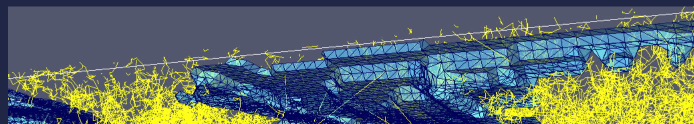
RANDOM-WALK SIMULATION METHODS FOR THE MODELING OF BALLISTIC/DIFFUSIVE HEAT AND MASS TRANSFER IN EVOLVING POROUS MEDIA

InterPore2026

Nantes, 20/05/2026



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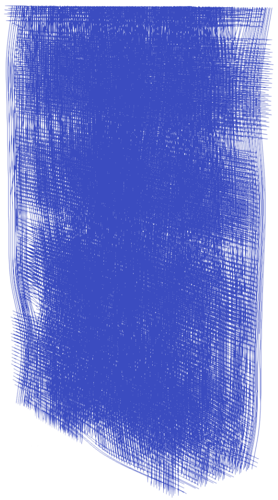
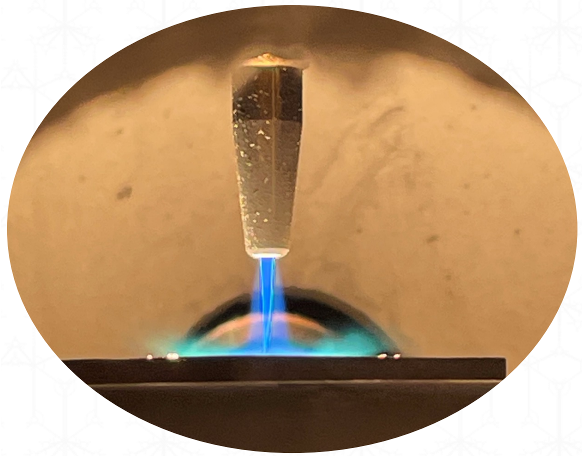
CONTEXT

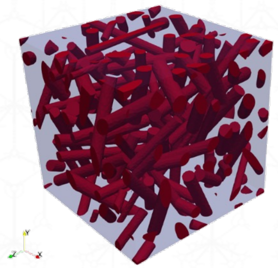
Laboratoire des Composites ThermoStructuraux

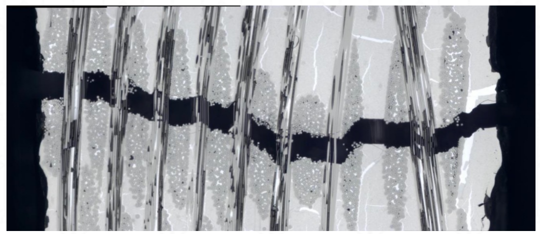
Laboratory for ThermoStructural Composites

