Willkommen
Welcome
Bienvenue

Empa
Materials Science and Technology

Simulation of Heat and Mass Transfer Phenomena in Additive Manufacture Open Cell structures for Automotive Catalyst Applications

P. Dimopoulos Eggenschwiler, Dr. sc techn. ETHZ, V. Papetti, Msc.

Milano, Two-day Meeting on Simulations Using OpenFOAM Technology, 13.02.2020

Additive Manufactured catalytic converters and microwave heating for zero environmental impact

Currently, major challenges are: Cold Starts and High Exhaust Mass Flow.

With contradictory requirements:

- lower catalyst thermal inertial (cold starts)
- bigger catalyst converter (high flow rate)

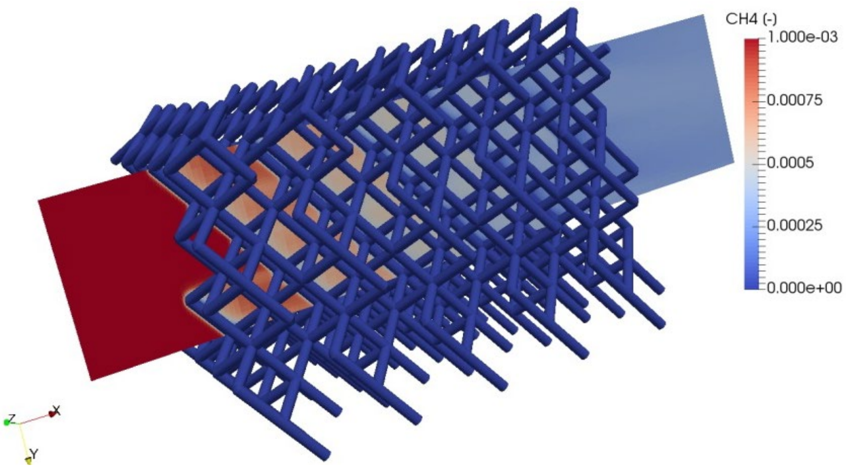
Further critical conditions are long low load operation, typical of hybrid powertrain systems

Focus: structures with high heat and mass transfer characteristics, as well as low flow through resistance

Catalyst performance under mass transfer limitation (steady state)

Simulations for geometrical optimization: CH_4 oxidation in air is studied

Empa
Materials Science and Technology



- Infinite fast Chemistry, mass transfer limited regime → Steady state
  → reactingSimpleFoam
- Single Region No CHT (<3°C),
  → T_{in}=700 K T_w=750 K
- Homogeneous reaction non considered,
- Heterogeneous reactions modelled as B.C.
  → Oxidation of methane

$$X_{sCH4} = 0$$

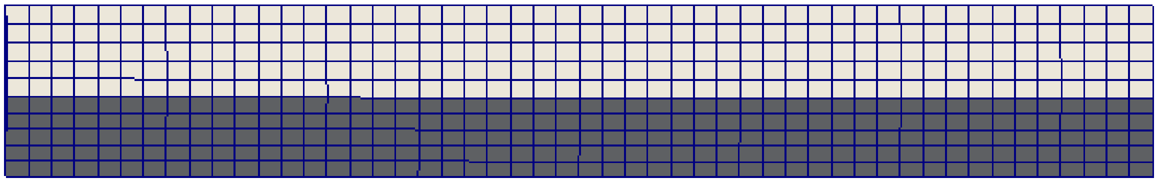
Other species :

$$\frac{\partial X_i}{\partial \boldsymbol{n}} = \alpha_i \frac{M_i}{M_{CH4}} \frac{\partial X_{CH4}}{\partial \boldsymbol{n}}$$

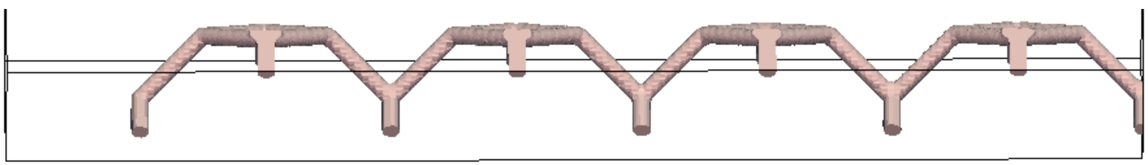
Inert specie: N_2

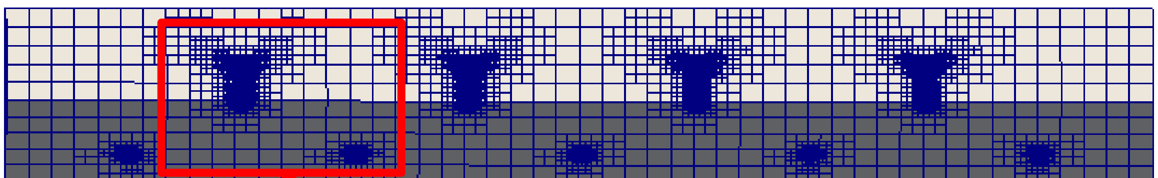
- 4x2x2 Cells + periodic B.C
- Wash coat not modelled

Standard Mesh with increasing resolution towards the surface

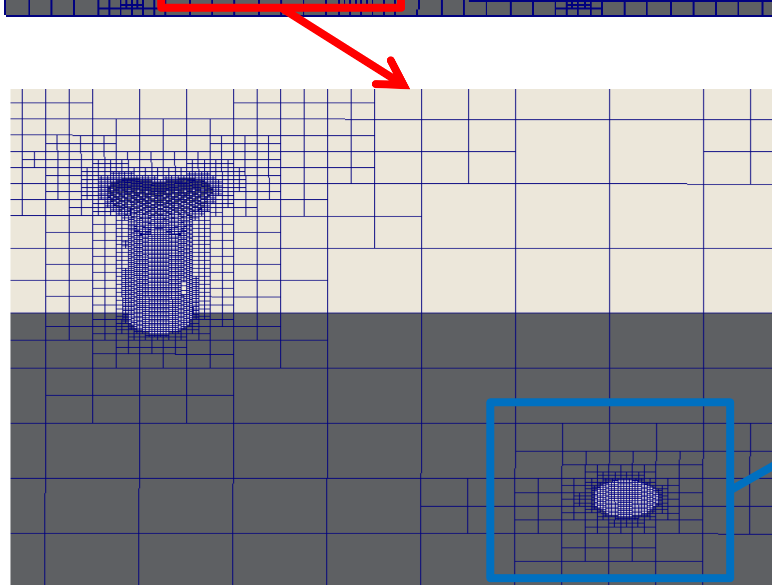


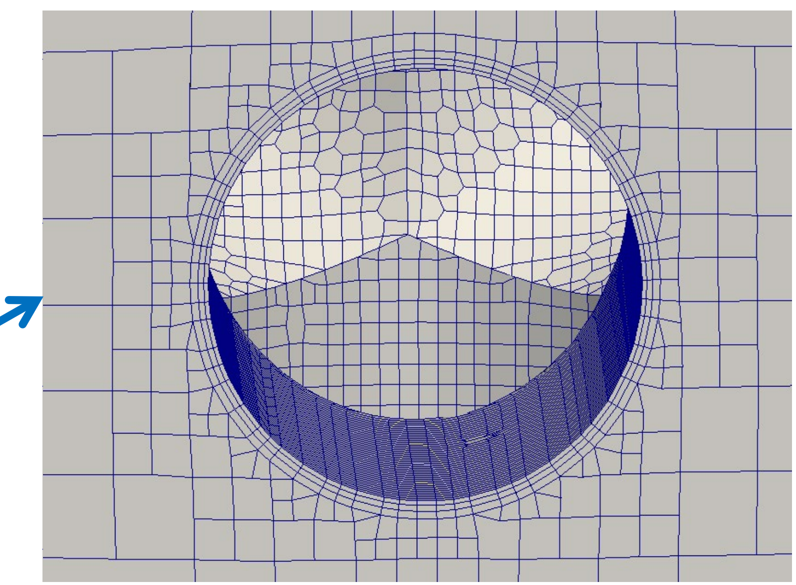
1. Cartesian Block Mesh
2. Foam Surface (STL file)
3. Castellate Mesh
4. Snapp to surface
5. Add Layer



