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PRINT CR3DIT

CHISA 2018 PRAGUE

PRES 2018

A CFD approach to study catalytic reactors filled with open cell foams

José Daniel Araújo, Daniel Direito and Manuel Alves

H2020: PRINTCR3DIT - Process Intensification through Adaptable Catalytic Reactors made by 3D Printing
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Computational Fluid Dynamics

Fluid Mechanics

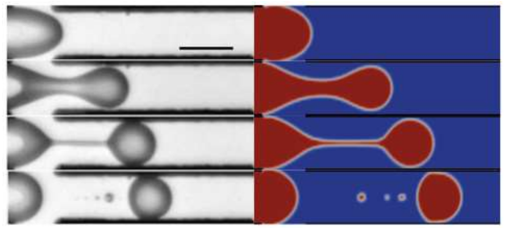
↓

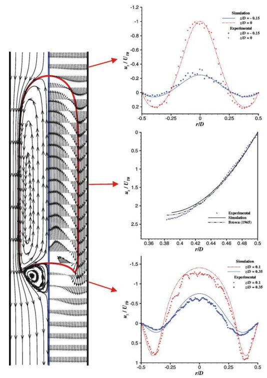
CFD

↙ ↘

Computer science

Mathematics





Main uses

- **Fundamental science: discover new phenomena**
- **Design and optimization: design and improve equipment**
- **Substitute for experiments and monitoring: modeling of existing equipment or natural phenomena**

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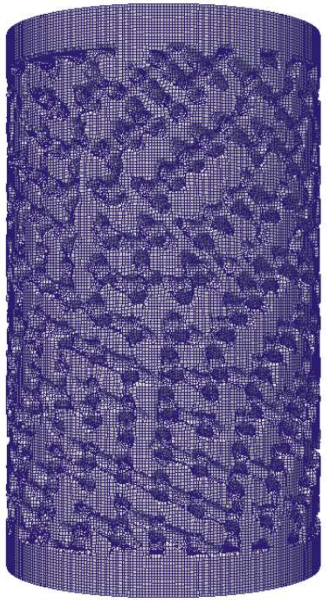
CFD simulations

Foam structure (solid part)

Domain (fluid part)

Computational mesh



Software: OpenFOAM

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CFD simulations – tracer tests