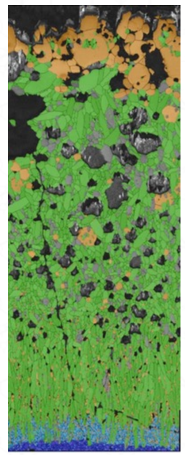
38 years of joint research & innovation











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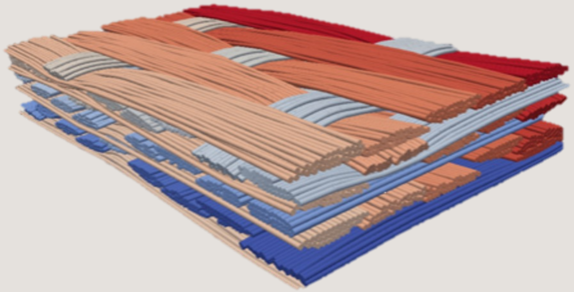
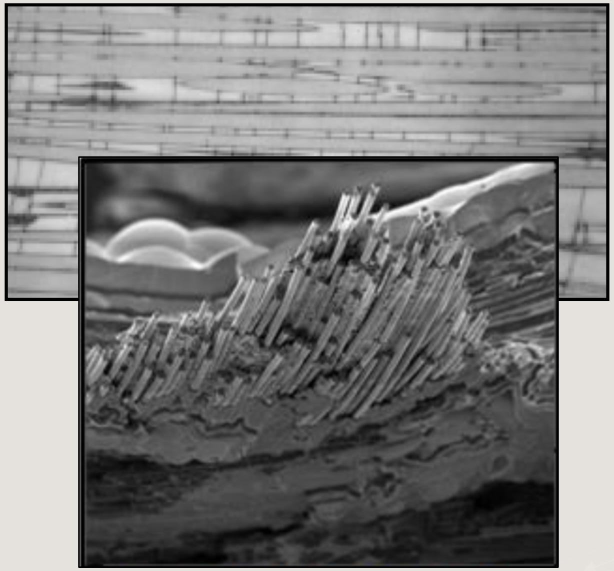
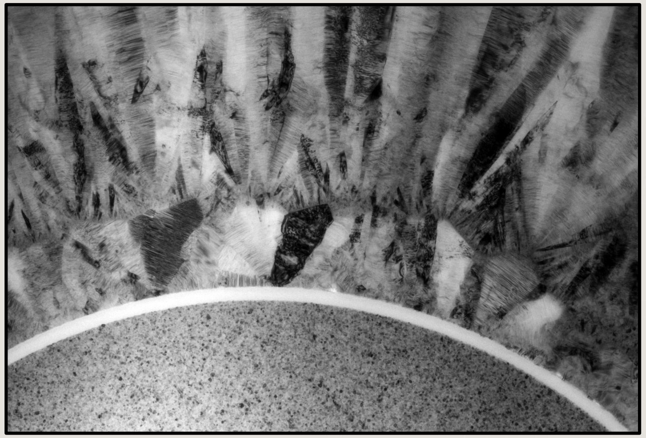
WHAT ARE THERMOSTRUCTURAL COMPOSITES ?

Ceramic-Matrix Composites(CMC)



Reinforced by ceramic fibers





Interphase between fibers and matrix

→ Non-brittle, even though having brittle components !

And, of course : stiff & refractory

APPLICATIONS

Current:

Space propulsion: nozzle throat, divergent

Brakes for aviation and racing cars

Thermal protection systems

Ionic propulsion

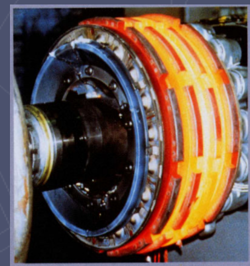
Industry

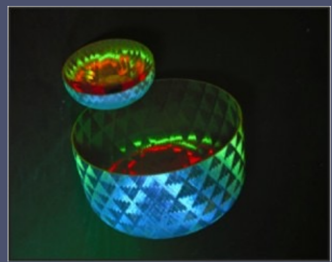
Future:

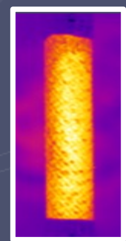
Aircraft propulsion

Nuclear (fission, fusion)