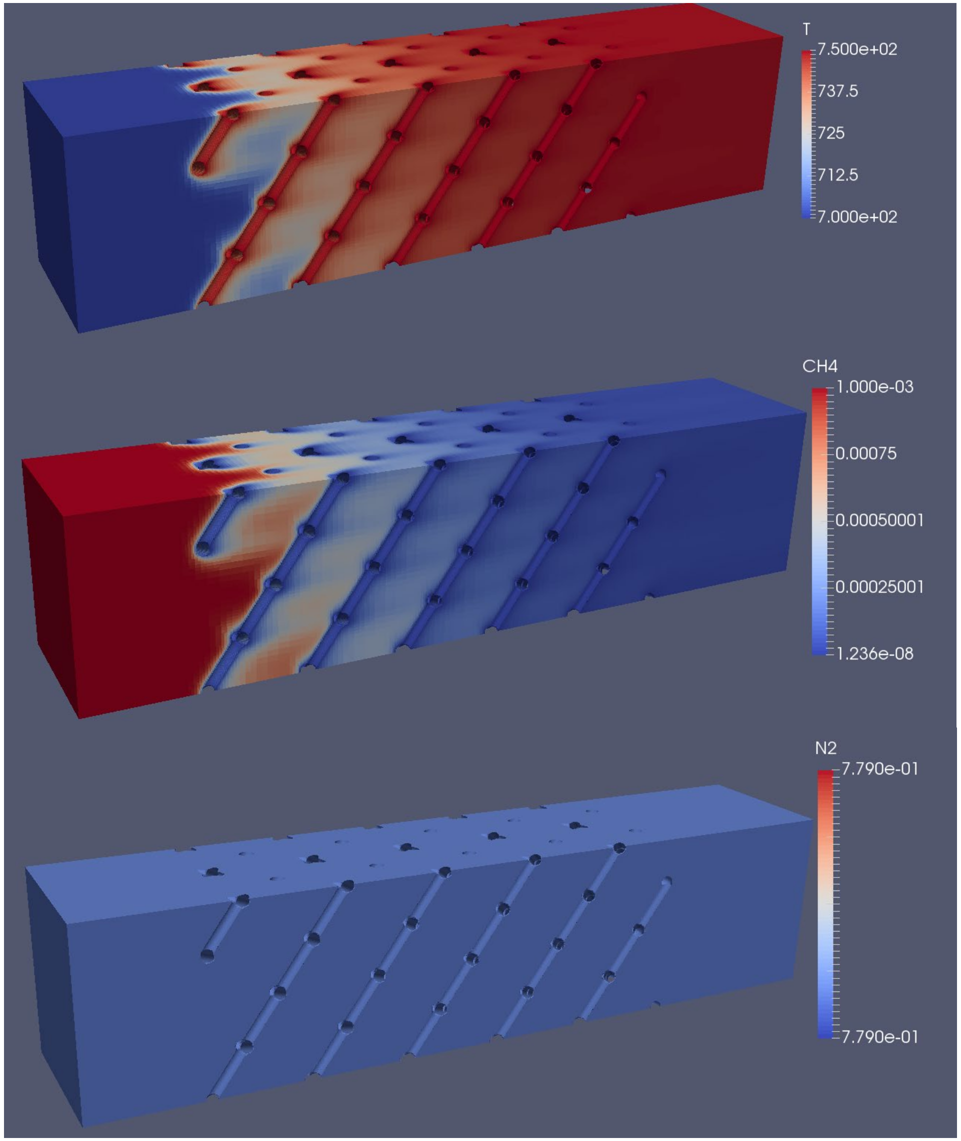


1 Case = (10^6) cells
12 hrs in 1CPU



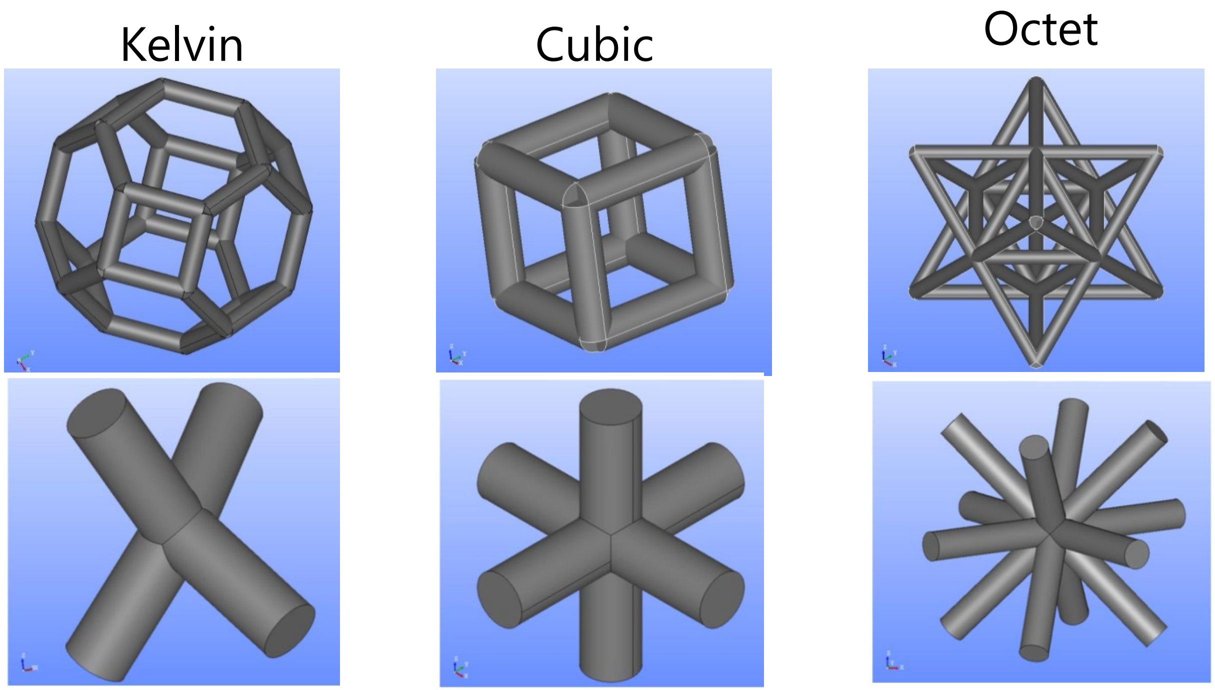


Sample Cubic 45 Cells results:



Inert Specie: N_2

Optimization of cell geometry



Cubic cells tested with 2 flow direction straight and at 45 degree

	CELL	ds	Ls	Lcell	ε	Sv
K2	Kelvin	0.5	2	5.66	0.95	416
C3	Cubic	0.5	3.4	3.36	0.95	416
O6	Octet	0.5	5.6	8.00	0.95	416

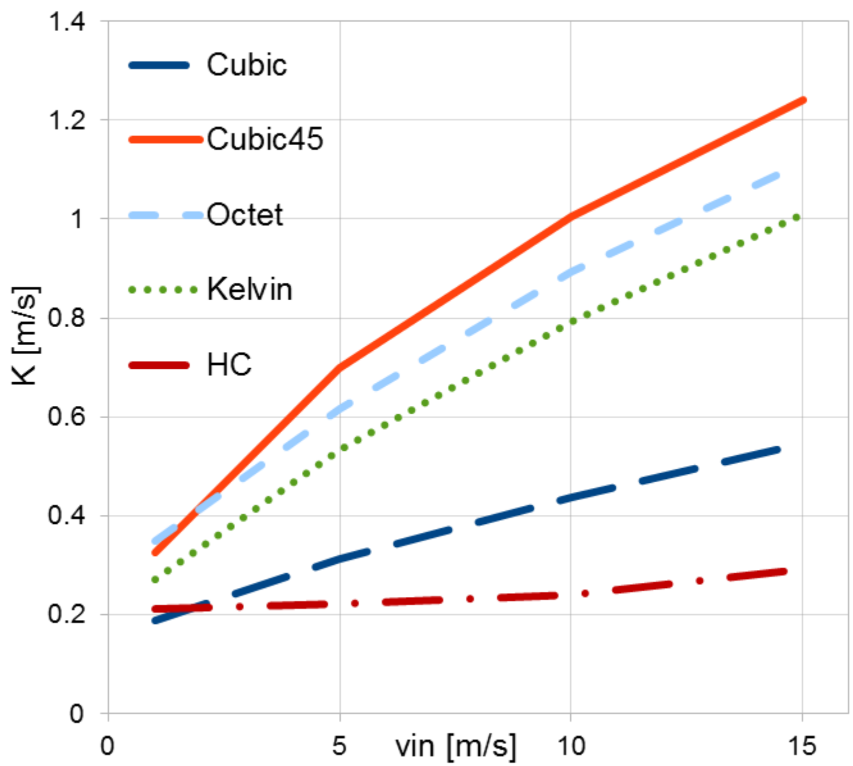
Manufacturing limit

Growing struts L

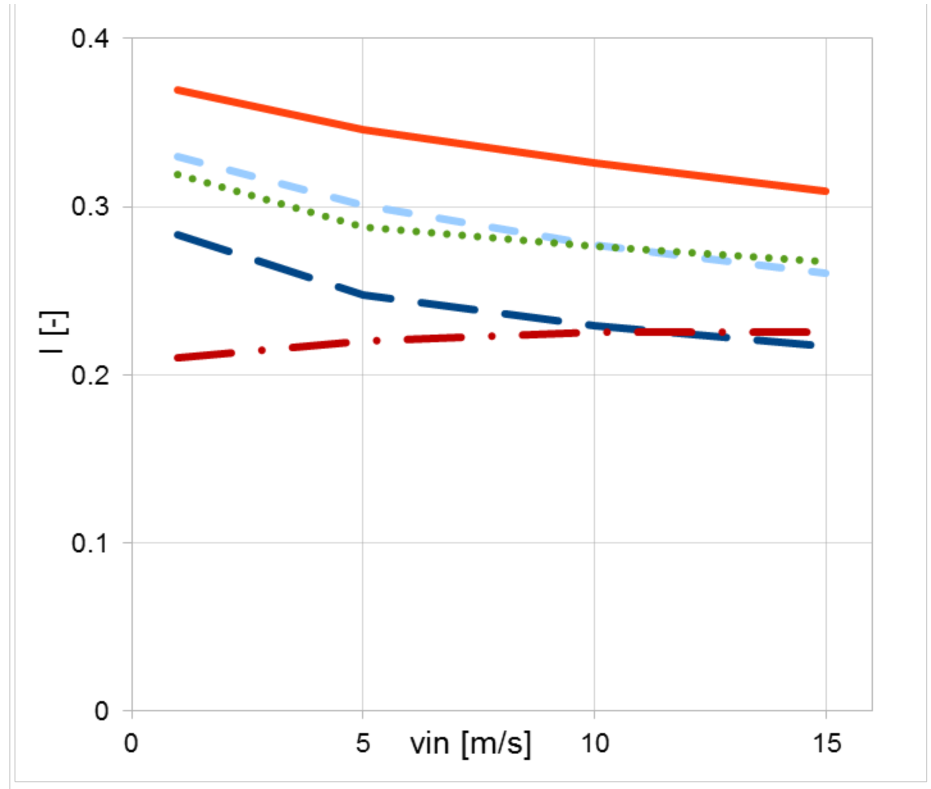
same ε and Sv

1. Rotated cubic cell is the optimal cell for a lattice structure, higher K and I at all velocities

Mass Transfer



conversion/pressure drop trade off



At vel=10m/s C45 requires 4 times less S_w than HC, but 3/2 bigger Volume ($S_{vHC} = 6S_{wCUBIC45}$)

