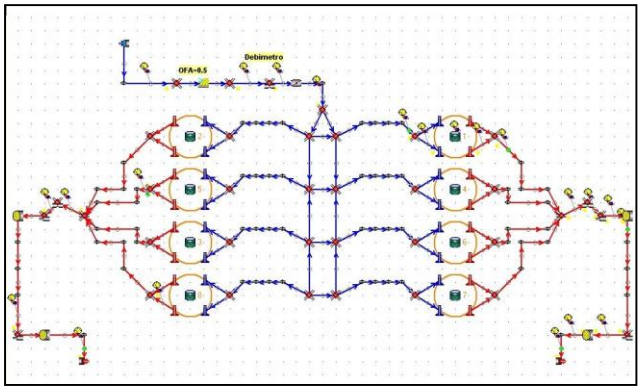


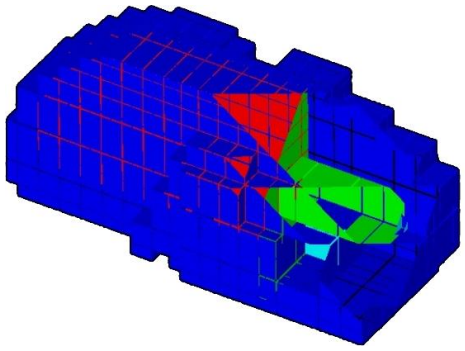
Stirling engine

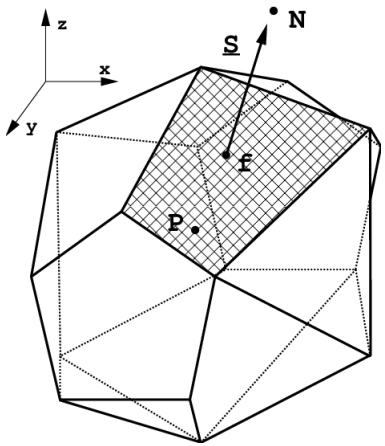


Development and application of simulations tools

GASDYN: simulation code developed at PoliMI for the simulation of ICE systems with 1D/quasi3D approaches

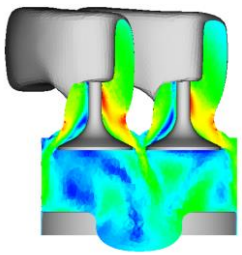


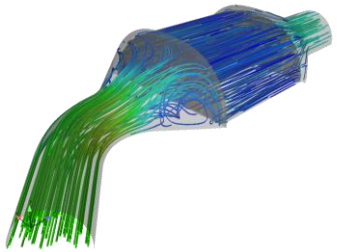


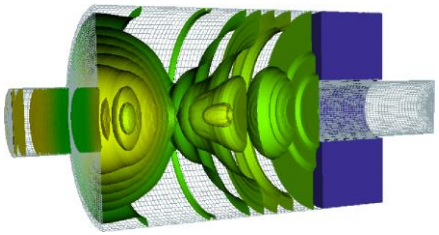


OpenFOAM®: Open-source CFD finite volume code written in object oriented C++

LibICE: A C++ library developed at PoliMI for the ICE simulation

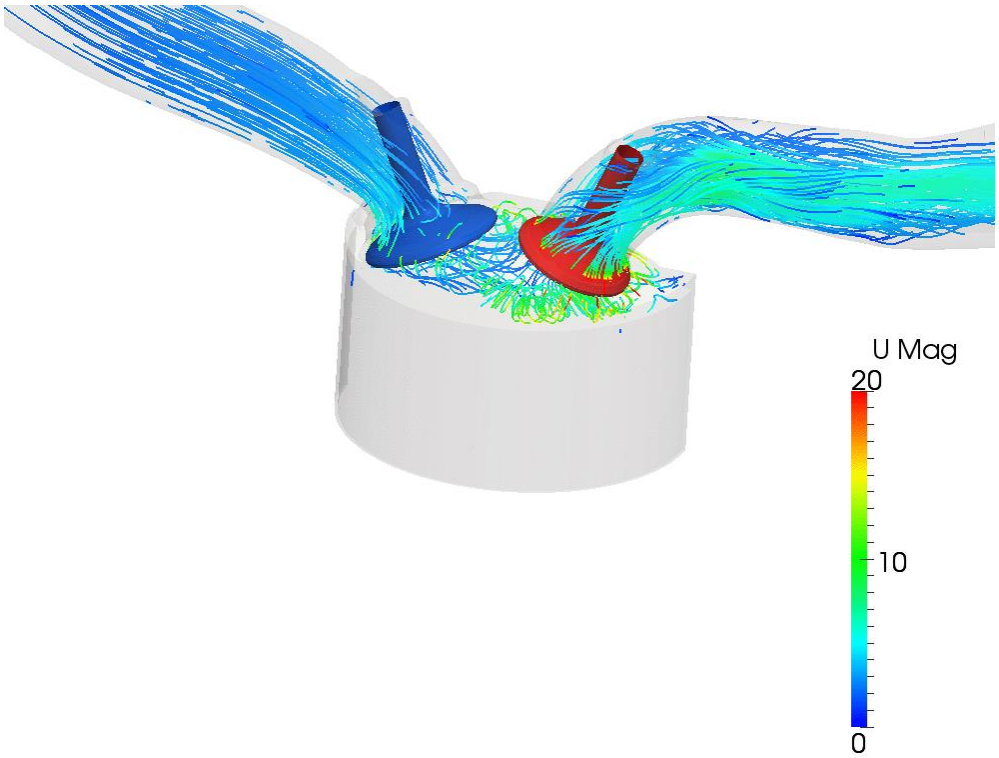






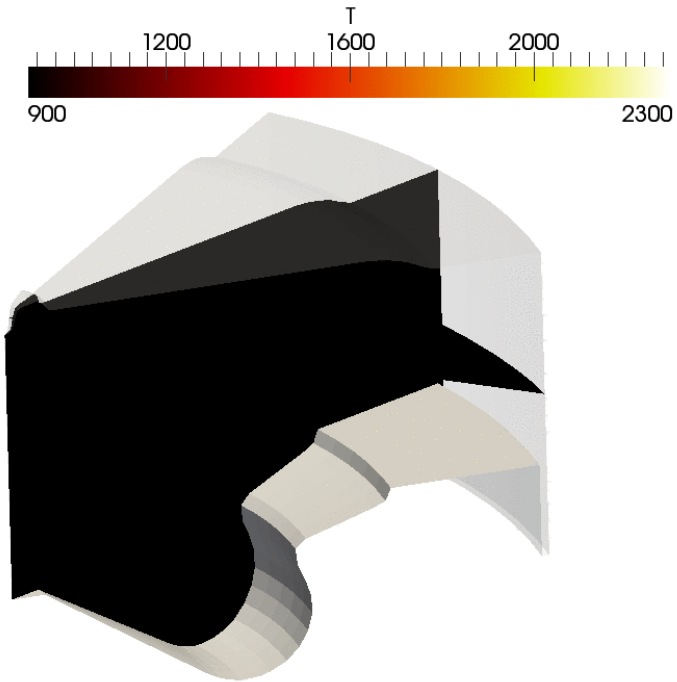
Cylinder modelling

Gas exchange



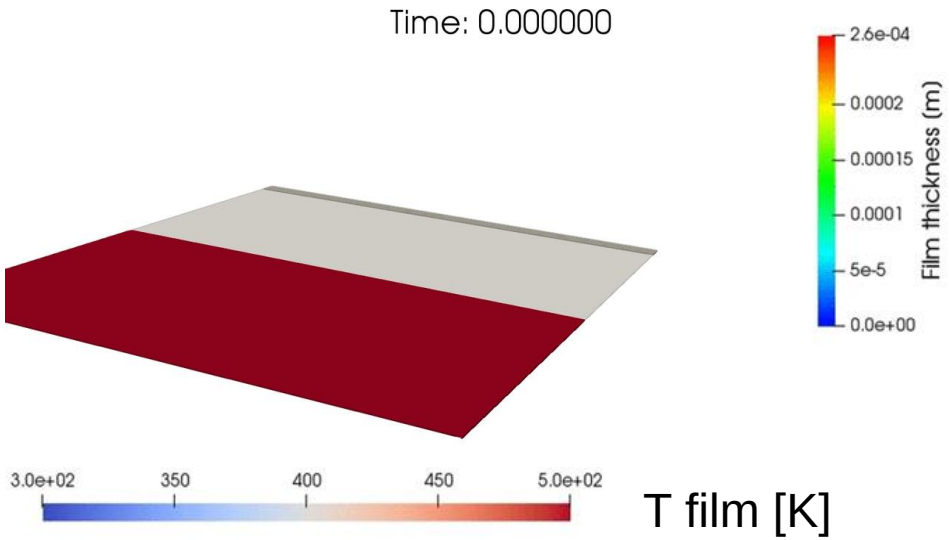
Time: 374.000000

Diesel combustion

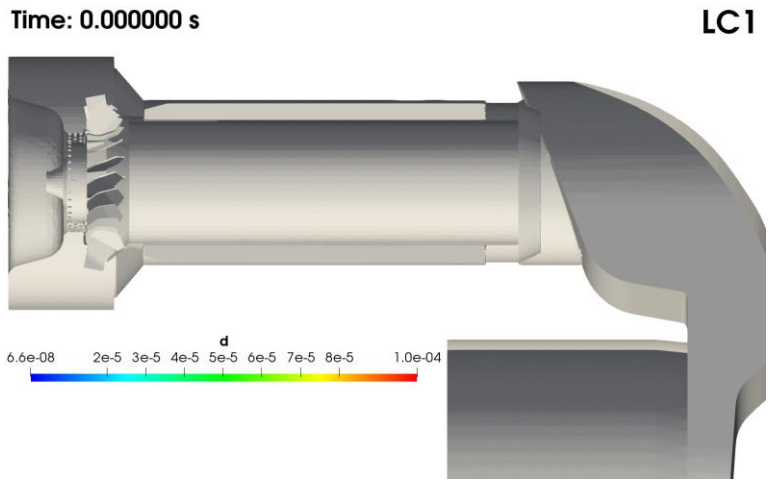


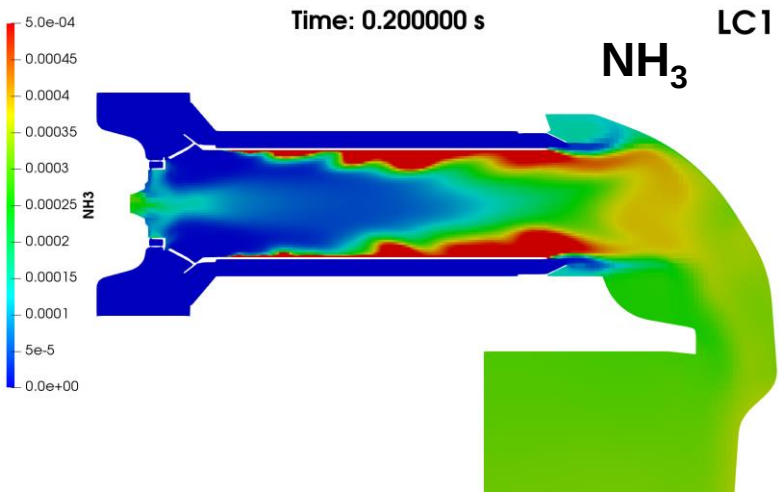
Time: -45.00

After-treatment system modelling



Simulation of urea injection process in SCR systems





Introduction

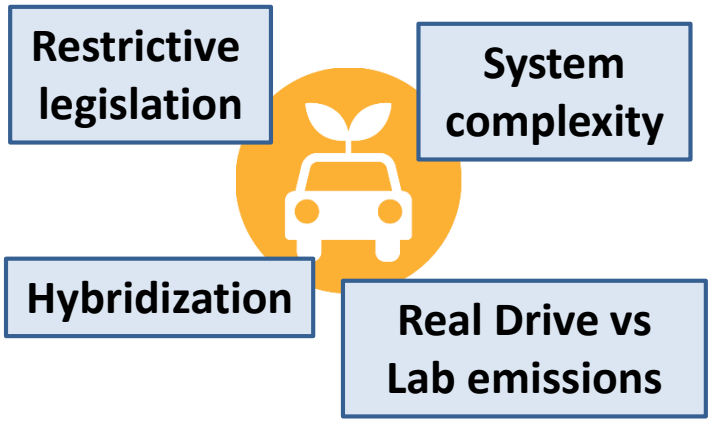
Acknowledgements

The work I am presenting today is the result of many contributors:

- ***Politecnico di Milano (IT):***
  - *ICE Group:* prof. G. Montenegro, prof. A. Onorati
  - *LCCP Group:* prof. E. Tronconi, prof. G. Groppi
- ***University of Exeter (UK):***
  - prof. G. Tabor, Dr. L. Wears
- ***EMPA Research Center (CH):***
  - Dr. P. Dimoupulos, Dr. F. Lucci, MSc V. Papetti
- ***SUPSI Technical University (CH):***
  - Prof. A. Ortona
- ***Università di Bologna (IT):***
  - Prof. G. Bianchi, prof. S. Falfari, Dr. F. Brusiani, MSc G. Micci

Background

Nowadays the control of pollutant emission from Internal Combustion Engine is an issue of extreme concern in the automotive field



Interest towards novel catalytic substrates as a substitute of traditional honeycombs

Requirements:

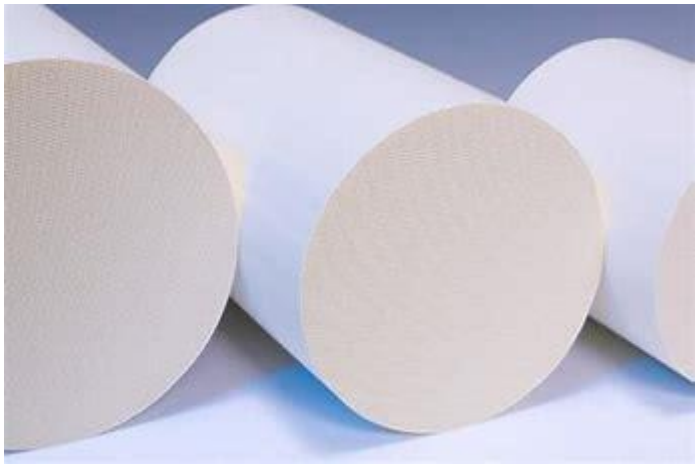
- High permeability
- High mass transfer coefficients
- Low thermal capacity

Goals:

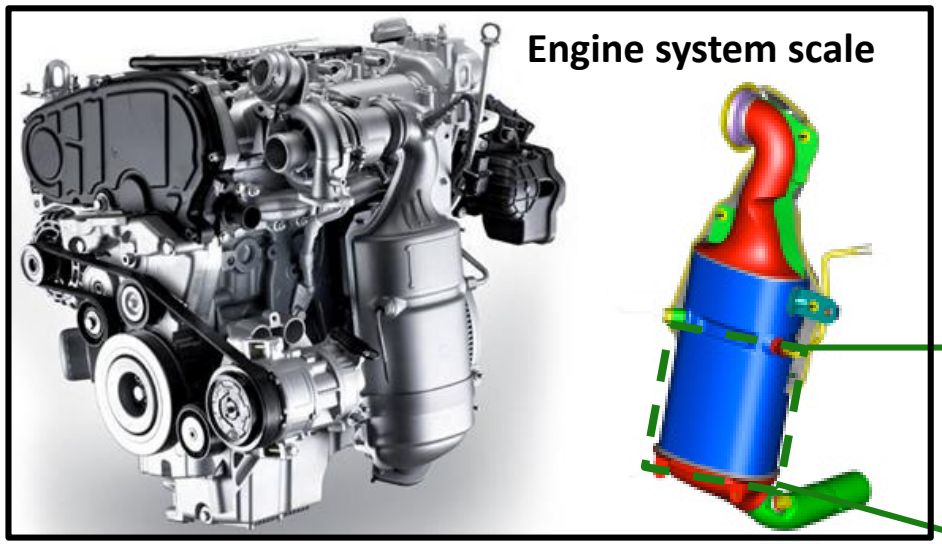
- Low pressure drop: fuel consumption
- Low catalyst loading: cost
- Fast light-off: transient response in hybrid powertrain

Background

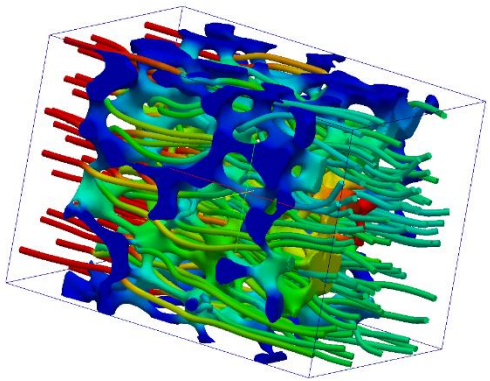
Can open-cell foams be a practical solution for the next generation of compact and efficient catalytic substrates?



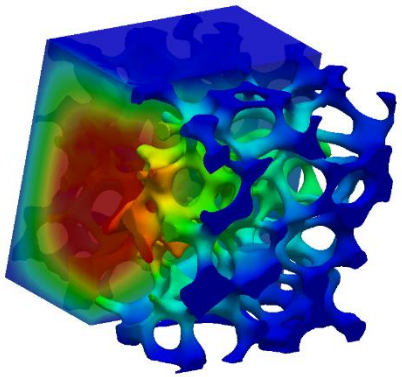
Overview of the scales involved



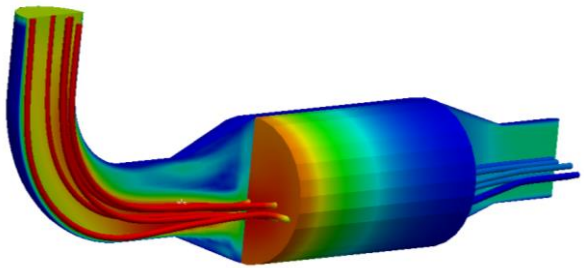
Micro-scale



Macro-scale



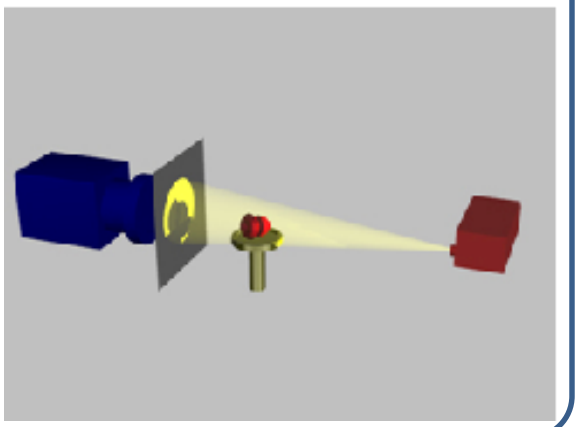
Component scale



The substrates

Micro-CT scanner

Micro-CT scanner



X-ray image

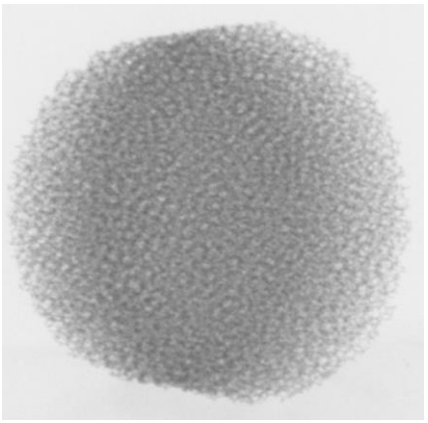
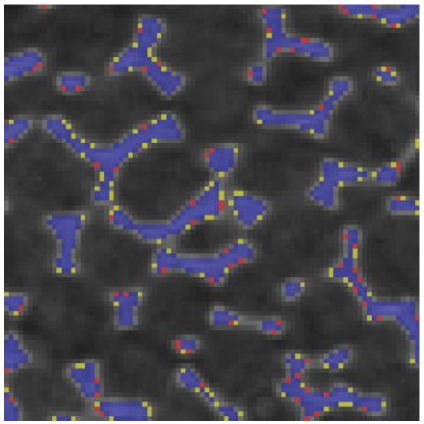
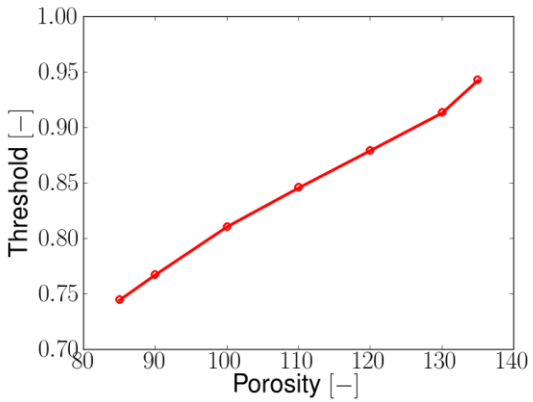
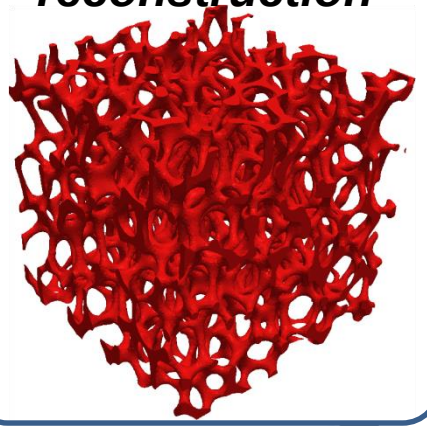


Image segmentation





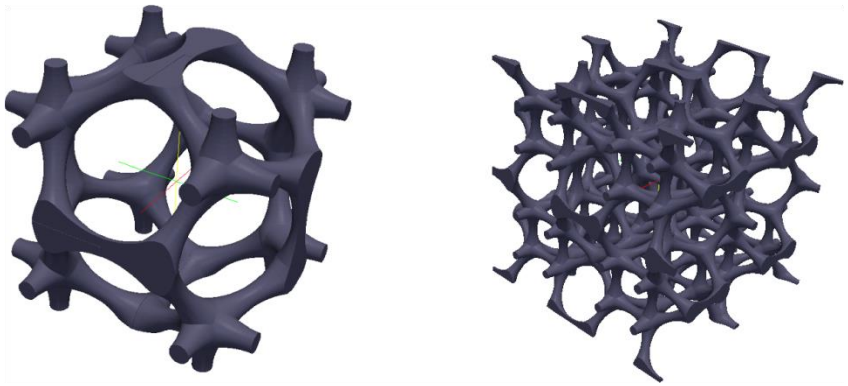
3D geometry reconstruction



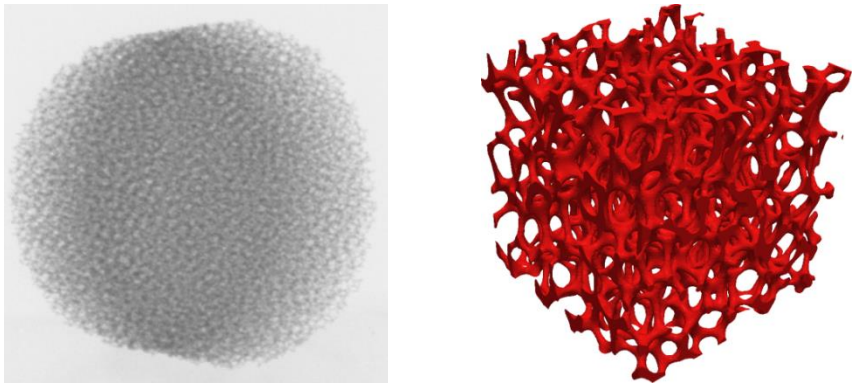
From the sample to the CFD model

Geometry reconstruction

Geometry idealization

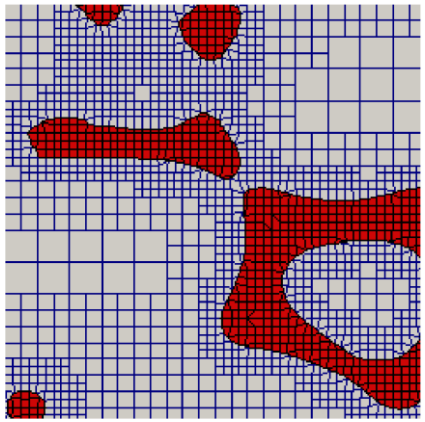


Micro-CT geometry reconstruction

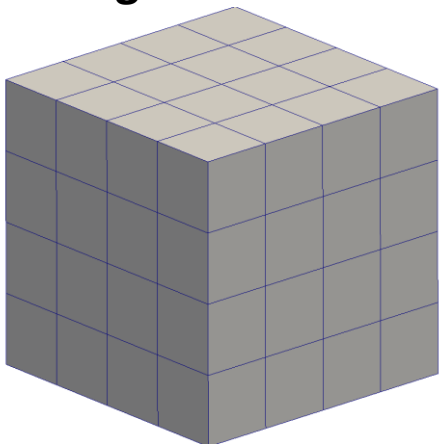


Mesh generation

snappyHexMesh



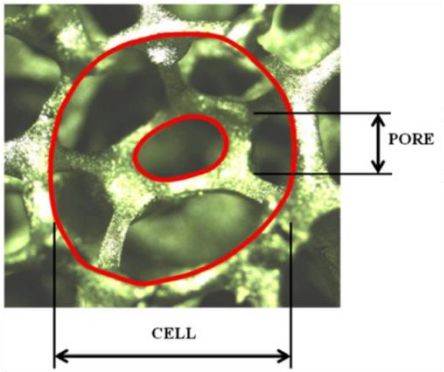
imageHexMesh

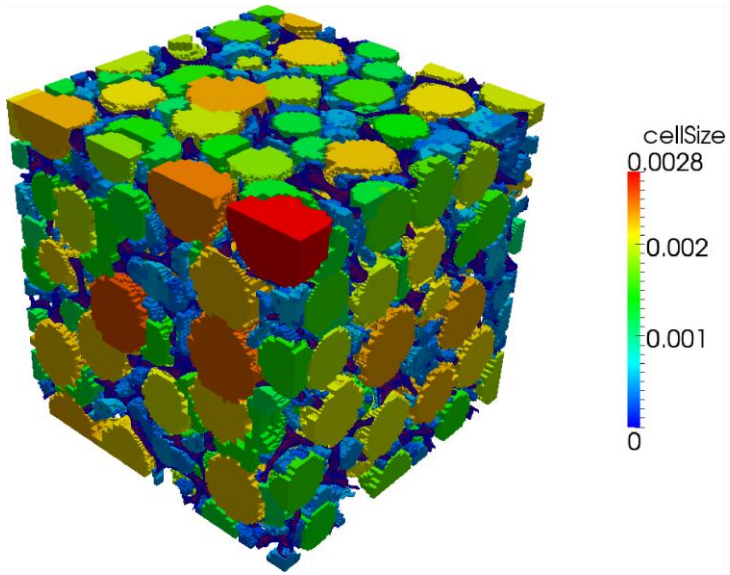


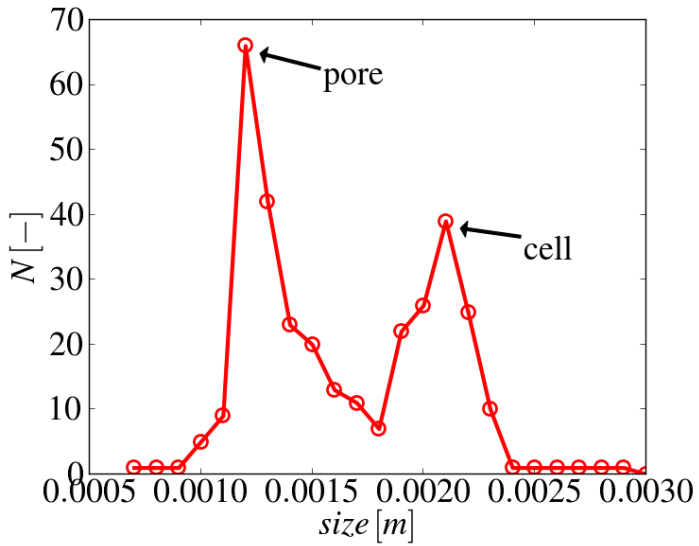
Geometry characterization

- 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 $[m]$	$1.2 \cdot 10^{-3}$	$3.1 \cdot 10^{-4}$	$1.6 \cdot 10^{-5}$





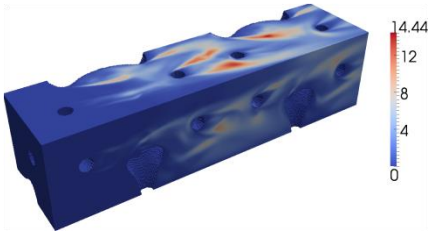


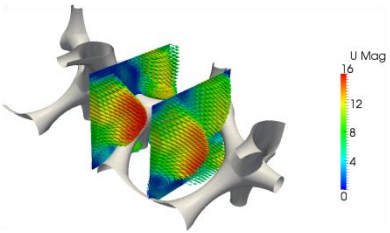
Methodology:
fluid-dynamics and heat-transfer at the micro-scale