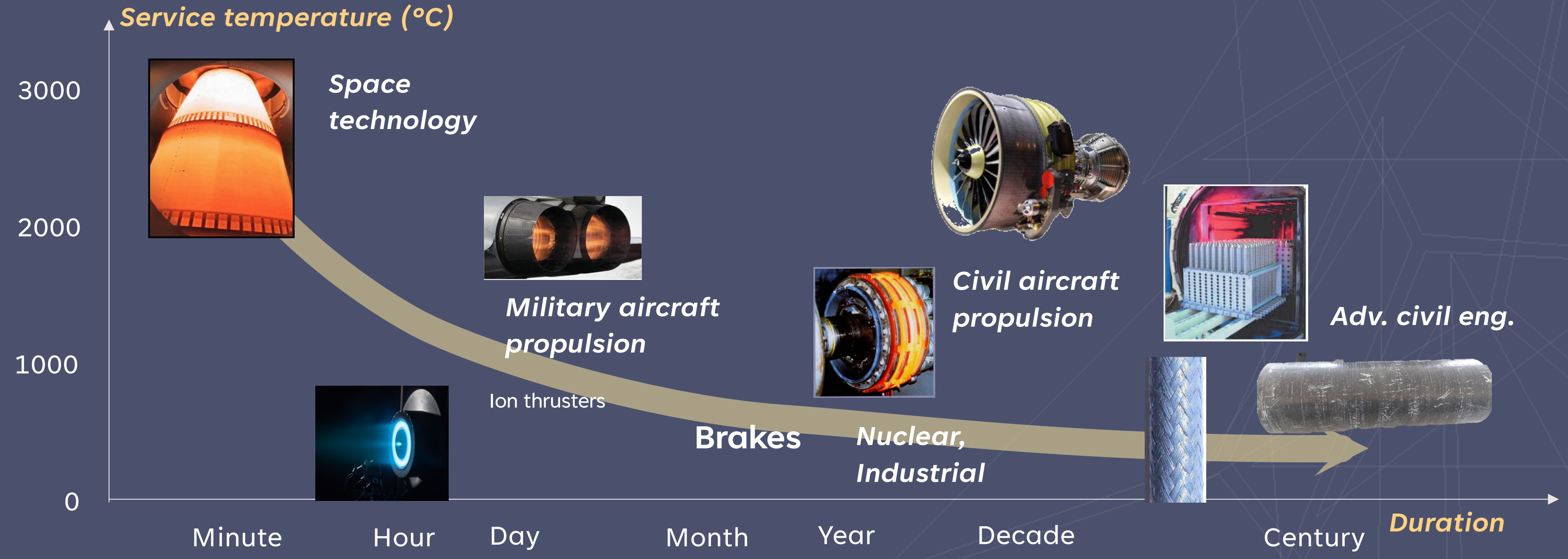
Other energies

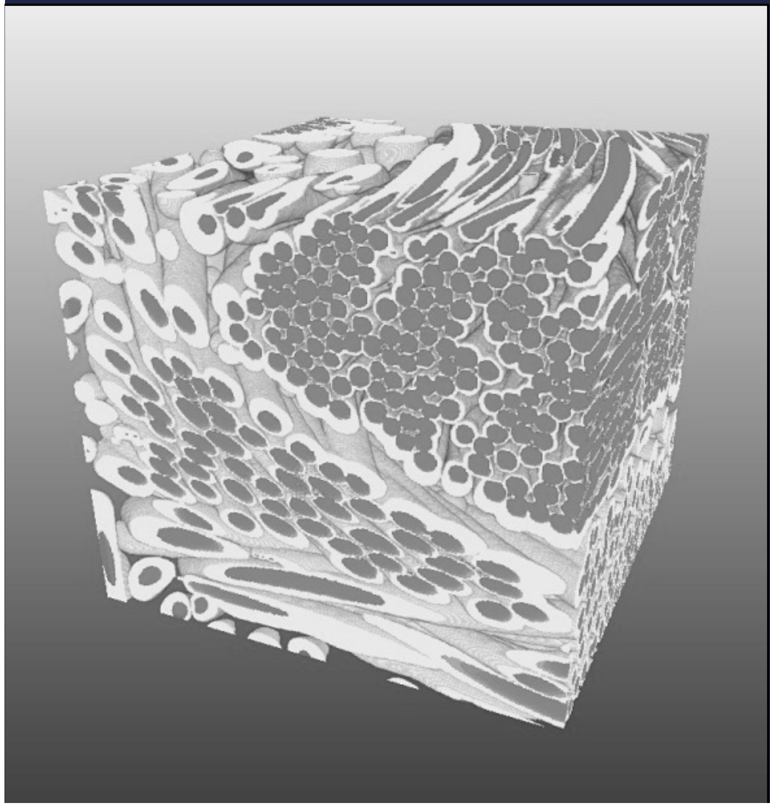






APPLICATION SPECTRUM OF CMCS





PROBLEMS

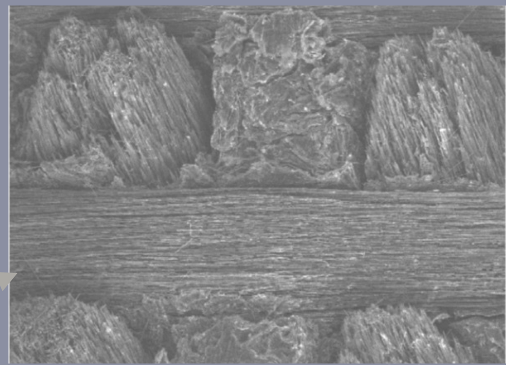
ABLATIVE C_F/C MATERIALS

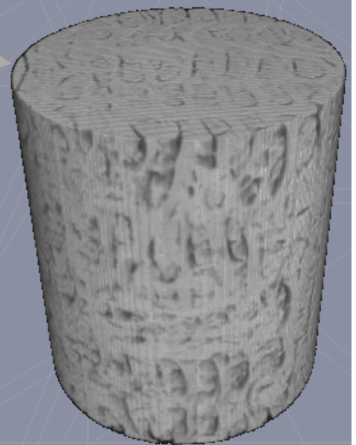