Performance index, I, according to Groppi:

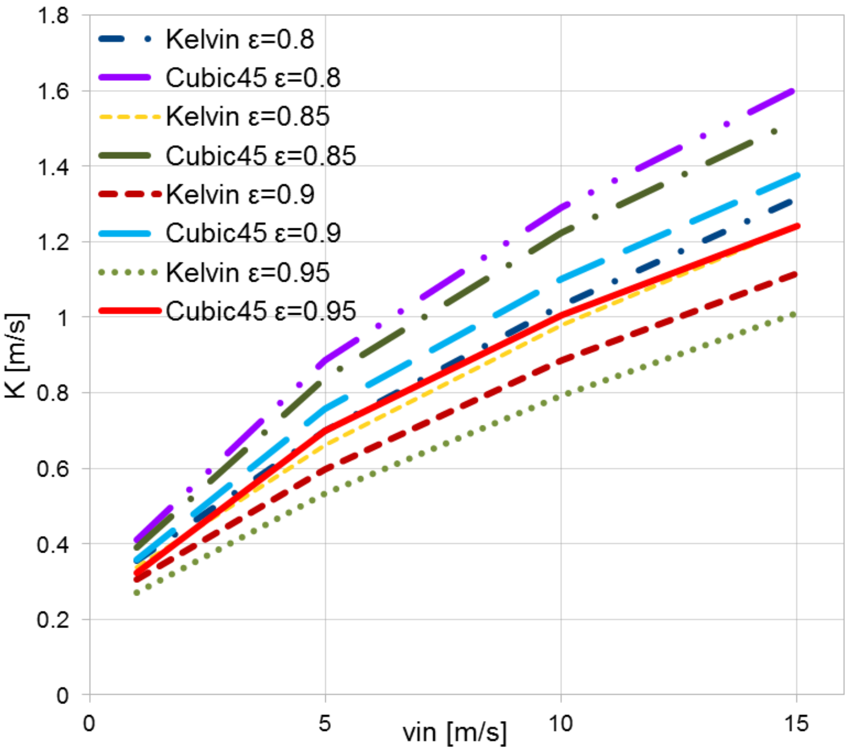
$$I = \frac{-\ln(1-\eta)}{\Delta P \cdot \rho \cdot U^2}$$

Papetti et al., IJoHaMT , (2018)

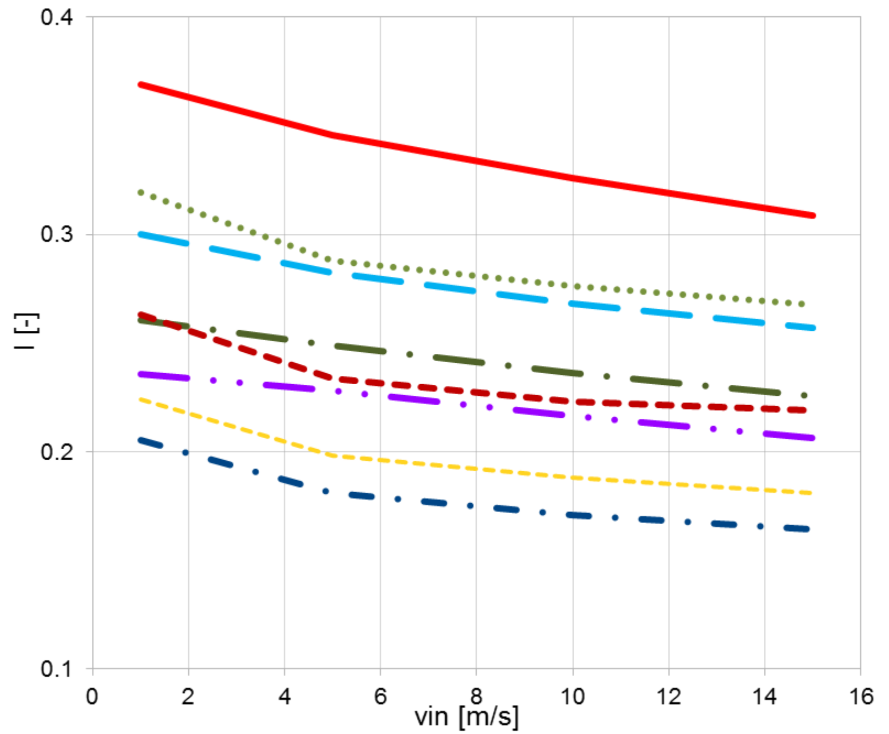
2. Rotated cubic cell is the optimal cell for a lattice structure at all ε,
Higher ε means lower K, but higher I

ε (0.8-0.95), same d_s

Mass Transfer



conversion/pressure drop trade off



$$K = -\frac{ln(1-\eta)}{S_v\, V/Q_{in}}$$

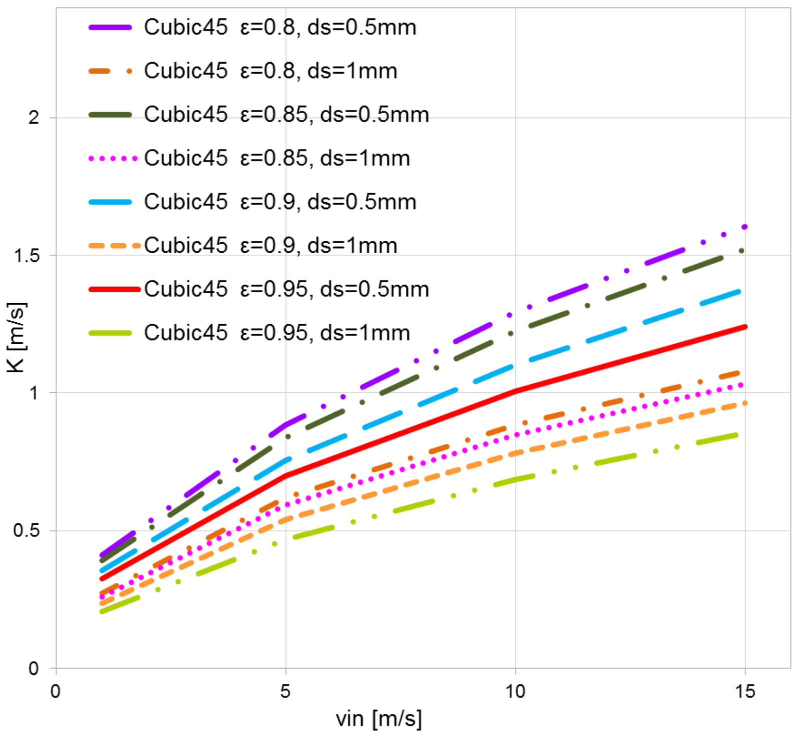
$$S_w = S_v V \propto 1/K$$

Papetti et al., IJoHaMT , (2018)

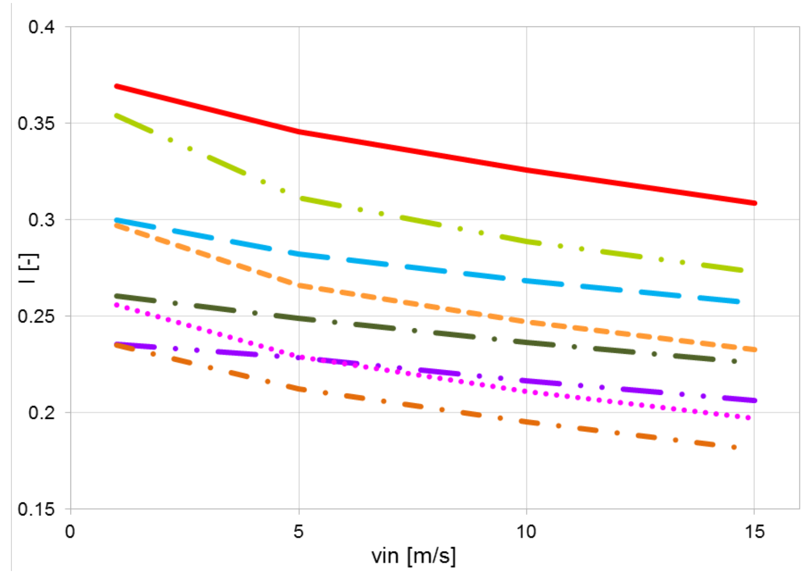
3. Lower ds means higher K and higher I

ε (0.8-0.95), ds (0.5-1) mm,

Mass Transfer



conversion/pressure drop trade off



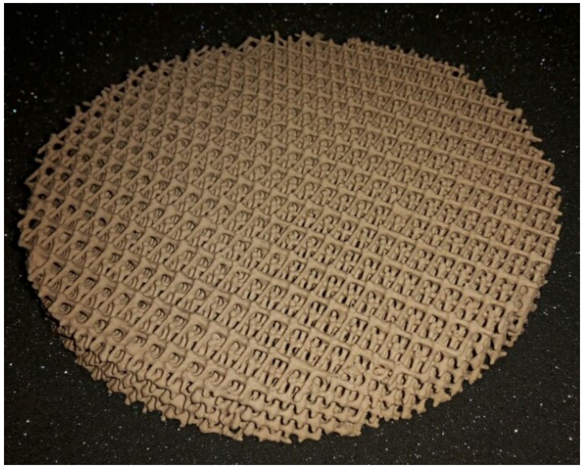
$$K = -\frac{ln(1-\eta)}{S_v V / Q_{in}}$$

$$S_w = S_v V \propto 1/K$$

BEST: Cubic45, higher ε, lower d_s

Papetti et al., IJoHaMT , (2018)