Fluid

Water properties

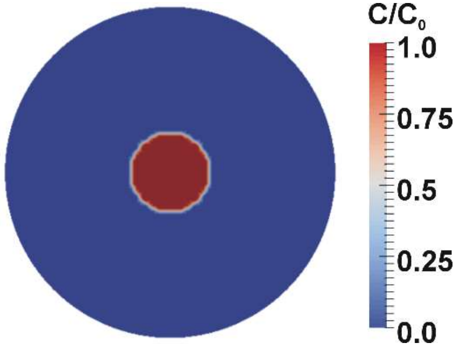
$D_m = 1 \times 10^{-9}\ m^2/s$

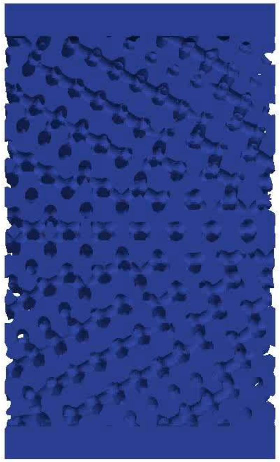
Domain

D = 2.08 cm

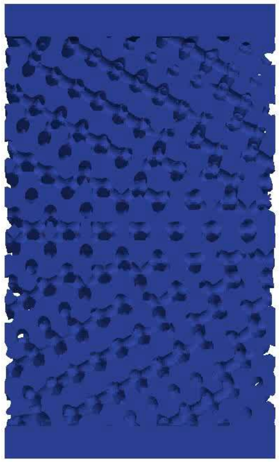
L = 3.50 cm

ε = 0.56

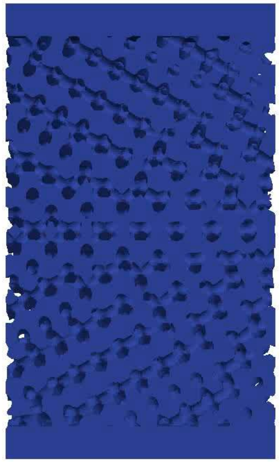




U_{sup} 0.3 m/s



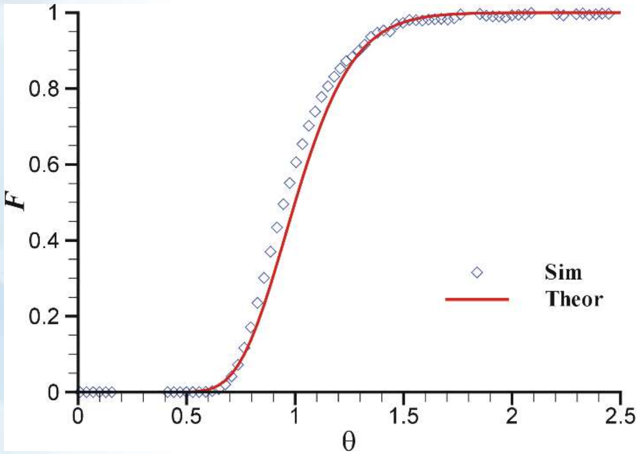
U_{sup} 0.03 m/s



U_{sup} 0.003 m/s

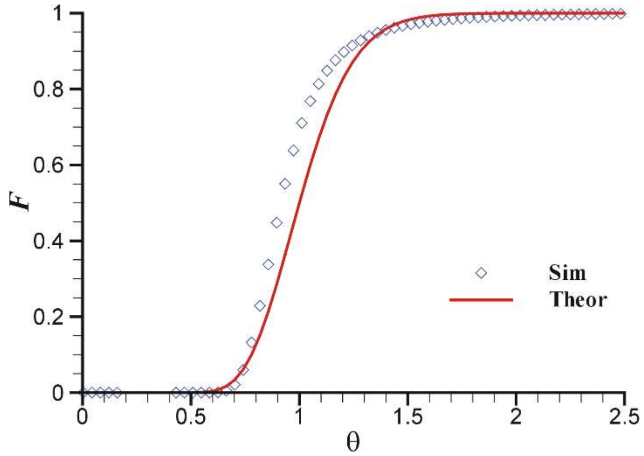
CFD simulations – tracer tests

U_{sup} = 0.3 m/s



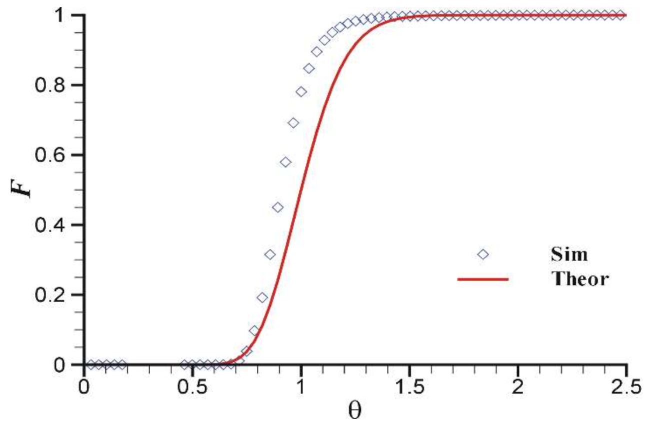
D_L (m²/s)
3.50x10^{-4}

U_{sup} = 0.03 m/s



D_L (m²/s)
3.04x10^{-5}

U_{sup} = 0.003 m/s



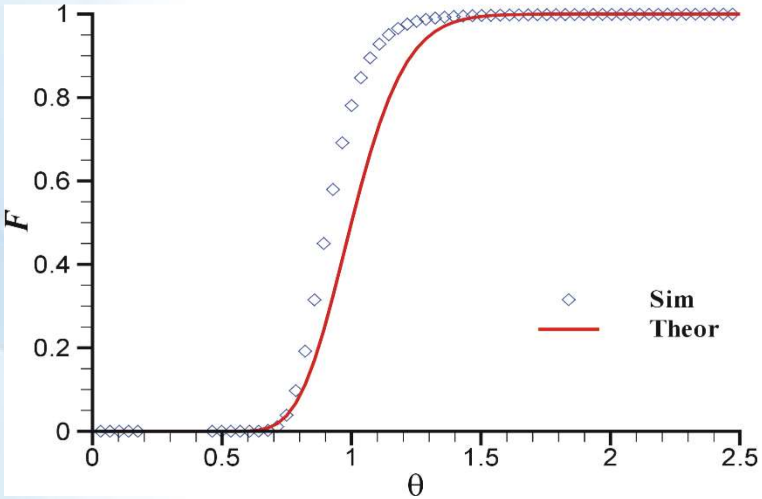
D_L (m²/s)
2.11x10^{-6}

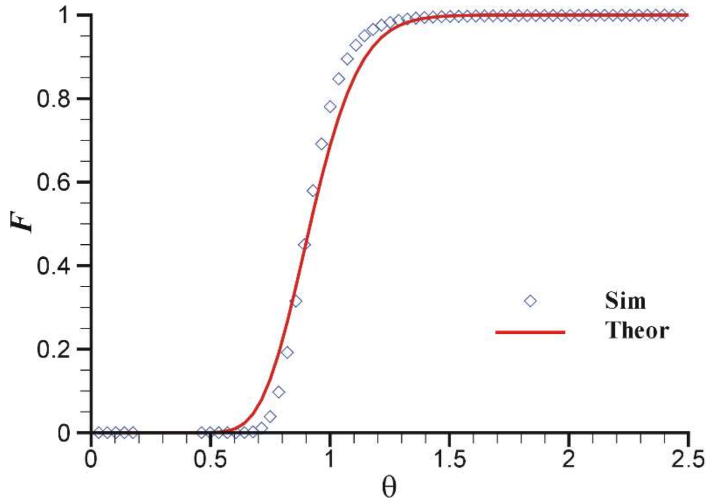
Danckwerts (1953)