Compact (almost non-porous) materials

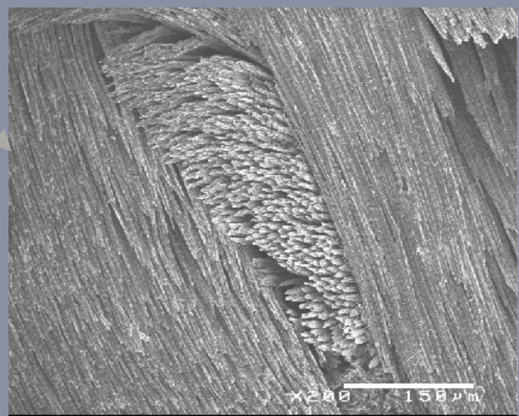
- 3D C/C
- Needle-punched « 2.5D » C/C

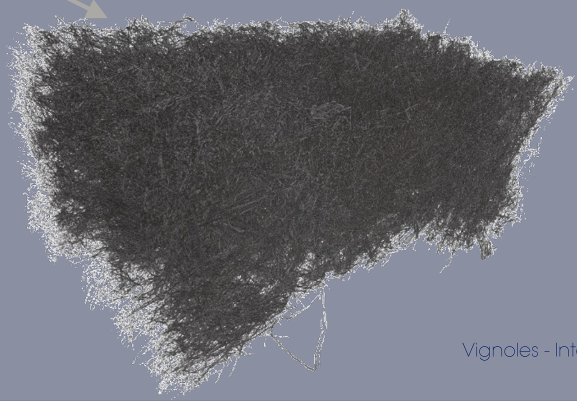
Porous ablators

- Pyrolyzed C/resin
- Felts (eg. Mersen's Calcarb ®)