Manufacturing, canning and testing of real size polyhedral catalyst substrates



- Manufacturing and stability constraints: restrict possible parameters

$\varepsilon \leq 0.9$
$d_s \geq 1$ mm

- Hybrid method: AM of the stamp, REPLICA method for the substrates

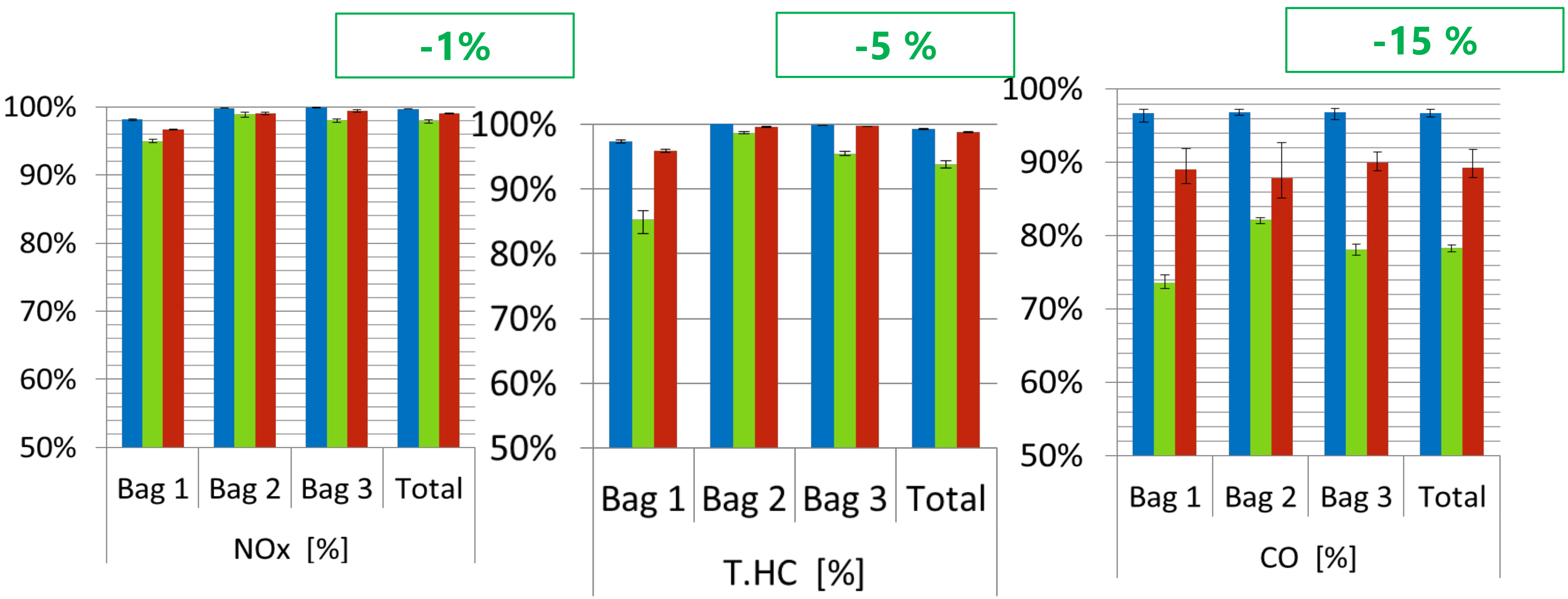
Ls = 3.9 mm
d_s = 1.2 mm
ε = 0.8
Sv= 743 m^2/m^3

We have succeeded in almost reaching the benchmark, the over years developed product has still superior performances

