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Benoit Rousseau, Salih Ouchtout, Jérôme Delmas, Christophe Le Bozec, Gwenael Biotteau, Steven Le Corre, Jérôme Vicente, Ludovic Charpentier, Cindy Schick, Eric Louradour, et al.

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# Finite Element Solver for Thermo-Hydraulic Optimization of Architected Ceramics (NExT I-Site industrial partnership program: OPTHOCERA): project overview

Benoit Rousseau<sup>1</sup>, Salih Ouchtout<sup>1</sup>, Jérôme Delmas<sup>1</sup>, Christophe le Bozec<sup>1</sup>, Gwenaell Biotteau<sup>1</sup>,  
Steven Le Corre<sup>1</sup>, Jérôme Vicente<sup>2</sup>, Ludovic Charpentier<sup>3</sup>, Cindy Schick<sup>4</sup>, Eric Louradour<sup>4</sup>,  
Christophe Chaput<sup>4</sup>

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CERAM SINTO Bonnac La Côte, France



September 27-30, 2022  
Albuquerque, NM, USA

28<sup>th</sup> SolarPACES Conference

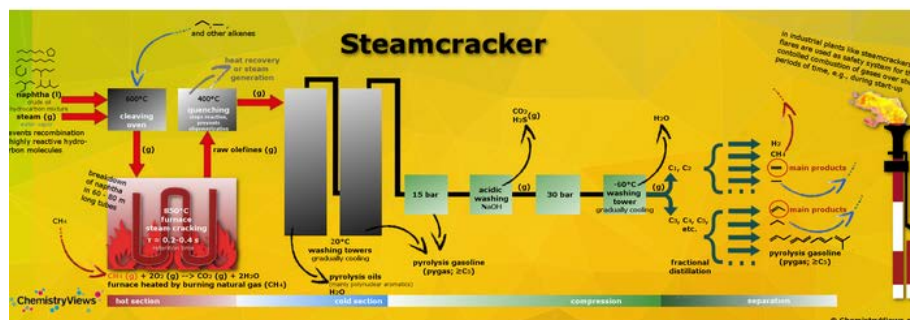
# Decarbonization of high-temperature industrial processes ( $T > 1,000^{\circ}\text{C}$ )

- Stabilization of global warming<sup>1)</sup> → net-zero emission of  $\text{CO}_2$  in human activities (industry, transport, residential sector...)
- Industry accounts for 32 % of the final energy consumption with 74 % of this component is required for heat production of which 90 % is provided by burning fossil combustible (coal, oil, gas)
- 48 % of energy consumption for producing industrial heat is due to high-temperature processes ( $T > 400^{\circ}\text{C}$ )

## Mineral sector



## Production of fuels and chemical commodities



Zimmermann in *Ullmann's Encyclopedia of Industrial Chemistry*, Wiley-VCH, Weinheim, Germany, 2009

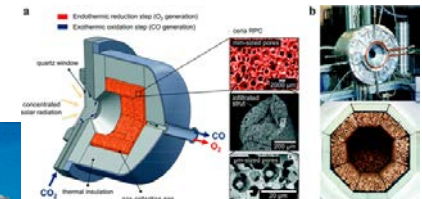
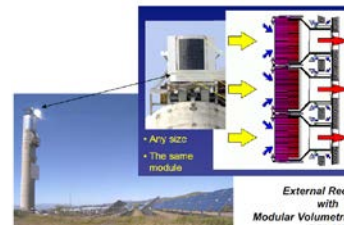
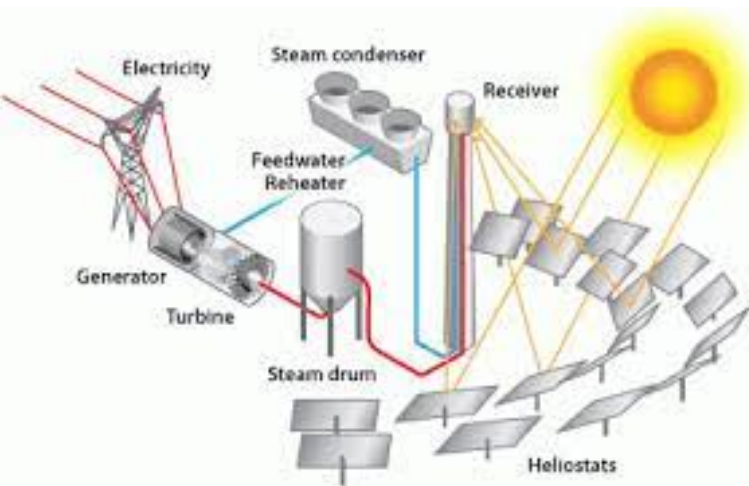
## Metallurgical sector



<sup>1)</sup> Masson-Delmotte et al., In: *Climate Change 2021 Contribution of Working Group I to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change*.

# Interest of high-temperature concentrated solar heat

- Solar energy → abundant : 1% of the  $3.8 \times 10^{24}$  joules of solar energy reaching the earth's surface every year → 40 times the electricity generated globally
- But dilute, geographically non uniform, temporally intermittent, variable
- Concentration<sup>2)</sup> of solar radiation (paraboloid dishes and solar towers) →  $1,000^\circ\text{C}$  ( with incident fluxes >  $1\text{MW}/\text{m}^2$ )

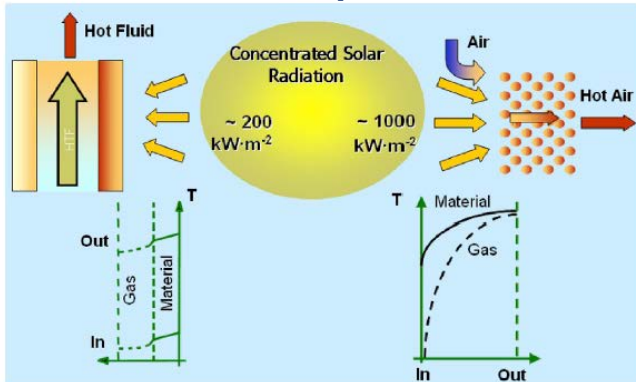


- Development of **high-temperature solar receivers with high solar-to-heat conversion efficiency and service life of 10,000 cycles under harsh conditions** → thermal, mechanical, material challenges

<sup>2)</sup> Romero, M., Steinfeld, A., 2012. Concentrating solar thermal power and thermochemical fuels. Energy Environ. Sci. 5, 9234–9245

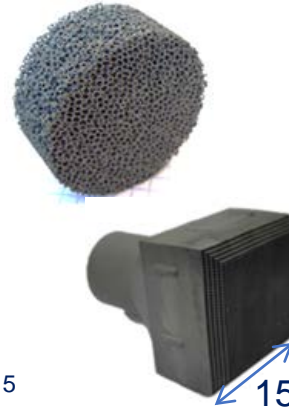
# Volumetric solar receivers = radiative-convective heat exchangers

## Principle



Avila-Marin et al., Renewable and Sustainable Energy Reviews, 2019, 111 15

## Conventional 3D geometries

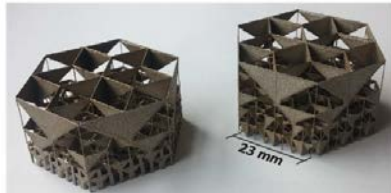
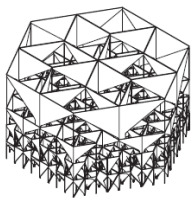


Refractory porous ceramics ( $\text{SiC}$ ,  $\text{Al}_2\text{O}_3$ ,...)

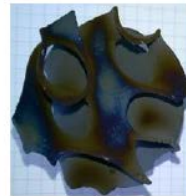
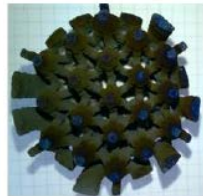
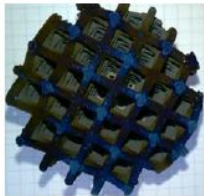
- High solar absorptance
- Good thermal conductivity
- High volumetric surface
- Low thermal emittance
- High thermal shock resistance

## New concepts based on additive manufacturing coupled with radiative transfer design

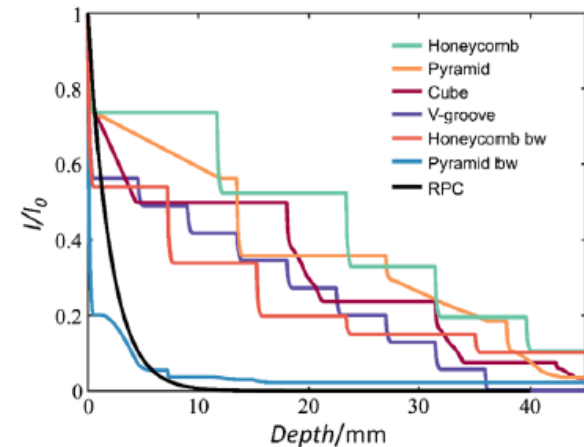
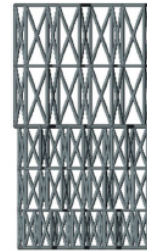
→ Improvement of the volume propagation of concentrated solar light, reduction of thermal emission