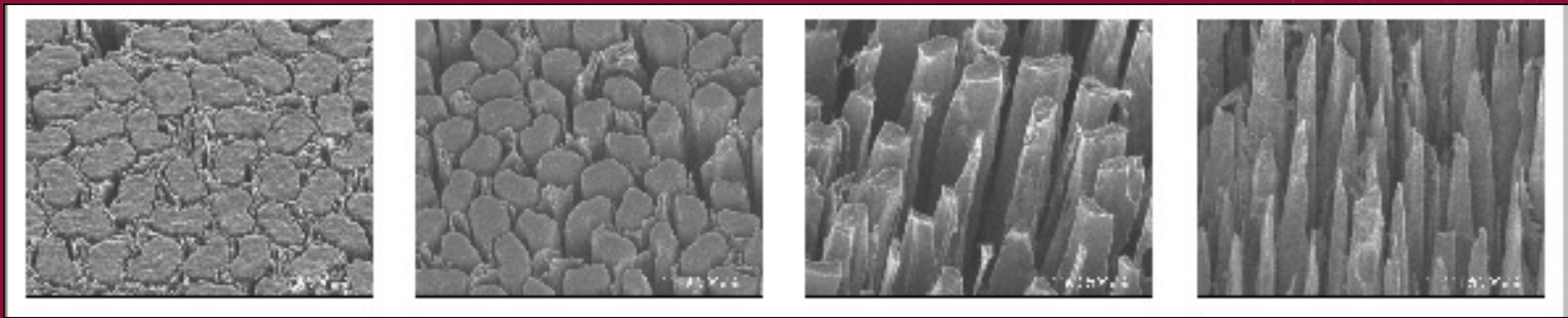




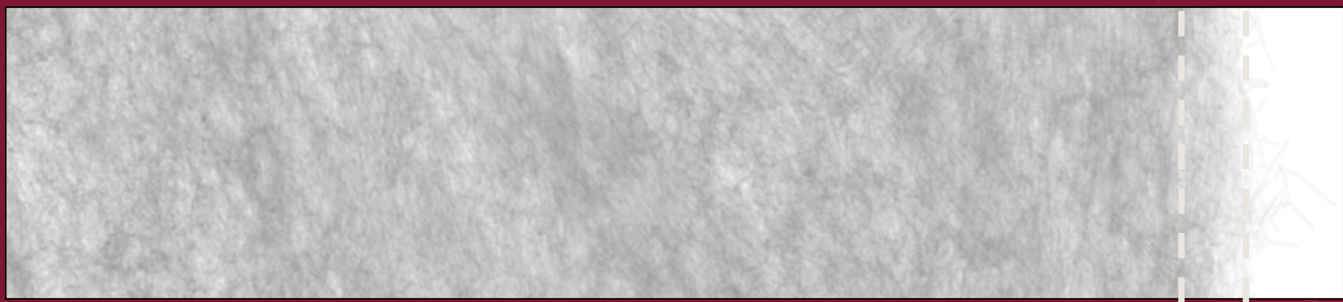


ABLATION

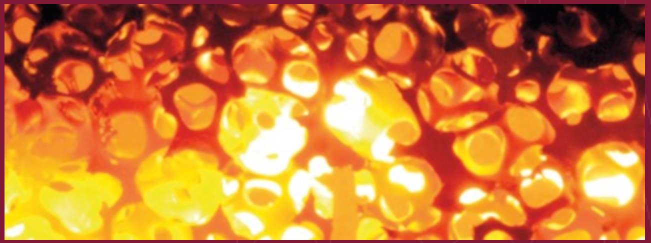
Surface becomes rough ➔ modifies fluxes and ablation rate



Porous ablators acquire an affected depth ➔ linked to effective rate



HIGH-TEMPERATURE HEAT TRANSFER

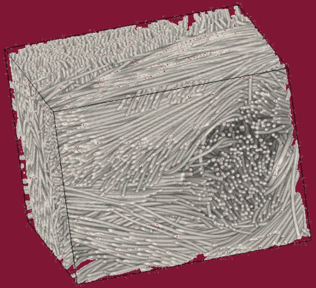


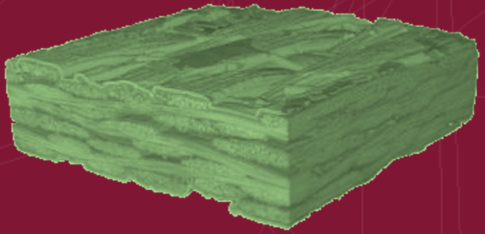
Applications

- Thermal gradients in CVI
- Thermal protection systems for atmospheric reentry
- Heat management in nuclear & CSP power plants