$$F = \frac{C_{out}}{C_{in}} = \frac{1}{2}\left[1 - erf\left(\frac{L - U_{sup}\cdot t}{2\cdot\varepsilon\cdot\sqrt{D_L\cdot t}}\right)\right]$$

CFD simulations – tracer tests

U_{sup} = 0.003 m/s





U_{sup} (m/s) 0.3 — D_L (m^2/s) 3.50×10^{-4}; V_{dead} (%) 3.4

U_{sup} (m/s) 0.03 — D_L (m^2/s) 3.04×10^{-5}; V_{dead} (%) 6.2

U_{sup} (m/s) 0.003 — D_L (m^2/s) 2.11×10^{-6}; V_{dead} (%) 8.2

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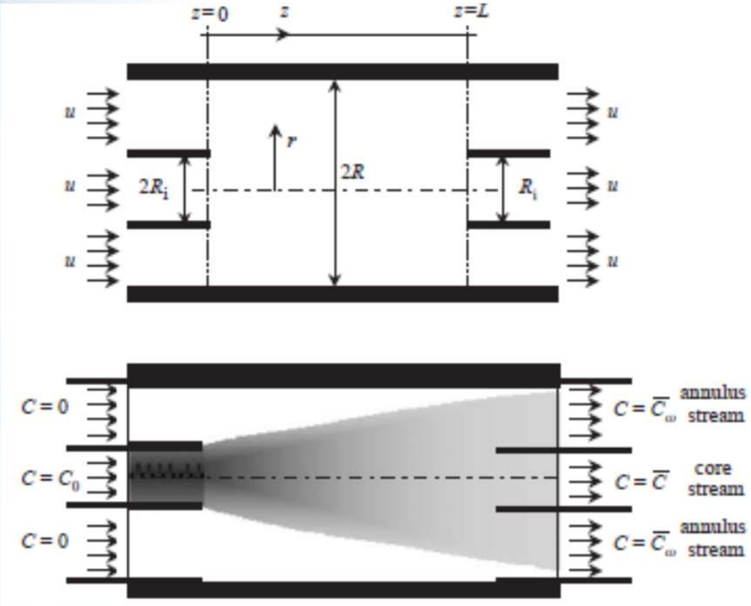
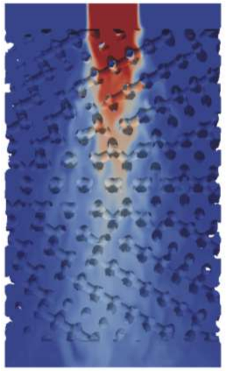
CFD simulations – tracer tests

Hiby and Schummer (1960)

$$\frac{C_{out,core}}{C_{in,core}} = 4\sum_{0}^{\infty}\frac{J_1^2\left(\lambda_n R_i/R\right)}{\lambda_n^2 J_0^2\left(\lambda_n\right)}\cdot\exp\left[-\frac{\varepsilon L\cdot D_T}{U_{sup}}\left(\frac{\lambda_n}{R}\right)^2\right]$$

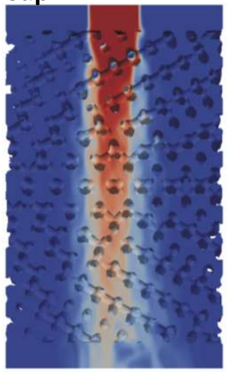


U_{sup} = 0.3 m/s



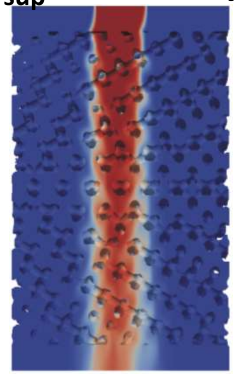
$D_T = 2.27\times10^{-4}$ m²/s

U_{sup} = 0.03 m/s



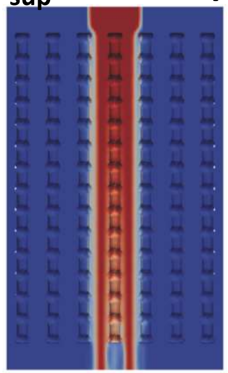
$D_T = 1.52\times10^{-5}$ m²/s

U_{sup} = 0.003 m/s



$D_T = 1.10\times10^{-6}$ m²/s

U_{sup} = 0.03 m/s



$D_T = 6.06\times10^{-6}$ m²/s

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CFD simulations – surface reaction