CFD simulations

Fluid phase: <u>Unsteady detailed numerical simulations</u>

Investigation of flow regimes occurring in open-cell foams



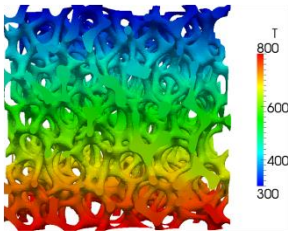


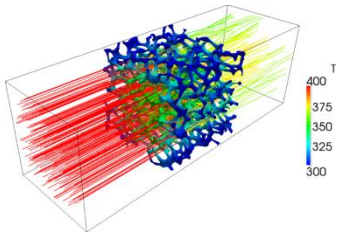
Fluid phase: <u>RANS numerical simulations</u>

Study of the effects of the geometry on the pressure drop

Solid phase: <u>Conductive heat-transfer simulations</u>

Characterization of the conductivity of the porous matrix

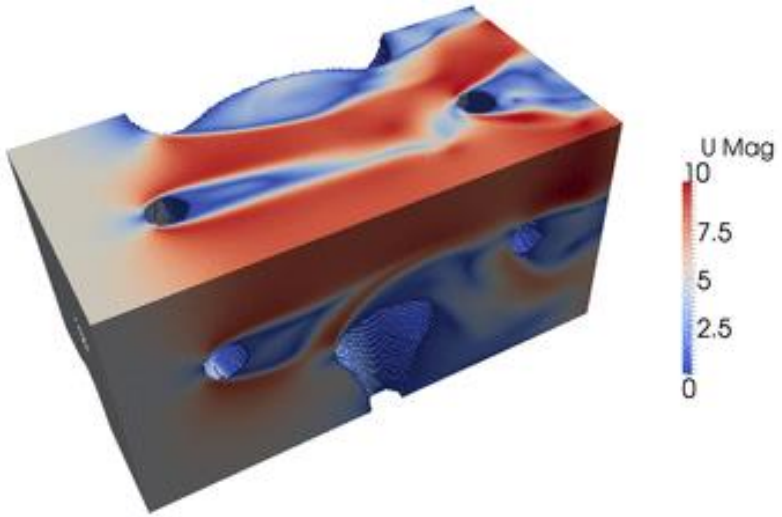




Fluid & solid phases: <u>Conjugate heat-transfer simulations</u>

Characterization of the inter-phase heat transfer

DNS: cold flow

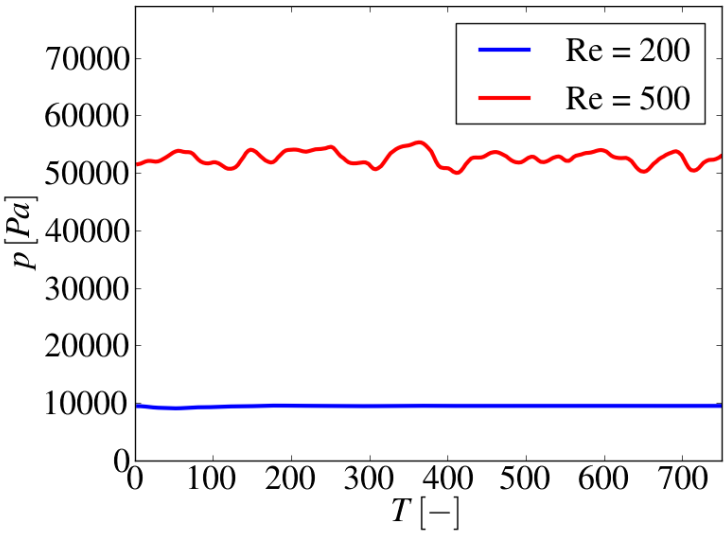


Numerical schemes accuracy:

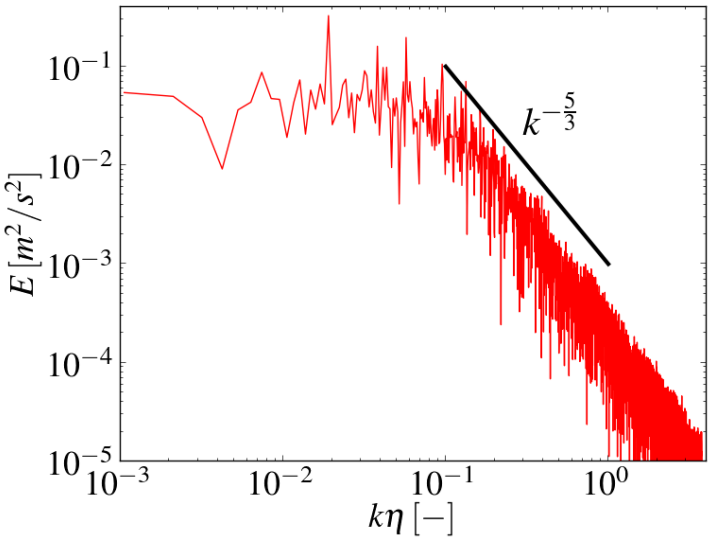
- ***Time:*** second order
- ***Space:*** third order

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

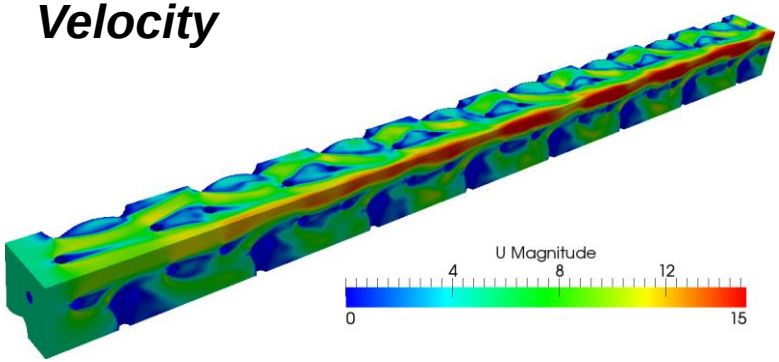


TKE spectrum

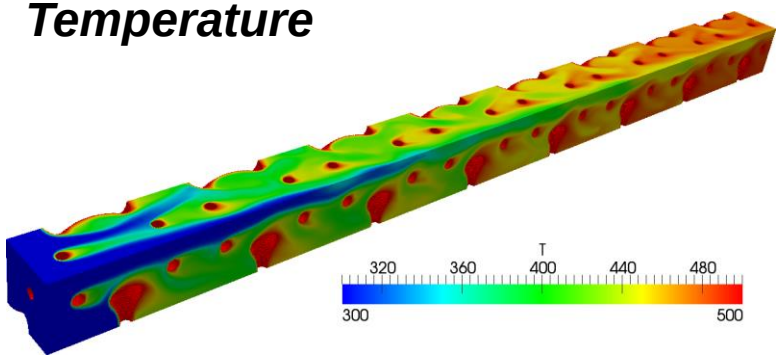


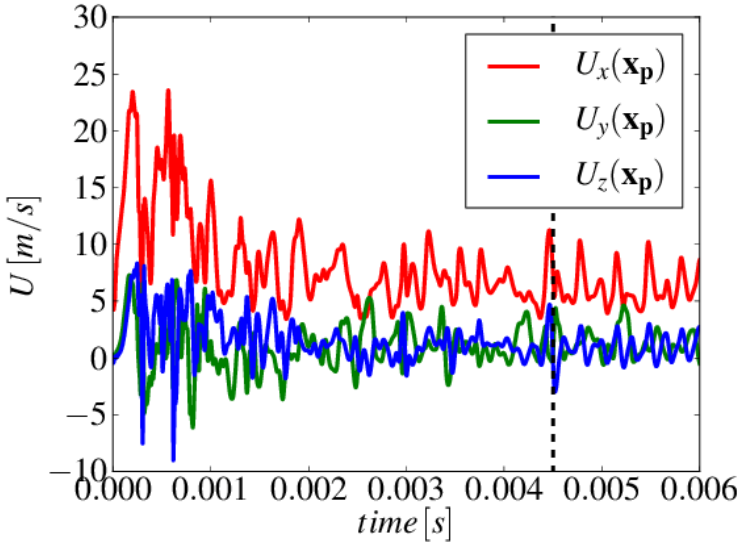
DNS: heat transfer

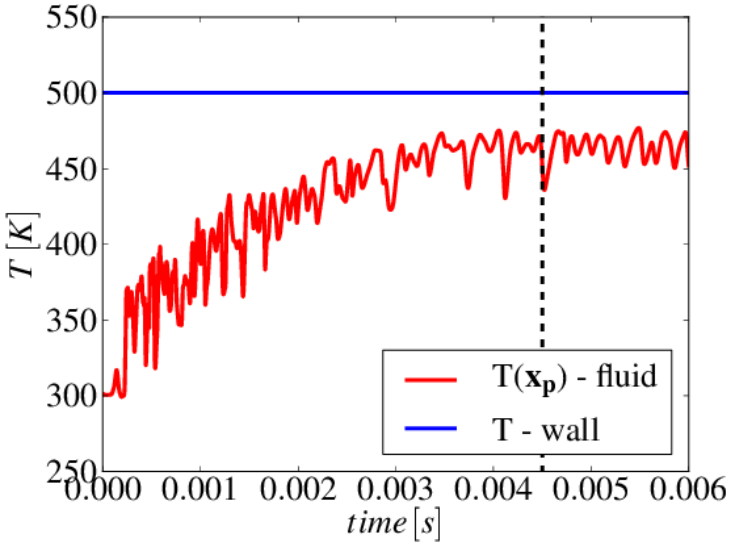
Velocity



Temperature

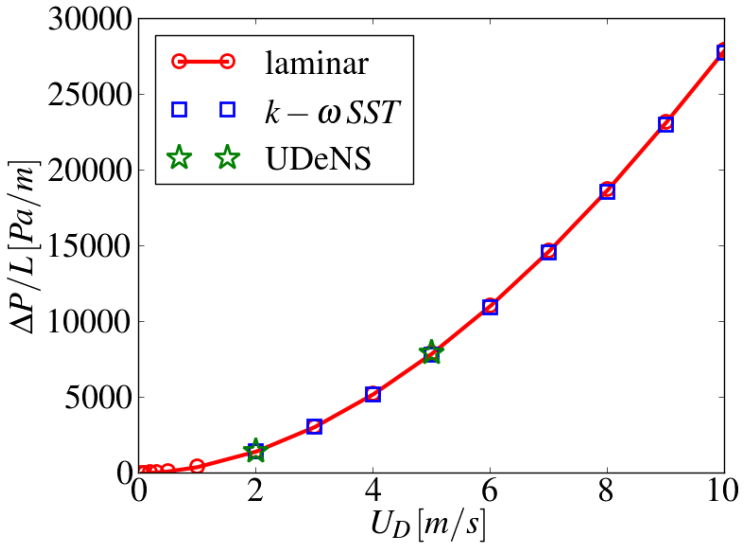




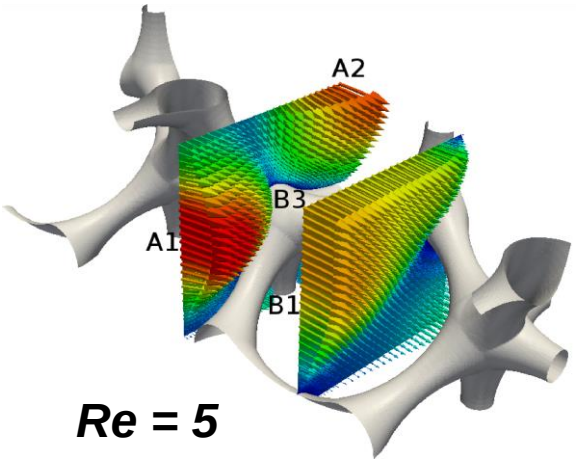


mesh: *16 mln cells* – runtime: *30 days on 16 processors*

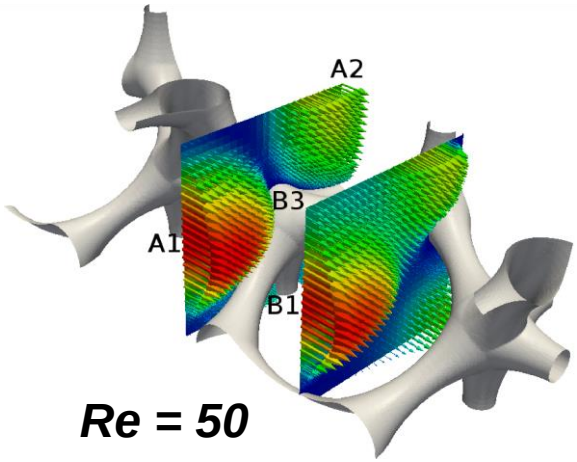
Cold flow RANS simulations: ideal foams



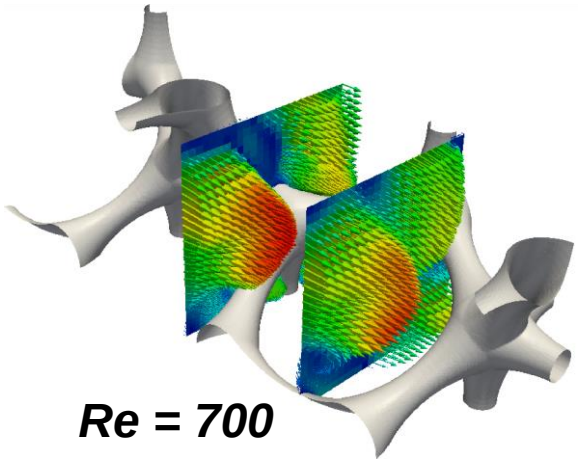
- Similar results obtained with:
  - ***Laminar*** simulation
  - ***RANS*** simulation
  - ***DNS*** simulation
- Investigation of the velocity field at different Reynolds



Re = 5



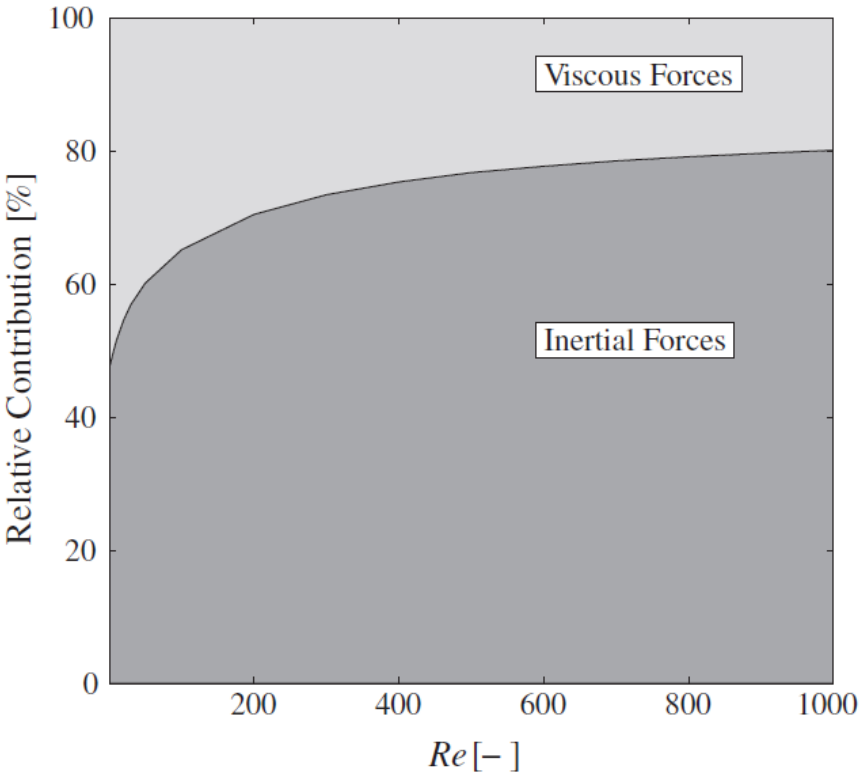
Re = 50



Re = 700

Cold flow RANS simulations: ideal foams

Contribution of viscous and inertial forces to the overall pressure drop:



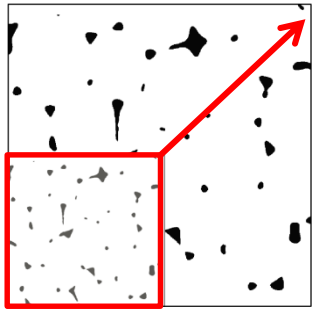
- At high Re numbers the contribution of inertial forces (form drag) is predominant.
- Viscous forces are predominant in the Darcy regime (Re < 10).
- This explains why turbulence has a negligible effect of the overall pressure drop.

Cold flow RANS simulations: real foams

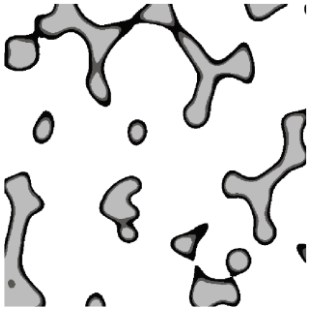
Mathematical transformations of the geometry of the real foam:

- ***Dilation:*** pore density modification
- ***Opening:*** porosity modification

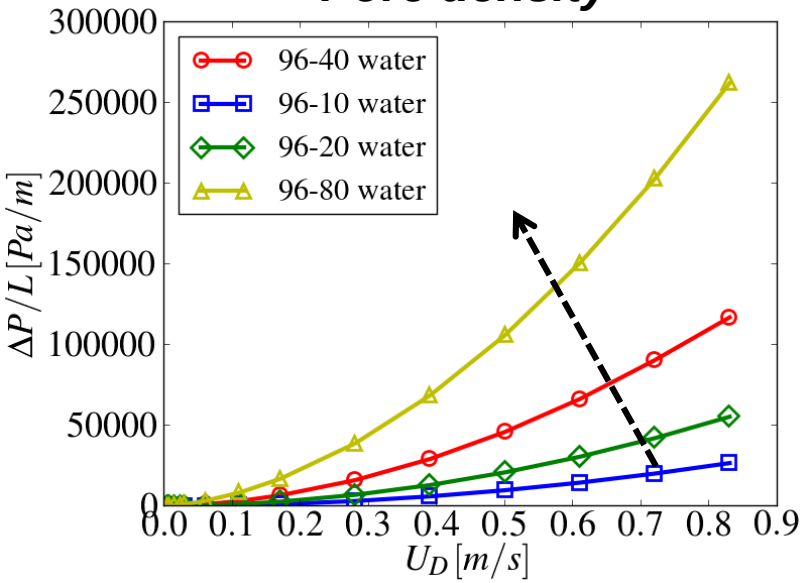
dilation



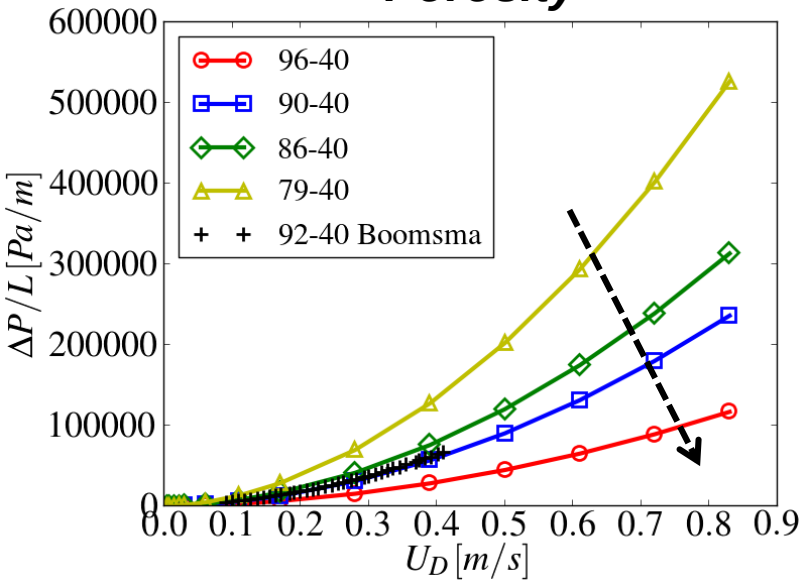
opening



Pore density



Porosity

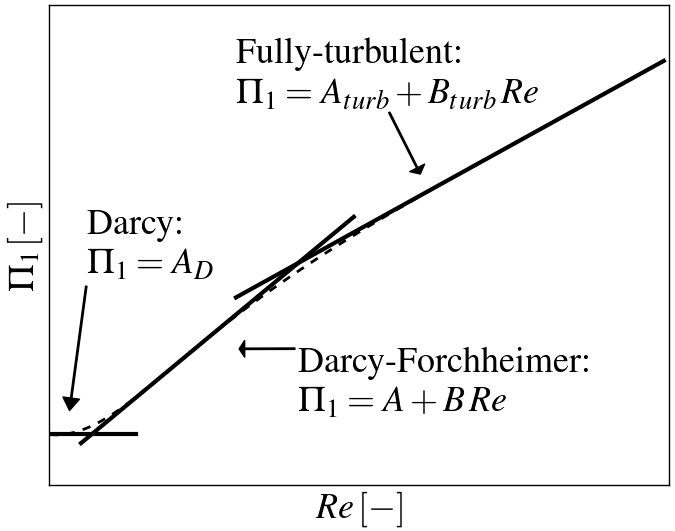


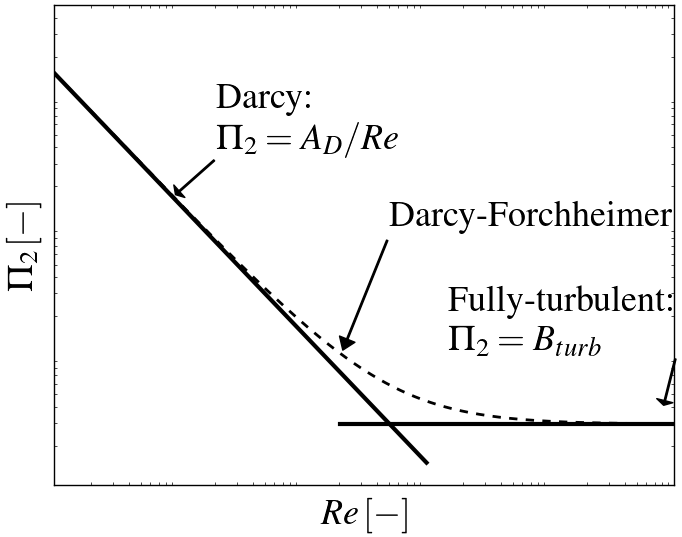
Cold flow RANS simulations: real foams

Analysis of flow regimes on the basis of non-dimensional relationships:

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

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



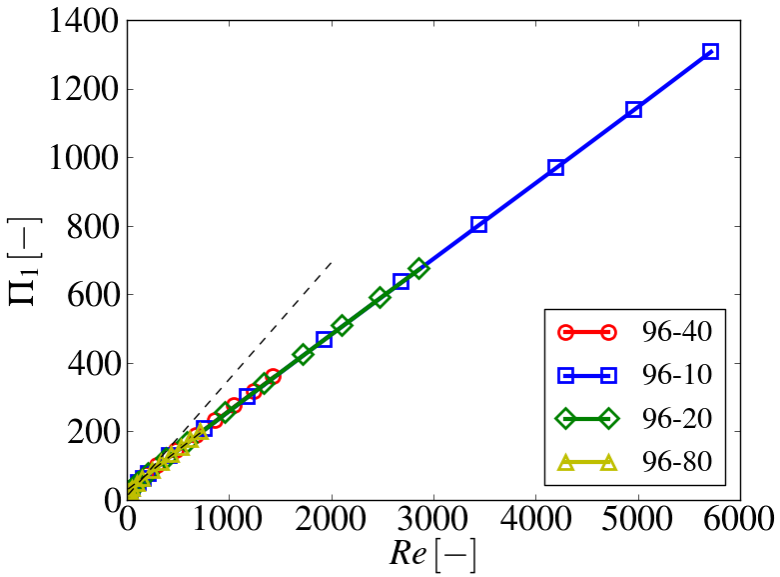


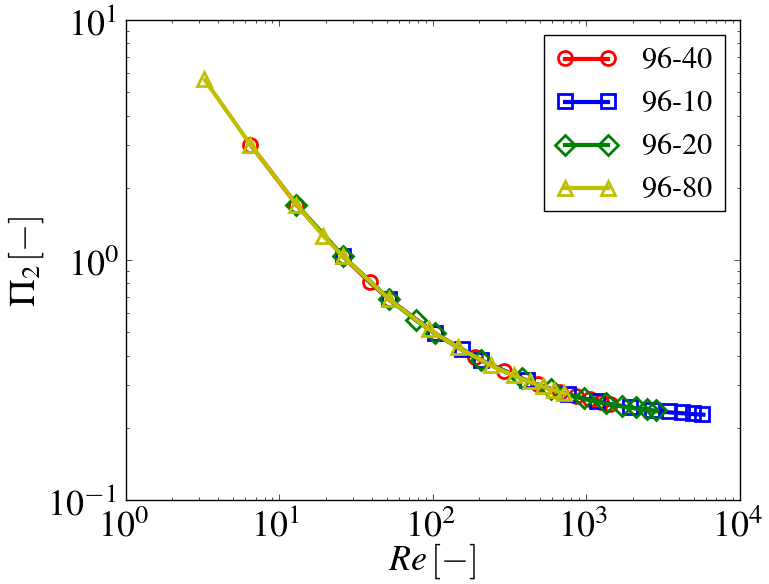
Cold flow RANS simulations: real foams

Analysis of flow regimes on the basis of non-dimensional relationships in case of pore-density variation (dilation):

$$\Pi_1 = \frac{\Re\, d_c^2}{\hat{\mathrm{U}}\,\hat{\mu}} = \mathcal{F}_{\Pi_1}\left(\mathrm{Re} = \frac{\rho\,\hat{\mathrm{U}}\,d_c}{\hat{\mu}}\right)$$

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



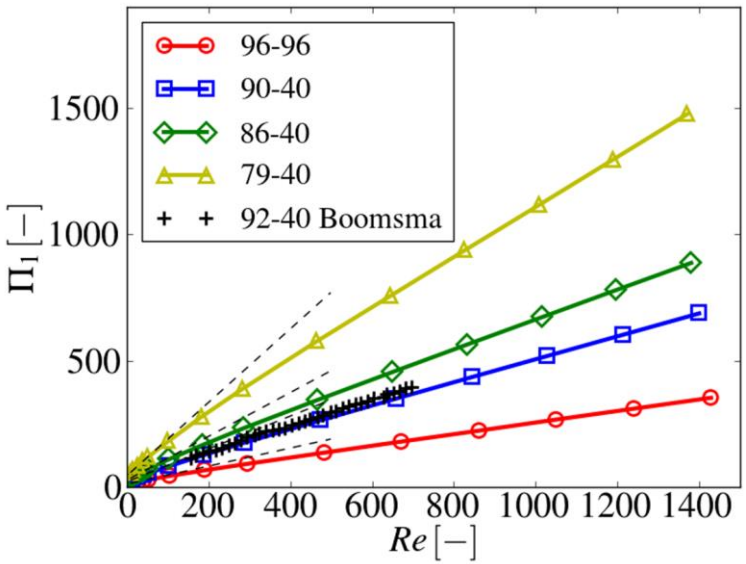


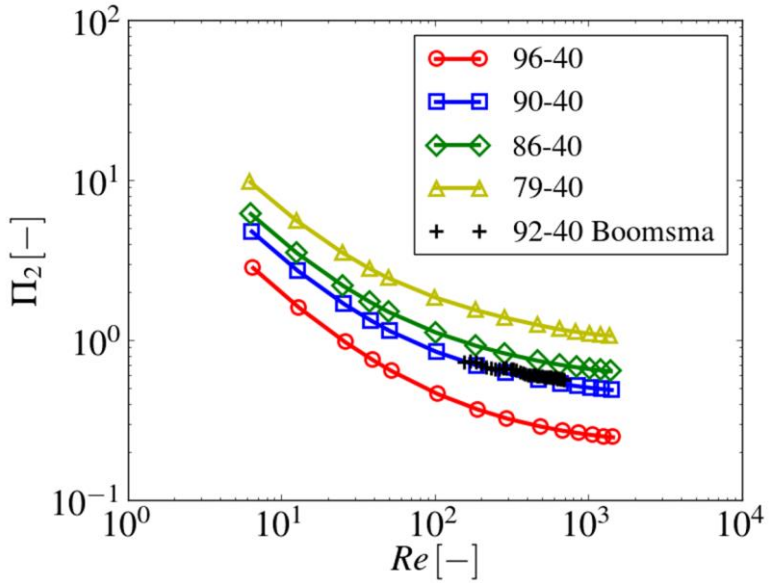
Cold flow RANS simulations: real foams

Analysis of flow regimes on the basis of non-dimensional relationships in case of porosity variation (dilation):

$$\Pi_1 = \frac{\Re\, d_c^2}{\hat{\mathrm{U}}\,\hat{\mu}} = \mathcal{F}_{\Pi_1}\left(\mathrm{Re} = \frac{\rho\,\hat{\mathrm{U}}\,d_c}{\hat{\mu}}\right)$$