Luque et al., Solar Energy, 2018, 174, 342

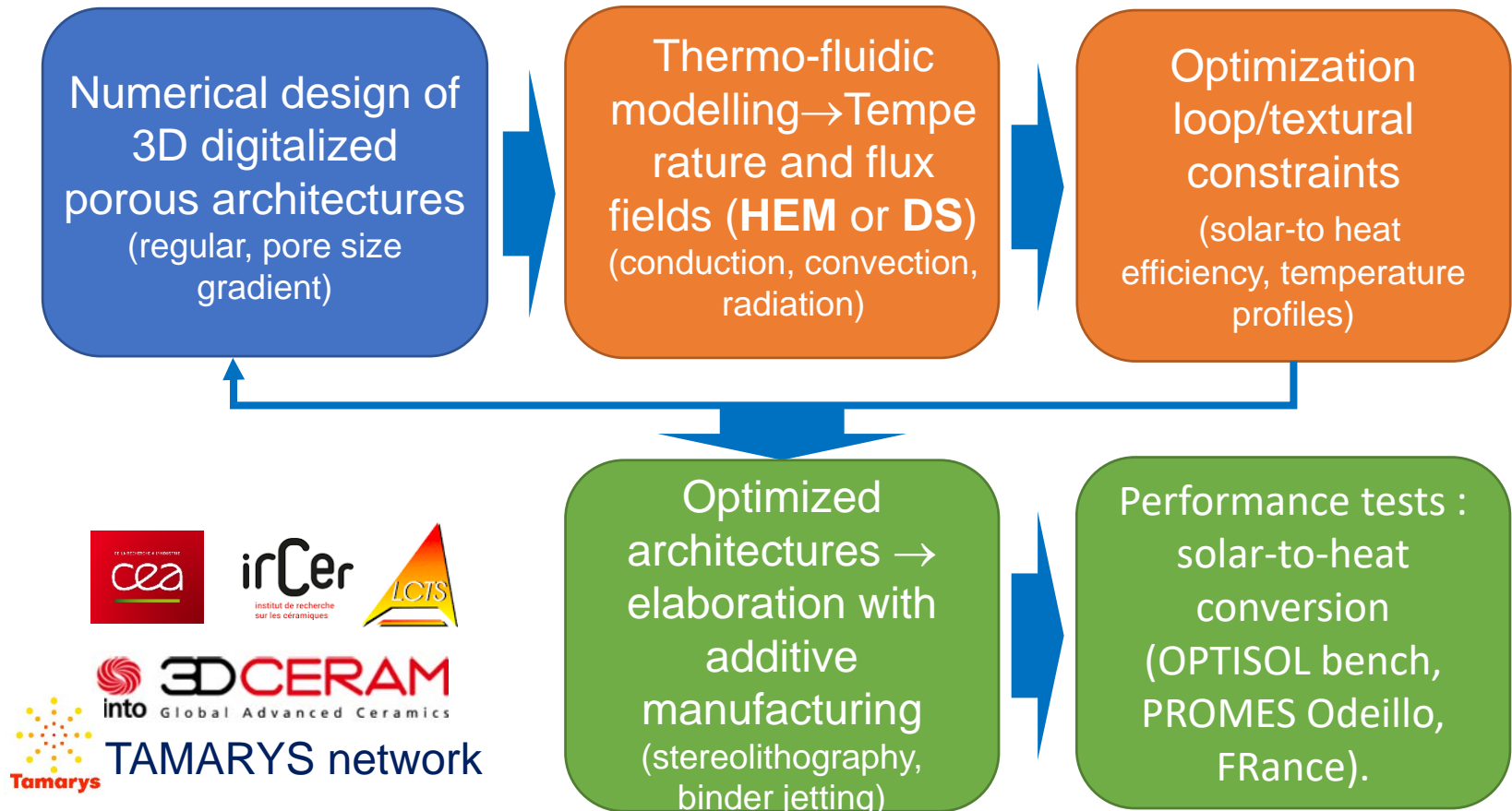


Heisel et al., Solar Energy Materials and Solar cells, 2021, 231, 111336



Hoes et al., Energy Technol. 2019, 7, 1900484

# Numerical design approach coupled with additive manufacturing



HEM : Homogeneous Equivalent Method → continuous scale approach  
DS : Detailed Simulation → pore scale approach

# OPTHOCERA program (1 year)



Numerical design of  
3D digitalized  
porous architectures  
(regular, pore size  
gradient)



Conductive-  
radiative  
modelling → Temper  
ature and flux fields  
(HEM and DS)



Selected  
architectures  
according to Planck  
number →  
elaboration by  
stereolithography

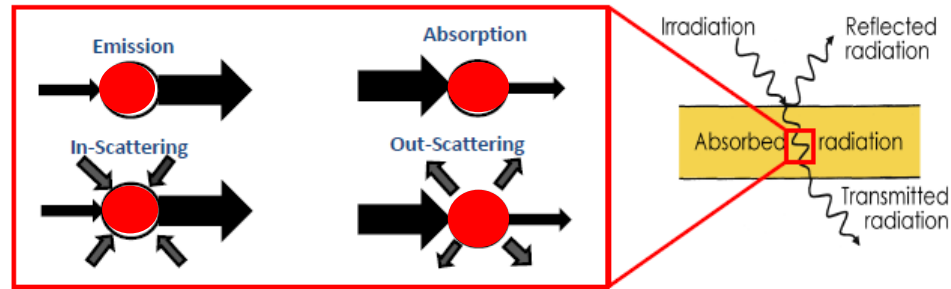
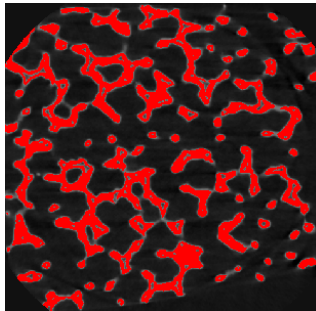


Performance tests :  
solar-to-heat  
conversion  
(OPTISOL bench,  
PROMES Odeillo,  
France).

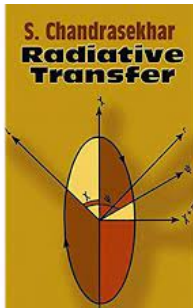
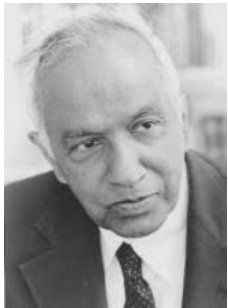


# Radiative Transfer Equation : modelling of volume propagation of thermal and solar radiations

- Macro-porous ceramics → semi-transparent media (absorption, scattering, emission)
- Valid if the medium is homogeneous, continuous and weakly spatially correlated



$$\hat{\Omega} \cdot \nabla I_\nu(s, \hat{\Omega}) + (\kappa_a + \kappa_s) I_\nu(s, \hat{\Omega}) - \kappa_s \int_{4\pi} I_\nu(s, \hat{\Omega}') P(\hat{\Omega}' \rightarrow \hat{\Omega}) d\hat{\Omega}' - \kappa_a I_{P\nu} = 0$$



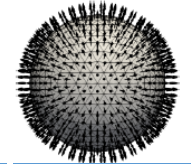
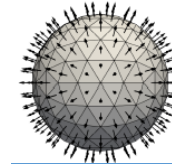
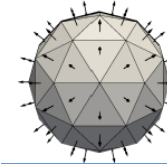
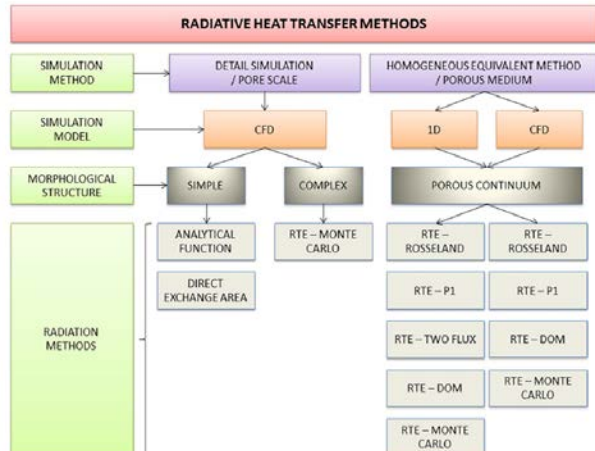
Chandrasekhar, Radiative Transfer, Dover, 1960

$$\nabla \cdot \dot{q}''(s) = \int_0^\infty \kappa_{av} 4\pi I_{bv}(T) d\nu - \int_0^\infty \int_{4\pi} \kappa_{av} I_\nu(s, \hat{\Omega}) d\Omega d\nu$$

$$\rho c_p \frac{\partial T}{\partial t}(s) = \nabla \cdot (k_{cond} \nabla T(s) - \dot{q}''(s))$$



# Methods for solving the steady-state RTE



~10<sup>7</sup> tetrahedral elements

80 directions

320 directions

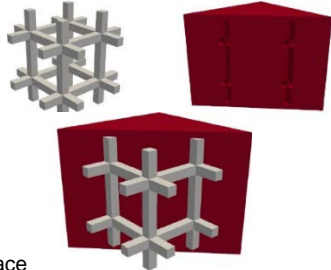
1280 directions

Fast, robust, accurate parallelized vectorial FEM solver

Badri et al., Journal of Computational Physics, 2018, 360, 74-92  
 Badri et al. Journal of Quantitative Spectroscopy and Radiative Transfer 212 (2018): 59-74