Empa
Materials Science and Technology

- Ref.Ka
- 3dKat
- Vergle

REF HC	AM	HC
V,	V,	1/5PGM
Sw,	1/5 Sw,	V,
PGM	1/5 PGM	Sw,
		1/5PGM

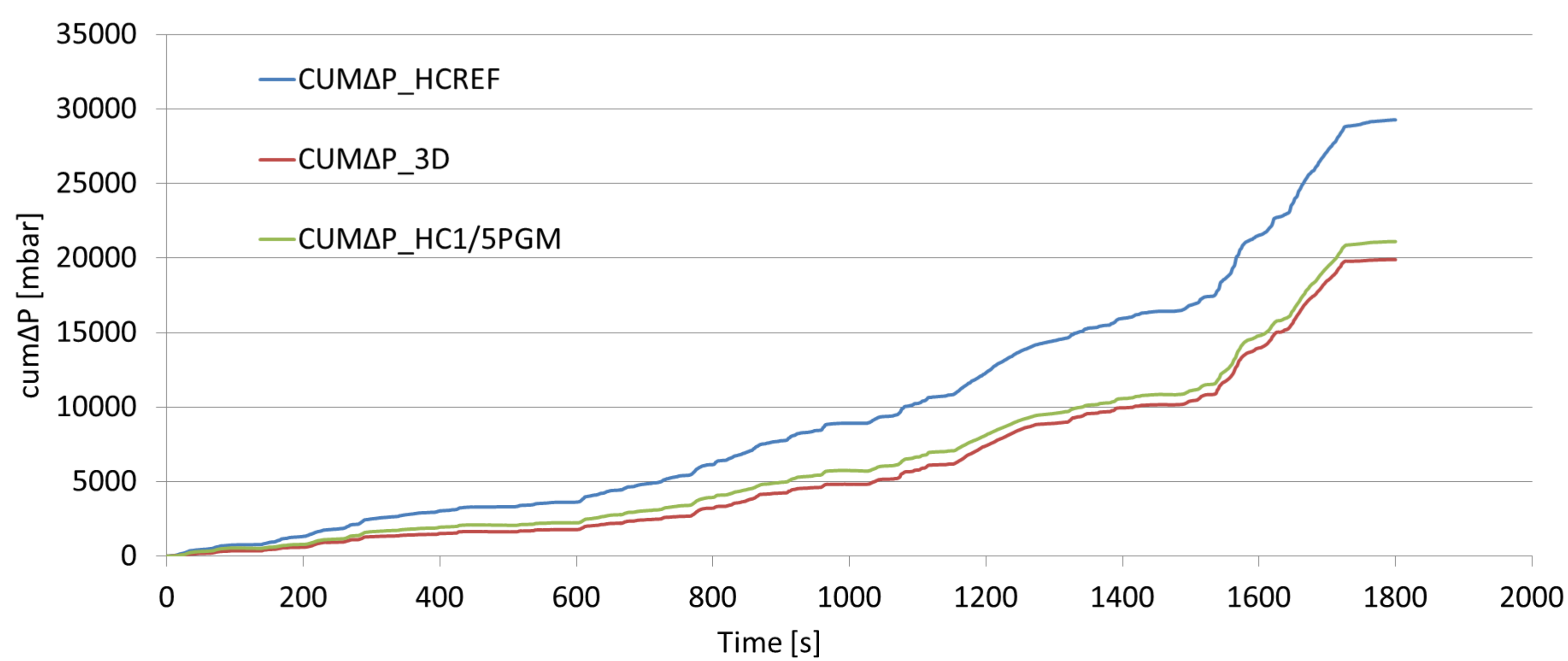


AM have lower pressure loss

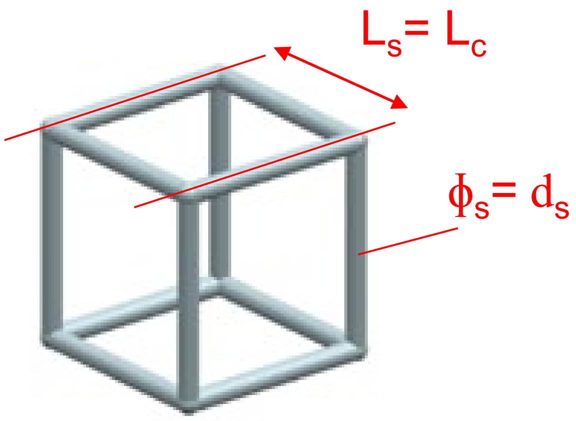
Empa
Materials Science and Technology

- Ref.Ka
- 3dKat
- Vergle

REF HC V, Sw, PGM	AM V, 1/5 Sw, 1/5 PGM	HC 1/5PGM V, Sw, 1/5PGM

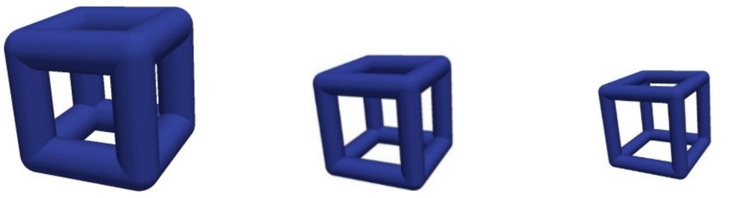


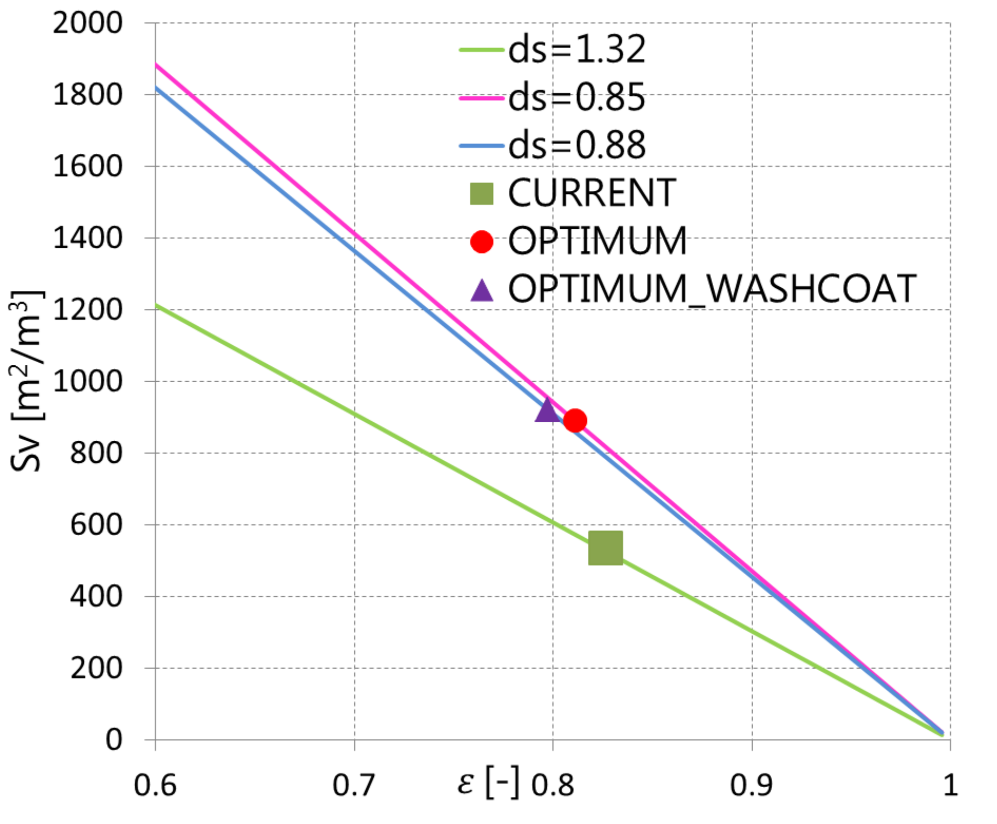
Manufactured Cordierite 3D catalysts had a higher strut diameter than anticipated



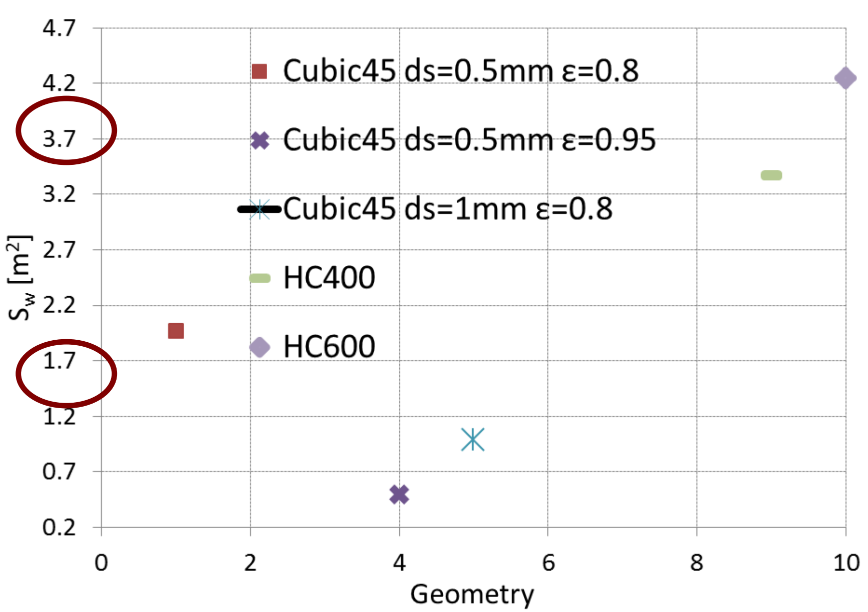
$$\varepsilon = \frac{V_o}{V_{TOTAL}}$$

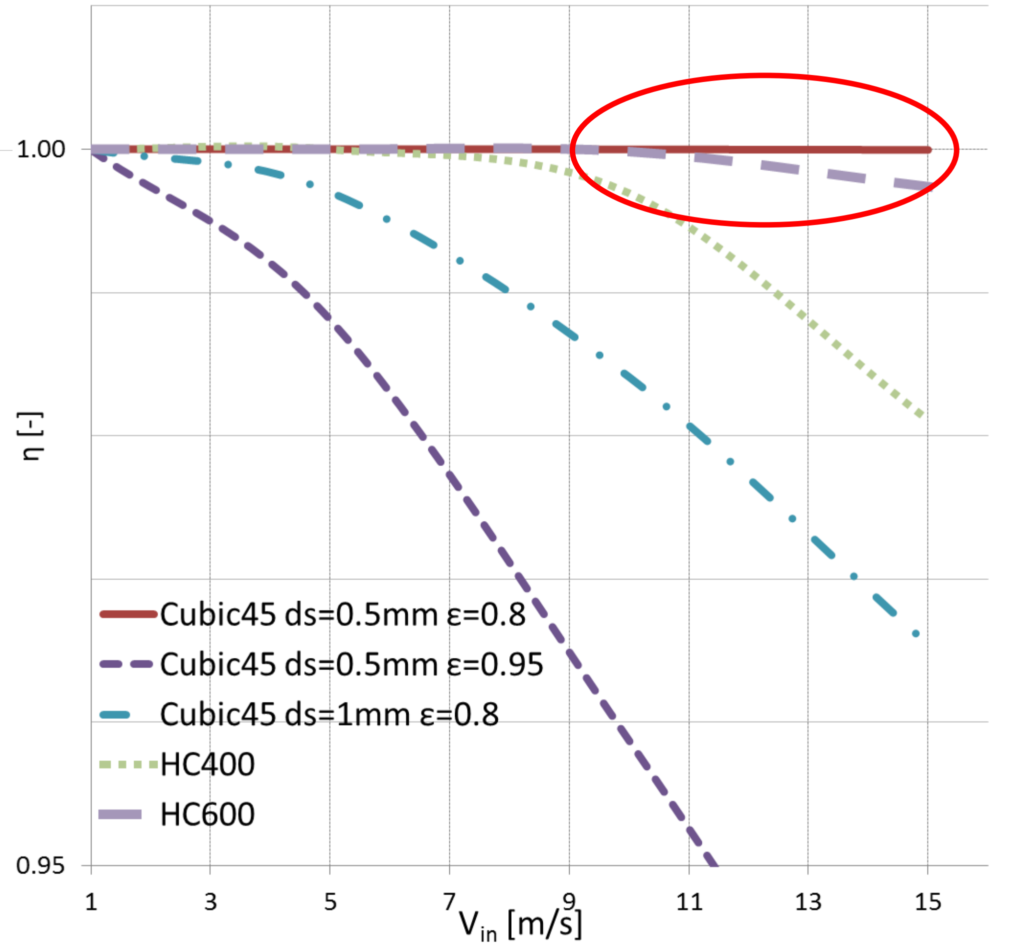
$$S_V = \frac{S_W}{V_{TOTAL}}$$



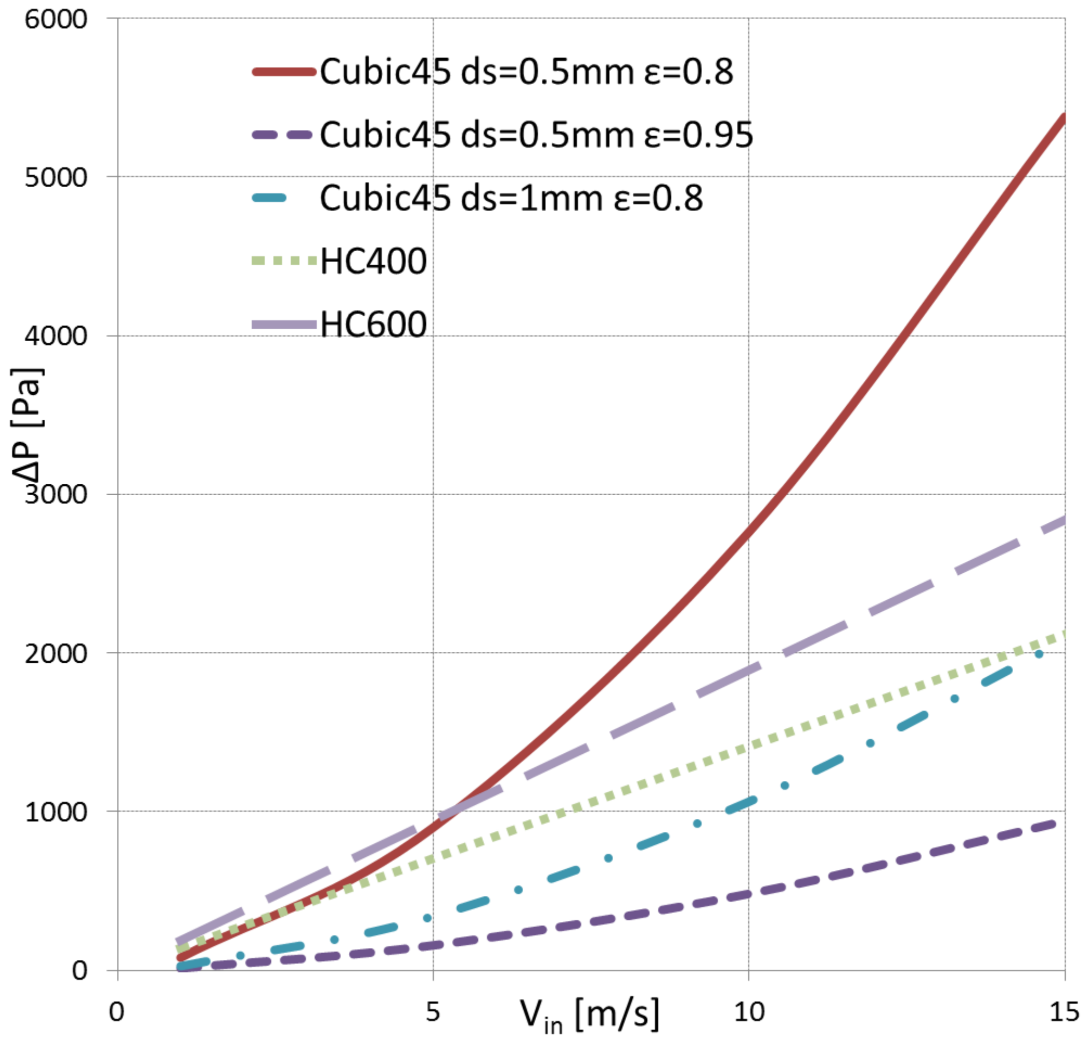


Comparison of entire catalysts with identical V: cubic45 higher conversion than HCs with 2 time less surface