Materials

- Ceramic foams
- Fibrous media
- Ceramic-matrix composites





Very porous, large pores

=> large contribution of radiation even at moderate temperatures

PURPOSE OF THE MODELING APPROACH

Work on 3D images → as close as possible to the « actual material »

Ablation :

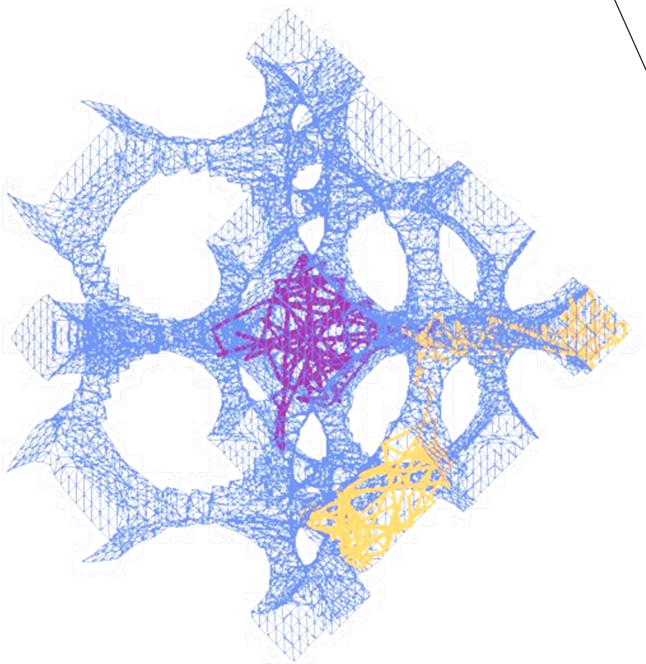
- Account for diffusion/reaction competition
- Describe morphological evolution of the material
- Obtain information on evolution kinetics & evolving effective properties

Heat transfer

- Account for radiation/conduction competition
- Obtain morphology/effective properties relationships

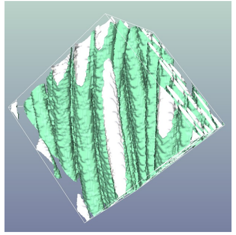
Large computational domains :
→ Memory requirements

Interest of Random-walks methods



METHODS

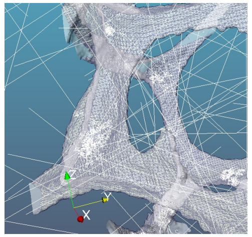
SCALES & PHENOMENA



Mass transfer :

- Solid/gas are clearly distinguished
- Gas may be rarefied => address kinetic theory of gases
- Ordinary diffusion : Brownian motion

- Deposition/ablation are interfacial phenomena
- Growth/recession: Moving fronts



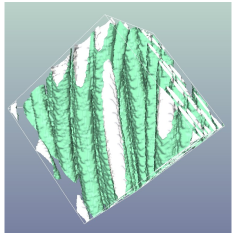
Heat transfer :

- Radiative cavities are distinguished
- Radiative transfer : analogous to rarefied gas transfer
- Conductive transfer : analogous to ordinary gas diffusion

- Exchange conditions between void and solid : analogous to « handling sticking events »

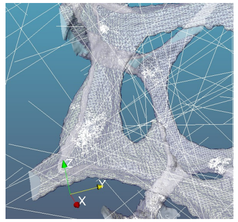
EQUATIONS AND METHODS

Mass transfer :



- Boltzmann kinetic equation: « Kinetic » (or Pearson) random walk
- Diffusion equation for solid : « Brownian » random walk
- Reaction: notion of « sticking probability »