Avila-Marin et al., Renewable and Sustainable Energy Reviews, 2019, 111 15

**Detailed Simulation (DS)**  
(discrete scale model)



**Rosseland model**

$$\nabla \cdot \left( \frac{16n^2\sigma_B}{3(\kappa_a + \kappa_s)} T^3 \nabla T \right) = \nabla \cdot k_R \nabla T$$

**Homogeneous Equivalent Model (HEM)**  
(continous scale model)

$$\widehat{\Omega} \cdot \nabla I(s, \widehat{\Omega}) + (\kappa_a + \kappa_s) - \kappa_s \int_{4\pi} I(s, \widehat{\Omega}') P(\widehat{\Omega}' \rightarrow \widehat{\Omega}) d\widehat{\Omega}' - \kappa_a \frac{1}{\pi} \sigma_B n^2 T^4 = 0$$

$$P(\widehat{\Omega}' \rightarrow \widehat{\Omega}) = \frac{1}{4\pi} \frac{1 - g^2}{(1 + g^2 - \widehat{\Omega} \cdot \widehat{\Omega}')^{3/2}}$$

$$\kappa_e = \kappa_a + \kappa_s = 4.8 \frac{(1 - p)}{d_{nom}} \quad \text{with} \quad \kappa_a = \varepsilon \kappa_e \quad \text{and} \quad \omega = \frac{\kappa_s}{\kappa_s + \kappa_a}$$

solid interface

$$\varepsilon n^2 \sigma_B (T_{S-V}^\partial)^4 - \varepsilon \int_{\widehat{\Omega} \cdot n_s > 0} I(\widehat{\Omega} \cdot n_s) |d\widehat{\Omega}| = 0$$

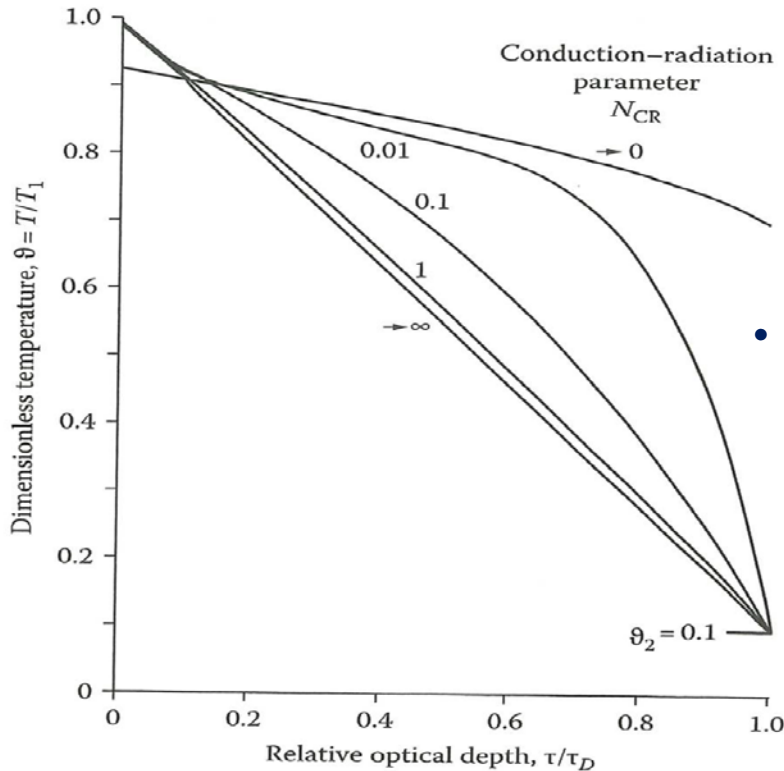
fluid phase

$$\widehat{\Omega} \cdot \nabla I(s, \widehat{\Omega}) = 0$$

Local radiative properties from the bulk

Effective radiative properties → porosity, nominal pore diameter and emissivity

# Use of the FEM solver for analyzing the coupling between conduction and radiation within a 1D slab sandwiched by a hot and a cold wall



Viskanta & Grosh JHT (1962)

- 1D layer of translucent conducting-radiating medium between two parallel black walls at temperature  $T_1$  et  $T_2$  with  $\theta = T/T_1$  et  $\theta_2 = T_2/T_1$

$$N = \frac{k_{cond}\kappa_a}{4\sigma_B T_1^3}$$

Planck or Stark number

$$N \rightarrow \infty$$

Pure conductive regime

$$N \rightarrow 0$$

Dominant radiative regime

For a porous ceramic with absorption and scattering phenomena



$$N = \frac{k_{cond}(\kappa_a + \kappa_s)}{4\sigma_B T_1^3}$$

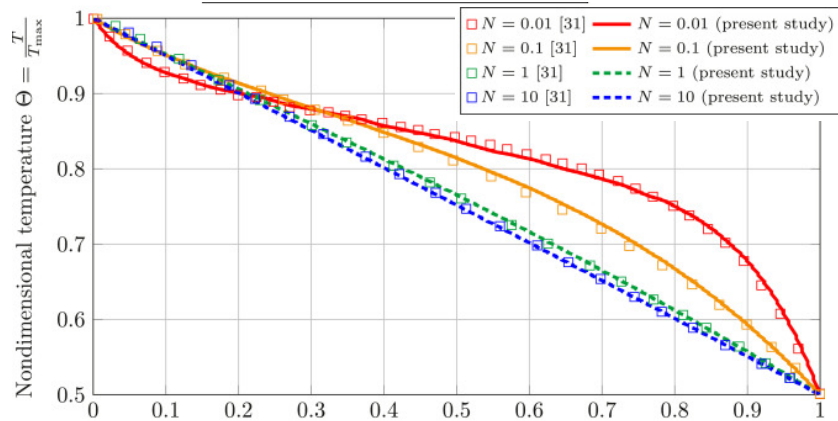
R. VISKANTA  
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Argonne National Laboratory,  
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Professor of Mechanical Engineering,  
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Lafayette, Ind.  
Assoc. Mem. ASME

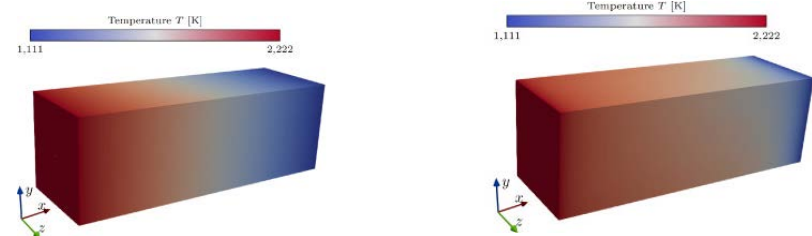
## Heat Transfer by Simultaneous Conduction and Radiation in an Absorbing Medium

*Heat transfer by simultaneous conduction and radiation in a thermal radiation absorbing and emitting medium is considered. Consideration is given to a one-dimensional system consisting of two, diffuse, nonblack, infinite, isothermal, parallel plates separated by a finite distance. The space between the plates is filled with a thermal radiation absorbing and emitting medium. The problem is formulated in terms of a nonlinear integro-differential equation and the solution is obtained by reducing it to a nonlinear integral equation. The numerical results are obtained by an iterative method. The temperature distributions and heat transfer are calculated. Two approximate methods for formulating radiant heat-transfer problems are presented and comparisons of the results are made with the most exact solution.*

# Comparison between HEM model/exact solution from Viskanta

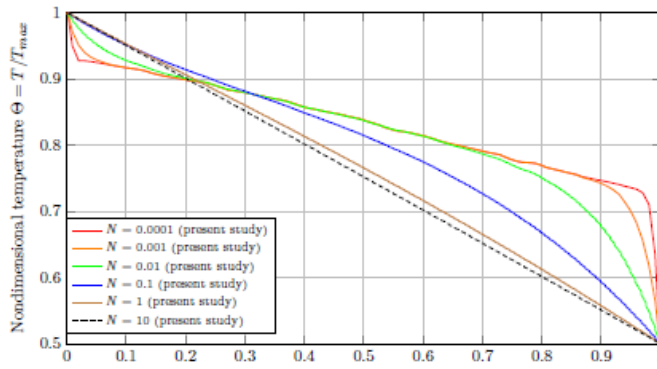


$\theta_2 = 0.5$ ;  $T_1 = 2,222$  K,  $T_2 = 1,111$  K,  $\kappa_a = 2,625$  m<sup>-1</sup>,  $\kappa_s = 0$



$N \rightarrow 0$

- Dominant radiative regime
- Increase of T near the cold wall
- $\tau = 0.9$  (+36 %)
- $\rightarrow$  @T=700 K, +252 K
- low  $\kappa_e$ : for a given  $p$ , high  $d_{nom}$  (low PPI)