For the simulated configurations, no evident disadvantages in pressure drop

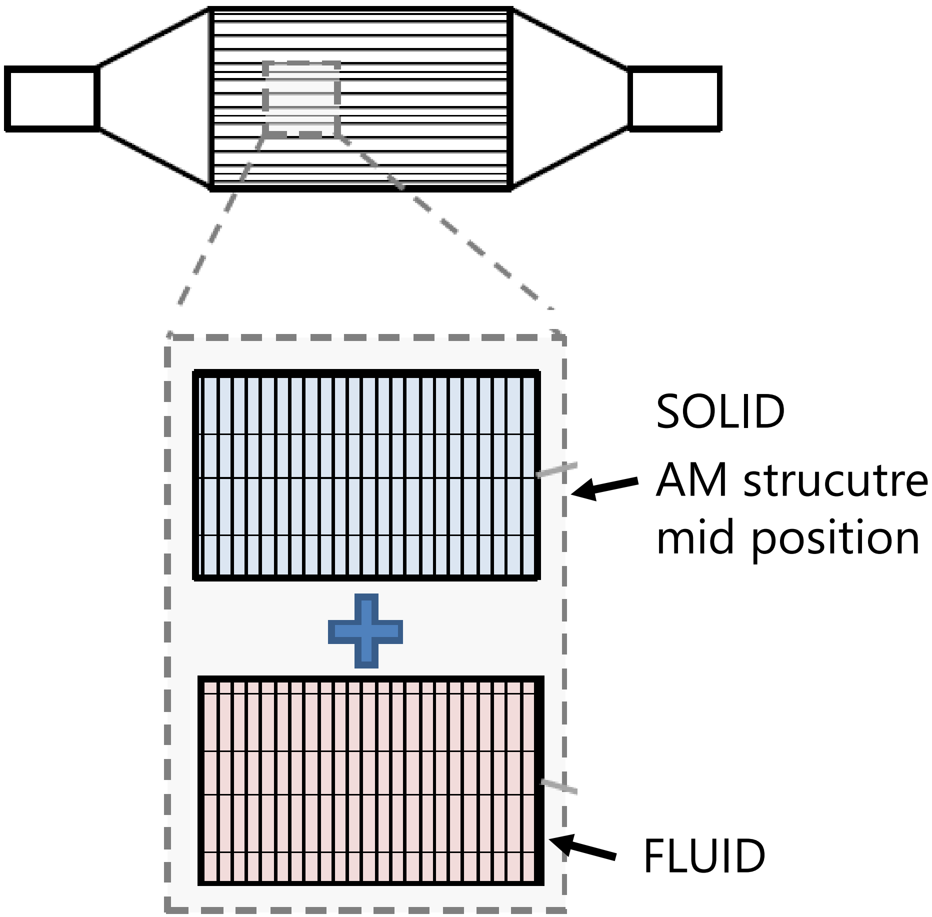


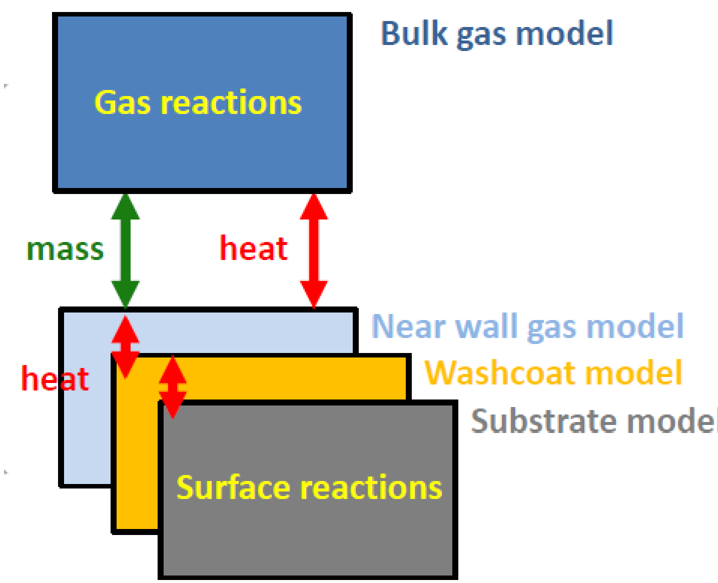
Catalyst performance in transient cold starts

OpenFOAM full-scale, multi region, converter SIMULATIONS: CO oxidation in DOC

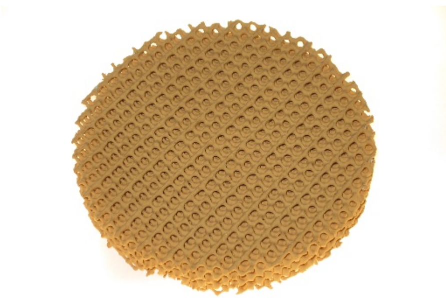
From micro scale simulations or experimental correlations:

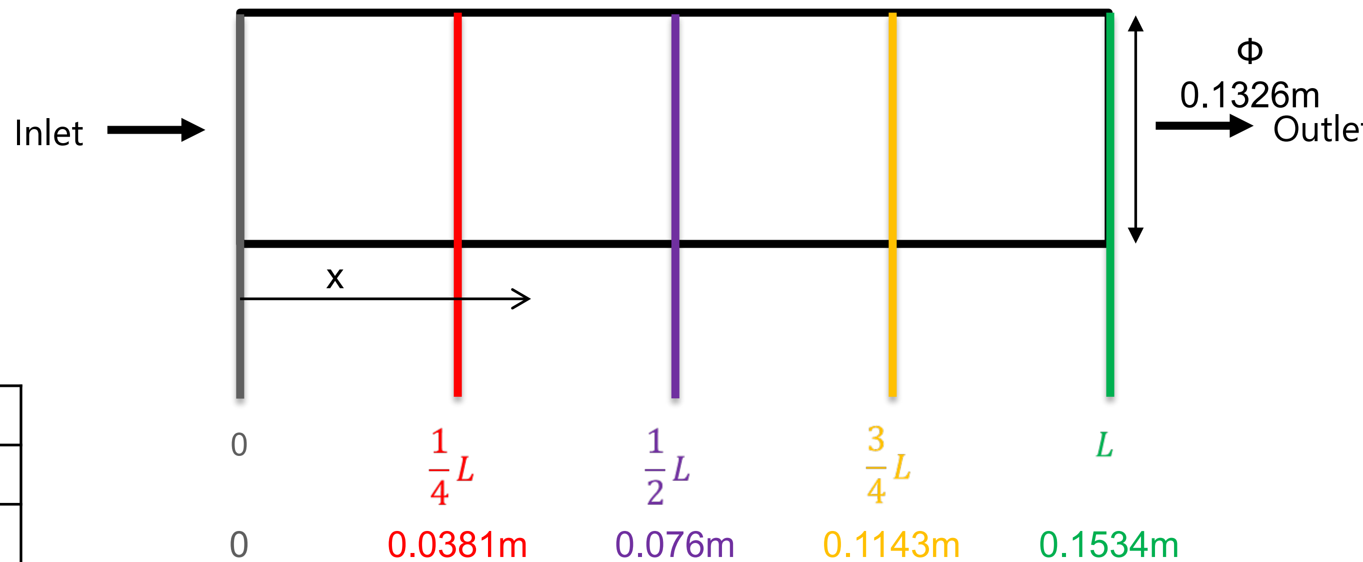
Coupled SOLID-FLUID
- Geometry model
- Permeability model
- Heat transfer models
- Mass transfer model
- Reaction models