U_{sup} = 0.03 m/s; k_r = 0.1 s^{-1}

Species

A – reagent
B – product

Reaction

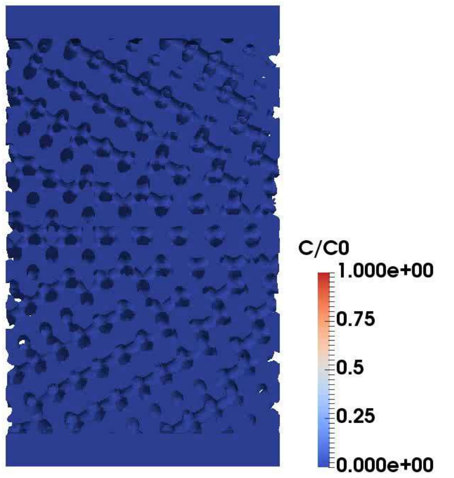
$$A \rightarrow B$$

$$r_A = -k_r \cdot C_A$$

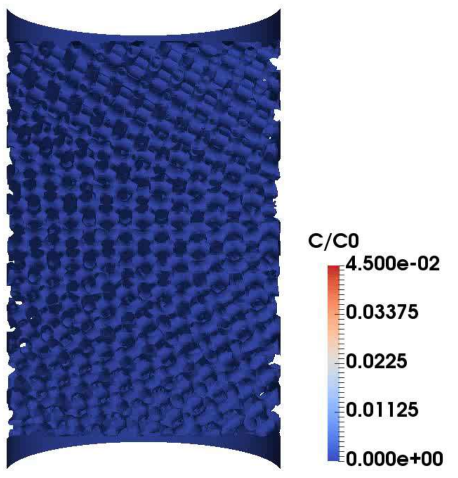
Fluid

Water properties
$D_m = 1x10^{-9}\ m^2/s$

A



B



SPIRE Sustainable Process Industry through Resource and Energy Efficiency

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CFD simulations – fluid phase reaction