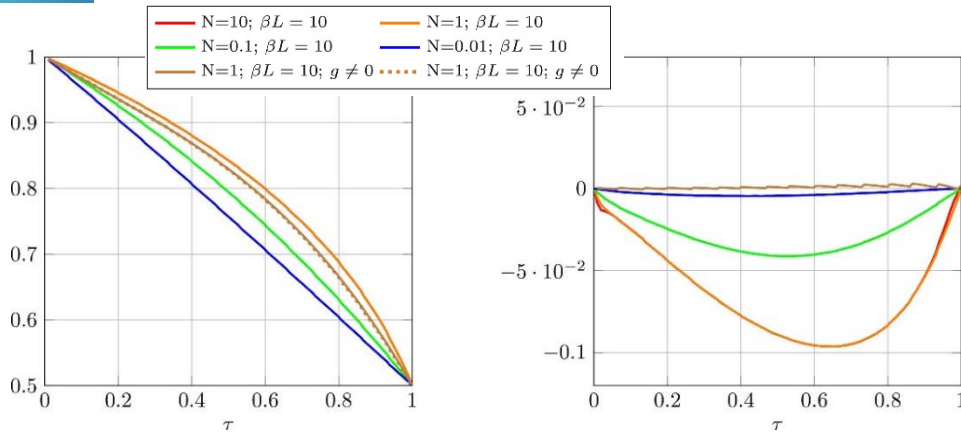
## Typical values of N for real ceramic-based open cell foams (T=1,300 K)

material	Thermal conductivity @1000°C [W/(m.K)]	Porosity=80 %, cell size = 2mm	Porosity=80 %, cell size = 4mm	Porosity=80 %, cell size = 8mm	Porosity=90 %, cell size = 2mm	Porosity=90 %, cell size = 4mm	Porosity=90 %, cell size = 8mm
alumina	~6.8	0,19652	0,09826	0,04913	0,09826	0,04913	0,02456
mullite	~3.2	0,09248	0,04624	0,02312	0,04624	0,02312	0,01156
cordierite	~1.5	0,04335	0,02167	0,01084	0,02167	0,01084	0,00542
silicon carbide	~50	1,44497	0,72249	0,36124	0,72249	0,36124	0,18062



Interest for semi-transparent porous ceramics with high  $p$  and high  $d_{nom}$

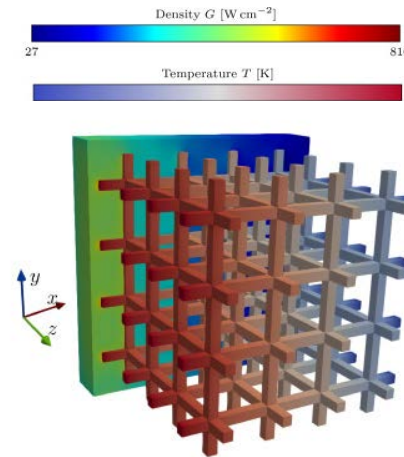
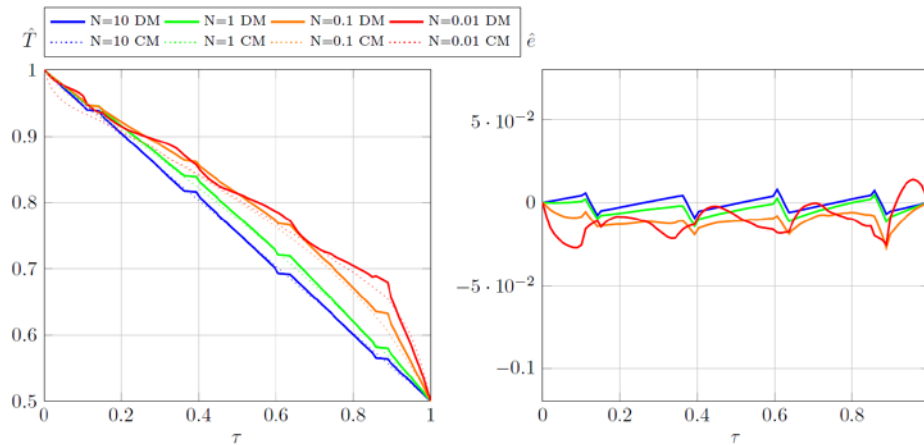
# Comparison of the Rosseland↔HEM model and of the HEM↔DS model



$$\hat{e}(u) = \frac{1}{L} \int_0^L u^2(x) dx$$

- Rosseland : less accurate model
- Up to 10 % of errors

$\theta_2 = 0.5 ; T_1 = 2,222 \text{ K}, T_2 = 1,111 \text{ K}, \kappa_a = 26,250 \text{ m}^{-1}, \kappa_s = 0$

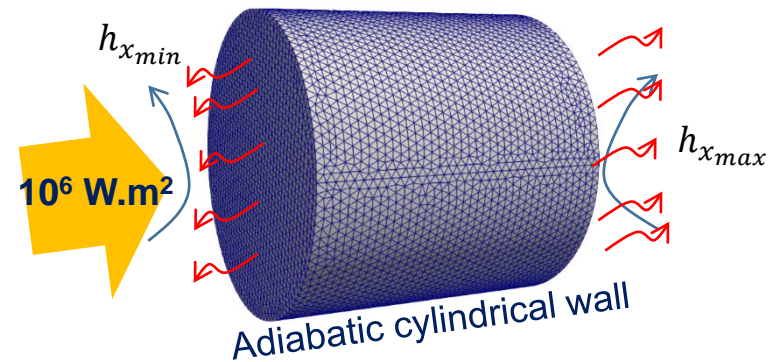


- HEM model : good approach for modelling thermal transfer and for performing future advanced (topology) optimisation process
- DS model : thermo-mechanical computation

Model Method	N = 10			N = 1			N = 0.1			N = 0.01		
	N-R	I F-P	F-P	N-R	I F-P	F-P	N-R	I F-P	F-P	N-R	I F-P	F-P
DS-CM	324 s	336 s	371 s	325 s	339 s	400 s	338	+∞	+∞	347	+∞	+∞
CS-CM	69 s	70 s	70 s	70 s	77 s	78 s	74 s	+∞	+∞	77 s	+∞	+∞
RM	9 s	-	10 s	10 s	-	13 s	11 s	-	17 s	11 s	-	+∞

331 860 tetrahedral elements for the solid phase and 1 753 680 elements for the fluid phase ; 62 processors, 128 directions

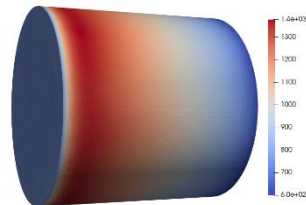
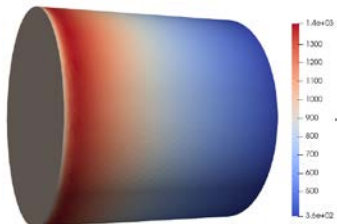
# Thermal behaviour of 4 fictitious alumina-based Kelvin Cell Foams exposed to a collimated concentrated solar beam ( $10^6 \text{ W.m}^2$ )



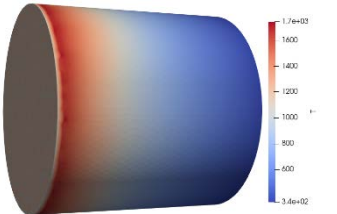
Porosity = 91 %,  $\varnothing = 5 \text{ cm}$ ,  $h = 5 \text{ cm}$

	$d_{nom}=0,004 \text{ m}$ without coating Case 1	$d_{nom}=0,008 \text{ m}$ without coating Case 2	$d_{nom}=0,004 \text{ m}$ with coating Case 3	$d_{nom}=0,008 \text{ m}$ with coating Case 4
$\beta_{eff} (\text{m}^{-1})$	108	54	108	54
$\kappa_{eff} (\text{m}^{-1})$	33.7	12,7	79	33
$\sigma_{eff} (\text{m}^{-1})$	74.3	41.3	29	21
$\varepsilon_{eff}$	0.31	0.24	0.73	0.61
$\lambda_{eff} (\text{W.m}^{-1}.\text{K}^{-1})$	0,33	0,33	0,33	0,33
$N_{P,\beta_{eff}}$	0,04422	0,02211	0,04422	0,02211
$\omega_{eff}$	0.67	0.76	0.27	0.39
$\rho_{eff} (\text{kg.m}^3)$	330	330	330	330
$C_{P,eff} (\text{J. Kg}^{-1}.\text{K}^{-1})$	1200	1200	1200	1200
$h_{x_{min}} = 10h_{x_{max}}$ ( $\text{W. m}^{-2}.\text{K}^{-1}$ )	10	10	10	10

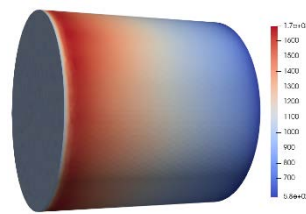
Case 1  $d_{nom}=0,004 \text{ m}$       Case 2  $d_{nom}=0,008 \text{ m}$