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

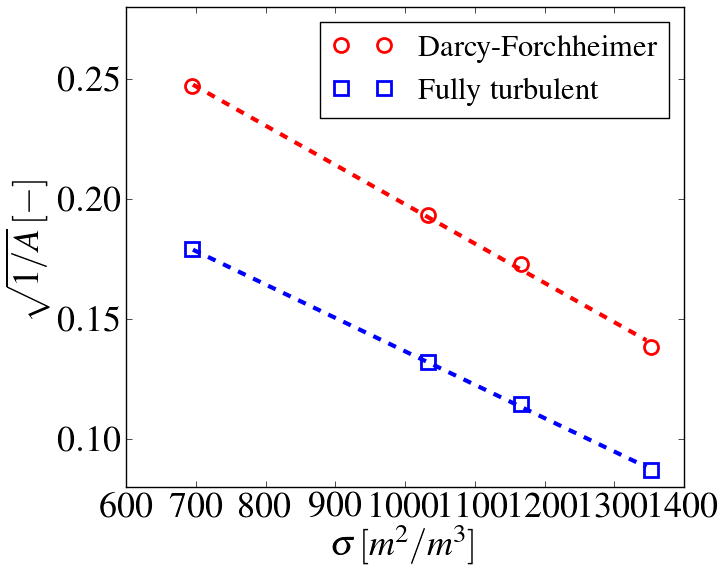


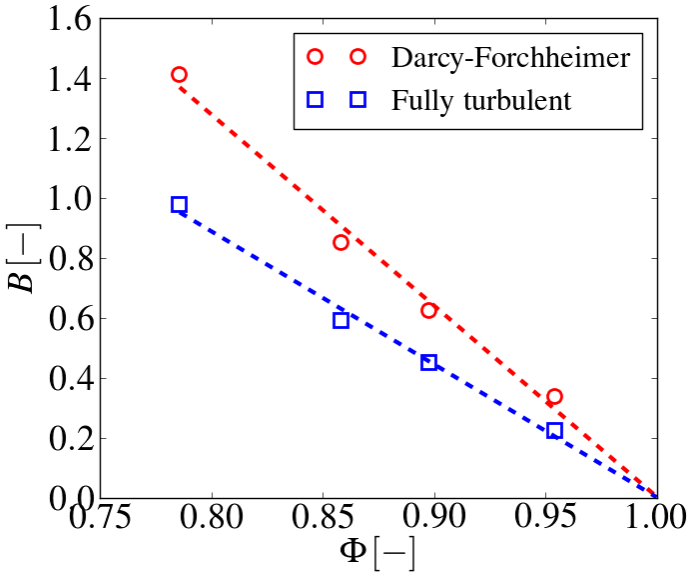


Cold flow RANS simulations: real foams

Dependency of permeability and Forchheimer coefficient on the geometrical properties of the foam:

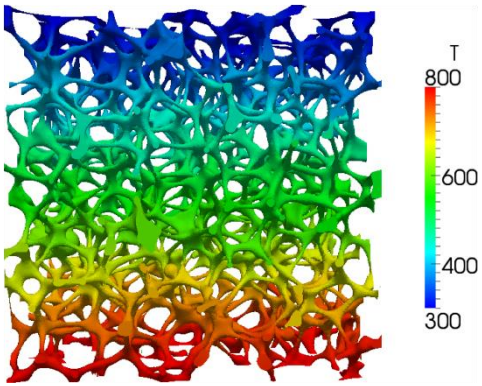
- Porosity
- Specific surface (i.e. pore-density)



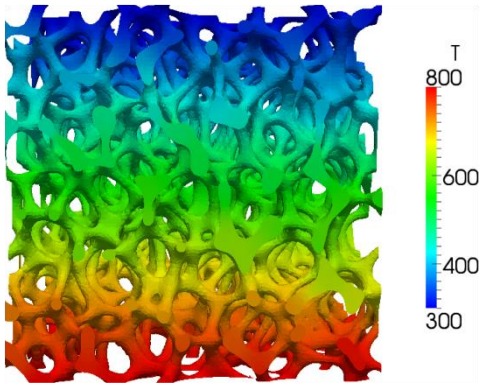


Conductive heat transfer simulation

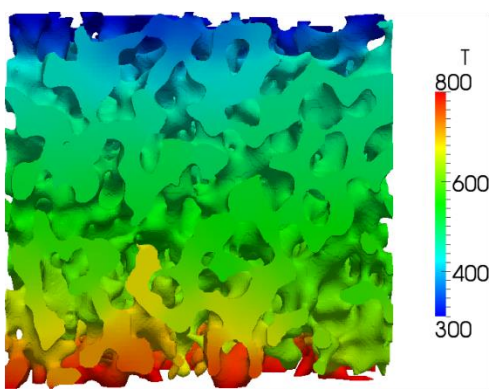
Al foam

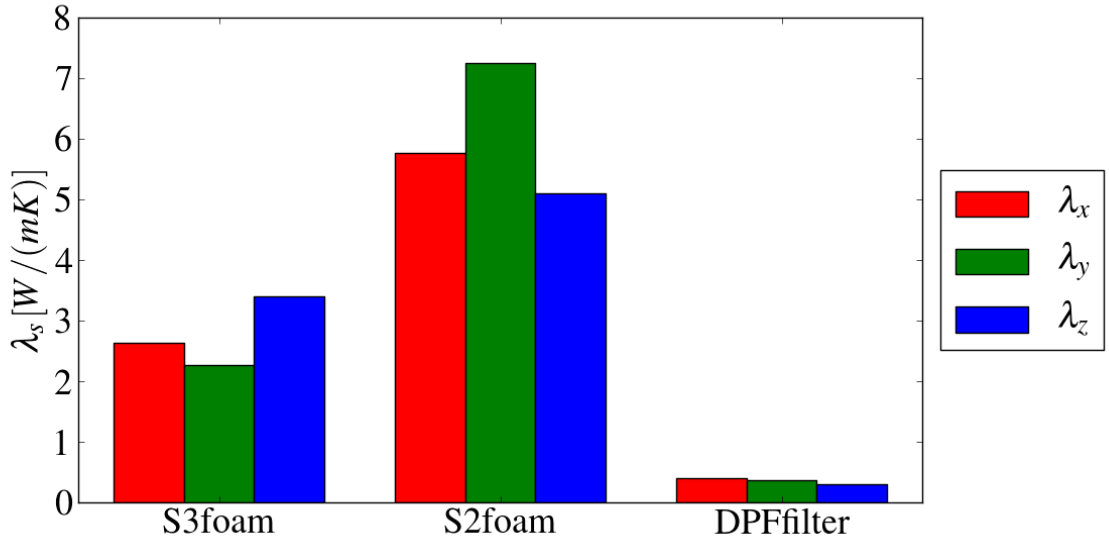


SiC foam



DPF filter

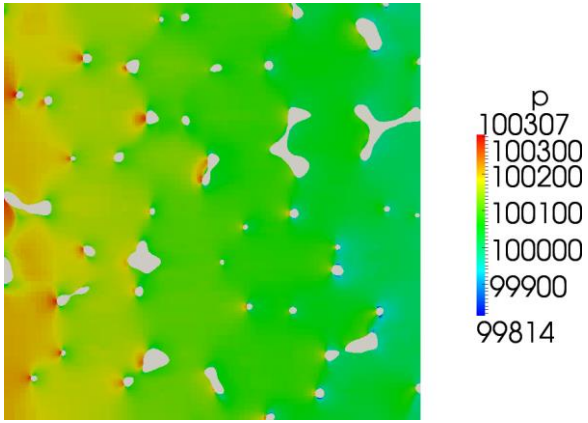


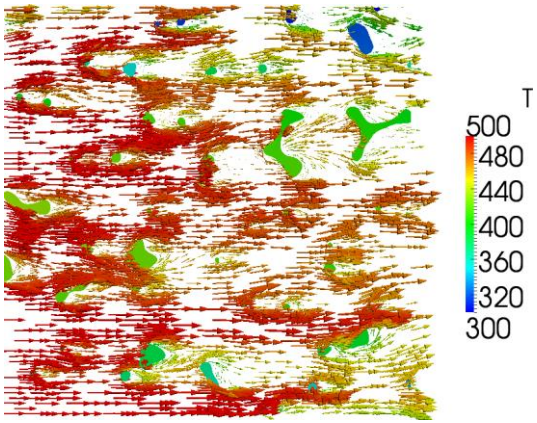


$$\lambda_{eff} = \frac{Q_{cond}}{A\,(T_h - T_c)}$$

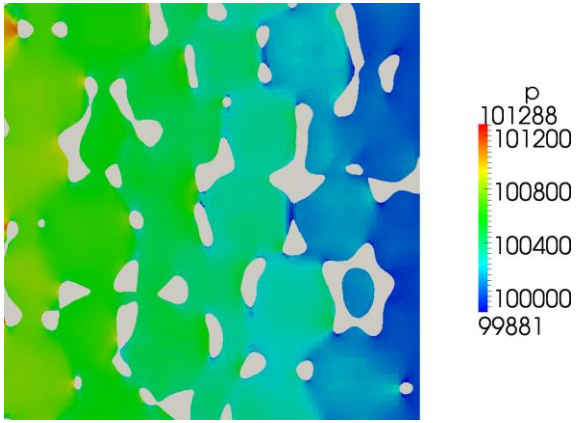
Conjugate heat transfer simulation

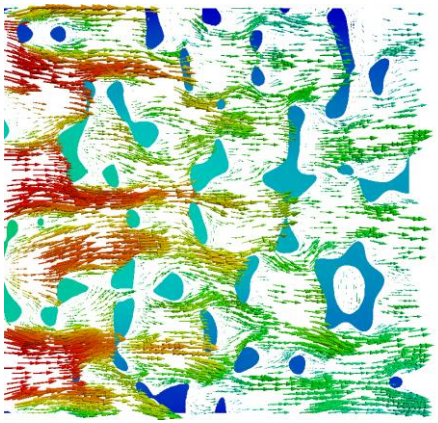
Al foam
10x10x10 mm
6.0 mln cells



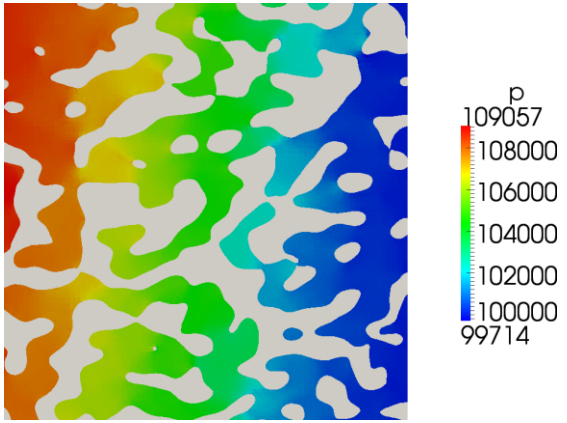


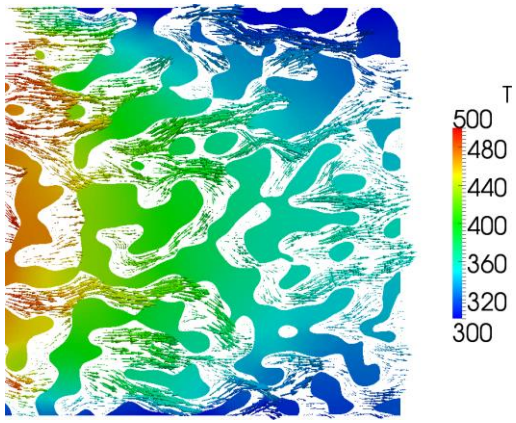
SiC foam
3x3x3 mm
2.1 mln cells





Cordierite
0.35x0.35x0.35 mm
3.2 mln cells

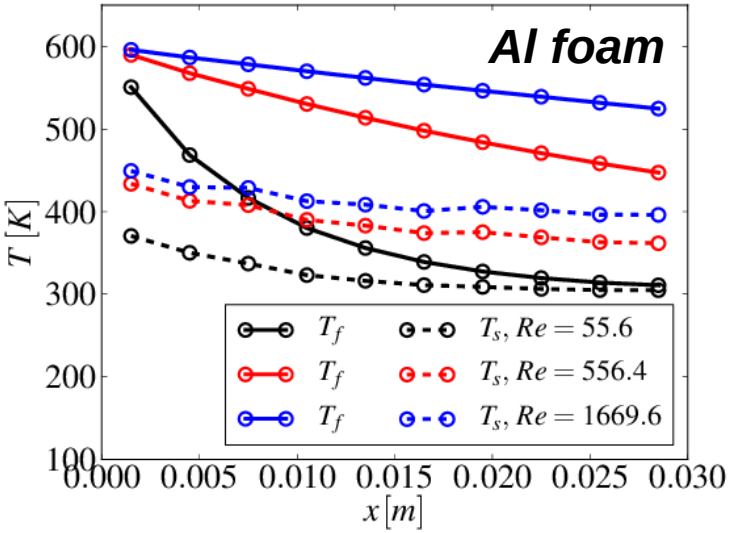


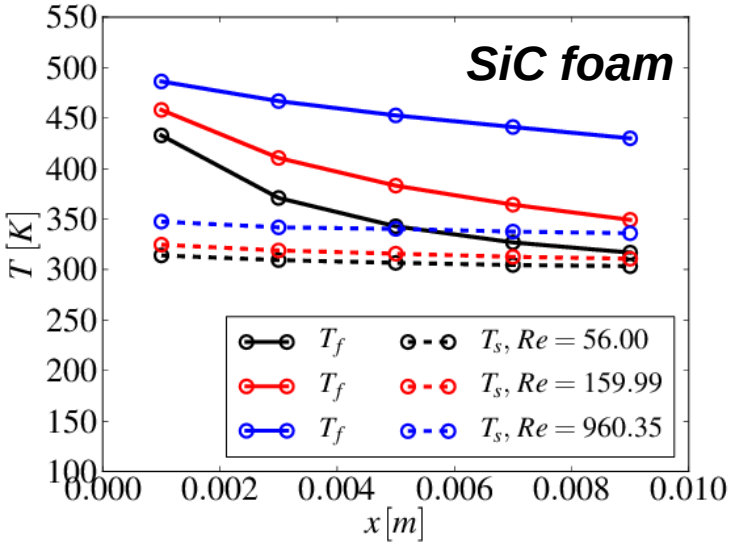


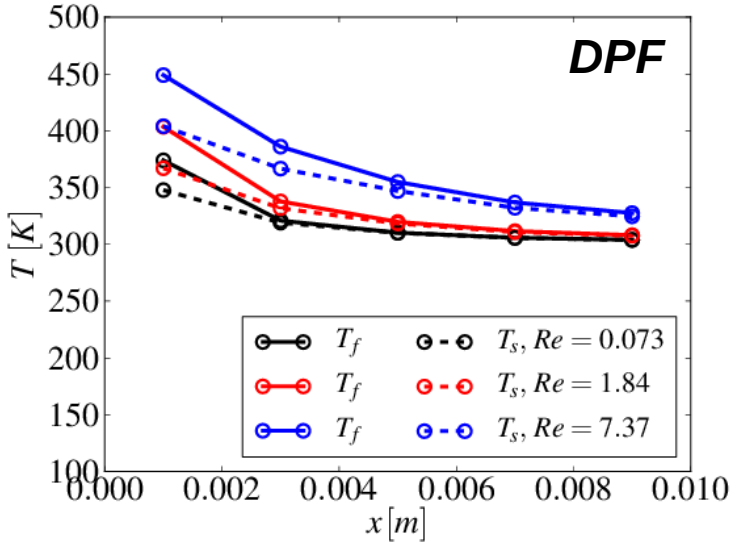
Micro-scale: conjugate heat-transfer

Temperature profiles of fluid and solid phases:

- At low Re: omogeneous temperatures
- At high Re: non-negligible temperature differences between phases





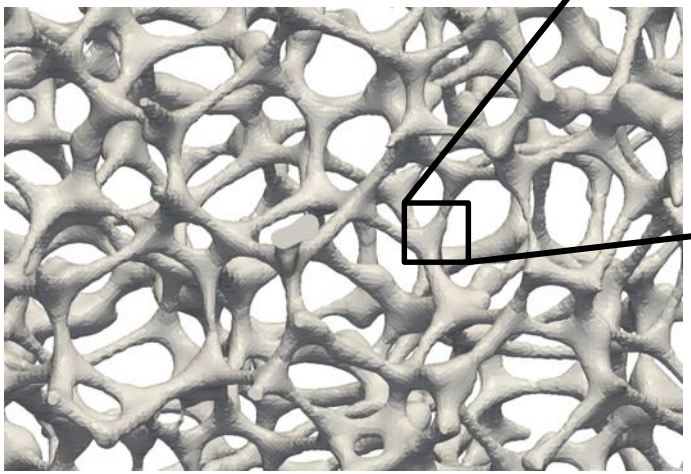


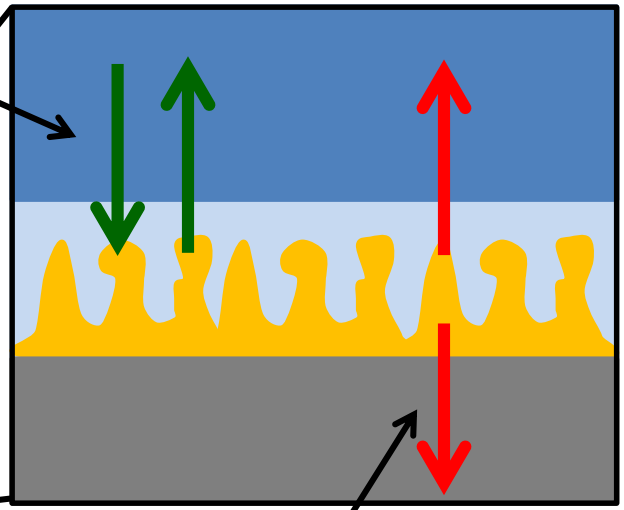
Methodology:
reacting flows simulation at the micro-scale

Micro-scale: modelling catalytic reactions

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

Mass transfer between gas phase and washcoat catalytic surface





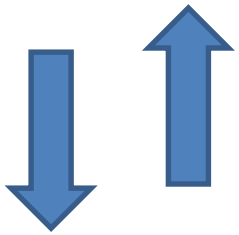
Reaction heat is released and transferred to fluid and solid phase

Micro-scale: modelling catalytic reactions

Finite Volume Solver

Fluid phase:
- Mass
- Momentum
- Chemical species balance
- Energy

Solid phase:
- Energy



Specie source terms
Energy source terms

Washcoat Solver (Finite Area)

Diffusion model

Mass transfer between gas and washcoat

Reaction model

Conversion of reactants into products & reaction heat release

Heat transfer model

Heat transfer to gas and solid phase

Micro-scale: modelling catalytic reactions

Washcoat solvers:

Baruah-like solver:
- Specie conversion rate is given by the minimum between reaction rate and diffusion rate
- Steady-state / transient simulations
- For diffusion limited problems, eg: CO catalytic reactions

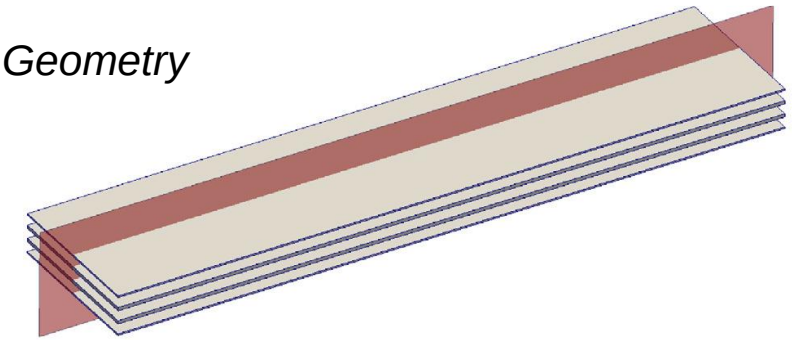
Single-step solver:
- Accumulation of mass and energy on the washcoat
- Transient simulations

ODE solver:
- Detailed solution of both diffusion and reactions
- Transient simulations

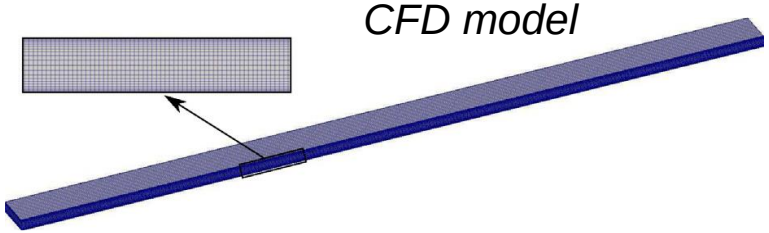
Micro-scale: reacting flow simulation

Validation on plate-type reactor: prediction of the light-off curve

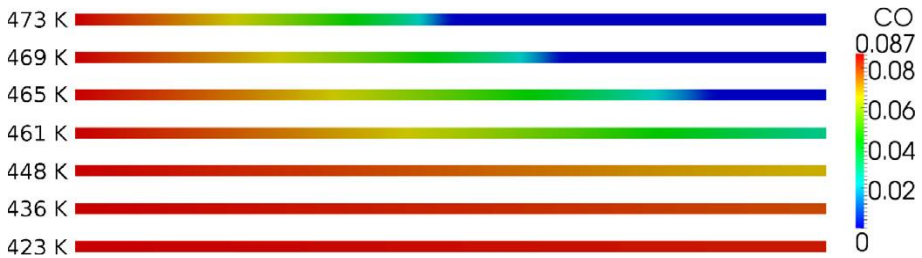
Geometry

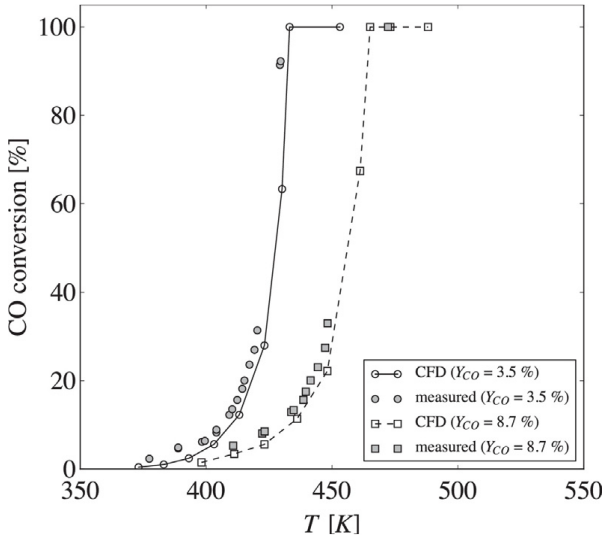


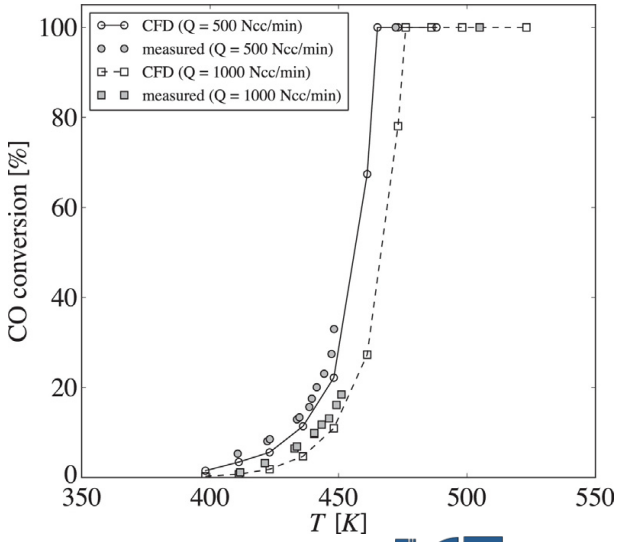
CFD model



CO evolution for different inlet T

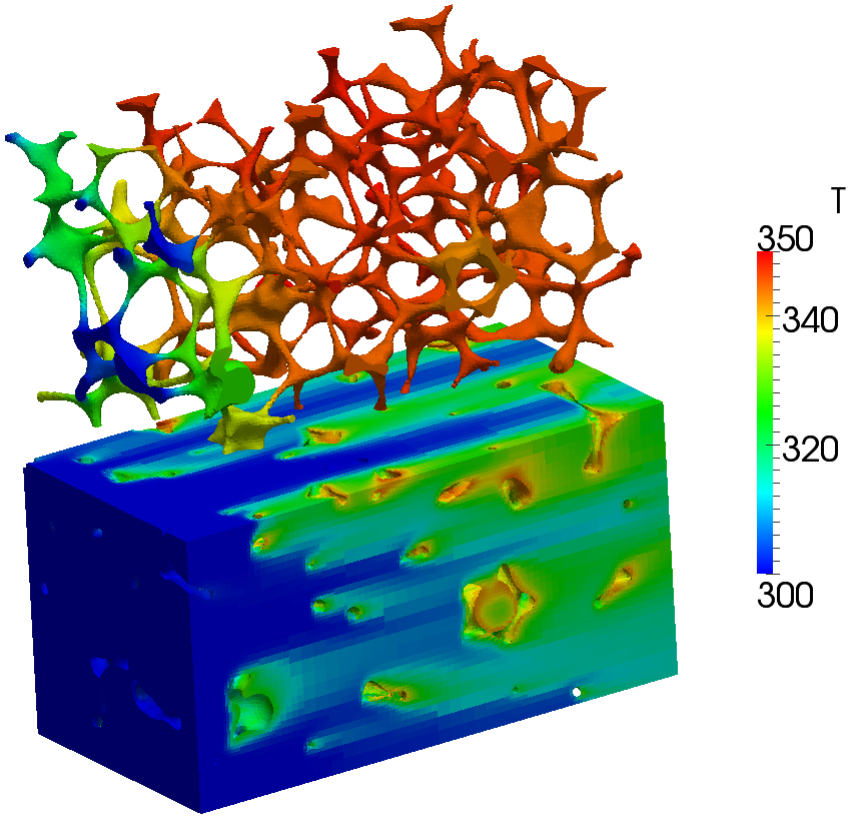






Micro-scale: reacting flow simulation

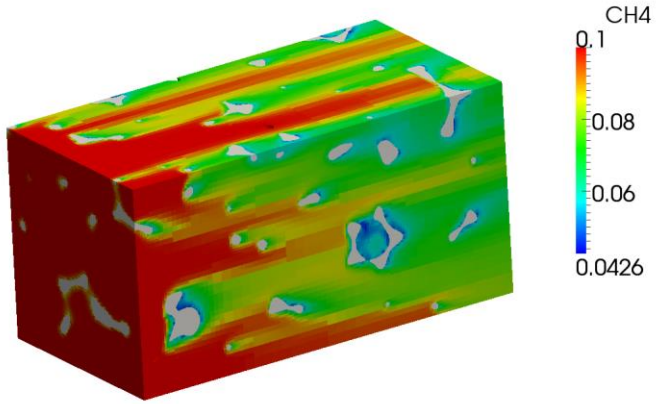
Al foam 95% porosity – 40 ppi / Micro-CT reconstruction

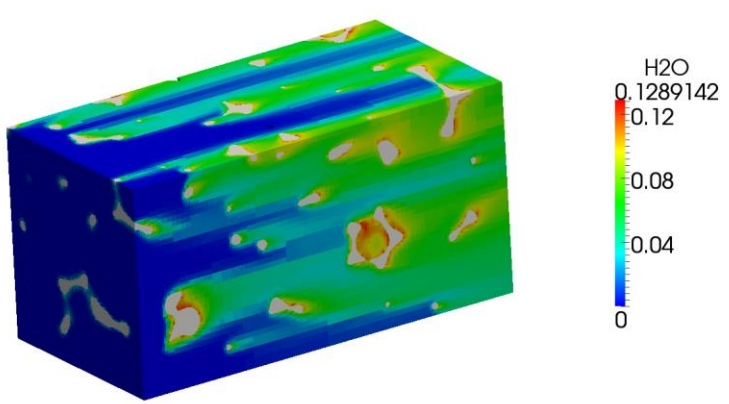


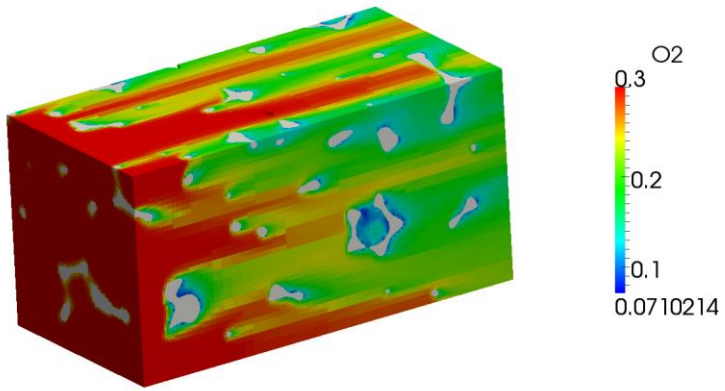
- Surface reaction on washcoat region
- Baruah-like solver
- Infinitely fast reaction model
- Conjugate heat transfer
- Fluid: inlet T=300K
- Solid: fixed T=300K on the inlet side, adiabatic elsewhere