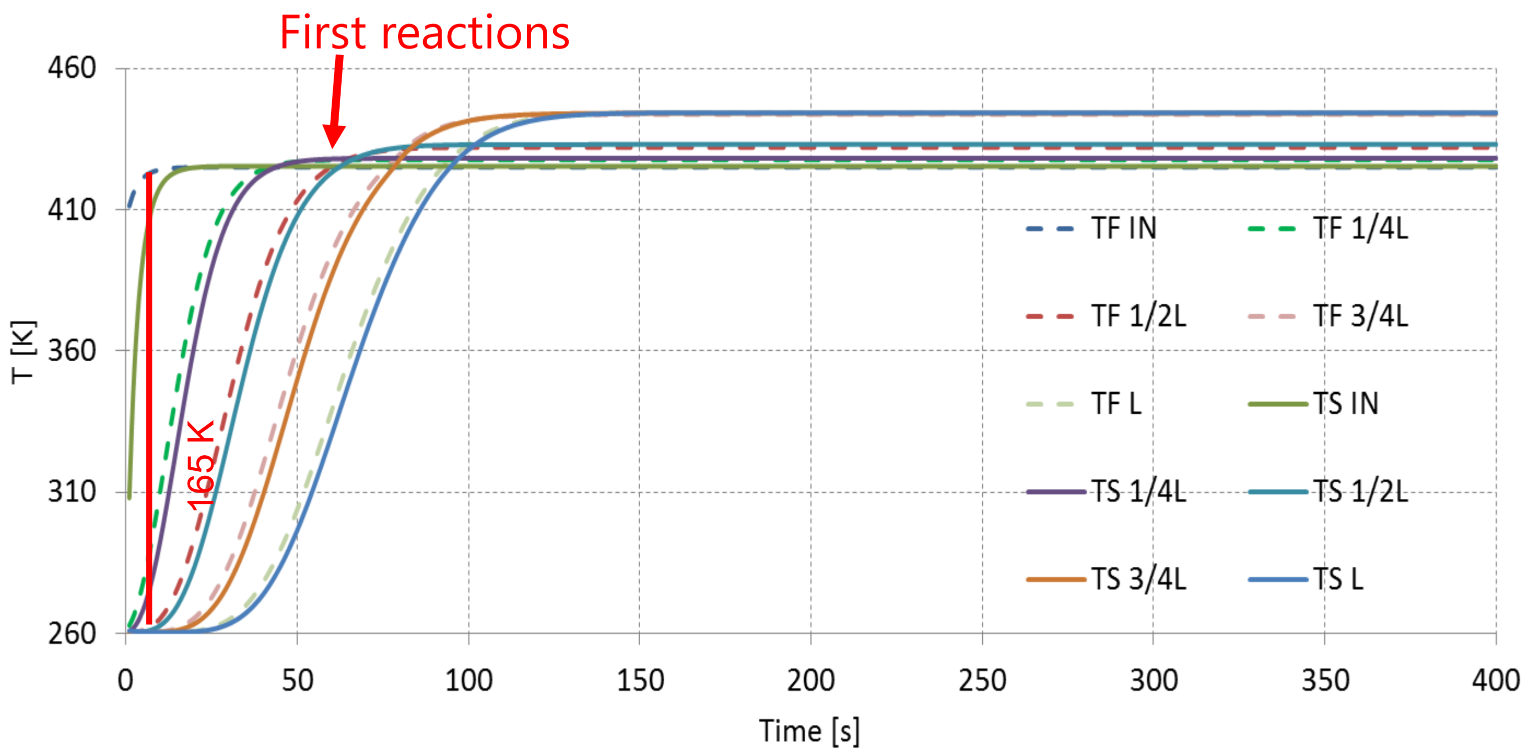
Case study: exhaust inflow mF=const with $TF_{in}(x=0,t)$=const >TS(t=0) 373K < $TF_{in}(x=0,t)$ < 410K 260K < TS(t=0)< 360K





Sv [m^2/m^3]	800
ε [-]	0.82
PGM [g/ft^3]	15
Mass [g]	752.01
Washcoat [g]	121.2
d_{WC} [μm]	30

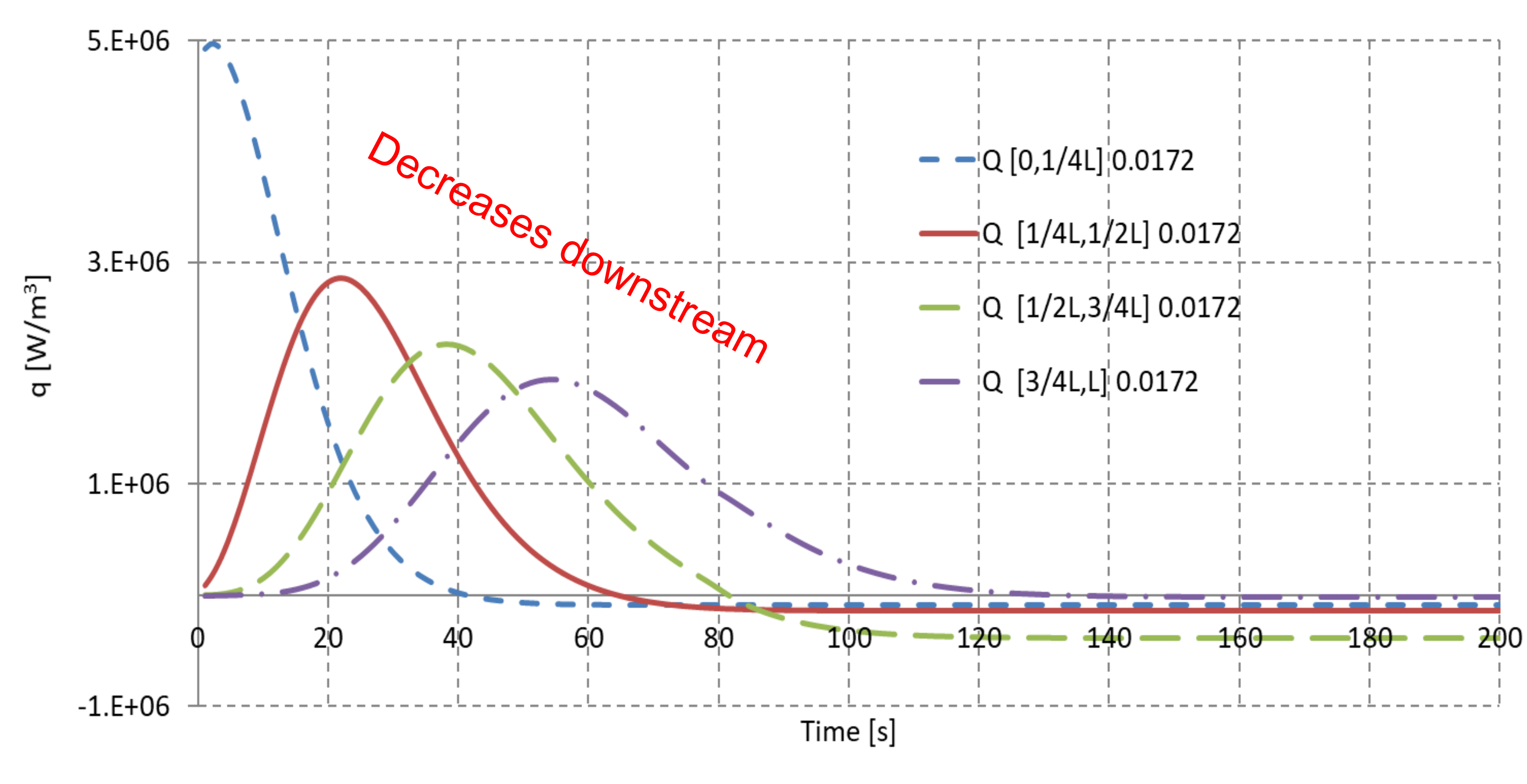
In the entrance, solid is heated up, downstream the fluid is cooled down



TF_{in}=425K TS(t=0s)=260K m_F=0.0172kg/s

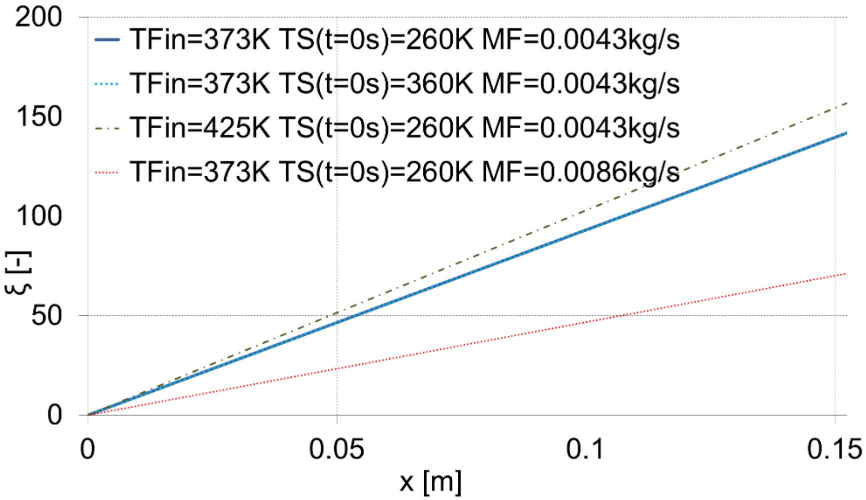
Heat convected is highest in the upstream, however the duration of the heat exchange increases in the downstream: almost homogeneous energy exchange

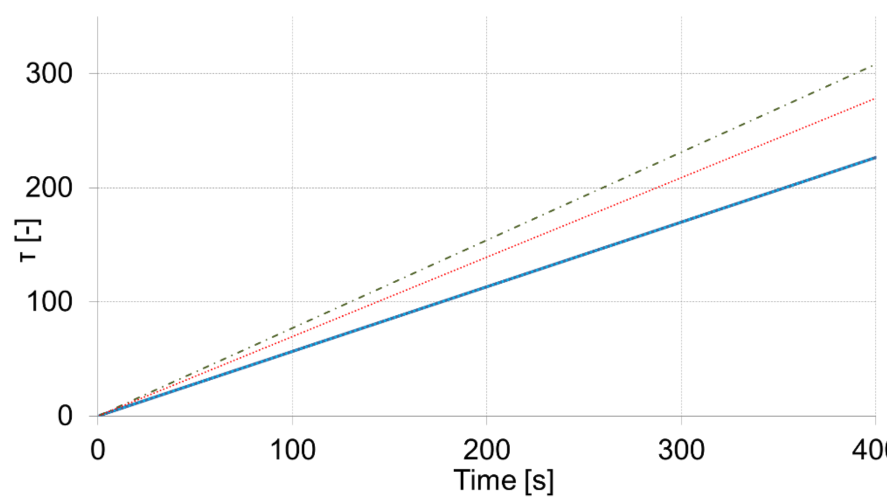
$$\dot{q}_{conv,i,t} = \frac{\dot{m}_F c_{PF}}{\Delta V}\left(T_{F,i,t} - T_{F,i+1,t}\right)$$