Case 3

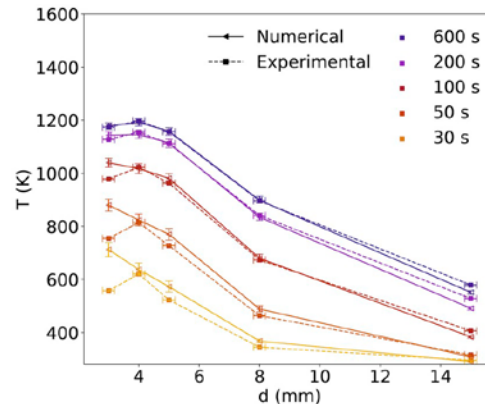
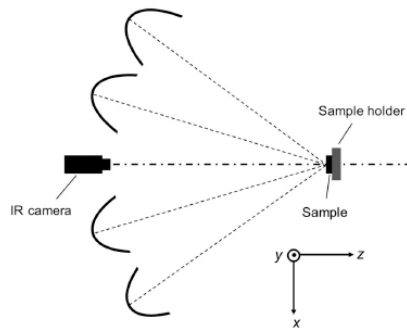
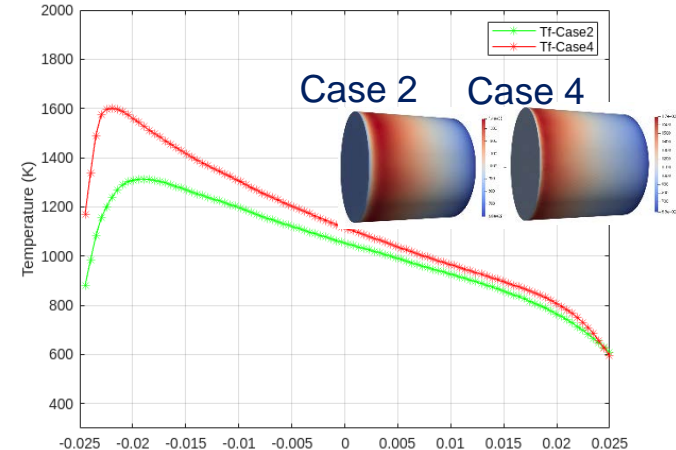
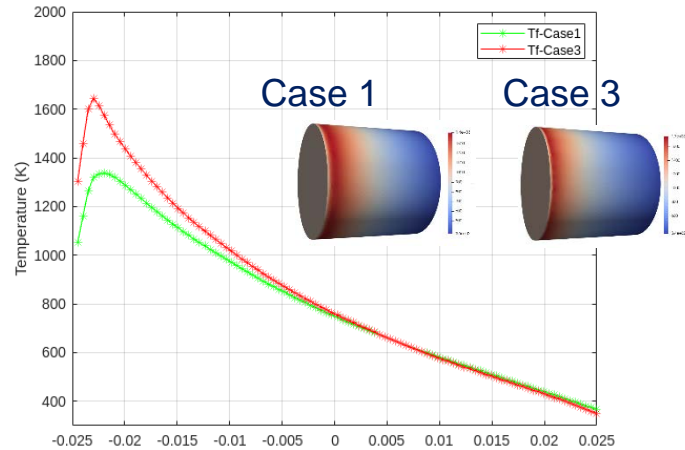


Case 4



Addition of an absorbing coating on the alumina ligaments

# Thermal behaviour of porous alumina ceramics exposed to a collimated concentrated solar beam ( $10^6 \text{ W.m}^2$ )



Similar temperature profile for alumina ceramics exposed to artificial concentrated solar flux.

Mora Monteros et al., *Ceramics International* 46 (2020) 2805–2815

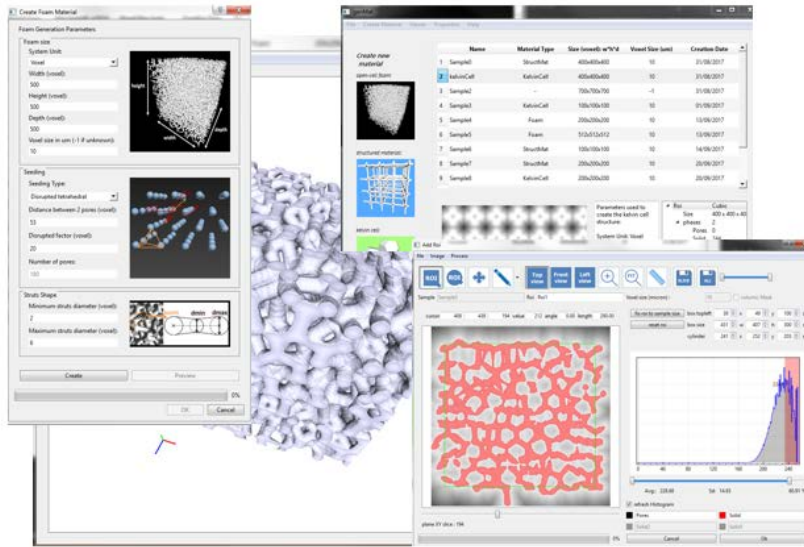
$$N_{P,\beta_{eff}}(1,3) = 2N_{P,\beta_{eff}}(2,4) \rightarrow \text{volume radiation effect more important}$$

$$\omega_{eff}(1,2) < \omega_{eff}(3,4) \rightarrow \text{volume radiation effect more important}$$

$$\varepsilon_{eff}(1,2) < \varepsilon_{eff}(3,4) \rightarrow \text{decreasing of the radiative losses at the front face}$$

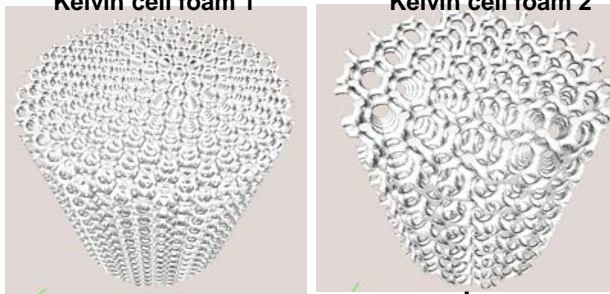
# From the numerical design of porous ceramics up to elaboration thanks to stereolithography

genMat  Qt



Kelvin cell foam 1

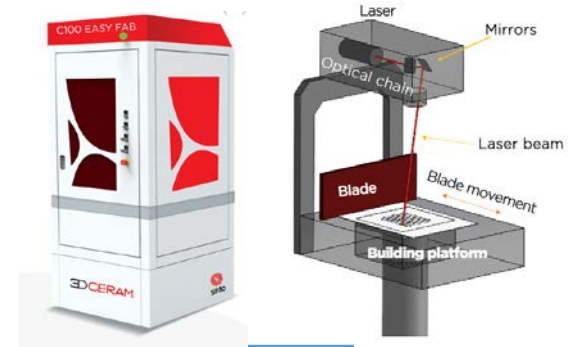
Kelvin cell foam 2



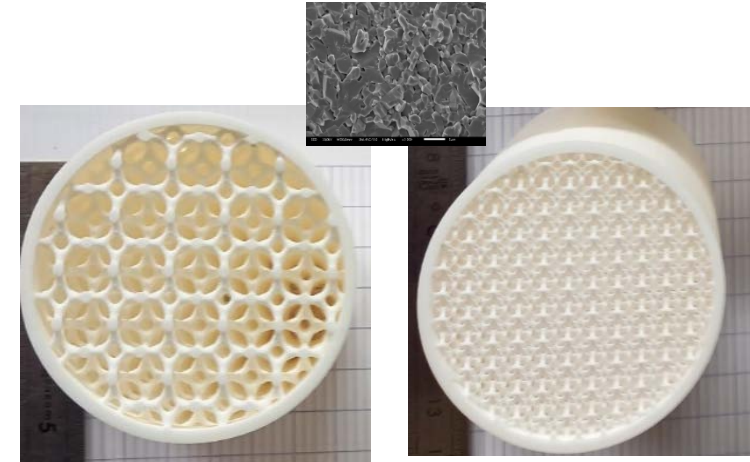
	Kelvin cell foam 1	Kelvin cell foam 2
$d_{nom}$ (m)	0.004	0.008
$p$	91 %	91%
$S_v$ (m <sup>-1</sup> )	704.288	314.751
$h$ (m)	0.05	0.05
$d$ (m)	0.05	0.05
$\beta_{eff}$ (m <sup>-1</sup> )	108	54