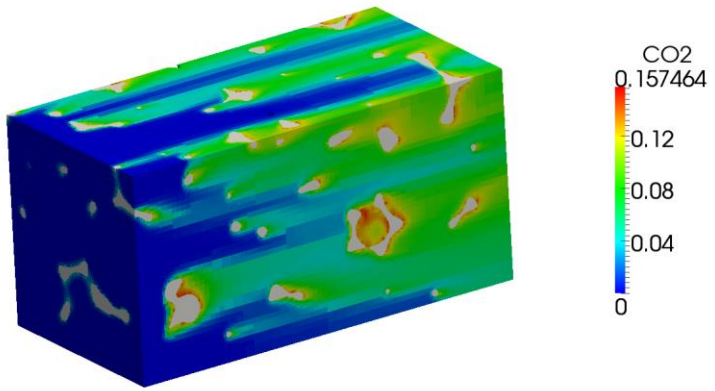
Micro-scale: reacting flow simulation

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





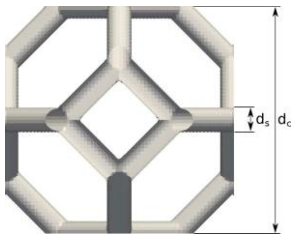


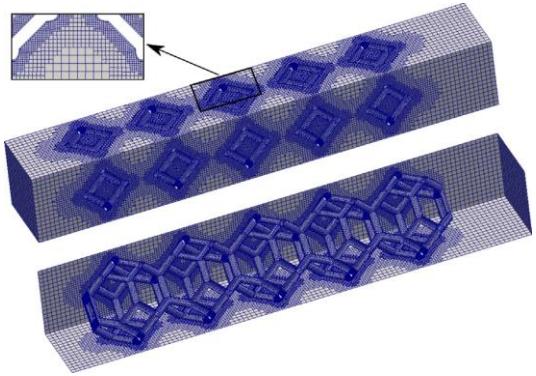


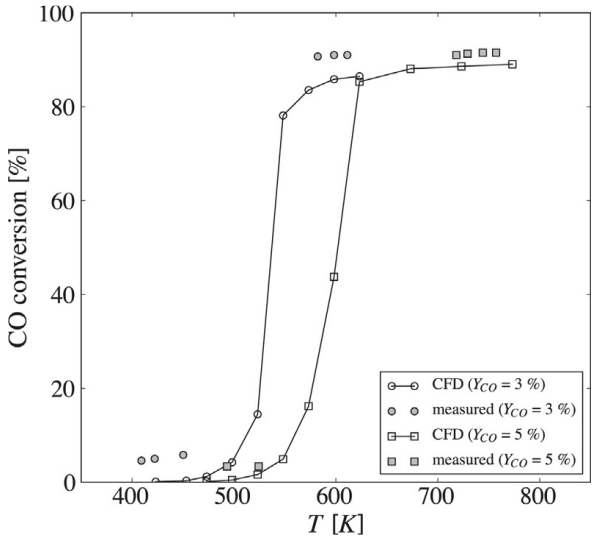
Micro-scale: reacting flow simulation

Validation on foam-type reactor: prediction of the light-off curve

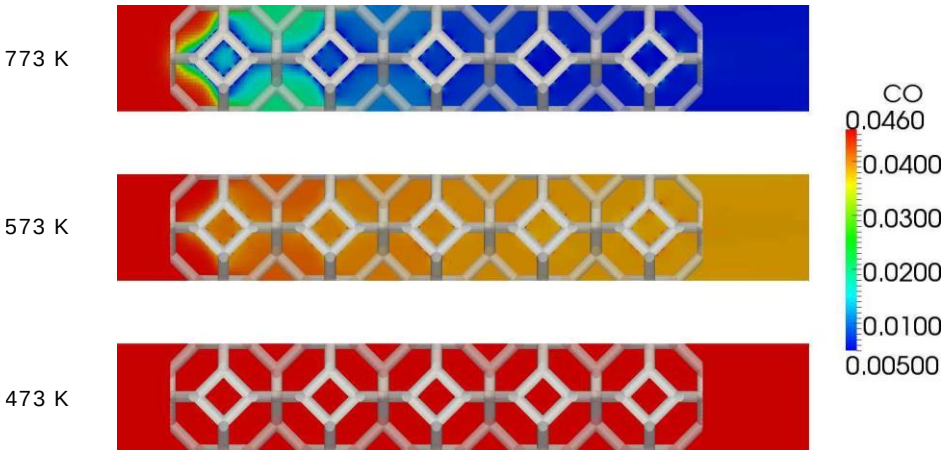
Kelvin cell

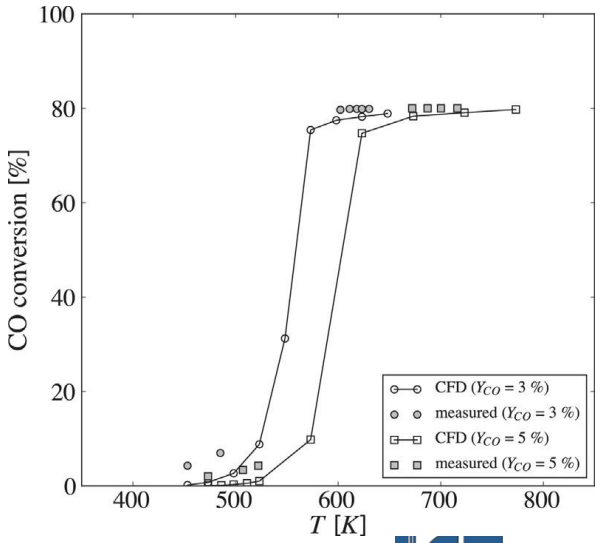






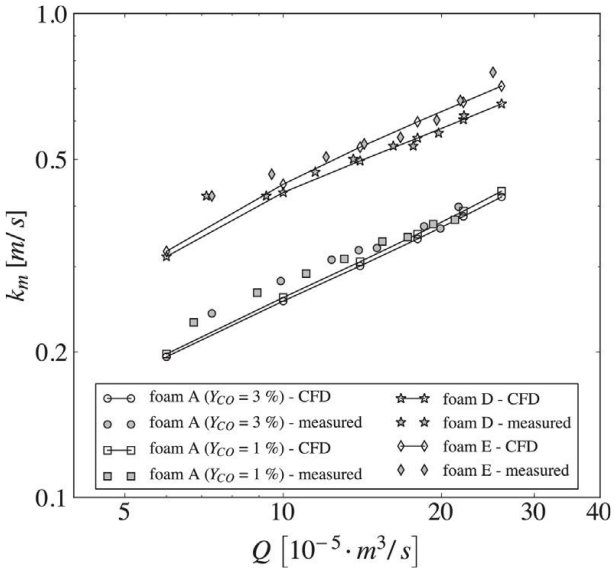
CO evolution for different inlet T





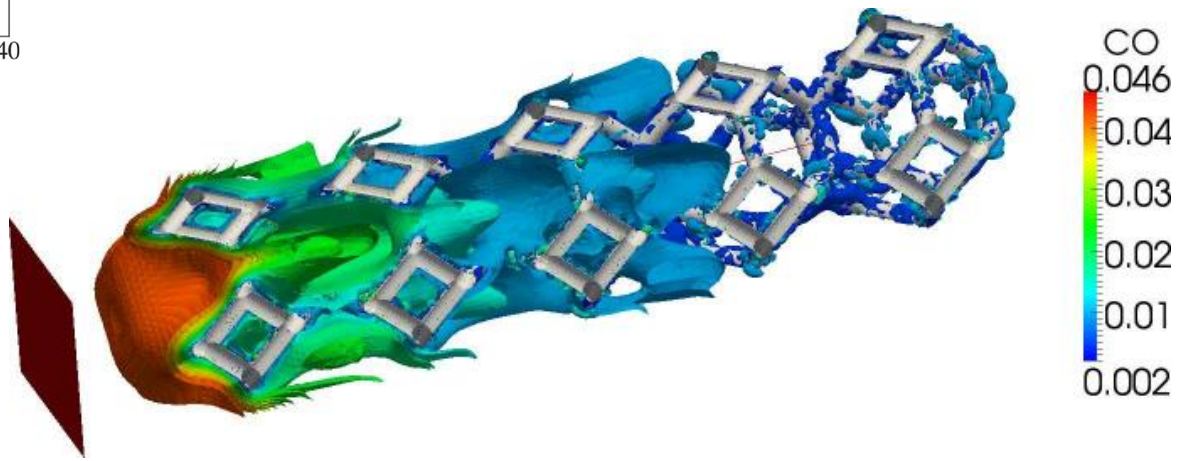
Micro-scale: reacting flow simulation

Validation on foam-type reactor: prediction of the mass transfer coefficient



Considering diffusion limited regime (i.e. high temperature) it is possible to evaluate the mass transfer coefficient:

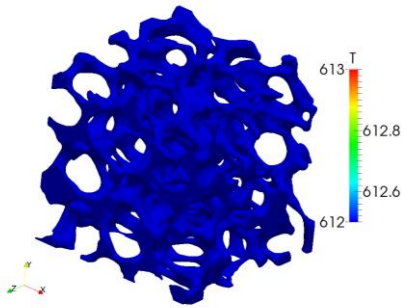
$$k_m = -\frac{\ln(1-\eta)}{S_V V/Q}$$



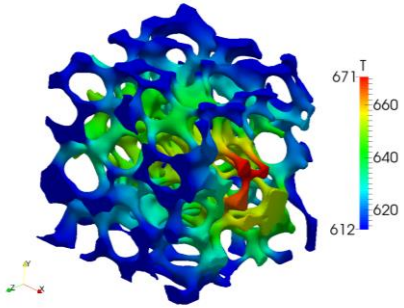
Micro-scale: reacting flow simulation

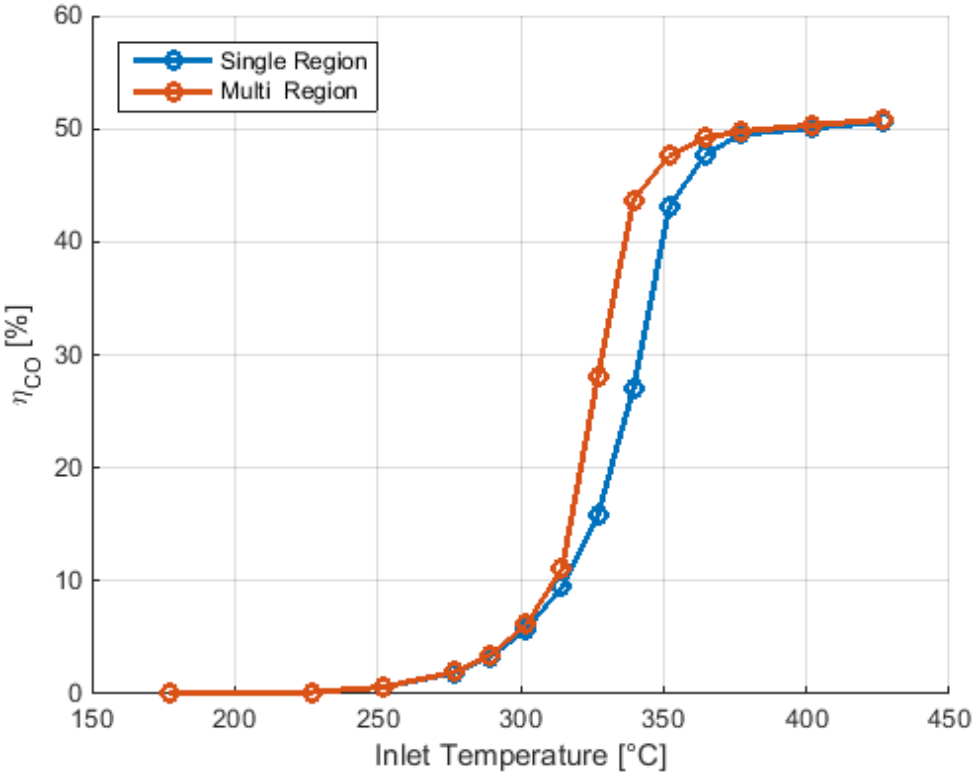
Effect of the temperature distribution on the light-off curve

Single-region simulation:
uniform temperature in the solid (i.e. infinite conductivity)



Multi-region simulation:
temperature imposed at the boundary of the solid



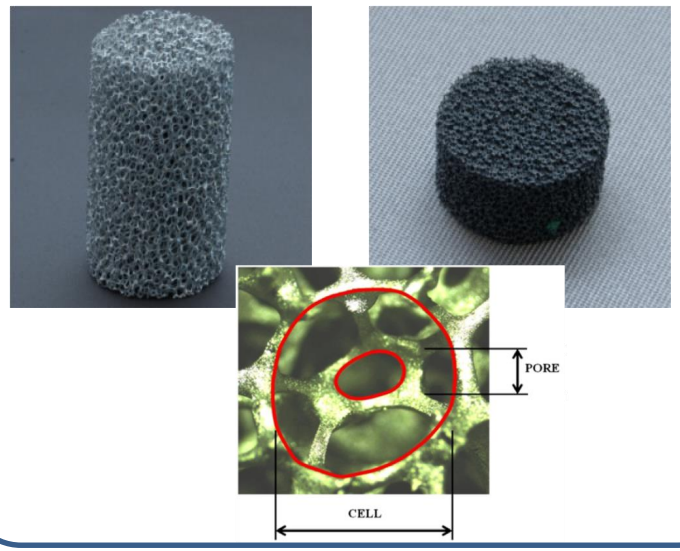


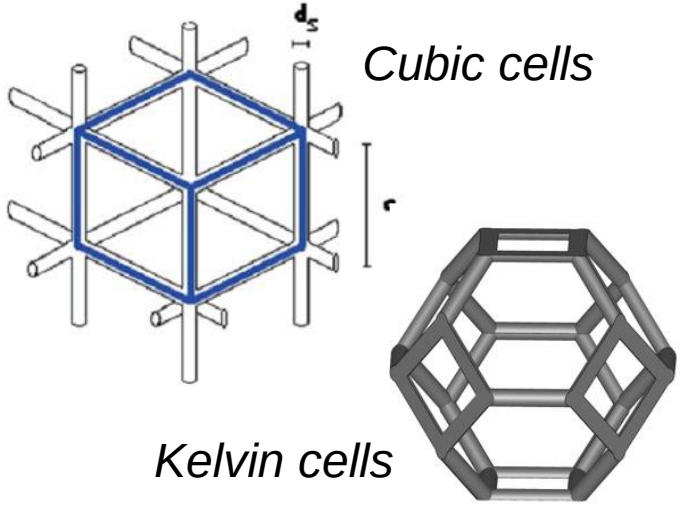
Methodology:
on the adoption of Kelvin-cells to model open-cell foam

Geometrical characterization: idealized structures

The micro-structure of real open-cell foam geometries needs sophisticated technology to be reconstructed.

Artificial idealized structures may be used as templates

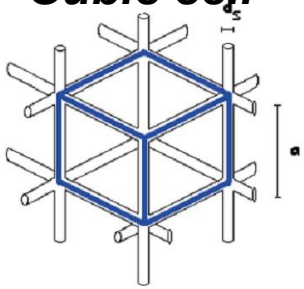


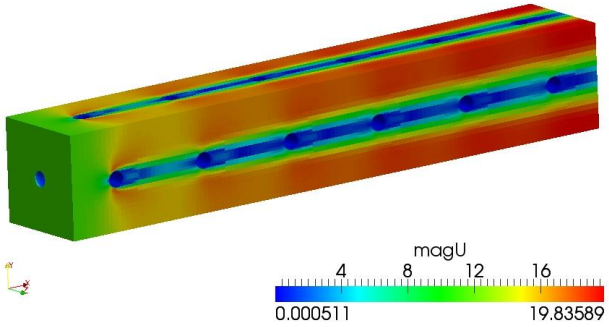


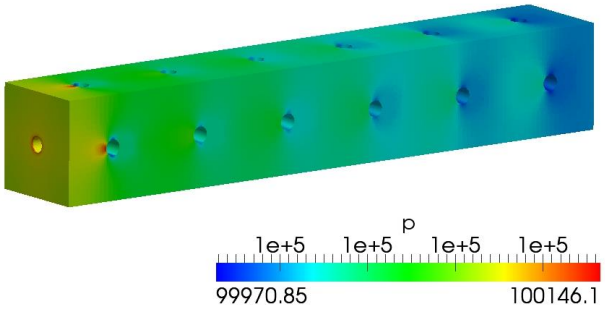
How much do these structure reproduce well the properties of open-cell foams?

Idealized structures: analysis of the flow field

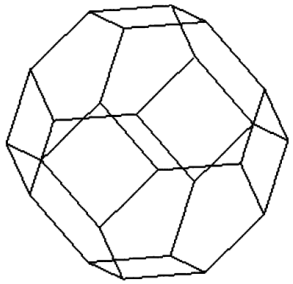
Cubic cell

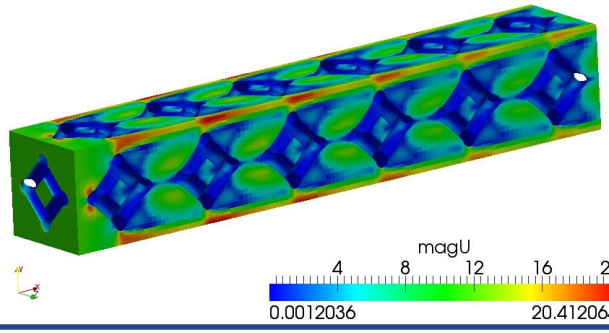


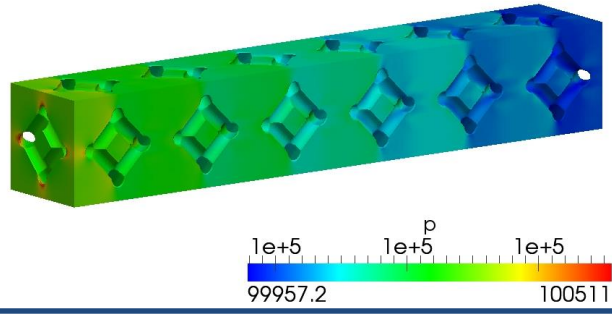




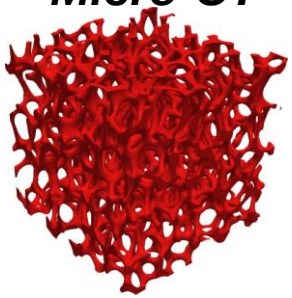
Kelvin cell

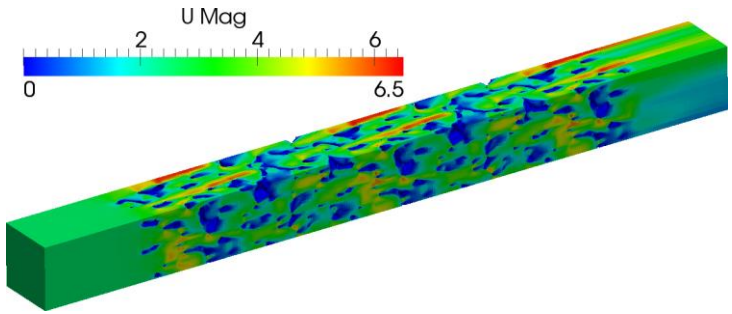


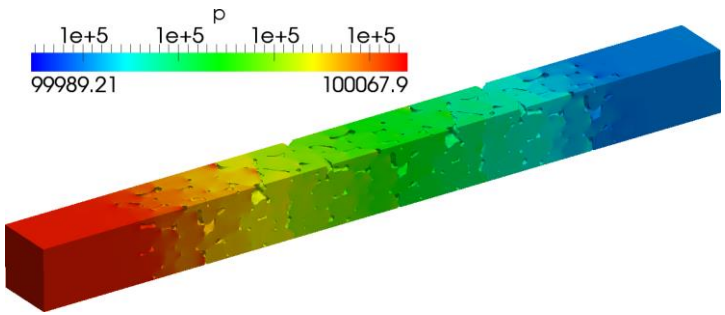




Micro-CT

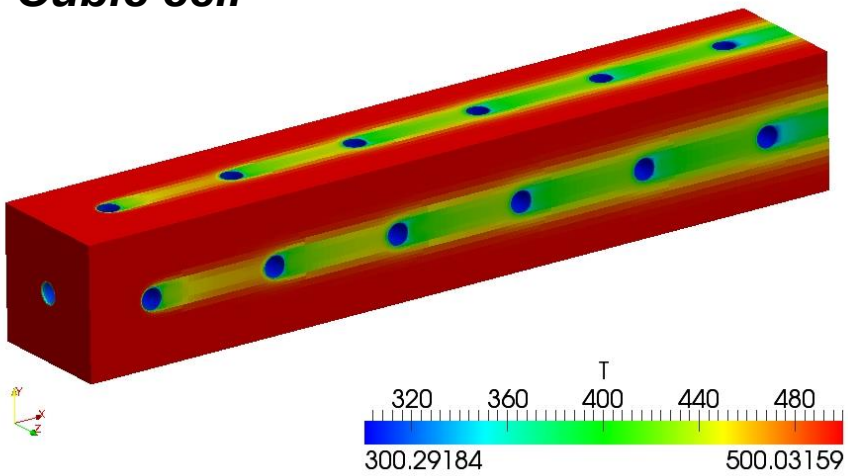


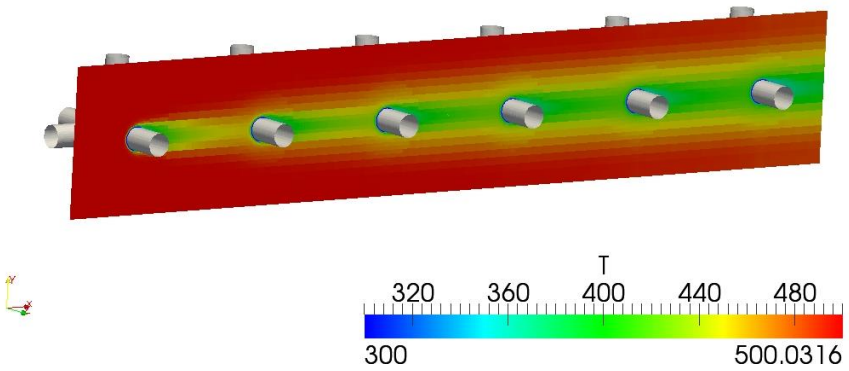




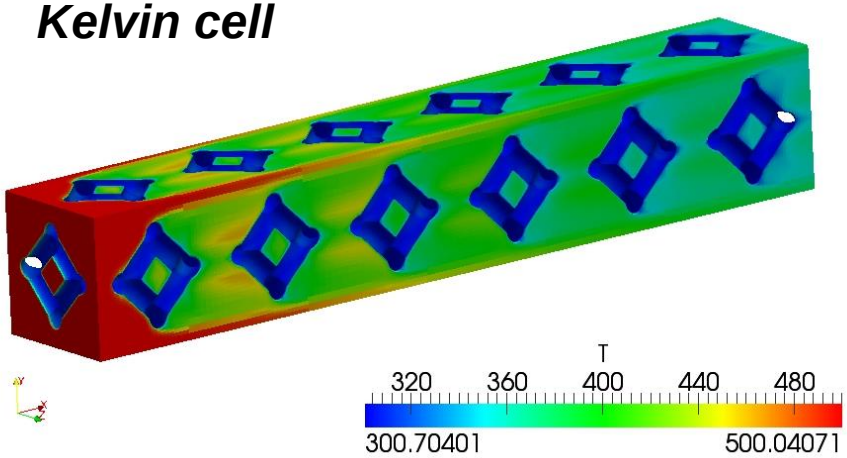
Idealized structures: analysis of the temperature field

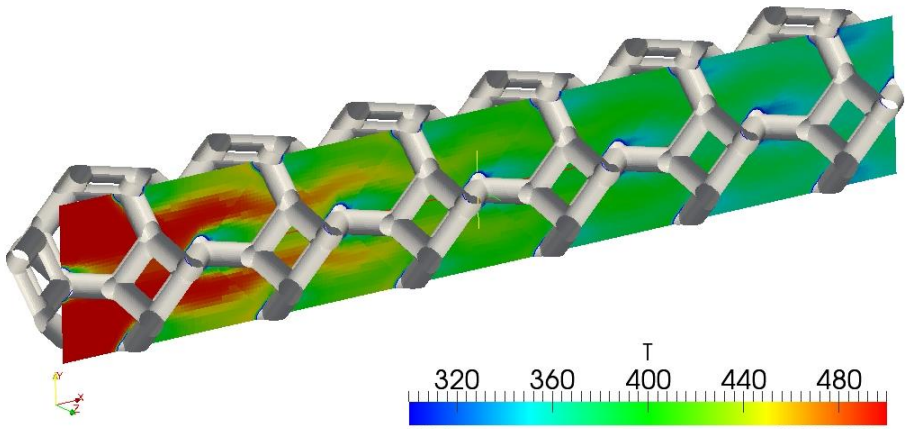
Cubic cell





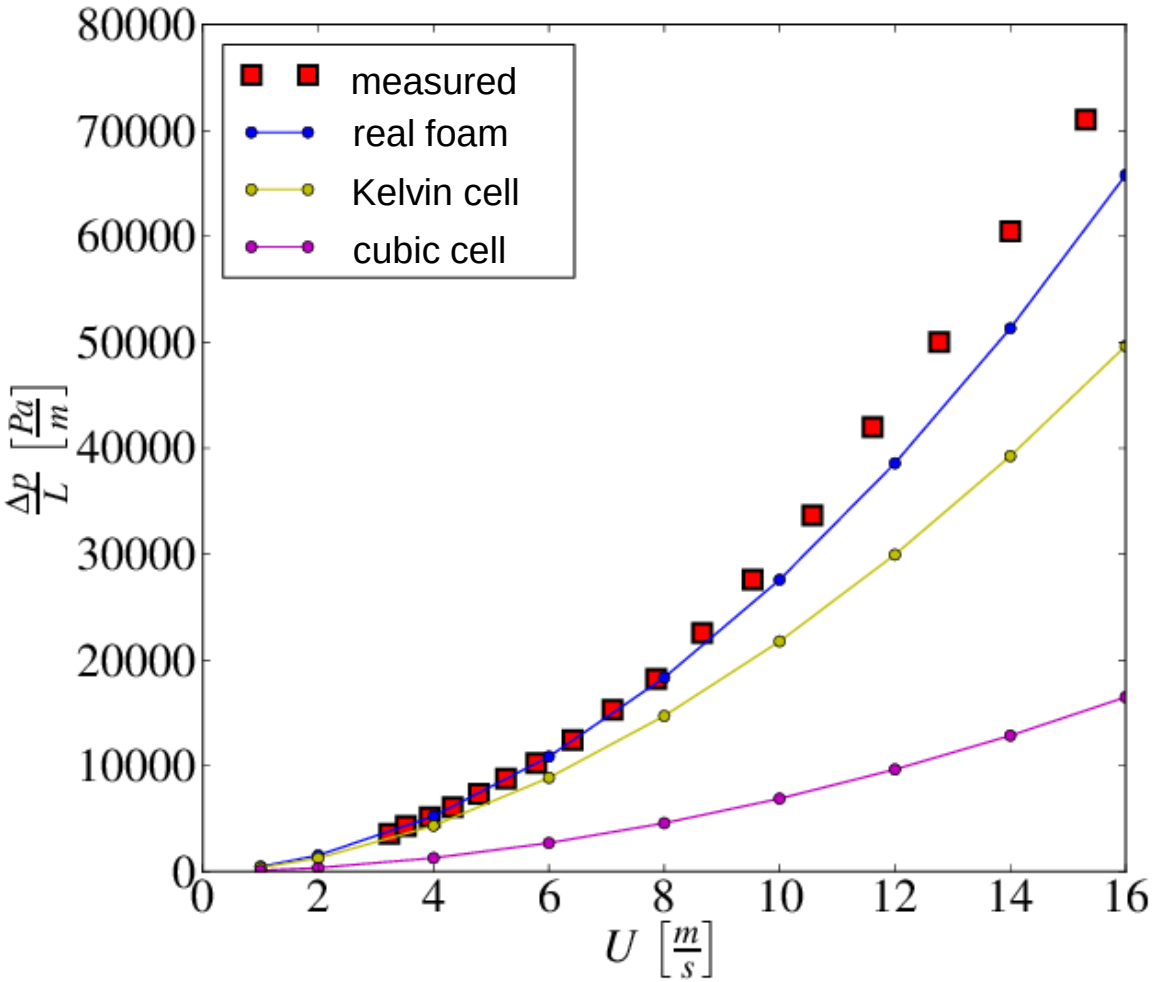
Kelvin cell

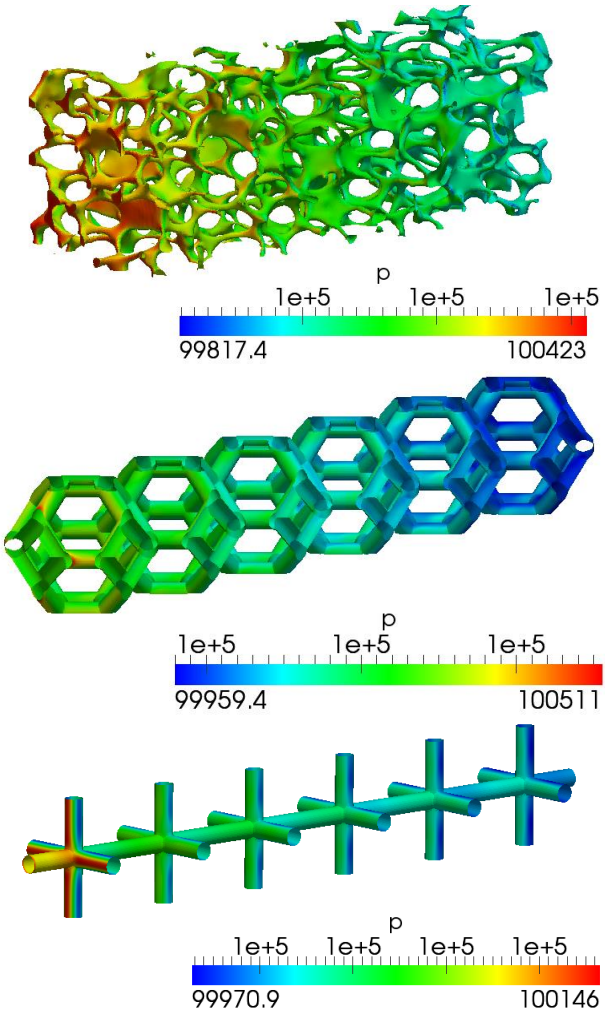




Idealized structures: comparison of pressure drop

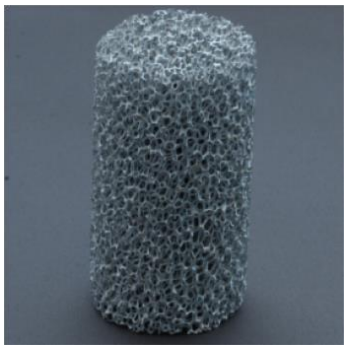
- Modeling criterium: **same porosity and same pore size**