Species

A – reagent
B – reagent
C – product
D – inert

Reaction

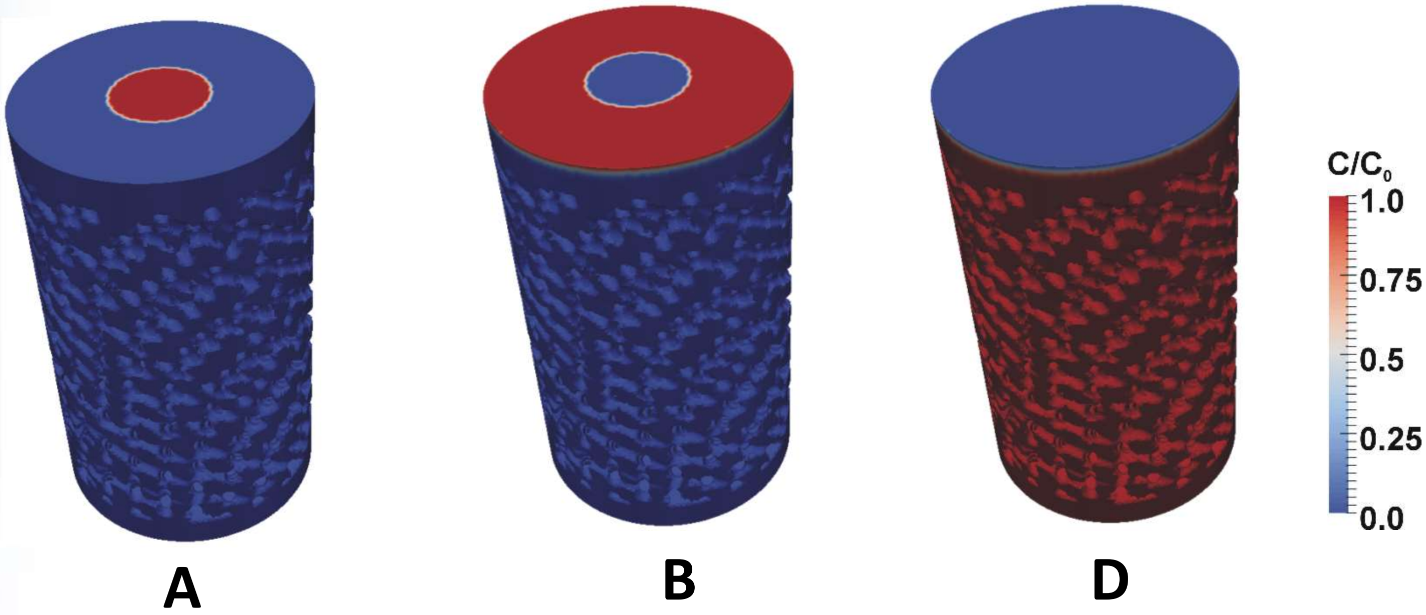
$$A + B \rightarrow C$$

$$r_A = -k_r \cdot C_A \cdot C_B$$

$$-\Delta H_r = 500 \text{ kJ/mol}$$

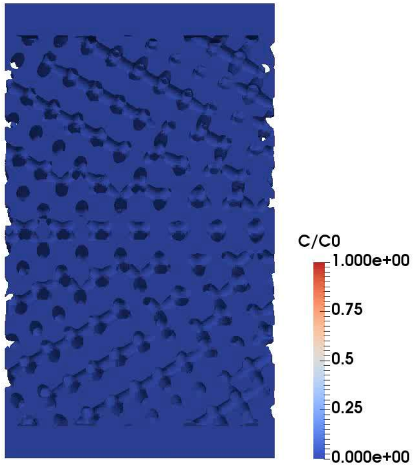
Fluid

Water properties
D_m = 1x10^{-9} m^2/s