genMat → stl files (100 Mo) → SOLIDWORKS

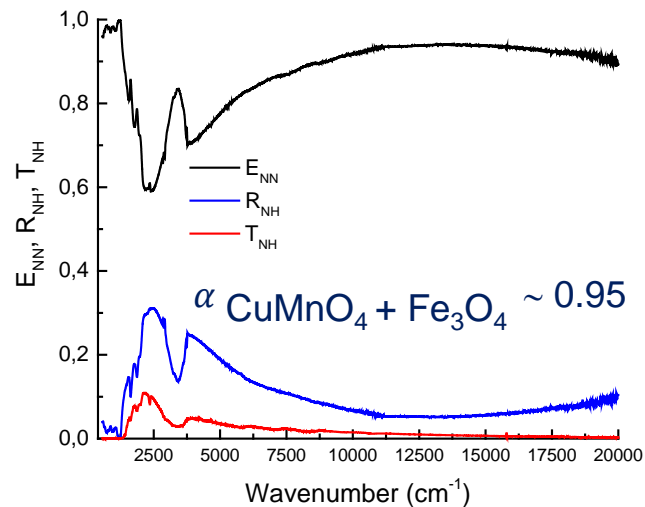
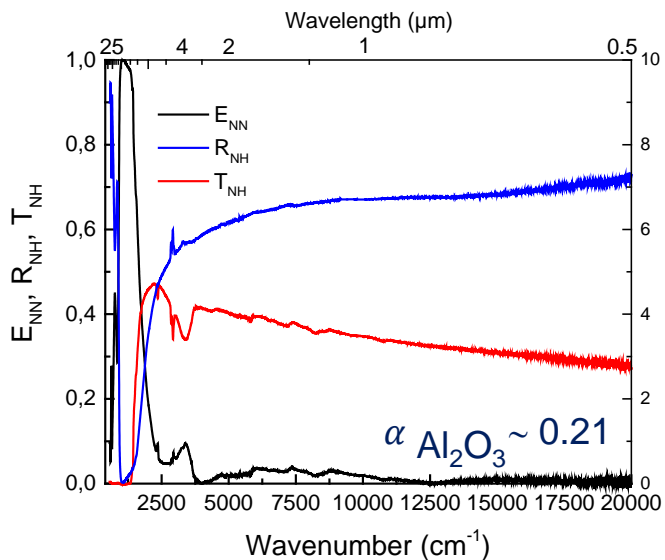
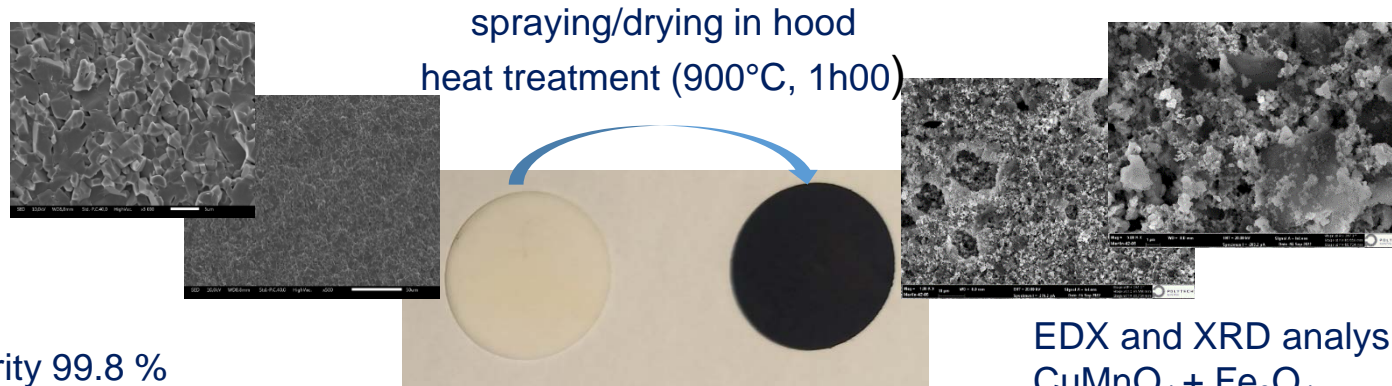
 **3DCERAM**  
Global Advanced Ceramics



Densification control – sintering 1700°C  
smooth surface state



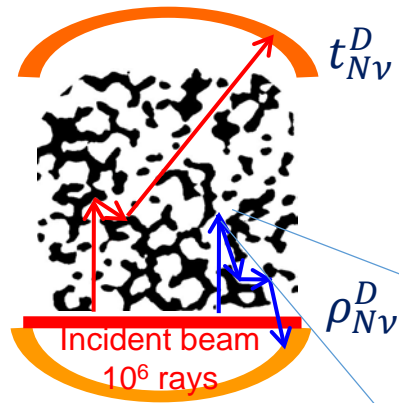
# Improvement of the solar absorptance of the alumina skeleton with a commercial refractory black coating





# Numerical computations of the Kelvin cell foams emissivities with genMat

Parallelized Monte Carlo Ray-Tracing code



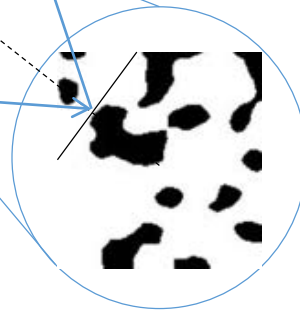
Mesoscopic scale :  
 $\sim 100 \mu\text{m}$

$\rho_{\text{Al}_2\text{O}_3} \sim 0.79$   
 $\rho_{\text{CuMnO}_4 + \text{Fe}_3\text{O}_4} \sim 0.05$

Macroscopic scale :  
 $100,000 \mu\text{m}$

Rousseau et al., JCPs, 2012

Guevelou et al., IJHMT 2016



8 mm without coating  
case 2

8 mm with coating  
case 4



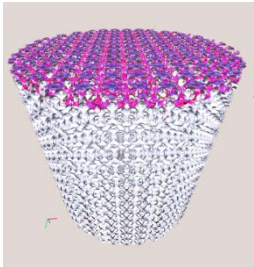
4 mm without coating  
case 1

4 mm with coating  
case 3

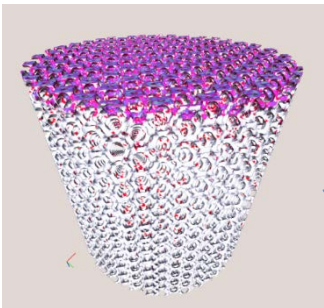
	$d_{nom}=0,004$ m without coating Case 1	$d_{nom}=0,008$ m without coating Case 2	$d_{nom}=0,004$ m with coating Case 3	$d_{nom}=0,008$ m with coating Case 4
$\epsilon_{eff}$	0.31	0.24	0.73	0.61

# Absorption length of the incident collimated beam : effect of $d_{nom}$

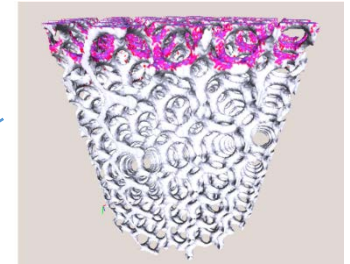
$d_{nom}=0,004$  m  
with coating  
case 3



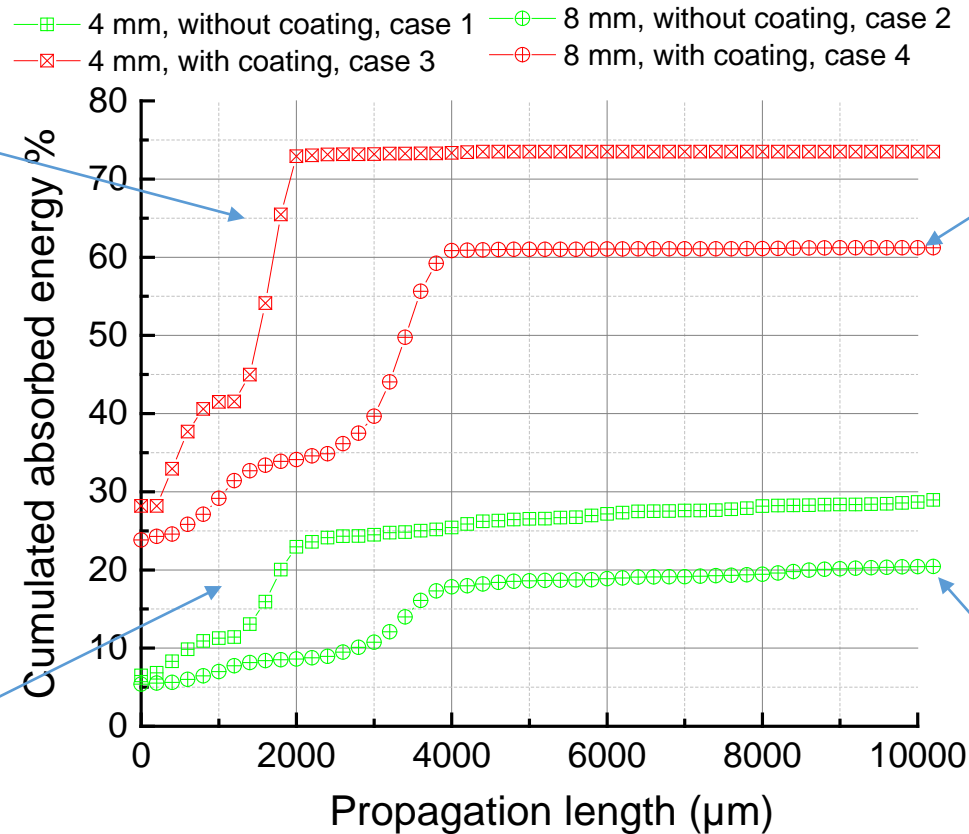
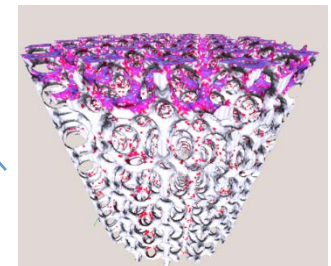
$d_{nom}=0,004$  m  
without coating  
case 1