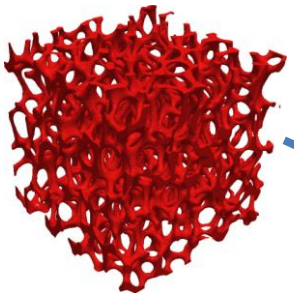


Idealized structures: correction of the KC model

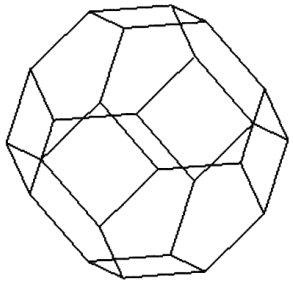
Same porosity and same pore size: underestimation of specific surface



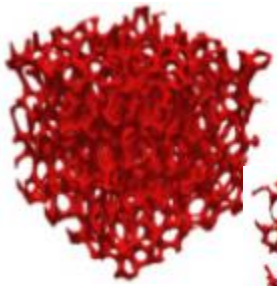
X-ray images



Porosity, Cell size

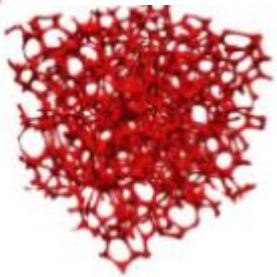


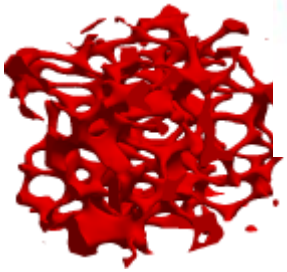
$$\frac{S_{V,real}}{S_{V,KC}} \approx 1.37$$



Si-C

Al





Cu

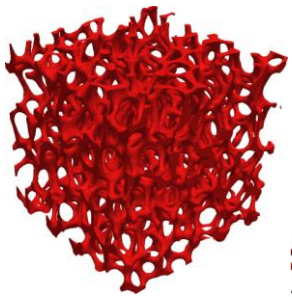
Test on 3 samples:

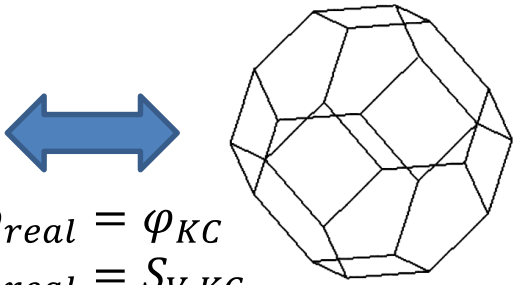
Sample	$L_c[m]$	$\epsilon[\%]$	$d_s[m]$	$S_V\,[m^2/m^3]$	$S_V/S_{V\,calc}$
Al foam	3.8×10^{-3}	96.0	0.34×10^{-3}	435.1	≈ 1.37
Si-C foam	1.0×10^{-3}	87.0	0.15×10^{-3}	2962	≈ 1.37
Campione F	4.6×10^{-3}	91.1	0.57×10^{-3}	555.2	≈ 1.37

Correction procedure to target the real SV:

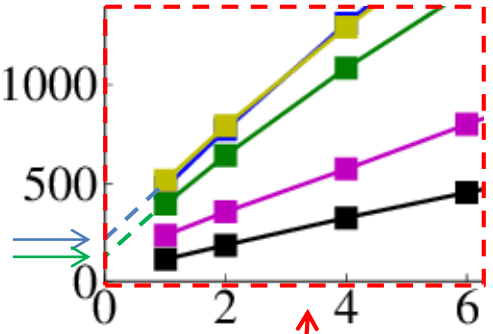
$$\varphi, d_c \longrightarrow KC \longrightarrow S_{V,KC} \longrightarrow \varphi, {d_c}^* \longrightarrow KC_{corr}$$

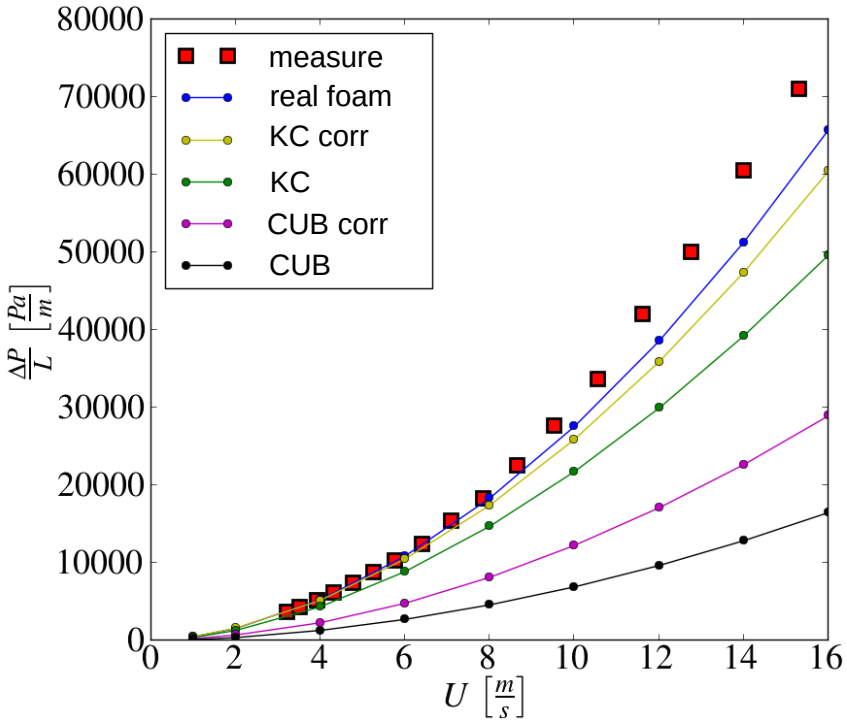
Correction of the KC model: pressure drop

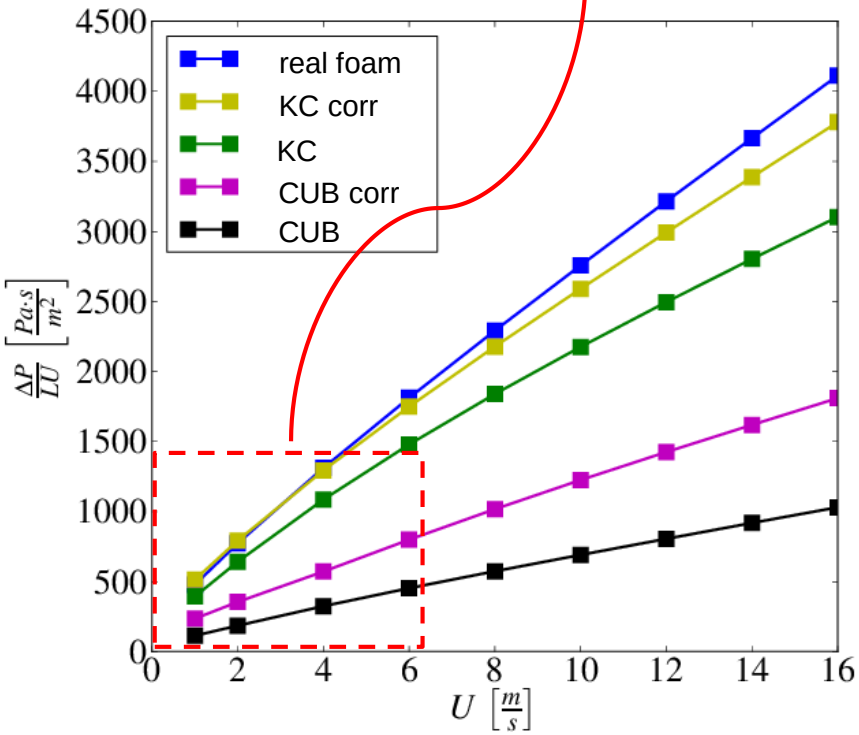




$$\varphi_{real} = \varphi_{KC}$$
$$S_{V,real} = S_{V,KC}$$

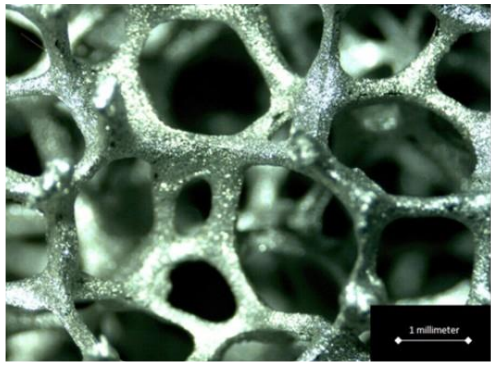




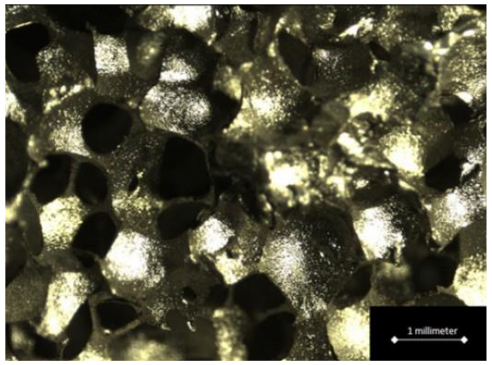


Comparison of pressure drop on different foams

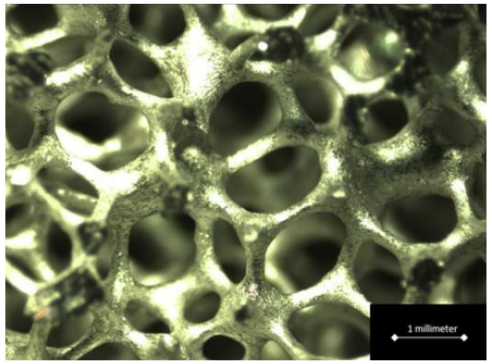
B



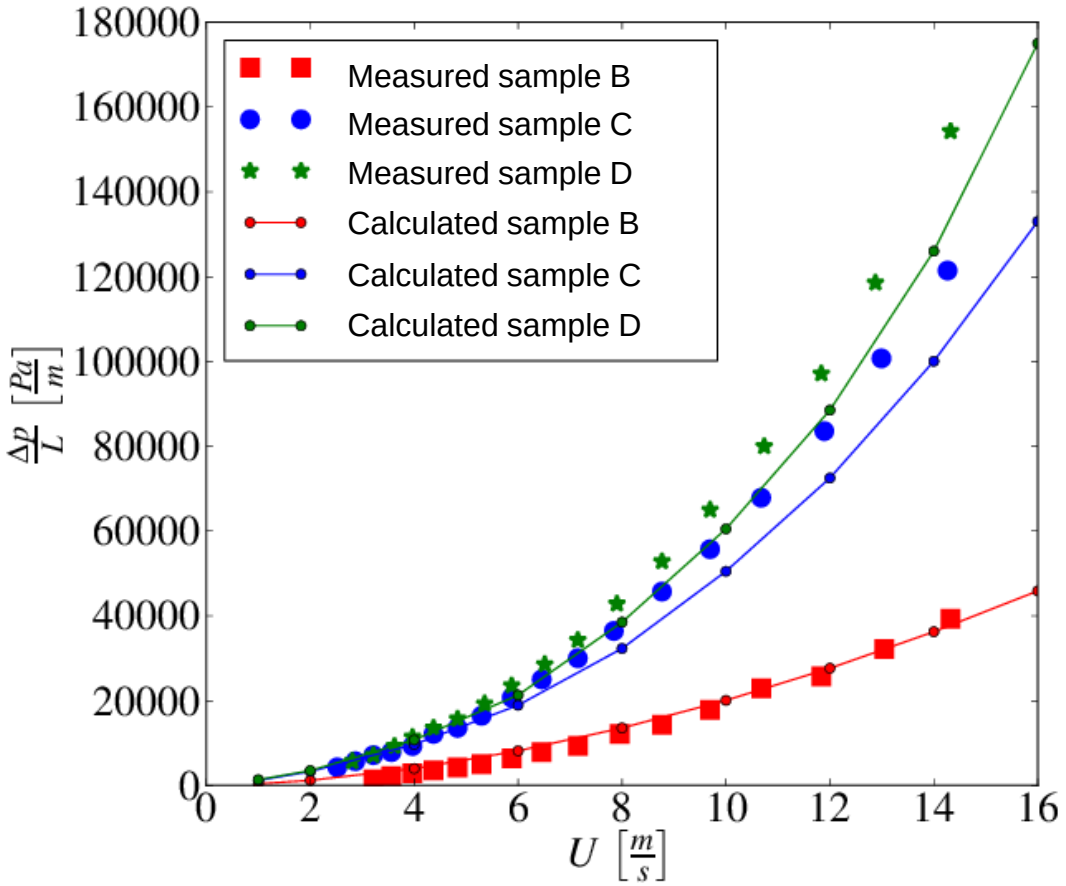
C



D

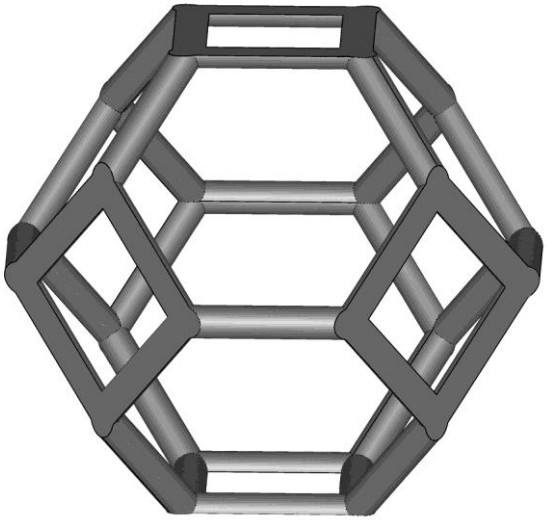


Reconstruction of real sample by Kelvin cell type idealized foam

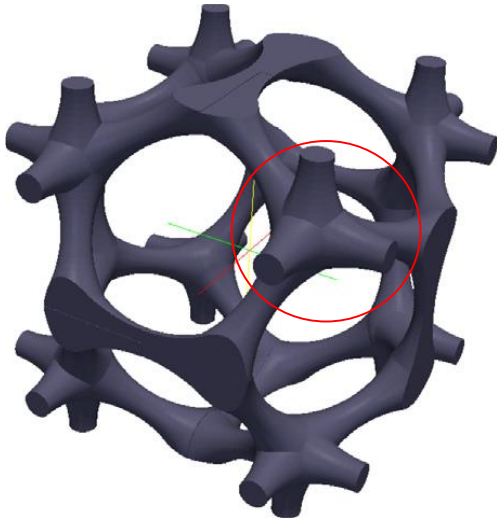


KC model: further enhancement

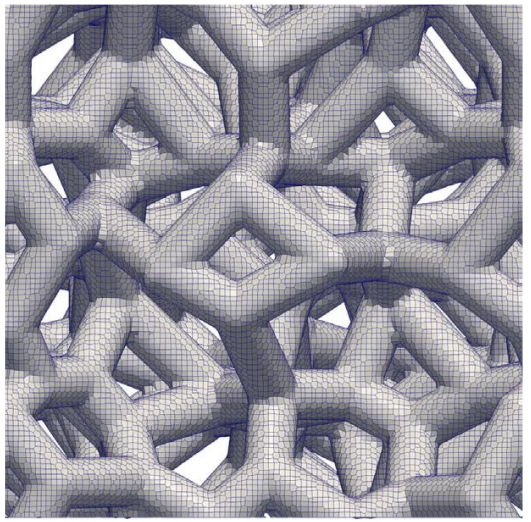
Introduction of an additional degree of freedom



Material clustering at cell vertexes

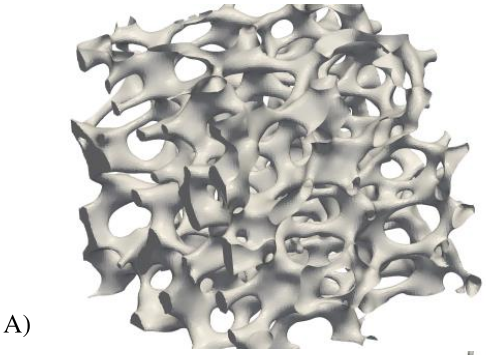


Randomization (edge length)

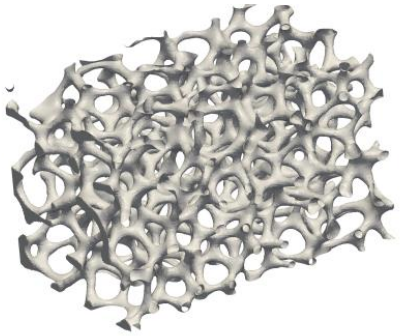


KC model enhancement: randomization

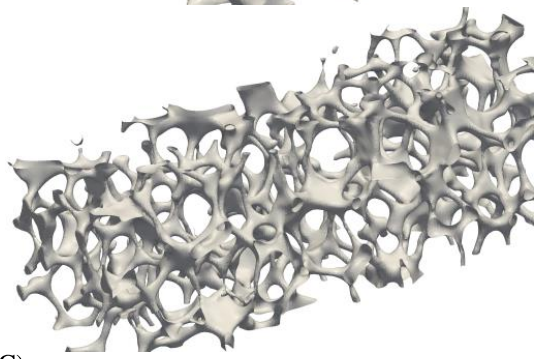
case	material	ε [-]	PPI [-]	S_v $[1/m]$	$2\varepsilon/S_v$ [mm]	$25.4/PPI$ [mm]	d_p [mm]	σ_{d_p} [mm]	d_w [mm]	σ_{d_w} [mm]
A	SiC	0.827	10	590	2.8	2.54	3.8	0.56	1.9	0.54
B	SiC	0.877	80	4120	0.42	0.32	0.51	0.047	0.27	0.058
C	Cu	0.897	20	820	2.2	1.3	2.2	0.29	1.3	0.23
D	Al	0.955	40	690	2.7	0.64	2.0	0.33	1.1	0.27



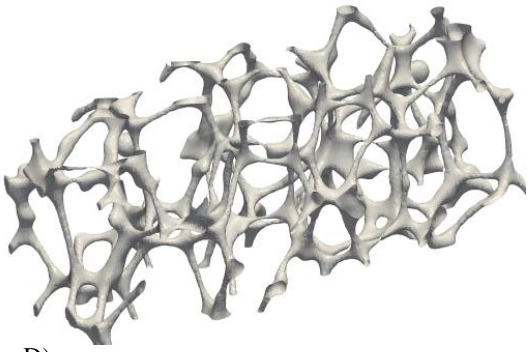
A)



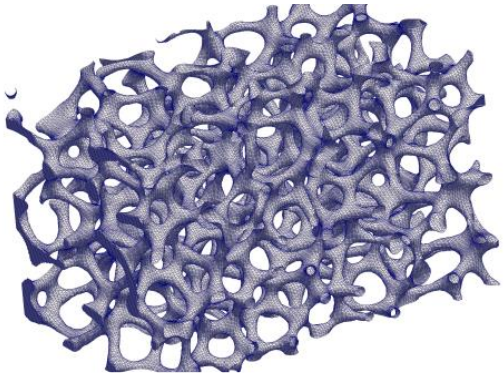
B)

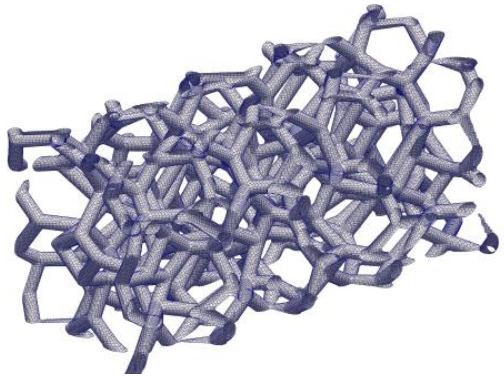


C)



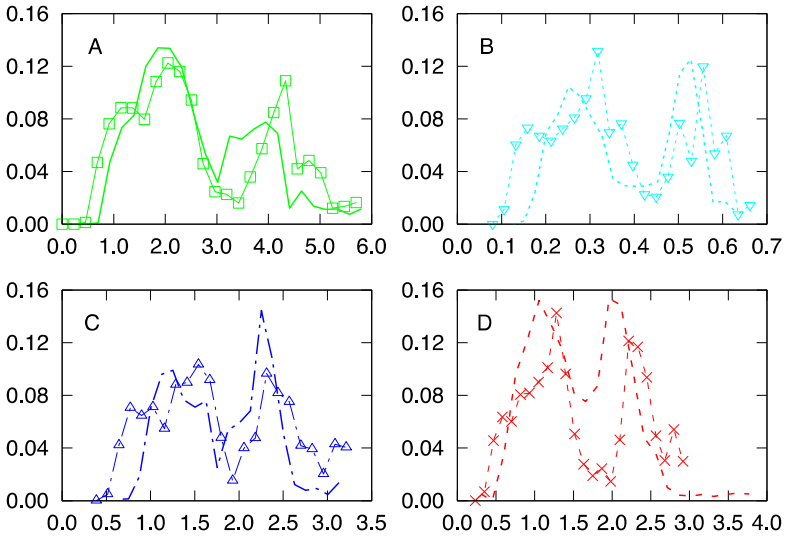
D)

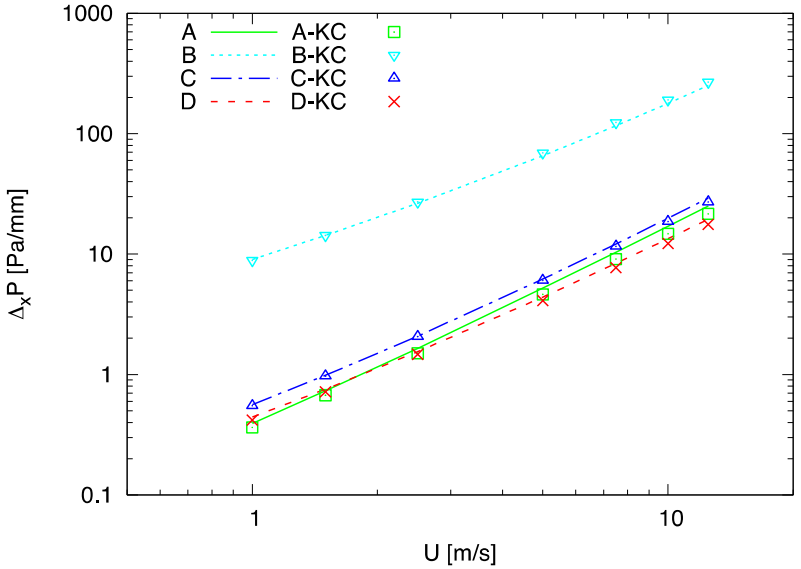


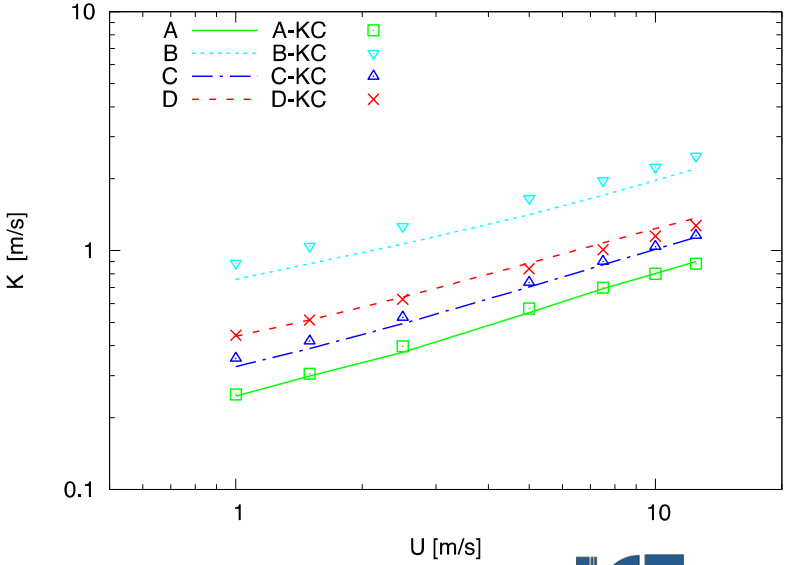


Characterization of the pore size, Δp and K

Diameter distributions for the four sample foams and the corresponding KC structures







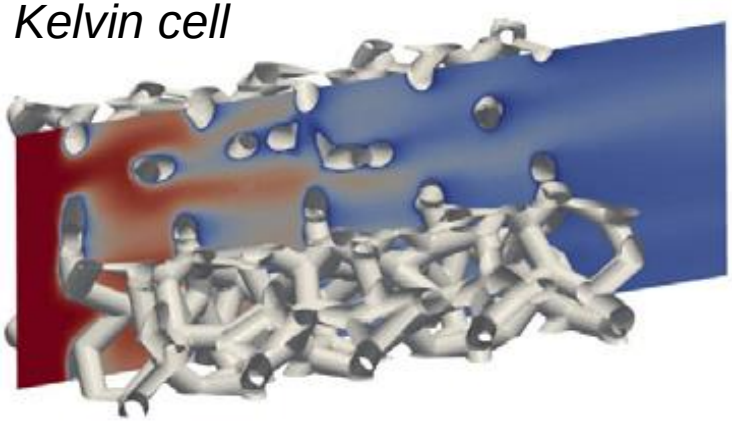
- Kelvin cells built by matching the porosity and the surface area of the foams resulted in having the pore diameter 15% bigger
- For high porosity foams, the KC structures are able to match the foam mass and momentum performance
- Pressure drops are predicted with a maximum error of 15%

Open-cells foams as catalytic substrates: Kelvin cells vs Honeycombs

Kelvin Cell vs honeycomb

In order to assess the **performances of open-cell foams for catalytic applications**, their properties should be compared with the state-of-the-art solution: **honeycomb.**

Kelvin cell

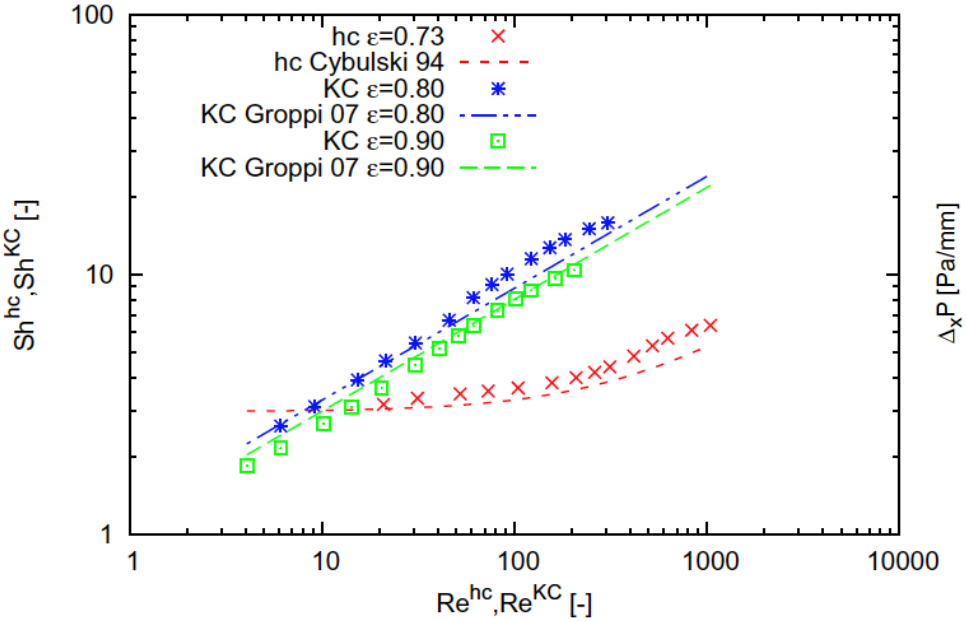


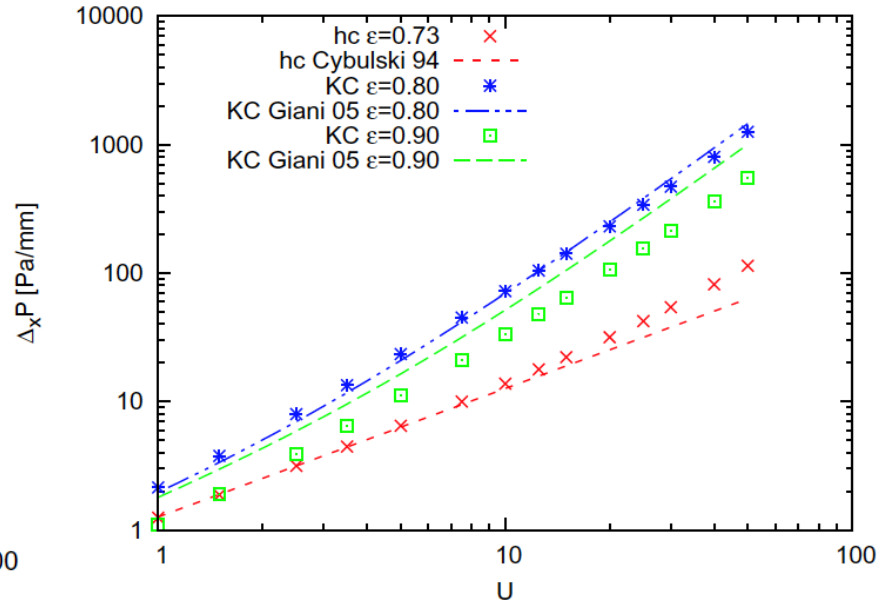
Main parameters:

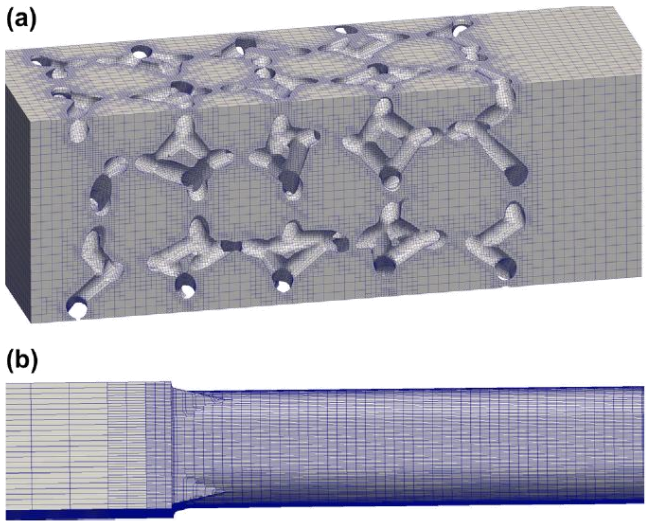
- *Pressure drop*
- *Heat-/mass-transfer*
- *Specific surface*
- *Volume*

Honeycomb

Kelvin Cell vs honeycomb

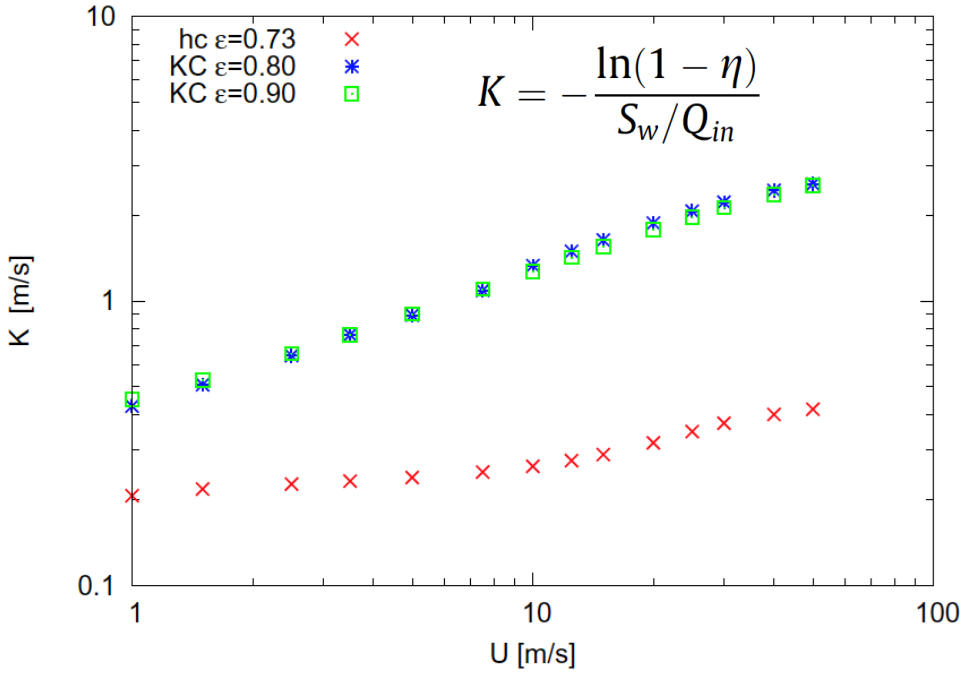






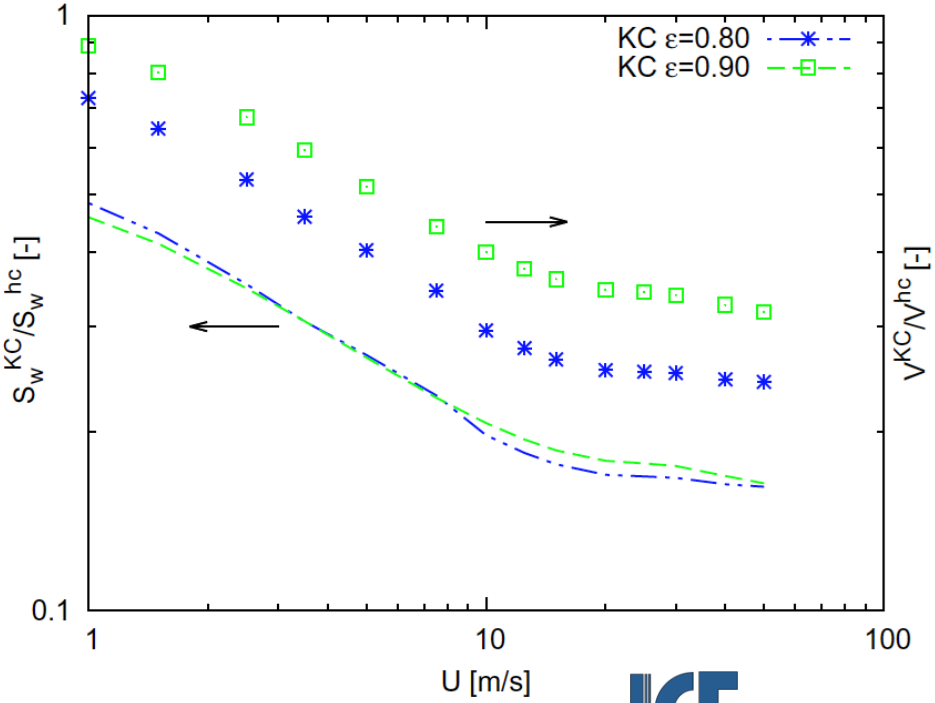
- The results of simulations compare fairly well with the correlations available in the literature
- There is still not agreement among authors in literature

Mass transfer: Kelvin Cell vs honeycomb

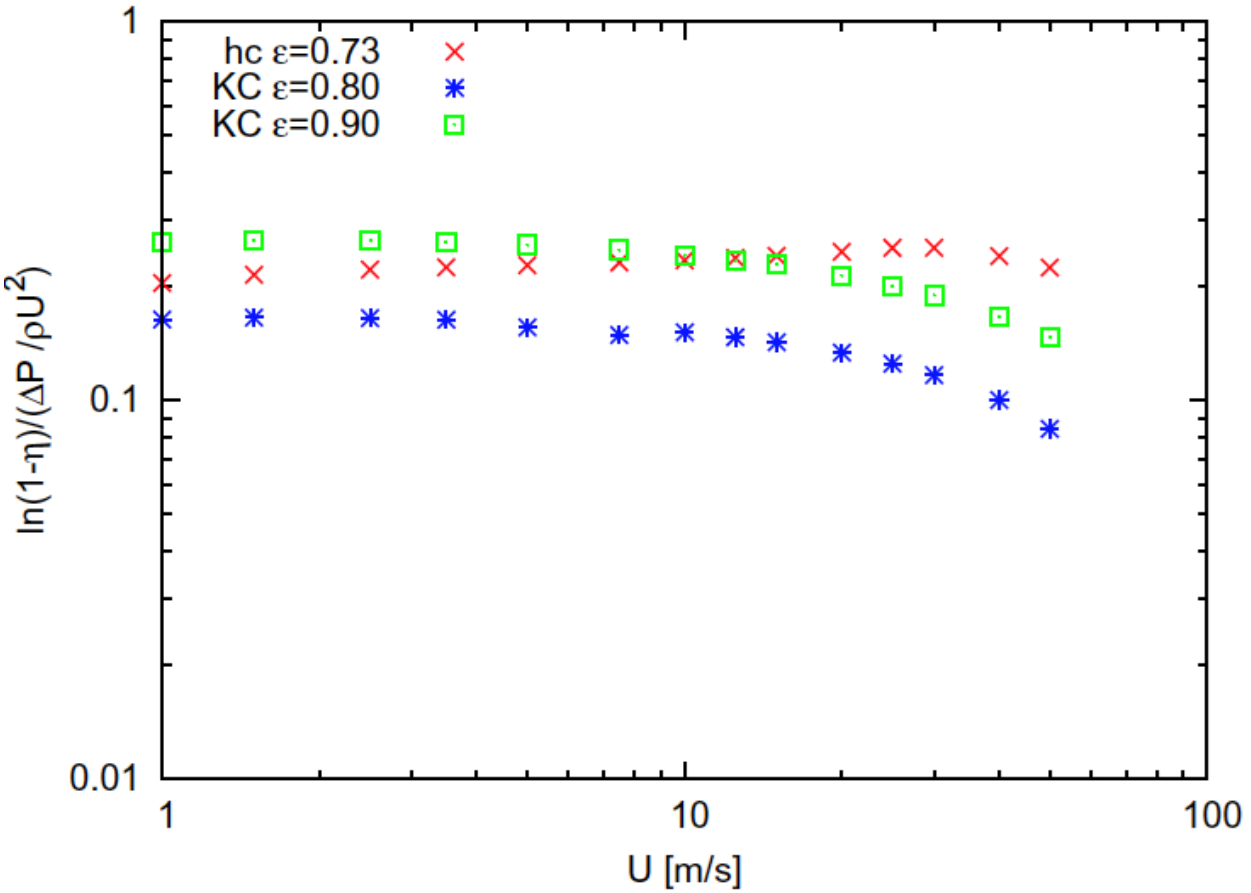


- At high flow velocity, KC structures need a smaller fraction of the honeycomb surface and volume
- It needs less surface to obtain the same conversion rate.

- KC structures have a higher mass transfer coefficient K
- It needs less surface to obtain the same conversion rate.



Performance index: Kelvin Cell vs honeycomb



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

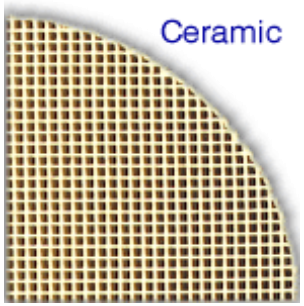
- The open cell foam exhibit a better performance if:
  - porosity is high
  - velocity is low (Darcean velocity)

Open-cells foams as catalytic substrates: design and optimization of an after-treatment system equipped with open-cell foams

Open-cell foams vs honeycomb: design optimization

In order to assess the **performances of open-cell foams for catalytic applications**, their properties should be compared with the state-of-the-art solution: **honeycomb.**

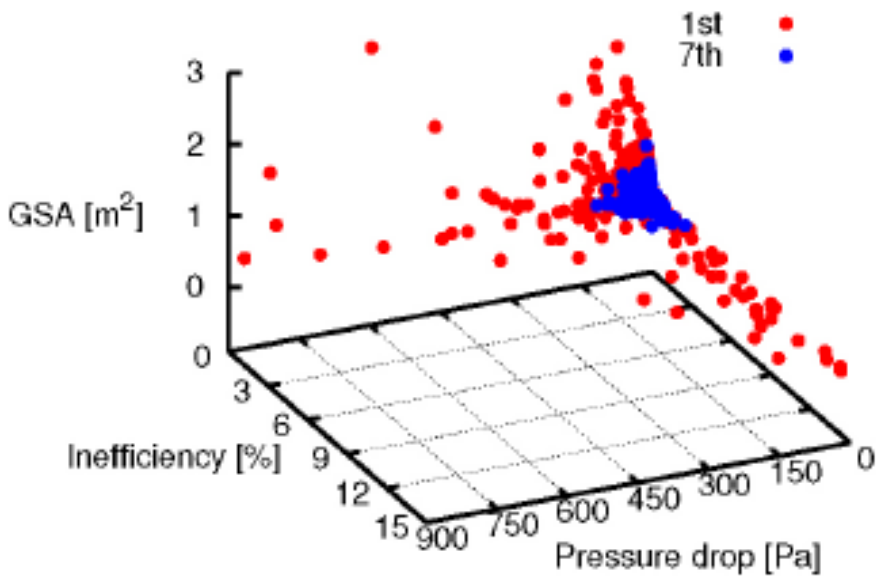
Input for foam-type substrate	
ϵ [%]	$84 \div 96$
d_p (ppi) [mm]	$0.635\,(40) \div 6.35\,(4)$
L [mm]	$30 \div 200$
D [mm]	$50 \div 150$



Input for honeycomb-type substrate	
ϵ [%]	$70 \div 90$
d_c (cpsi) [mm]	$0.733\,(1200) \div 1.27\,(400)$
L [mm]	$30 \div 200$
D [mm]	$50 \div 150$

Open-cell foams vs honeycomb: design optimization

The optimization was performed using Genetic Algorithms



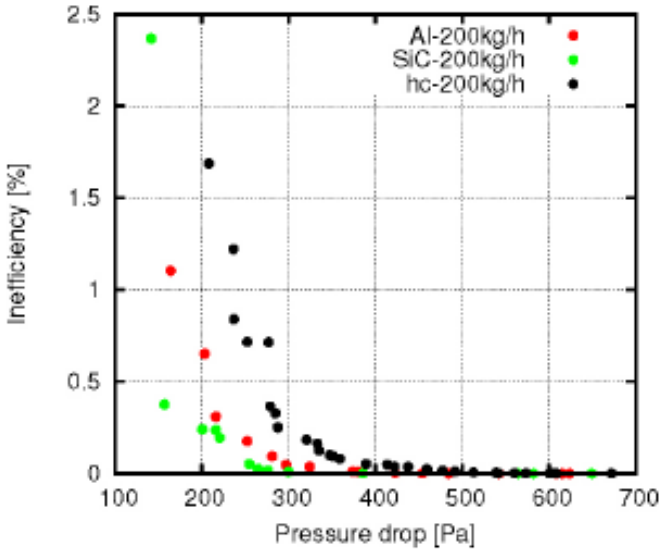
Design variables:

- Lenght of the catalyst
- Diameter of the catalyst
- Porosity
- Pore size

The objective of the optimization is the minimization of:

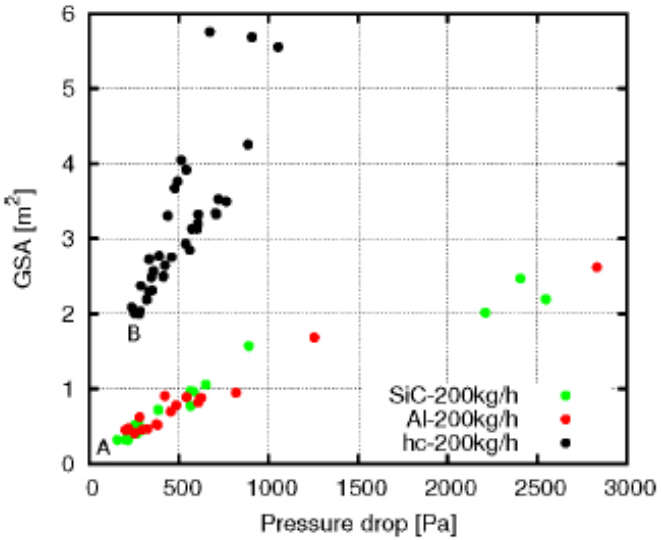
- Pressure drop
- Conversion inefficiency
- Catalytic surface

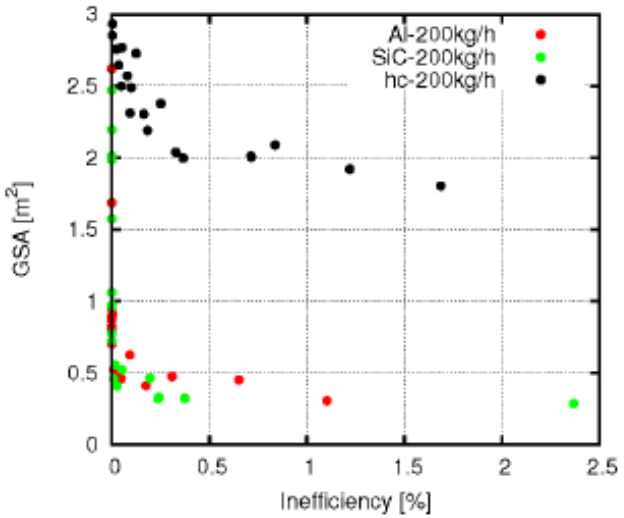
Open-cell foams vs honeycomb: design optimization



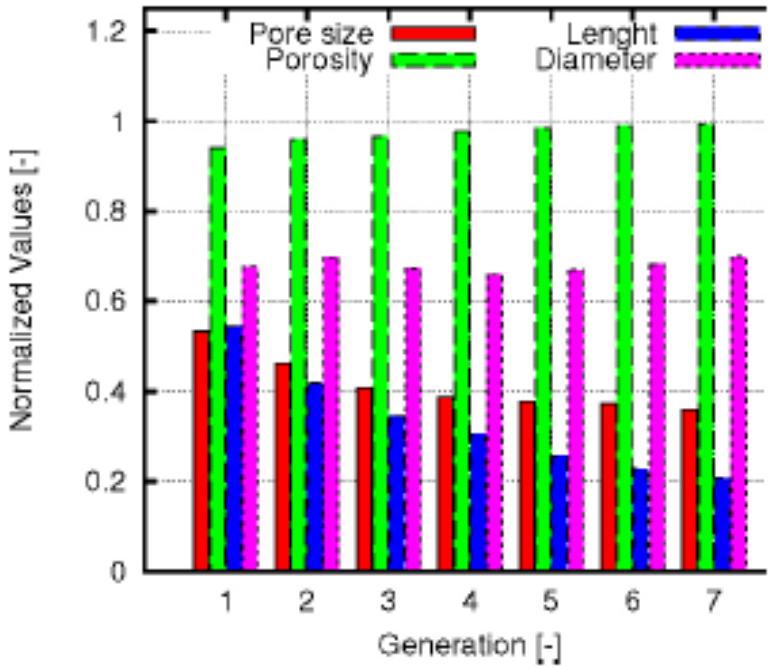
Open-cell foams vs homeycomb:

- Lower inefficiency for the same pressure drop
- Lower surface for the same inefficiency





Open-cell foams vs honeycomb: design optimization

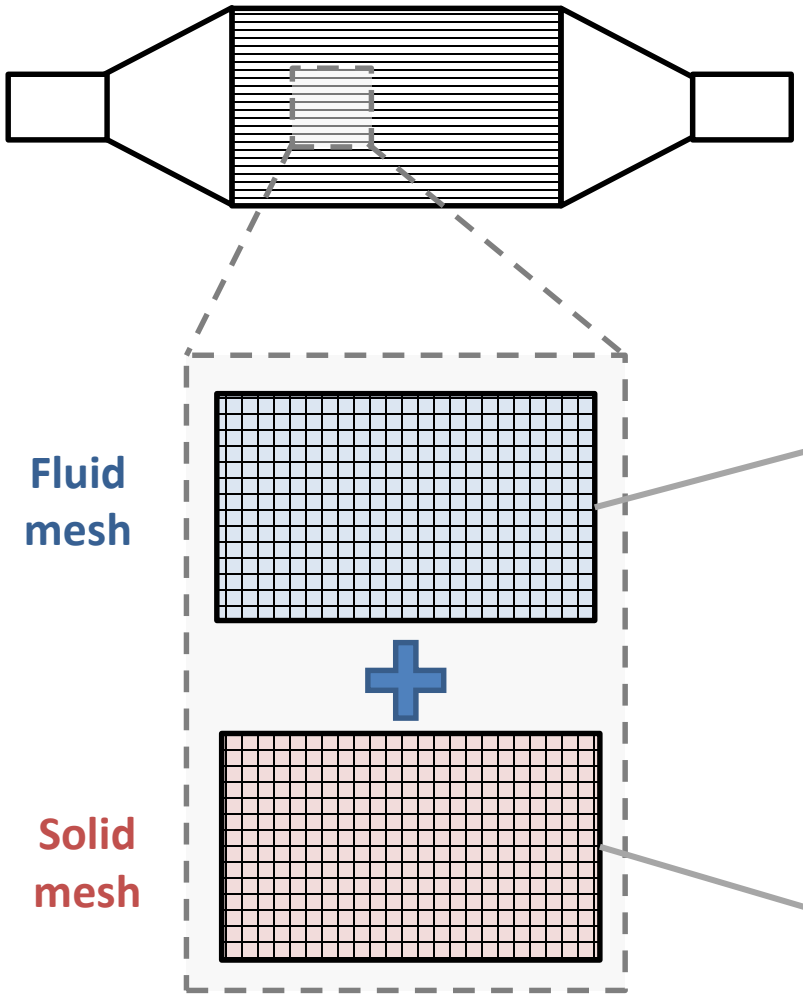


Guidelines for the optimization:

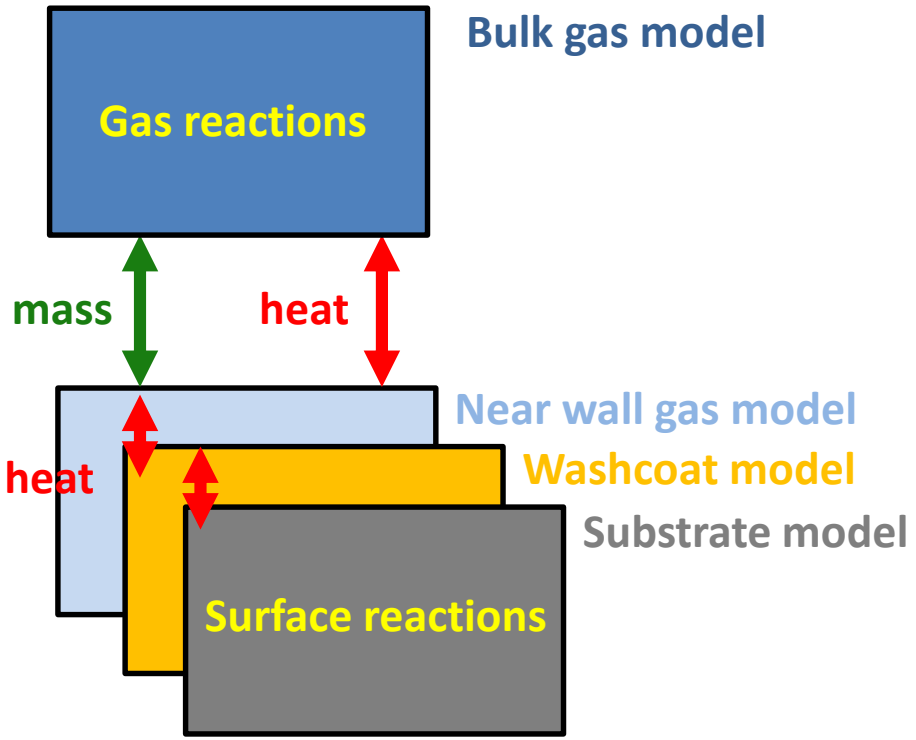
- Increase the porosity
- Increase the diameter
- Descrease the lenght
- Choose the pore size as a compromise between pressure drop and amount of catalytic surface

Open-cells foams as catalytic substrates: full-scale simulation of ATS equipped with open-cell foam substrates

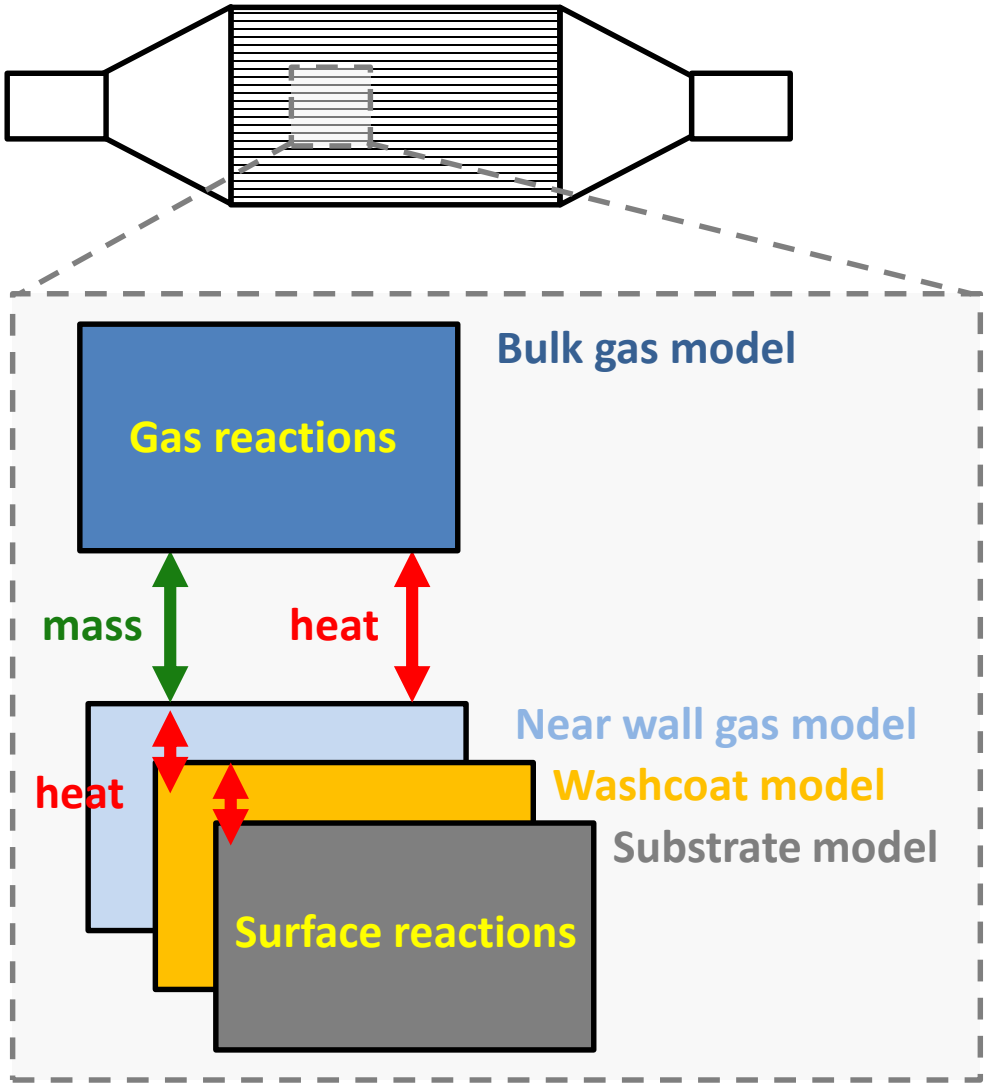
CFD macro-scale model for ATS simulations



- 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:

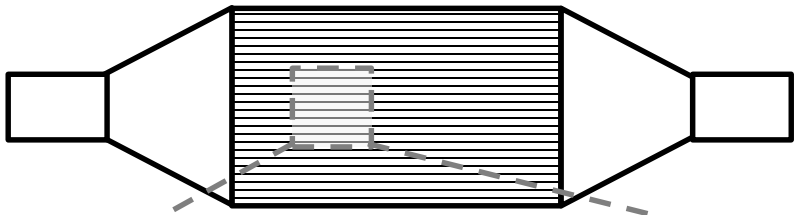
- *multi-region framework*
- *coupling between zones on different fluid or solid meshes*

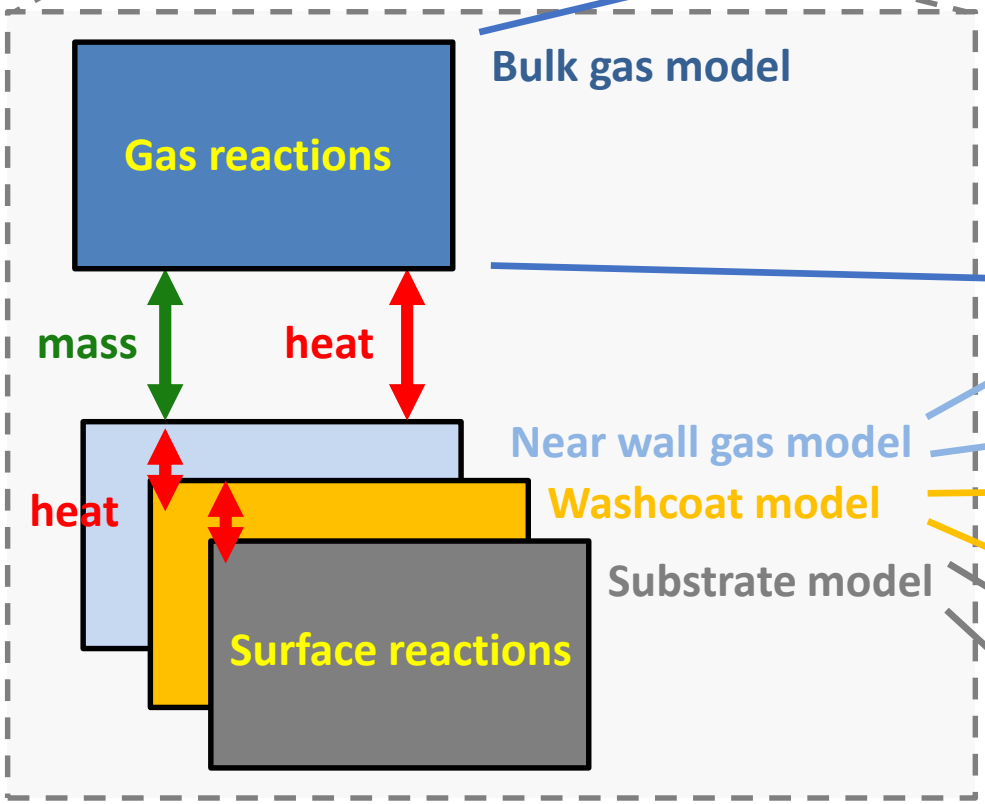
Coupling between fluid and solid regions requires specific models:

- *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.