T_{in} = 373 K

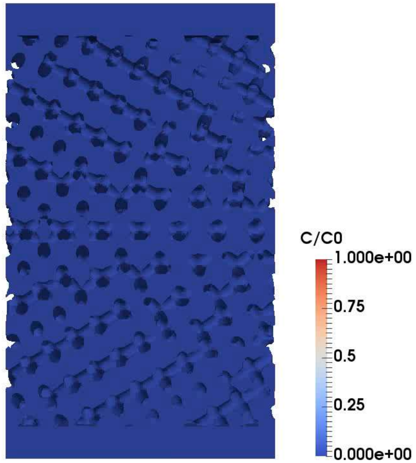


CFD simulations – fluid phase reaction

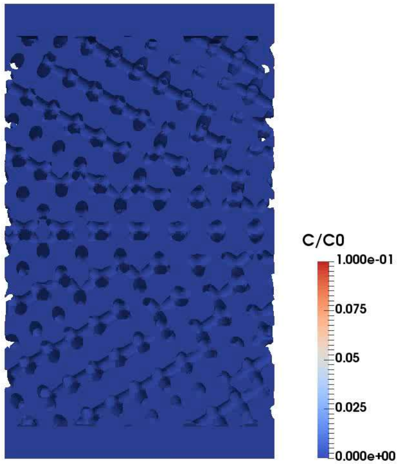
A



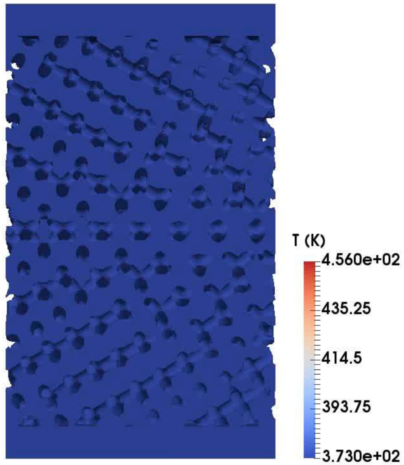
B



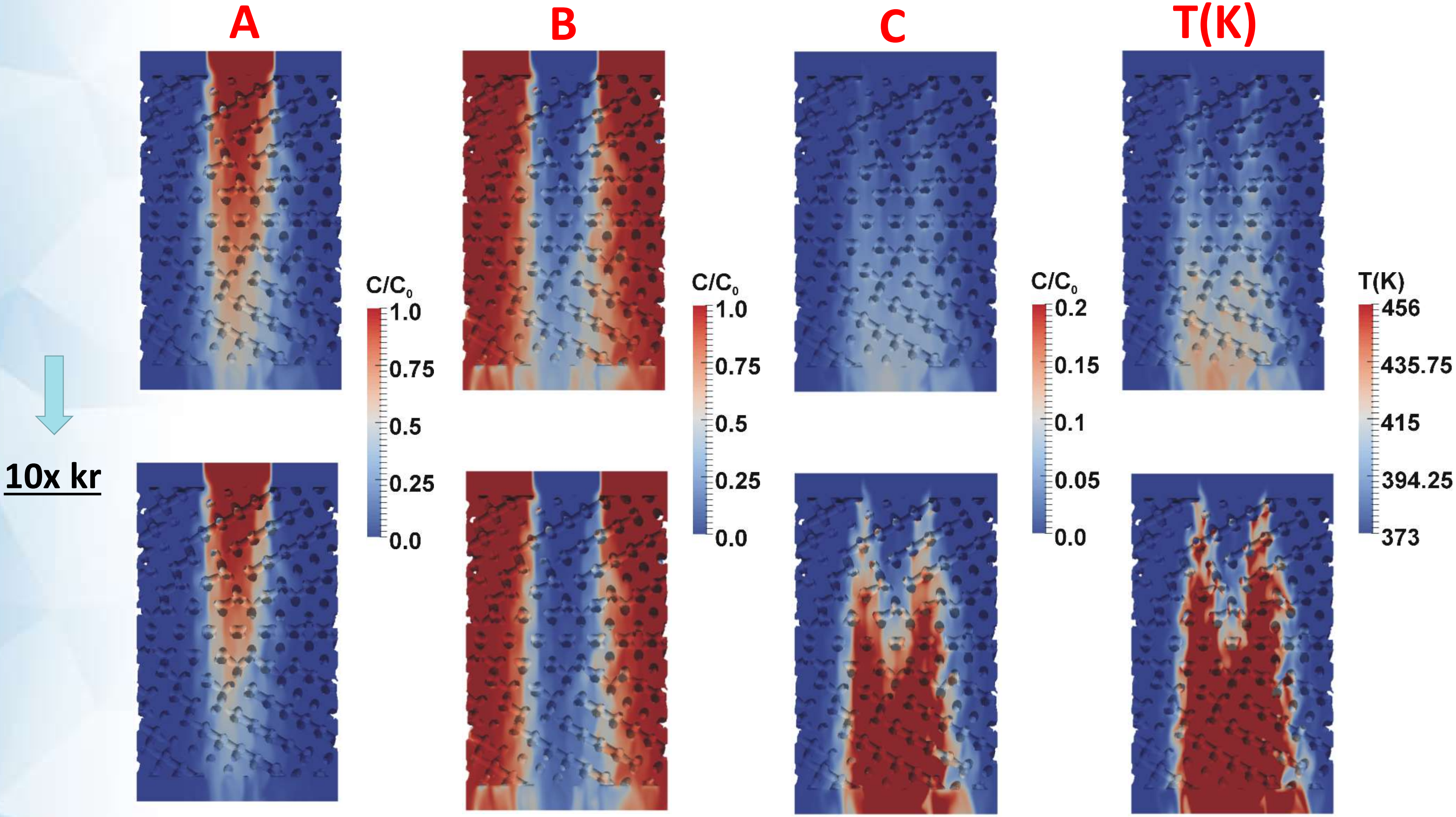
C



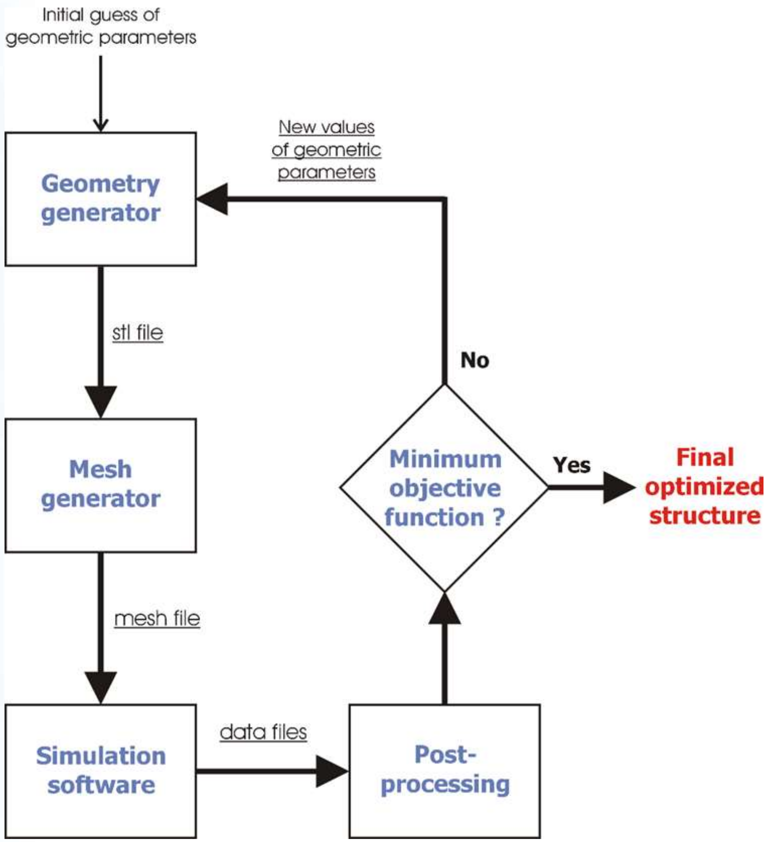
T(K)