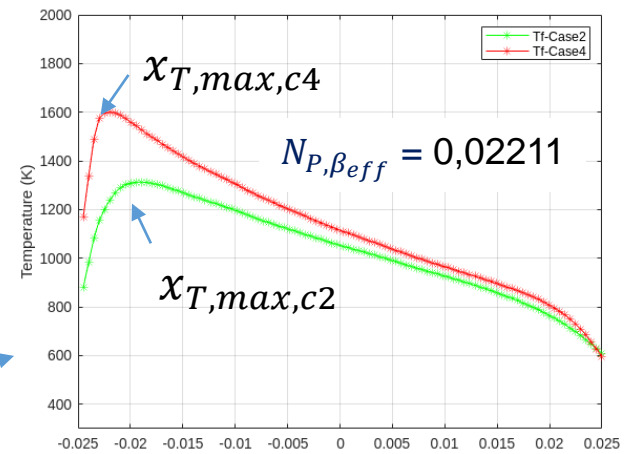
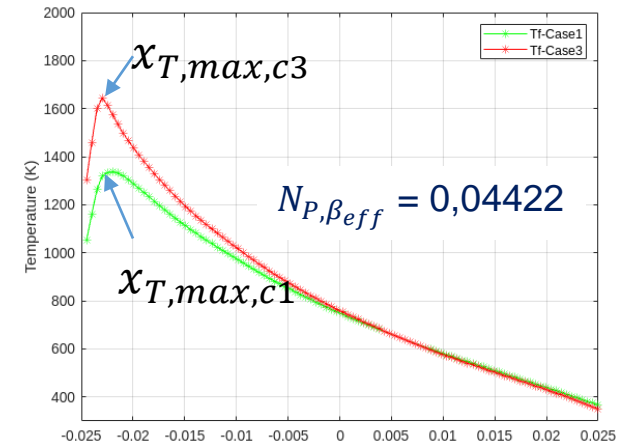
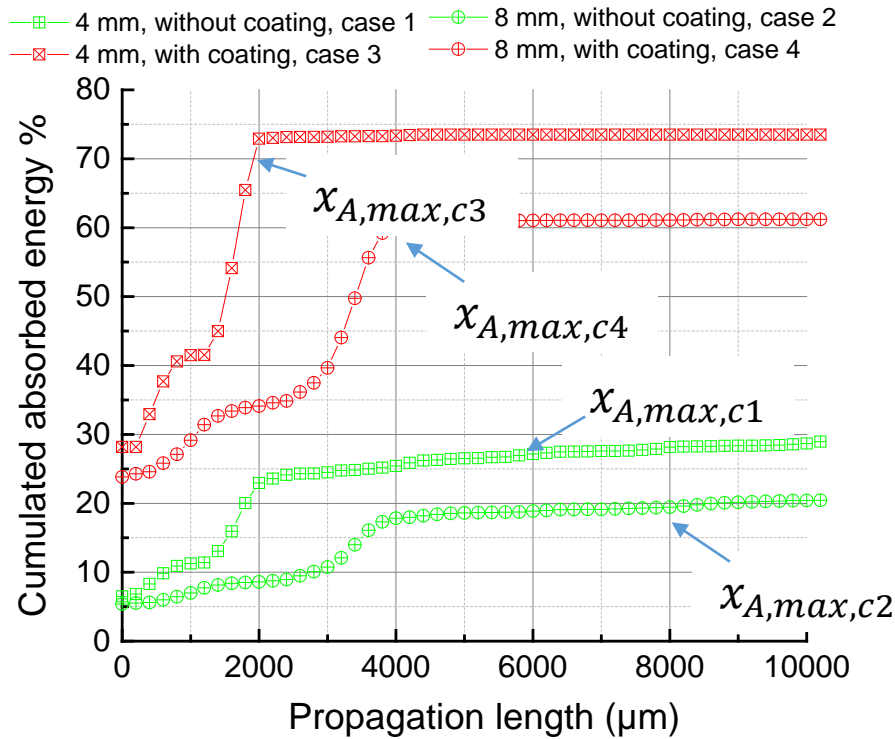
$d_{nom}=0,008$  m  
with coating  
case 4



$d_{nom}=0,008$  m  
without coating  
case 2



# Impact $d_{nom}$ on the absorption of the incident radiative flux and the position of $T_{max}$

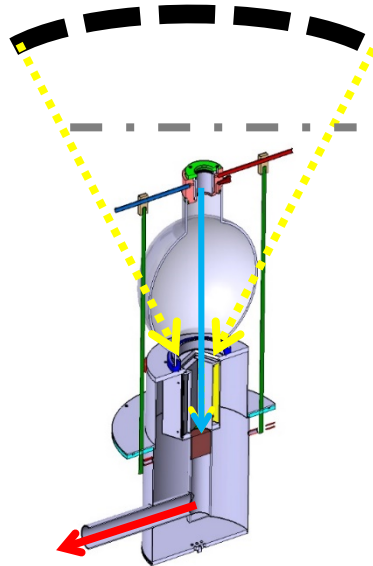
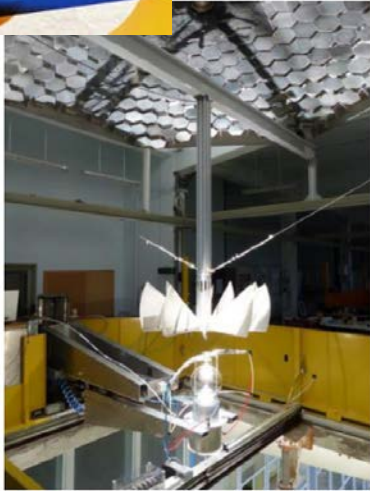


**Similar effect**

Radiation transport is stopped at the first rank of cell : after conductive (convective) heat transfer

# Solar-to-heat performances : OPTISOL bench

PROMES



Mey-Cloutier et al., Solar Energy 136 (2016) 226–235

Qualitative agreement but some experiments must still be explained

$$\eta_{ST,1} < \eta_{ST,2} \leftrightarrow N_{P,\beta_{eff},1} > N_{P,\beta_{eff},2}$$

$$\eta_{ST,4} < \eta_{ST,3} \text{ but } N_{P,\beta_{eff},3} > N_{P,\beta_{eff},4}$$

$$\eta_{ST,4} < \eta_{ST,3} \leftrightarrow \omega_{eff,3} < \omega_{eff,4}$$

**Modification of the front face for case 4 ?**  
**Heat exchange coefficient?**

$d_{nom}=0,004$ m without coating : case 1			
DNI (W/m <sup>2</sup> )	q air (g/s)	T out (° C)	$\eta_{ST}$
1017	3	219	0,39
1020	2	270	0,33
1022	1	387	0,24
$d_{nom}=0,004$ m with coating : case 3			
DNI (W/m <sup>2</sup> )	q air (g/s)	T out (° C)	$\eta_{ST}$
1014	3	423	0,82
1024	2	574	0,75
1014	1	838	0,57
$d_{nom}=0,008$ m without coating : case 2			
DNI (W/m <sup>2</sup> )	q air (g/s)	T out (° C)	$\eta_{ST}$
1027	3	307	0,56
1028	2	368	0,46
1024	1	490	0,32
$d_{nom}=0,008$ m with coating : case 4			
DNI (W/m <sup>2</sup> )	q air (g/s)	T out (° C)	$\eta_{ST}$
1022	3	382	0,72
1034	2	507	0,64
1034	1	731	0,48

Experimental data

$$N_{P,\beta_{eff}} = 0,04422$$

$$\omega_{eff} = 0.67$$

$$N_{P,\beta_{eff}} = 0,04422$$

$$\omega_{eff} = 0.27$$

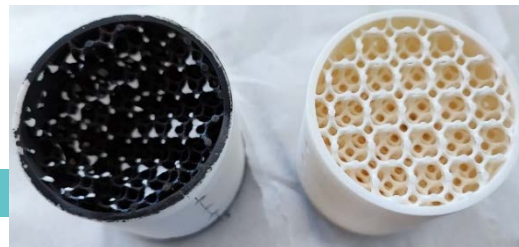
$$N_{P,\beta_{eff}} = 0,02211$$

$$\omega_{eff} = 0.76$$

$$N_{P,\beta_{eff}} = 0,02211$$

$$\omega_{eff} = 0.39$$

Conduction-to-radiation number



# Conclusions & outlook

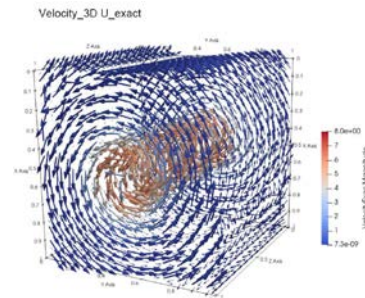
- Fast and robust FEM solver for conduction-radiation heat exchange modelling through HEM and DS method
- Validation of HEM-DS ↔ Viskanta model (hot and black wall) for a porous structure with a regular lattice (cubic cells)
- Volume propagation of radiation locally increases  $T \rightarrow$  interest for developing VSR
- Numerical design and elaboration of 4 based-alumina VSR ( $\varnothing = 5$  cm,  $h = 5$  cm) with stereolithography
- Performance tests with the OPTISOL bench
- Best VSR : porosity 91 %, nominal pore diameter 4 mm with a coating of high solar absorptance
- Planck number not sufficient for following volume propagation within VSR : need to introduce a trapping effect number.



Finite element framework for modeling conducto-radiative transfers within heterogeneous media at both discrete and continuous scales

S. Ouchtout, B. Rousseau, Y. Favennec\*

Nantes Université, CNRS, Laboratoire de thermique et énergie de Nantes, LTEn, UMR 6607, Nantes F-44000, France



- Coupling with fluid transport (Darcy-Forchheimer - HEM/ Navier-Stokes - DS) → ANCRE SdBE FATHERCASE program (2022-2023) with IFPEN and GeM
- PRC ANR ORCHESTRA (2022-2026) with LTEn-GeM-IFPEN-IRCER
- Topology optimization →
- Thermal shock resistance modelling
- Elaboration of SiC lattice with binder jetting...