Submodel for ATS simulations





Bulk gas model

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

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

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

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

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

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

Submodel for ATS simulations

Geometry model: *Description of substrate definition for **unstructured** (e.g. foam type) or **structured** (e.g. honeycomb, metallic)*

Permeability model: *Description of the fluid-dynamic resistance on the basis of **correlations** or data derived from **upscaling** results of micro-scale simulations.*

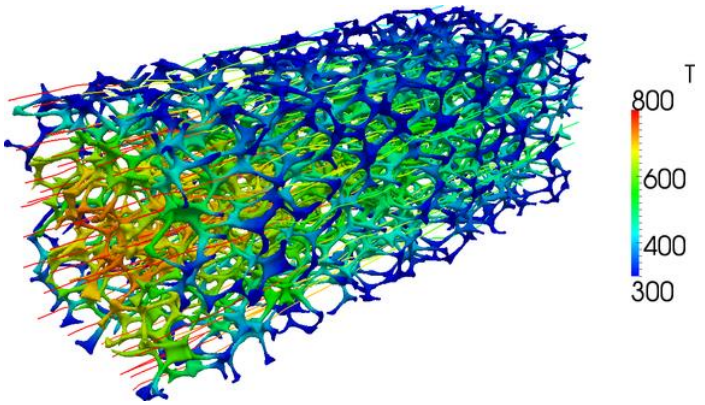
Heat transfer model: *Description of heat transfer by **convection** (fluid-solid) and **conduction** (washcoat-substrate and across the monolith in the 3 directions) on the basis of correlations or data derived from upscaling results of micro-scale simulations.*

Diffusion model: *Description of the diffusion of chemical species between gas and washcoat (**reactants / products**) on the basis of correlations or data derived from upscaling results of micro-scale simulations.*

Reaction model:

- *Description of the reaction mechanism occurring in the washcoat and integration of the **reaction rate** by means of ODE solvers.*

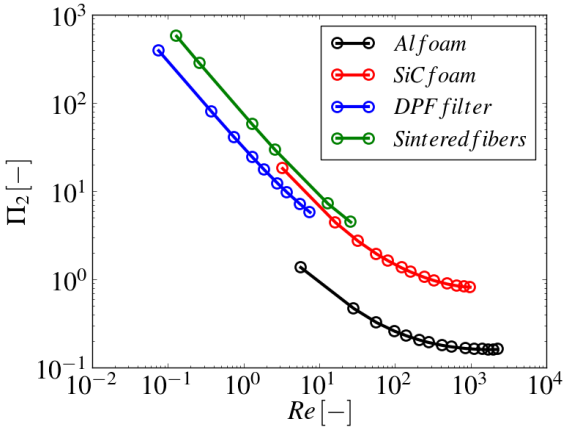
Submodel: flow resistance, heat and mass transfer



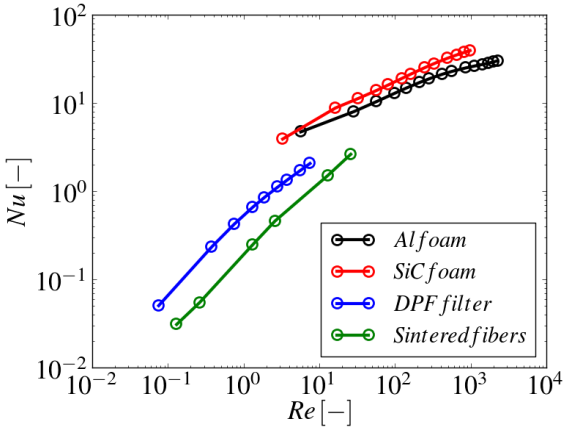
Specific correlations can be exploited to specify the transfer of **heat/mass** or the **flow resistance** on the basis of:

- empirical correlations
- detailed CFD analysis of the microstructure

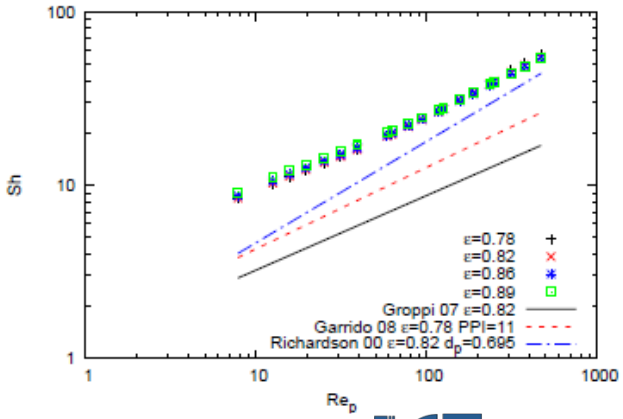
$$\mathcal{R} = \mathcal{F}\left(\mathrm{Re}, d_f\right)$$



$$\mathcal{Q}^{w\to g} = \mathcal{F}\left(\mathrm{Nu} = \mathcal{G}\left(\mathrm{Re}, \mathrm{Pr}\right)\right)$$



$$\mathcal{J}^{wg\to g} = \mathcal{F}\left(\mathrm{Sh} = \mathcal{G}\left(\mathrm{Re}, \mathrm{Sc}\right)\right)$$



Submodel: chemistry

$$\alpha A + \beta B \rightarrow \gamma C + \delta D$$

$$r_i = k_{r,i} \frac{C_{s,A}\, C_{s,B}}{G_i} Eq_f$$

$$k_{r,i} = A_{r,i}\, e^{-\frac{E_{r,i}}{RT_w}}$$

$$G_i = T_w\left(1 + k_{a,1} C_{s,A} + k_{a,2} C_{s,B}\right)^2$$

$$k_{a,i} = A_{a,i}\, e^{-\frac{E_{a,i}}{RT_w}}$$

$$Eq_f = 1 - \frac{C_{s,C}^{\gamma}\, C_{s,D}^{\delta}}{C_{s,A}^{\alpha}\, C_{s,B}^{\beta} K_p(T)}$$

- Langmuir-Hinshelwood to account for the competition of the chemical species on the active sites
- Inhibition factor takes into account the adsorption and desorption of reactants and products on the active sites.
- Eq_f is for reactions that exhibit a reversible behavior

Example:
reaction scheme for DOC

R1: $CO + \frac{1}{2} O_2 \rightarrow CO_2$

R2: $H_2 + \frac{1}{2} O_2 \rightarrow H_2O$

R3: $C_3H_6 + \frac{9}{2} O_2 \rightarrow 3\, CO_2 + 3\, H_2O$

R4: $C_3H_8 + 5\, O_2 \rightarrow 3\, CO_2 + 4\, H_2O$

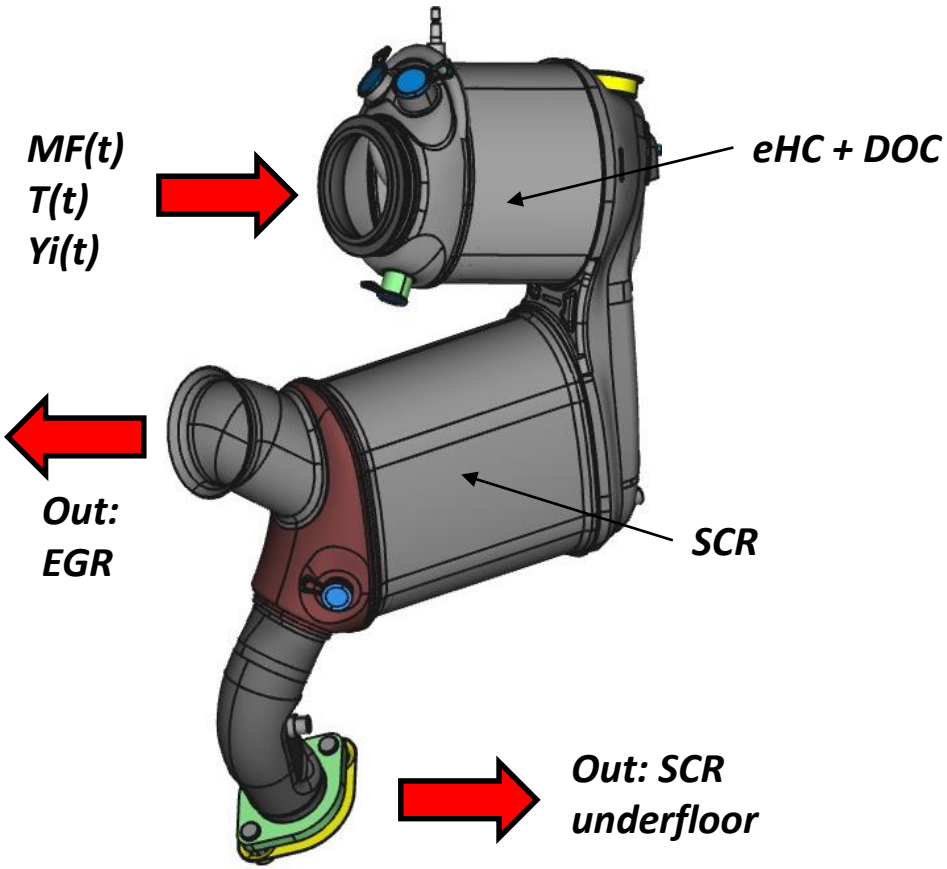
R5: $\frac{1}{3} C_3H_6 + H_2O \rightarrow CO + 2\, H_2$

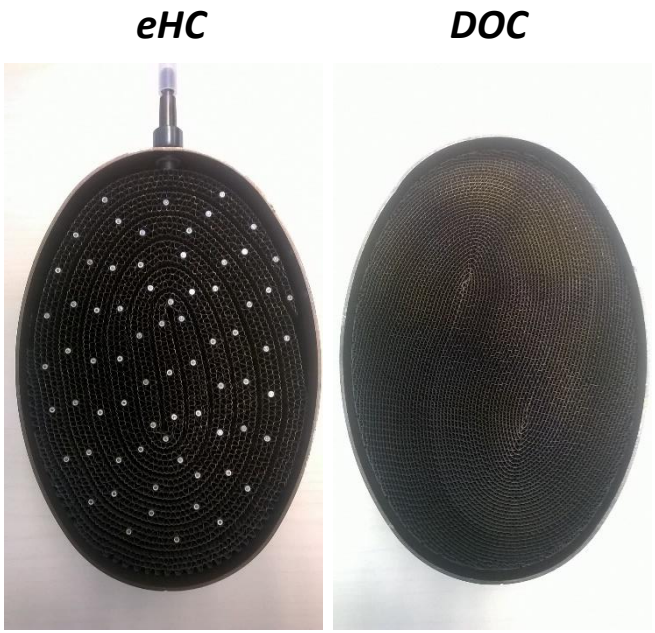
R6: $\frac{1}{3} C_3H_8 + H_2O \rightarrow CO + \frac{7}{3} H_2$

R7: $CO + H_2O \rightarrow CO_2 + H_2$

ATS with electrical heated catalyst

After-treatment system for Diesel engine including DOC monolith, electrical heating and integrated SCR-DPF





Example of application

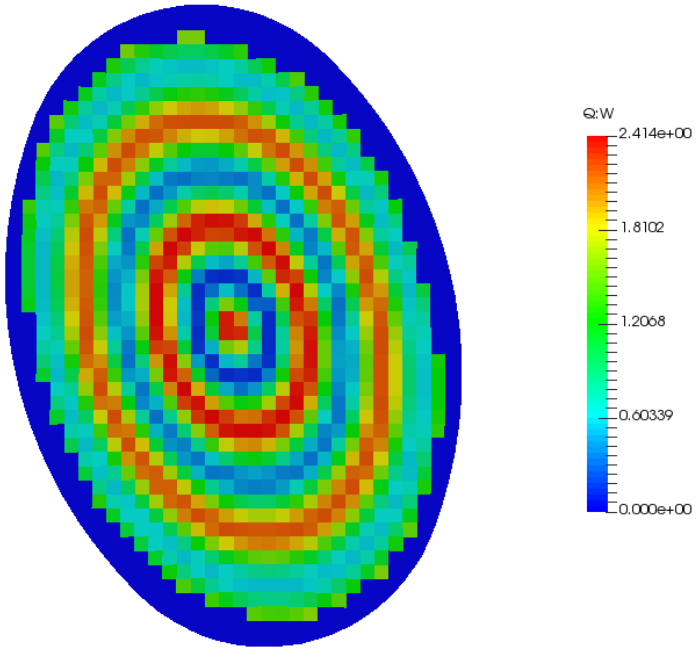
ATS with electrical heated catalyst

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

Phenomenological model:

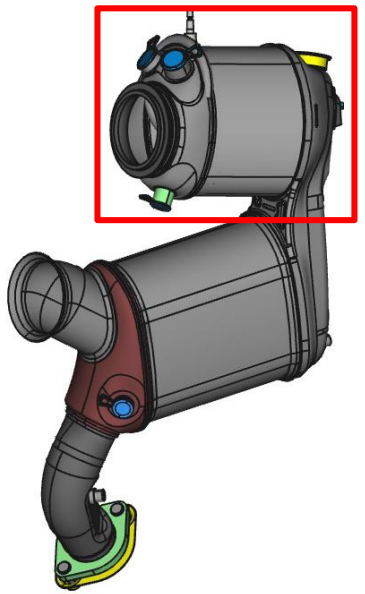
- Each spiral has a high T side and a low T side
- Non-uniformity decreases from center to boundary
- No heating at the boundary (short circuit)

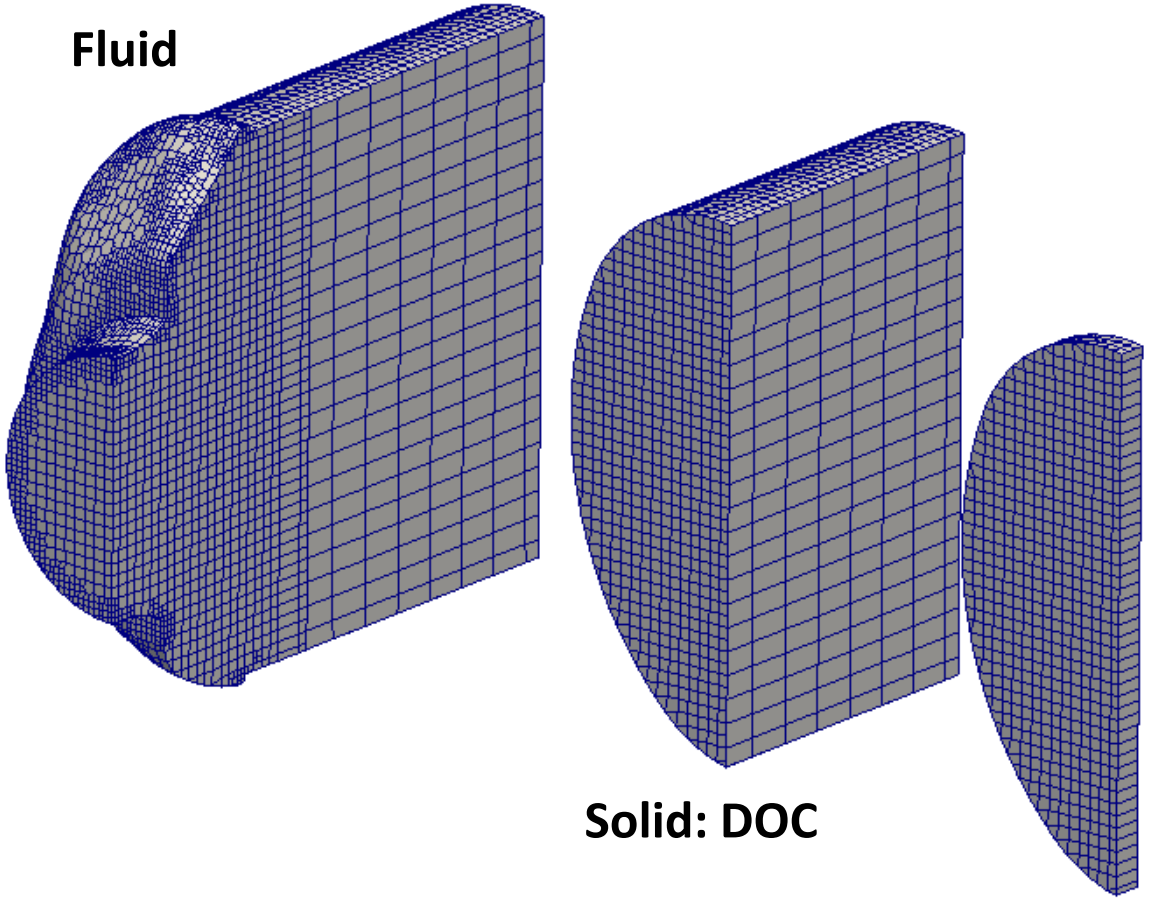
Spatial distribution for the heat release



ATS with electrical heated catalyst

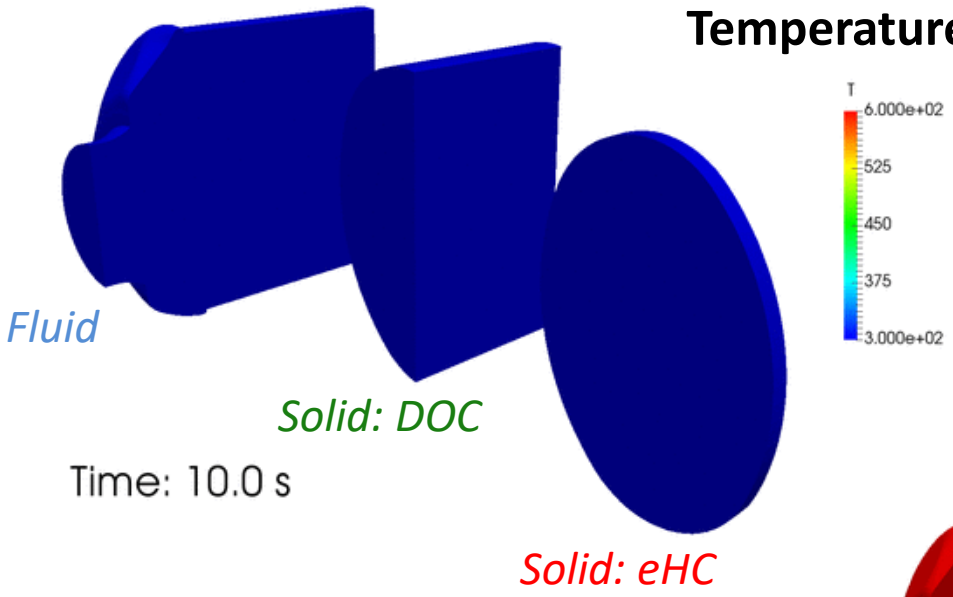
Fully-3D CFD model of the DOC section of the ATS





Example of application

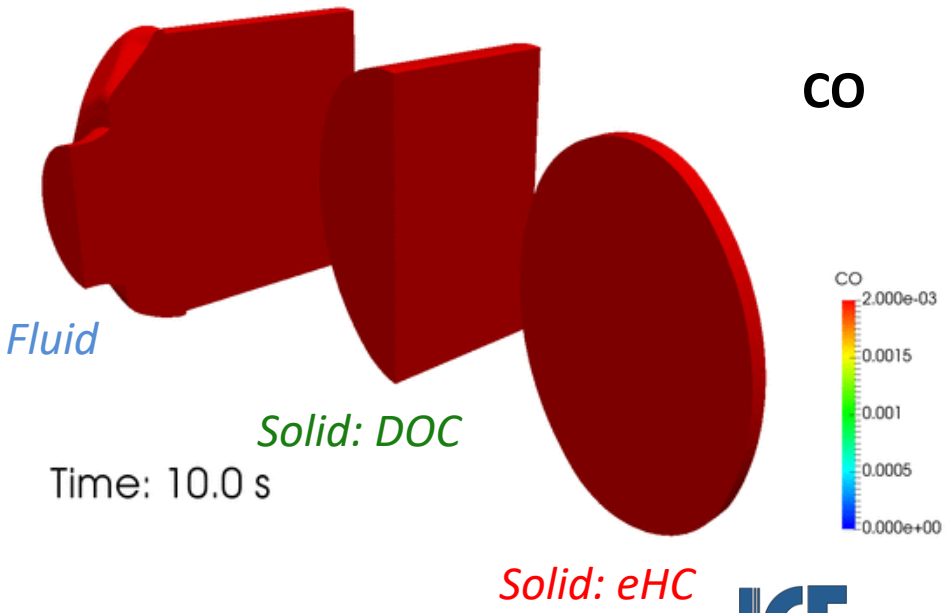
ATS with electrical heated catalyst



Non-uniform heating

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

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



Non-uniformity of the heating generates hot spots

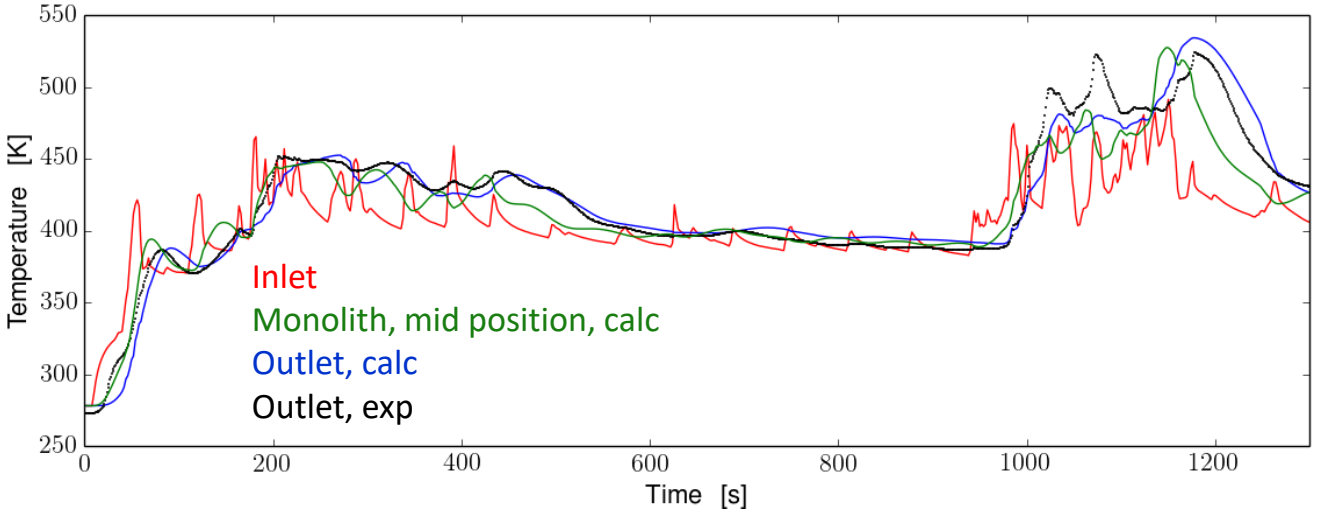
→ **earlier light-off**

Example of application

ATS with electrical heated catalyst

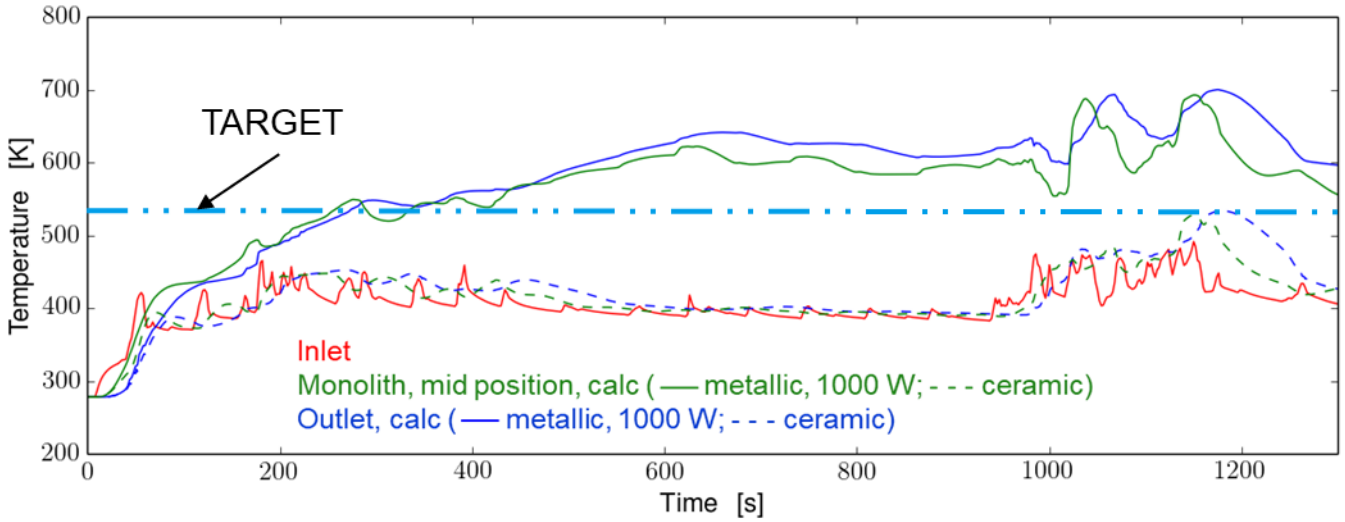
Baseline:

- ceramic substrate
- without electrical heating



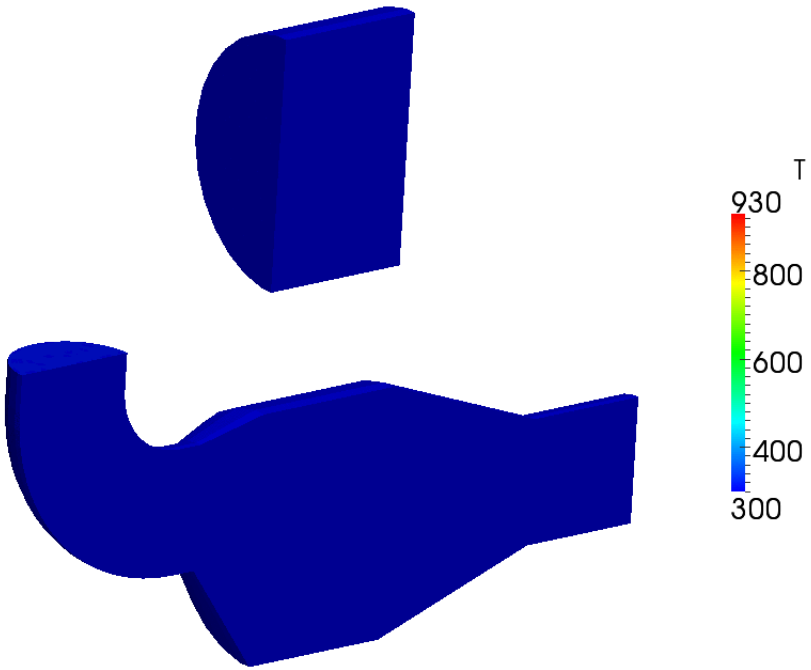
Alternative:

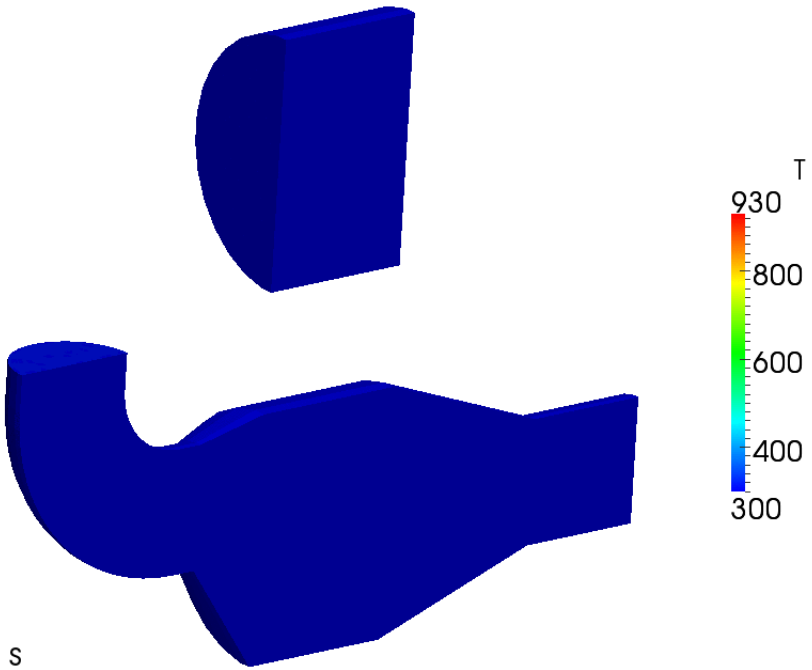
- metallic substrate
- with electrical heating



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.