CFD simulations – fluid phase reaction



Optimization procedure



Fully automatic

Input – initial parameter values

Output – stl file with optimized shape

Couples several tools

Geometry generator

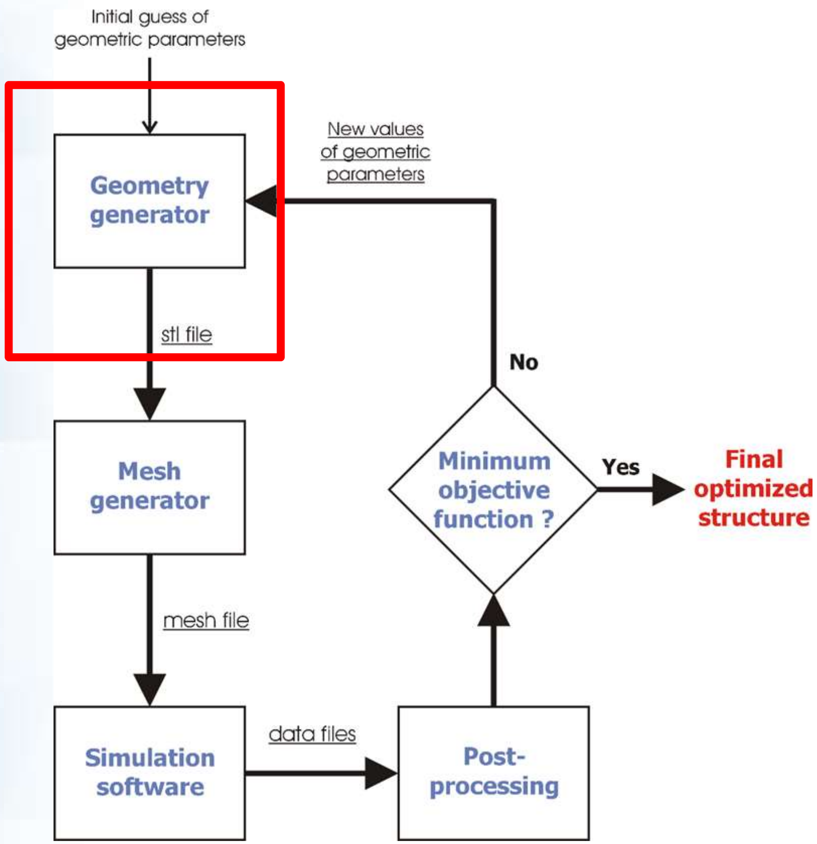
CFD software

Optimizer

Versatile

Useful for optimization of different types of systems and process units

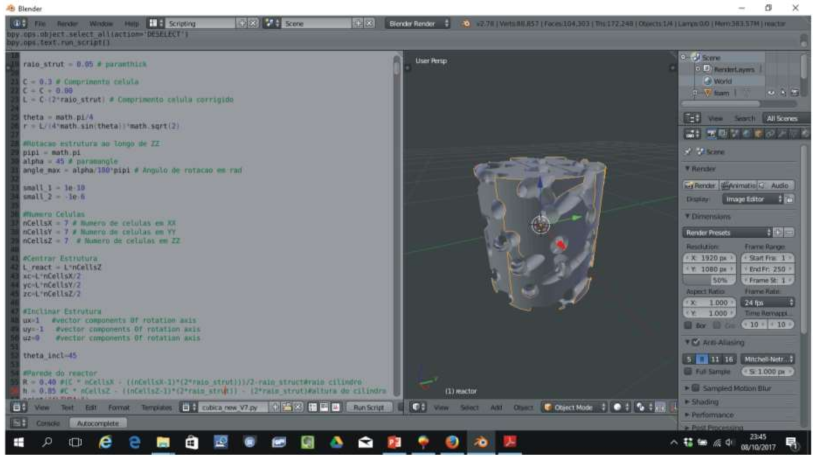
Optimization procedure



1 - Shape generation

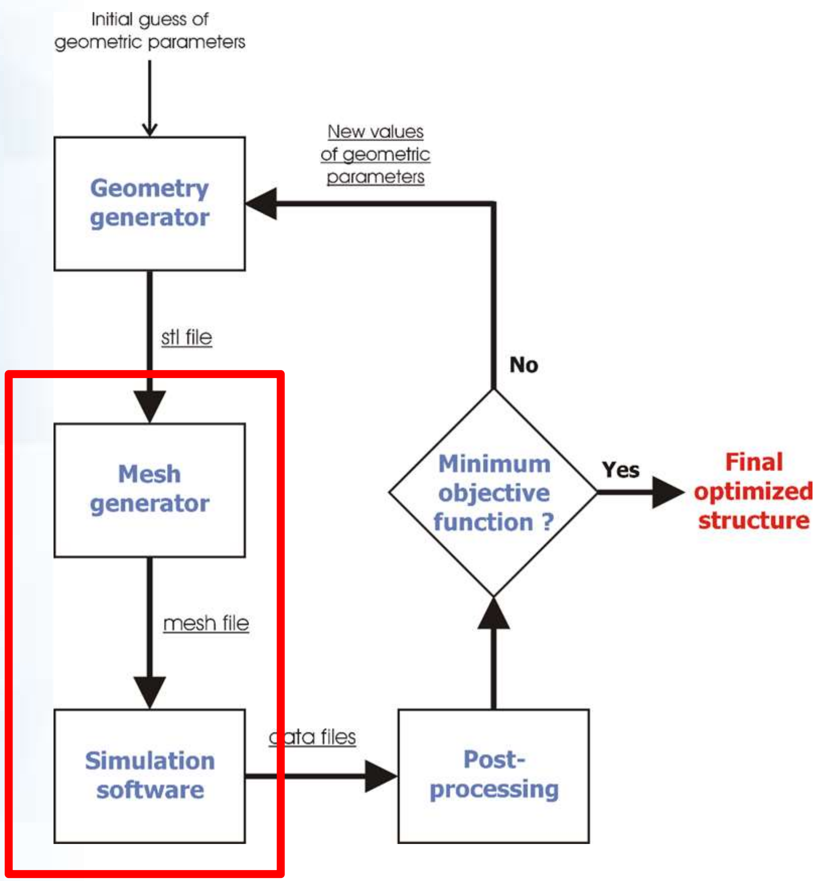
Blender® software (freeware)

Python script (each one for a different topology)



Stl files

Optimization procedure



2 – CFD tools

OpenFOAM® software (freeware)

Communication with other blocks – application of bash scripts

Language – C++

Meshing – cfMesh or snappyHexMesh tools