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ET ENERGIE DE NANTES  
UMR 6607

GeM  
Institut de Recherche en  
Géométrie et Mécanique

ifp  
Energies  
nouvelles

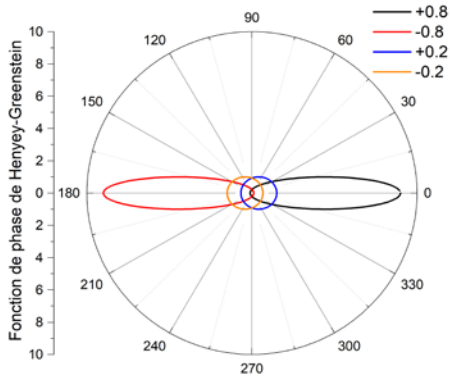
irCer  
Institut de recherche  
sur les céramiques



Thank you for your attention !  
benoit.rousseau@univ-nantes.fr



# Influence of the anisotropy factor

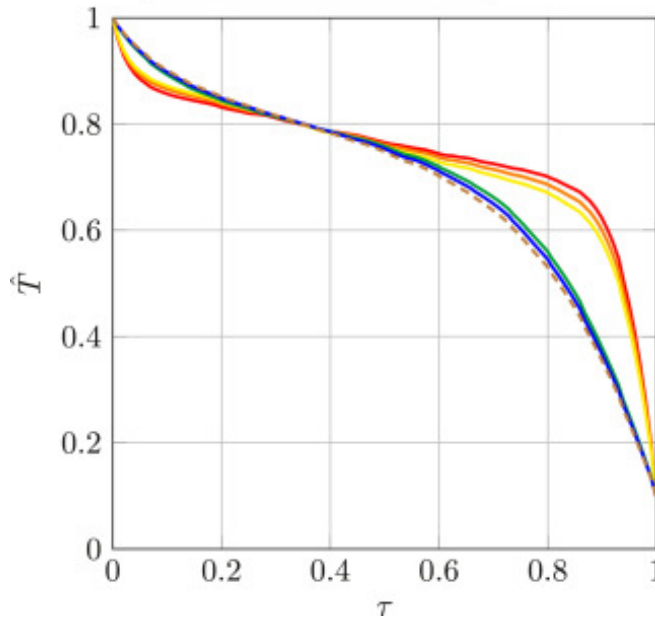


$$P(\hat{\Omega}' \rightarrow \hat{\Omega}) = \frac{1}{4\pi} \frac{1 - g^2}{(1 + g^2 - \hat{\Omega} \cdot \hat{\Omega}')^{3/2}}$$

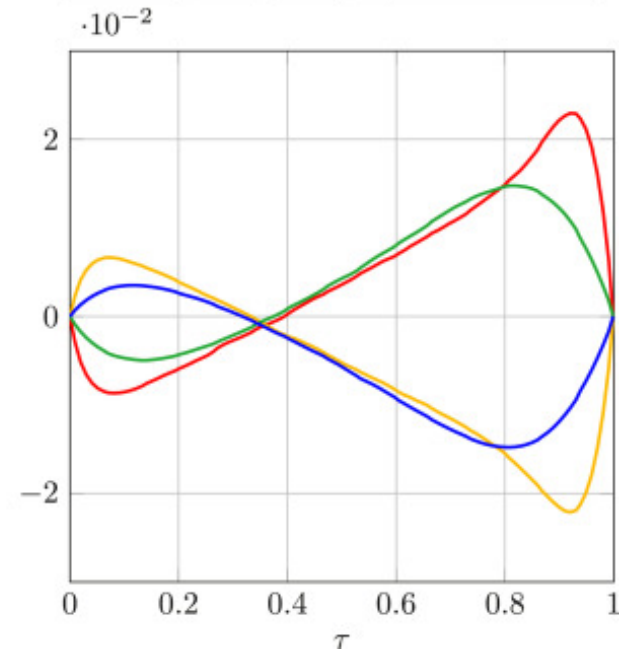
Key quantities

$\kappa_a$     $\kappa_s$

- $N = 0.001$  &  $g = 0.9$
- $N = 0.001$  &  $g = 0$
- $N = 0.001$  &  $g = -0.9$
- $N = 0.01$  &  $g = 0.9$
- $N = 0.01$  &  $g = 0$
- - -  $N = 0.01$  &  $g = -0.9$

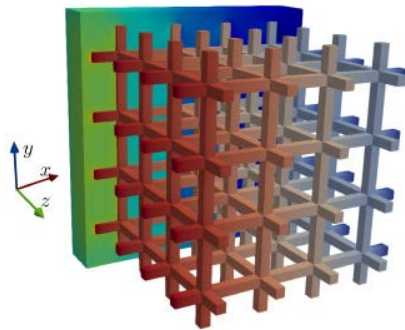
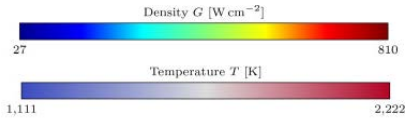


- $\hat{T}_{(g=0.9)} - \hat{T}_{(g=0)}$  &  $N = 0.001$
- $\hat{T}_{(g=-0.9)} - \hat{T}_{(g=0)}$  &  $N = 0.001$
- $\hat{T}_{(g=0.9)} - \hat{T}_{(g=0)}$  &  $N = 0.01$
- $\hat{T}_{(g=-0.9)} - \hat{T}_{(g=0)}$  &  $N = 0.01$

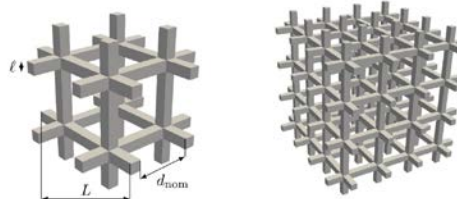




# From macro-scale to meso-scale



macro → meso

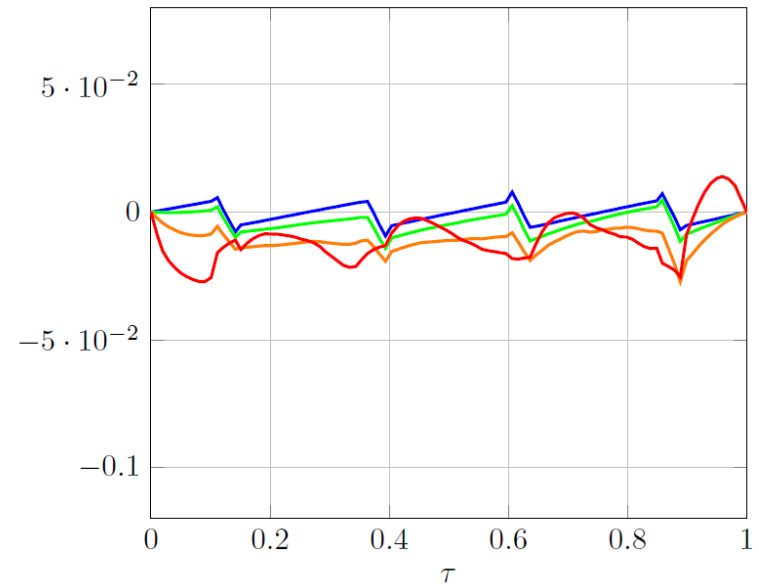
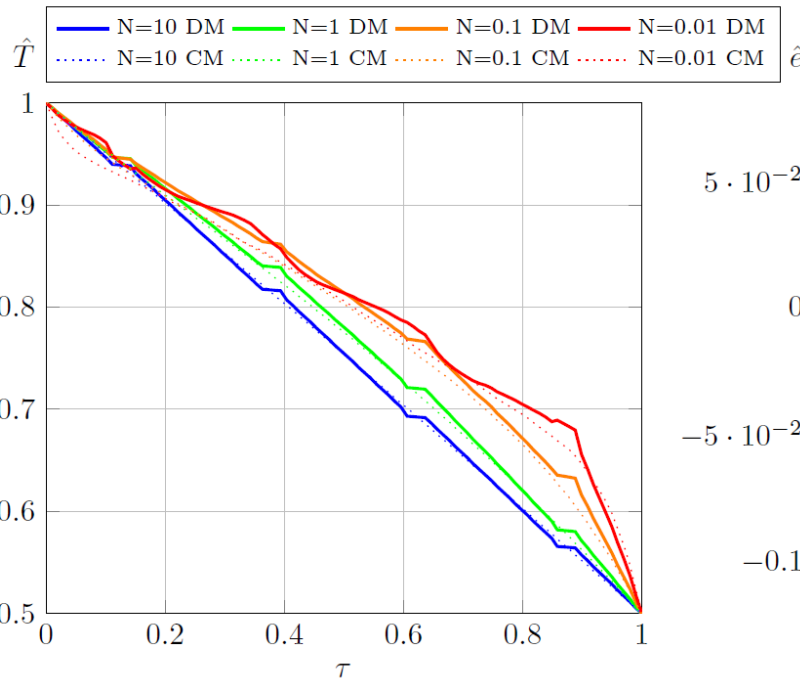


$$p(\ell) = \frac{L^3 - 12\ell^2L + 16\ell^3}{L^3}; \quad d(\ell) = \frac{L - 2\ell}{2}$$

$$k_{cond,s} = 3 \frac{k_{cond,eff}}{1 - p}$$

$$\varepsilon_s = 1 - \frac{1 - \varepsilon_{eff}}{1 - \frac{4}{5}p}$$

S. Guévelou et al., Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 189, 329-338



# Influence of the albedo