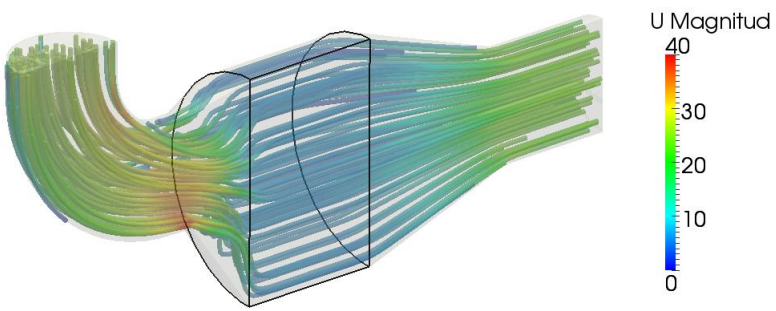
Time: 0 s

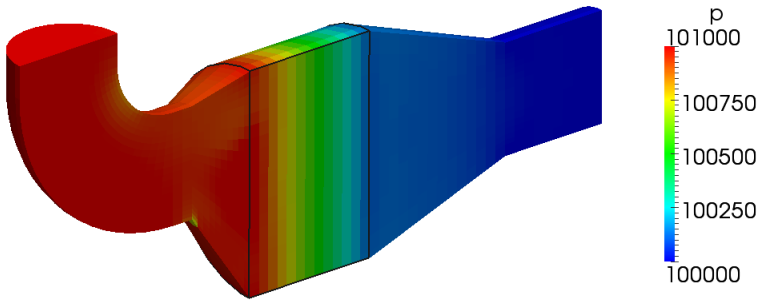
HONEYCOMB

OPEN CELL FOAM

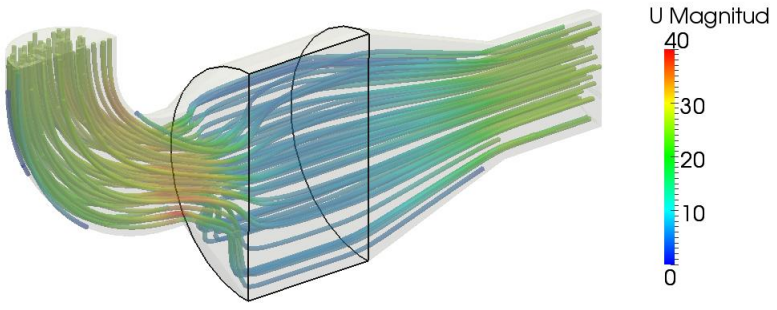
Honeycomb vs open-cell foam

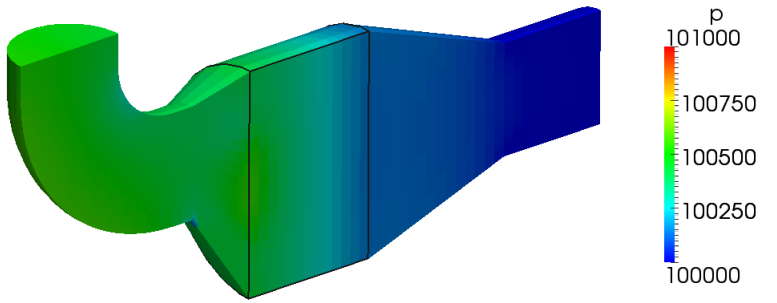
HONEYCOMB





OPEN CELL FOAM





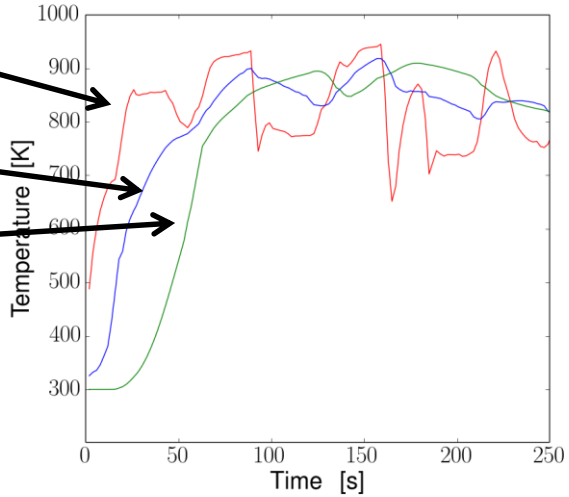
Honeycomb vs open-cell foam

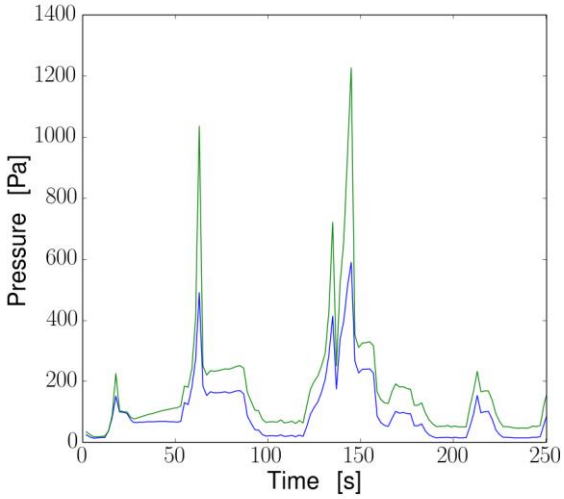
- NEDC cycle (first 250 seconds) with two different technologies

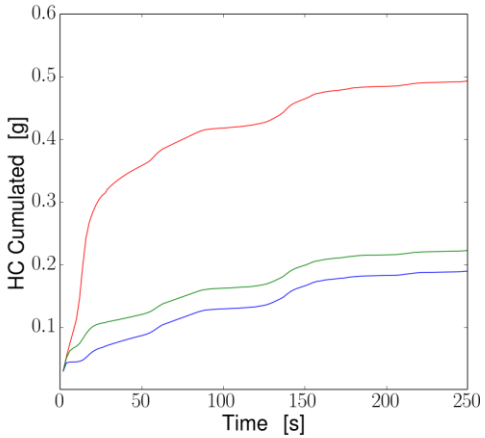
Inlet measured

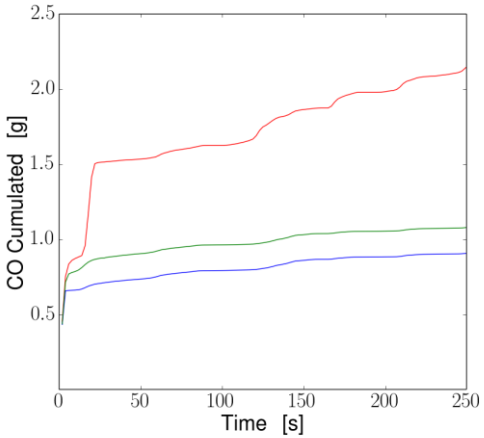
Open cell

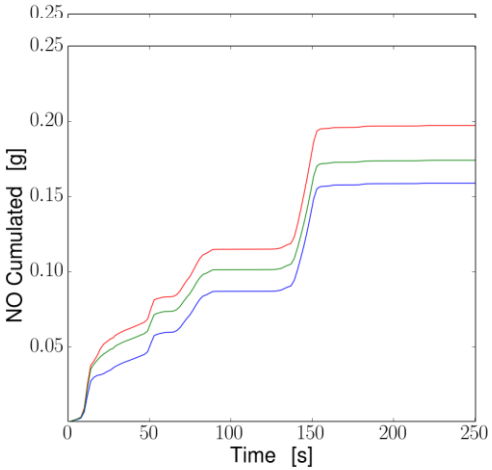
Honeycomb









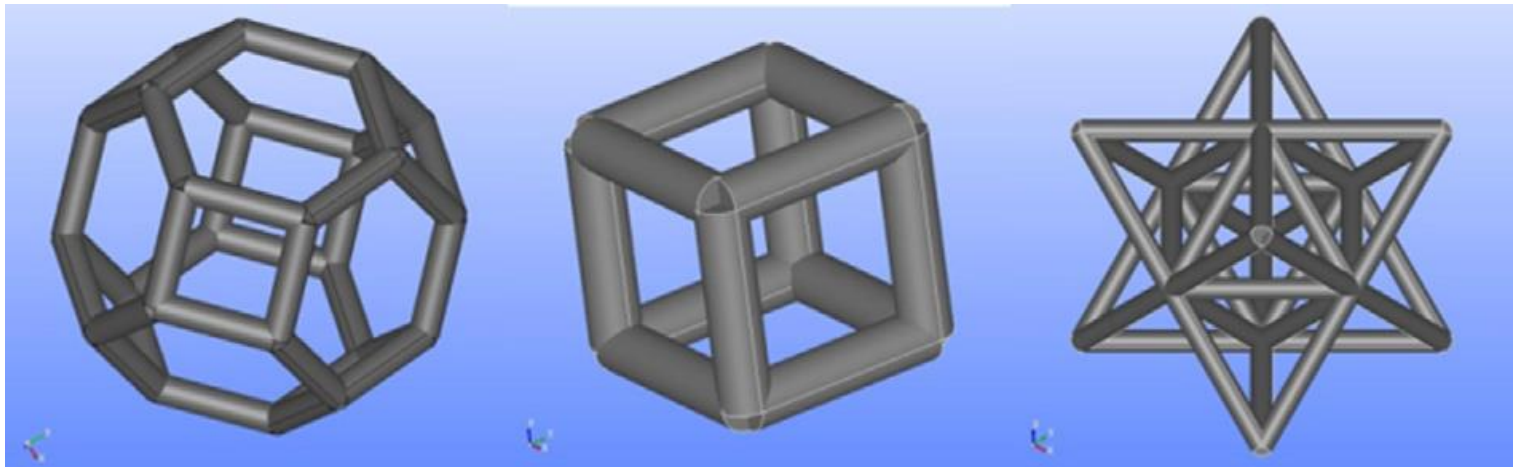


Towards future solutions:
additive layering manufacturing of structured substrates

Additive Layer Manufacturing polyhedral structures

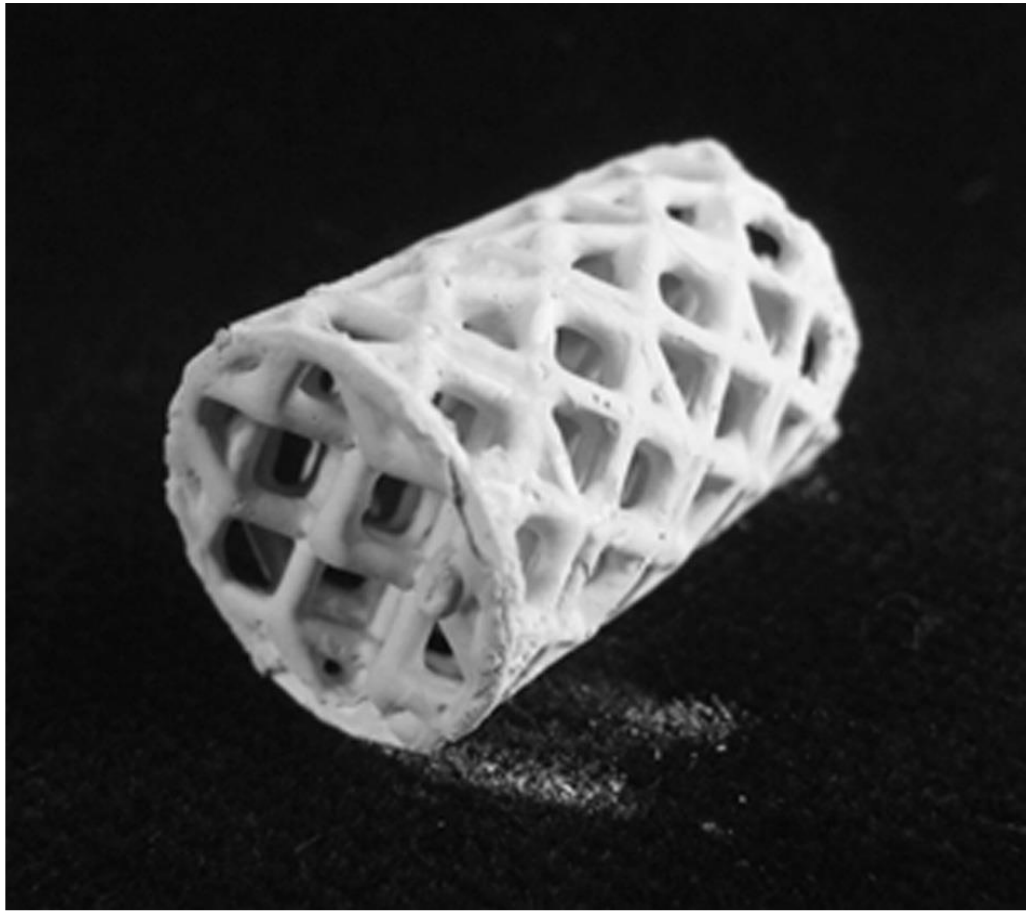
ALM technology offers the possibility to design and manufacture optimized polyhedral structures.

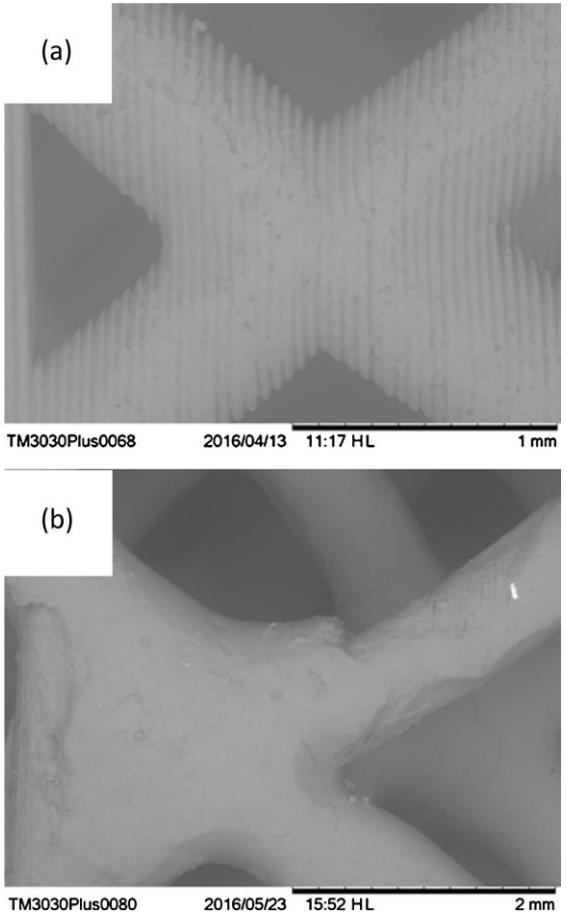
Kelvin cell *Cubic cell* *Octet cell*



Additive Layer Manufacturing polyhedral structures

Example: cubic cell, rotated 45° with respect to the flow direction.





Additive Layer Manufacturing polyhedral structures

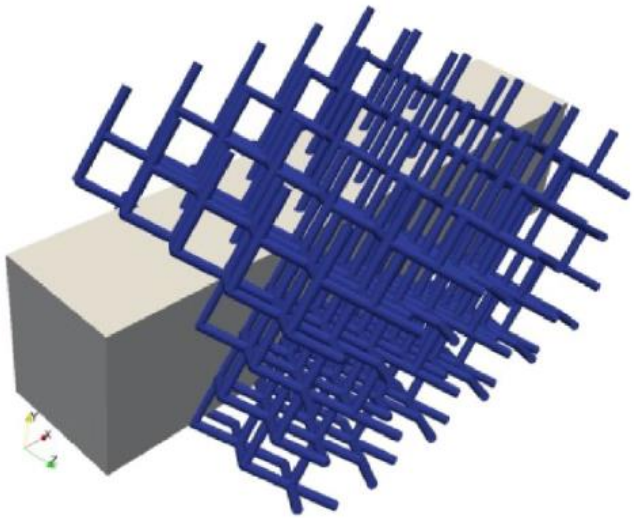
Comparison between different structures: geometrical parameters

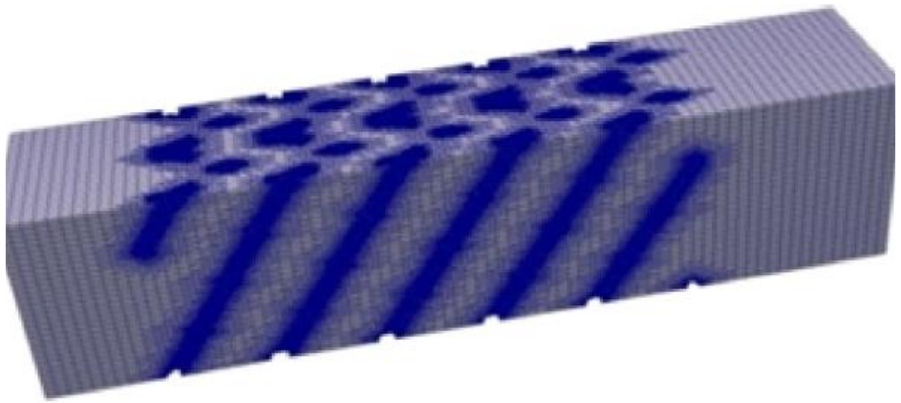
Honeycomb

ε [–]	CPSI [–]	D_c [mm]	d_c [mm]	r_c [mm]	L_c/D_c [–]	S_v [m^2/m^3]
0.73	400	1.25	1.125	0.375	30	2480

Artificial polyhedral structures

Cell geometry	ε [–]	d_s [mm]	L_s [mm]	L_c [mm]	S_v [m^2/m^3]
Kelvin	0.95	0.5	2.04	5.77	400
Cubic/Cubic45	0.95	0.5	3.43	3.43	400
Octet	0.95	0.5	5.77	8.17	400

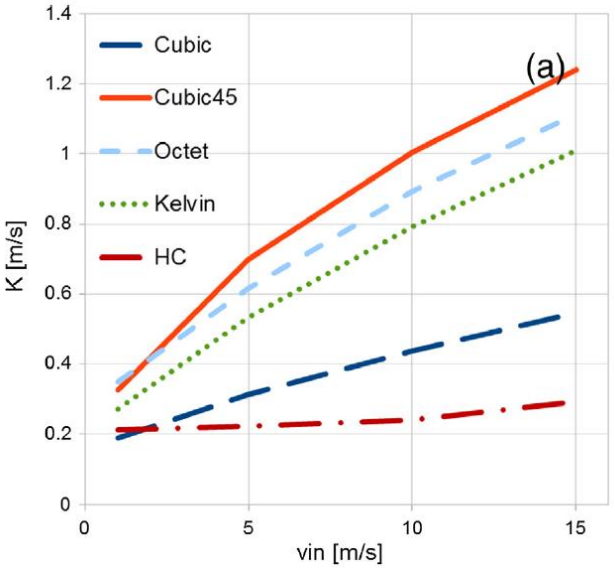




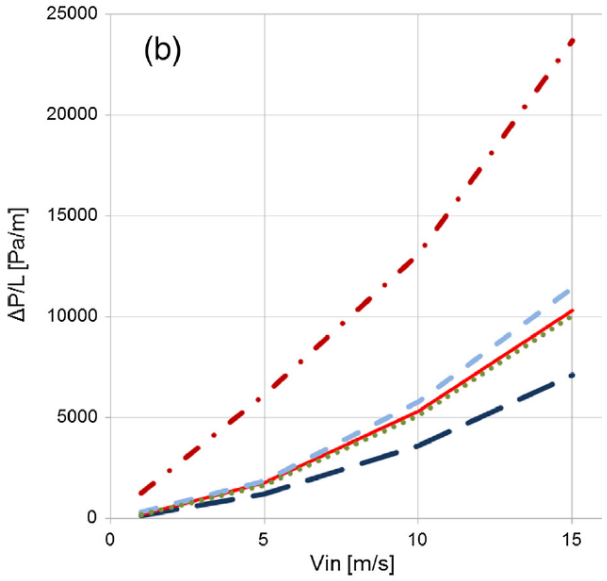
Additive Layer Manufacturing polyhedral structures

Comparison between different structures: computed performances

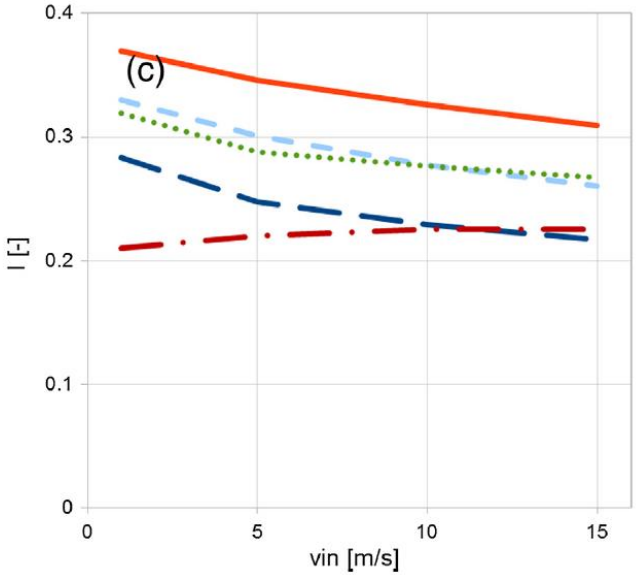
Mass transfer



Pressure drop



Performance index



- Cubic 45 shows the best performances with respect to the other artificial structures.
- In the comparison with HC, it should be taken into account that high porosity structures are considered.

Additive Layer Manufacturing polyhedral structures

Cubic 45: analysis with different **porosity** and **strut diameter**

Cell geometry	ε [–]	d_s [mm]	$L_s = L_c$ [mm]	S_v [m^2/m^3]
Cubic45	0.8	0.5	1.72	1600
Cubic45	0.8	1	3.43	800
Cubic45	0.85	0.5	1.98	1200
Cubic45	0.85	1	3.96	600
Cubic45	0.9	0.5	2.43	800
Cubic45	0.9	1	4.85	400
Cubic45	0.95	0.5	3.43	400
Cubic45	0.95	1	6.86	200

*Range of **porosity** and **strut diameters** compatible with practical applications with **washcoat**.*

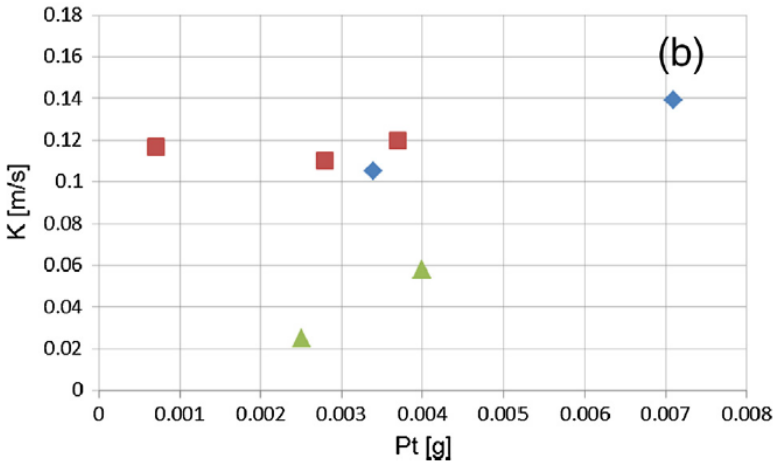
Cubic45/HC	K (~$1/S_w$)	S_v	V	I
ε = 0.95, d_s = 1 mm	2.8	1/12	4.3	1.4
ε = 0.85, d_s = 1 mm	3.5	1/4	1.2	1.0
ε = 0.95, d_s = 0.5 mm	4.1	1/6	1.5	1.6
ε = 0.85, d_s = 0.5 mm	5.1	1/2	0.4	1.2

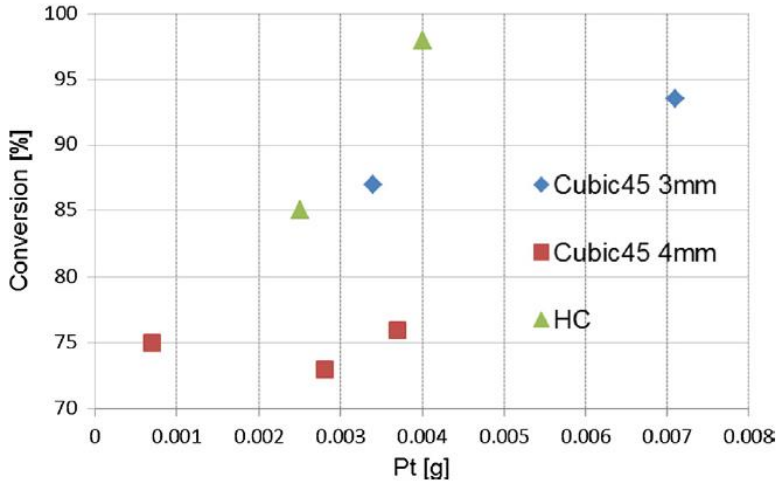
Comparison with HC, for the same conversion and flow rate:

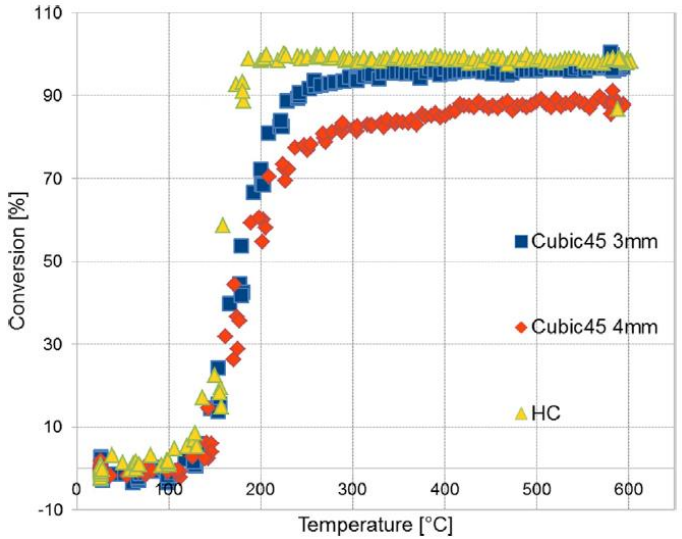
- CC45 exhibits higher K with respect to HC
- CC45 has lower SV, requiring higher volume
- CC45 has higher performance index I

Additive Layer Manufacturing polyhedral structures

Cubic 45: experimental results







- CC has higher K
- CC requires lower catalyst loading
- Pore diffusion has a great impact on the conversion

Conclusions

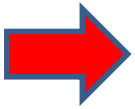
Summary: Open-cell foam VS Honeycombs

A) Conversion Efficiency ***AND*** *Pressure Drop* **- +**

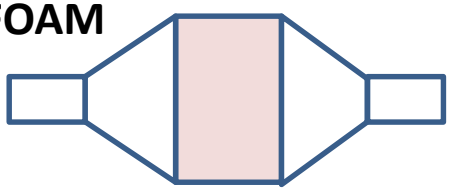
The advantage is not huge, however better performances can be obtained with a **proper design** of the foam substrate.

- ***High D***
- ***Low L***
- ***High porosity***

HONEYCOMB



FOAM



B) Catalytic Surface **+ +**

Foam substrates requires **low catalytic surface** to achieve the same conversion efficiency: **low amount of catalyst loading**

C) Light-off time **+**

Foam substrates **if optimized** acccording to A) exhibits a **lower light-off time**

Thank you very much for your attention!

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- S. Falfari, G.M. Bianchi, G. Micci, A. Della Torre, G. Montenegro, A. Onorati, S. Negro, “Geometric and Fluid-Dynamic Characterization of Actual Open Cell Foam Samples by a Novel Imaging Analysis Based Algorithm”, (2017) SAE International Journal Of Engines, vol. 10, p. 1-13, ISSN:1946-3944, doi: 10.4271/2017-01-9288.

- F. Lucci, A. Della Torre, G. Montenegro, R. Kaufmann, P. Dimopoulos Eggenschwiler, “Comparison of geometrical, momentum and mass transfer characteristics of real foams to Kelvin cell lattices for catalyst applications”, (2017) International Journal Of Heat And Mass Transfer, vol. 108, p. 341-350, ISSN: 0017-9310, doi: 10.1016/ j.ijheatmasstransfer.2016.11.073.

- Della Torre A., Lucci F., Montenegro G., Onorati A., Dimopoulos Eggenschwiler P., Tronconi E., Groppi G. (2016), “CFD modeling of catalytic reactions in open-cell foam substrates. Computers & Chemical Engineering” (2016), vol. 92, p. 55-63, ISSN: 0098-1354, doi:10.1016/j.compchemeng.2016.04.031.

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- Lucci, F., Della Torre, A., Montenegro, G., Dimopoulos Eggenschwiler, P. On the catalytic performance of open cell structures versus honeycombs (2015) Chemical Engineering Journal, 264, pp. 514-521.

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- A. Della Torre, G. Montenegro, A. Onorati, G. Tabor, CFD Characterization of Pressure Drop and Heat Transfer Inside Porous Substrates, Energy Procedia, Volume 81, December 2015, Pages 836-845, ISSN 1876-6102