Solver – Single-phase flow with heat and mass tranfer

Cyclic BC – to benefit from the periodicity of flow field in open channel structures

data files

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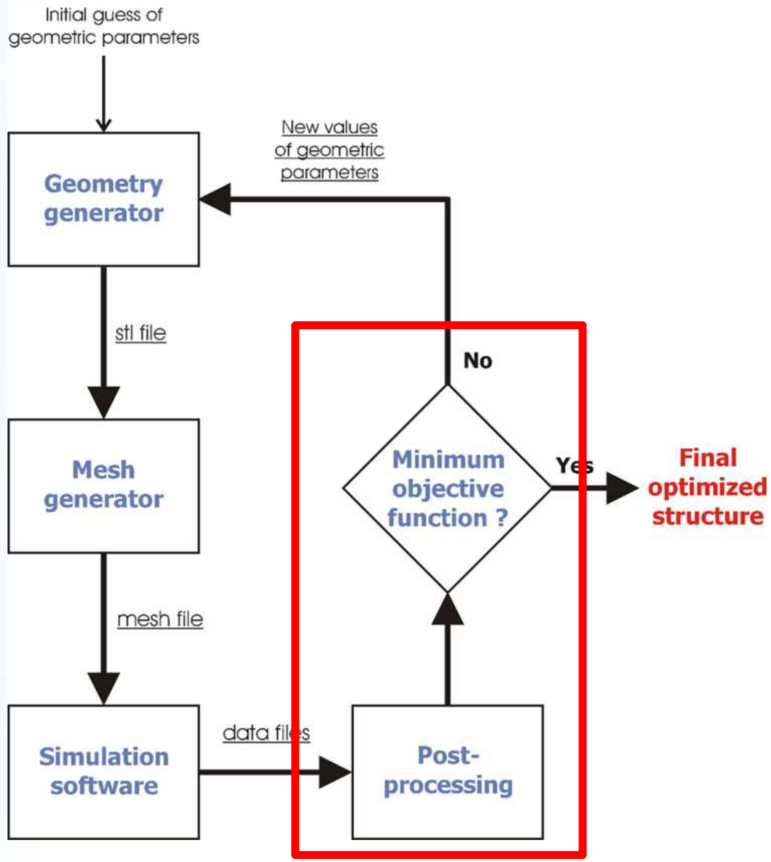
Optimization procedure



3 – Post-processing

Evaluation of an objective function that synthetizes the limitations and/or goals of the process

★ $$F_{obj} = w_C \cdot \frac{\sum \left| C_{out} - \bar{C}_{out} \right|}{\sum C_{out}} + w_T \cdot \frac{\sum \left| T_{out} - \bar{T}_{out} \right|}{\sum T_{out}} + w_P \cdot (P_{in} - P_{out}) + w_A \cdot \frac{V_{total}}{A_S}$$

↓

Nomad® optimizer (freeware)

↓

new parameter values

Acknowledgements

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