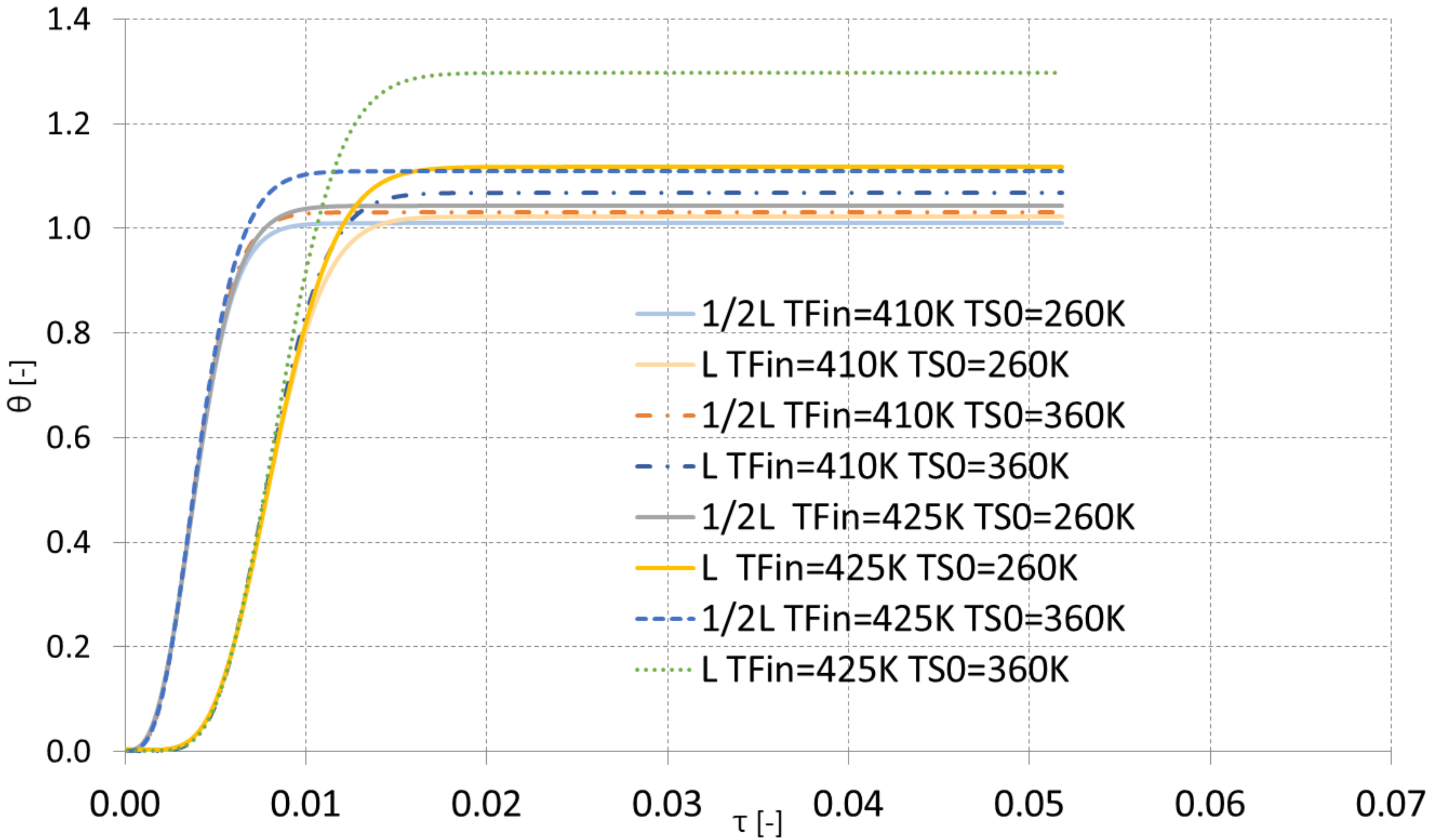
Introduction of dimensionless time, space and temperature differences

$$\theta_S = \frac{T_S - T_0}{T_{F,in} - T_0} \qquad \theta_F = \frac{T_F - T_0}{T_{F,in} - T_0} \qquad \xi = \frac{4Nu\lambda_F x}{\dot{m}_F c_{PF}} = NTU_\theta \qquad \tau = \frac{4Nu\lambda_F t}{A_{S,FRONT}\, \rho_S\, c_S}$$





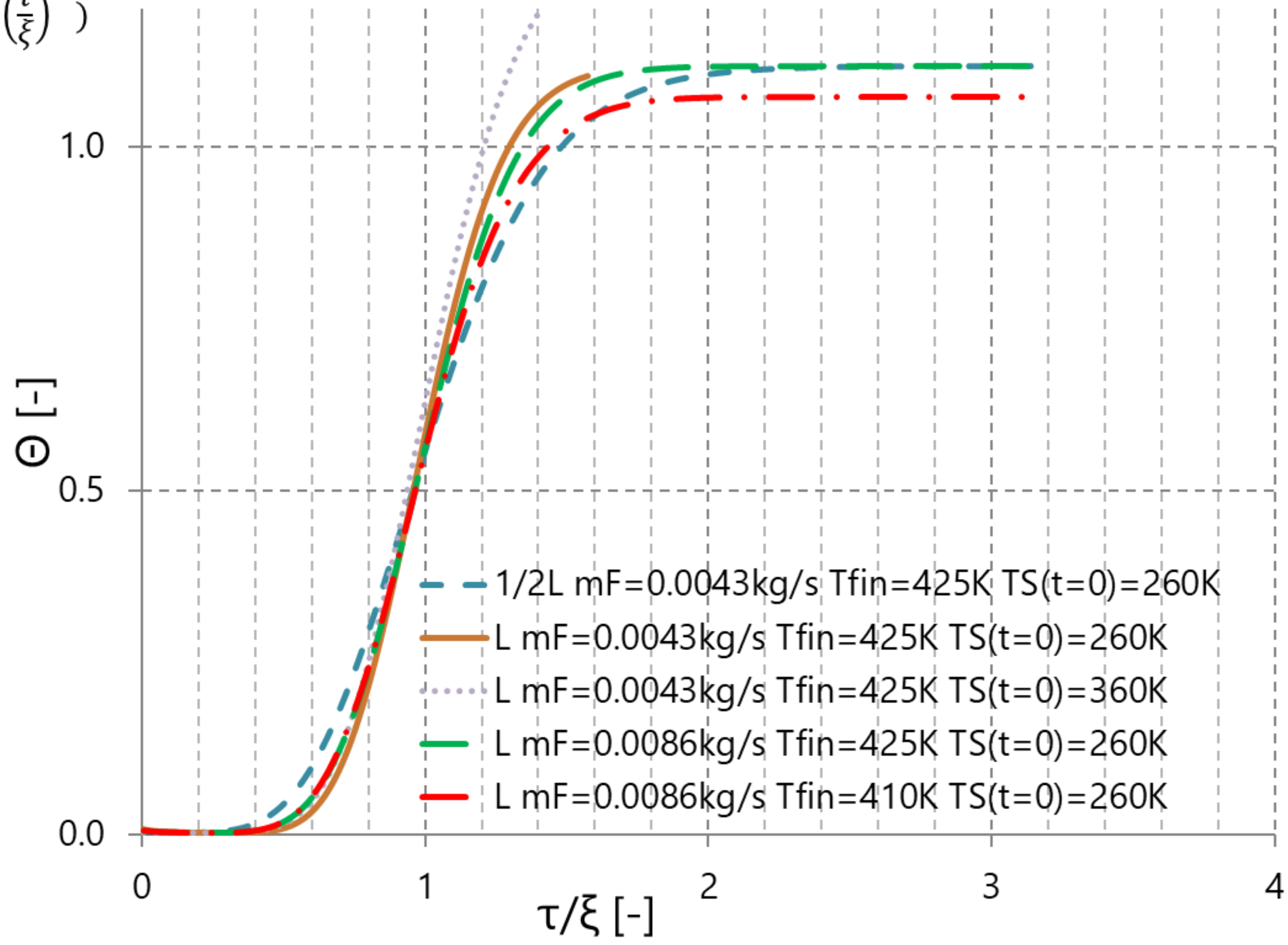
θ_F is neither a function of $T_S(t=0)$ nor T_{Fin}, θ_F is a function of length and m_F



Heat up can be described as an exponential function of τ/ξ

Empa
Materials Science and Technology

$$\theta = \theta\left(\frac{\tau}{\xi}\right) = 1 - e^{\left(-k\left(\frac{\tau}{\xi}\right)^{m}\right)}$$



Numerical Simulations lead to new catalyst structures in combination with new manufacturing techniques

Empa
Materials Science and Technology

- Worldwide first AM manufactured catalyst converter has been tested on a vehicle (manufacturing, coating, mechanical stability, integration)
- Conversion characteristic with 1/5 of precious metals is good almost on the level of the benchmark HC
- Flow resistance lower than benchmark HC
- Experiments confirmed simulation results

Understanding the heat up inside the catalyst is important for cold start reduction

Empa
Materials Science and Technology

- In the entrance, solid is heated up, downstream the fluid is cooled down
- The introduction of dimensionless temperature differences, time and space evidences the self similarity of the catalyst heat up before reactions start
- The catalyst heat up can be approximated analytically with a double logarithmic function in dimensionless coordinates
- Evaluation and assessment of preheating strategies

Empa
Materials Science and Technology

Thank You!

Questions?