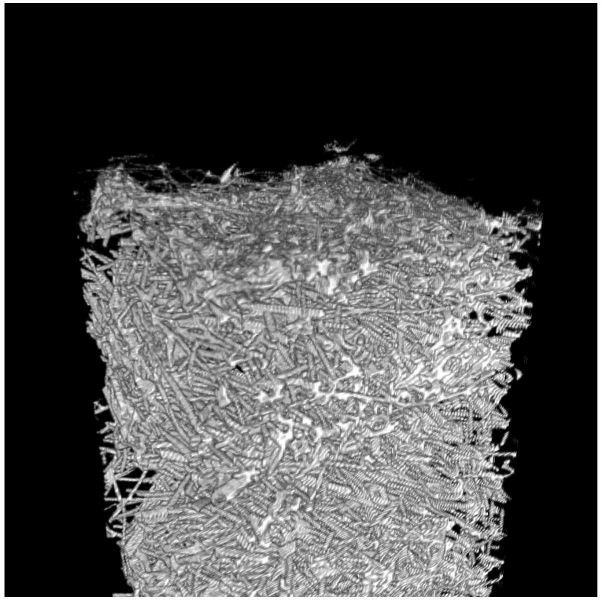
Heat transfer :



- Kinetic equation for radiation : « Kinetic » random walk (or simple ray-tracing)
- Diffusion/conduction equation for solid : « Brownian » random walk
- Rad./Cond. exchange: « transition probability »

RESULTS - PART 1

ABLATION OF A FIBROUS PREFORM



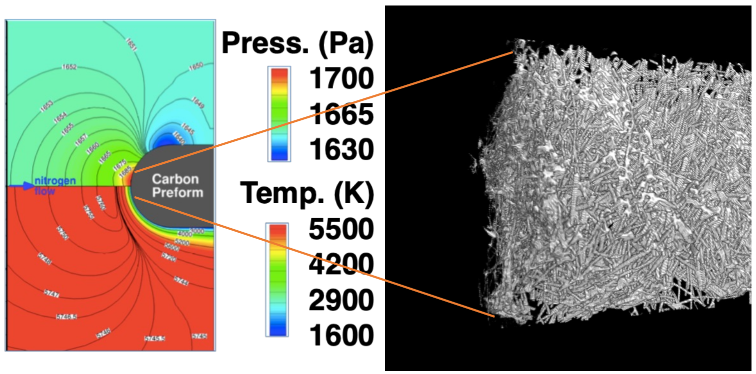
G. L. VIGNOLES et al., *Carbon* (2018), vol. **134**, pp. 376–390.

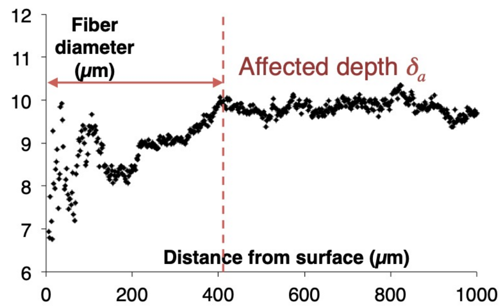
ABLATION SIMULATIONS: POROUS FELTS

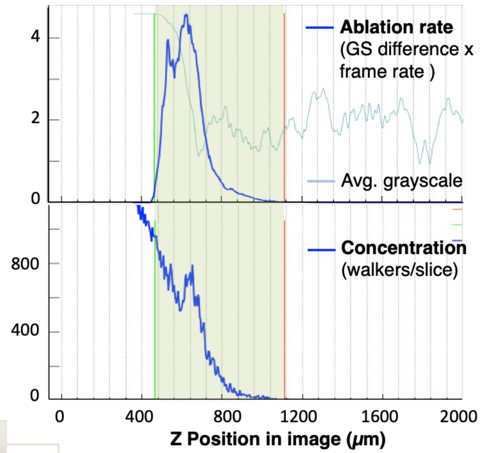
esa SAPIENZA UNIVERSITÀ DI ROMA VON KARMAN INSTITUTE FOR FLUID DYNAMICS

Nitrogen plasma ablation testing on carbon preforms

New analytical and numerical models







Affected depth observation & measurement

Rebuilt flow conditions

Measured recession rate

Effective rate constants

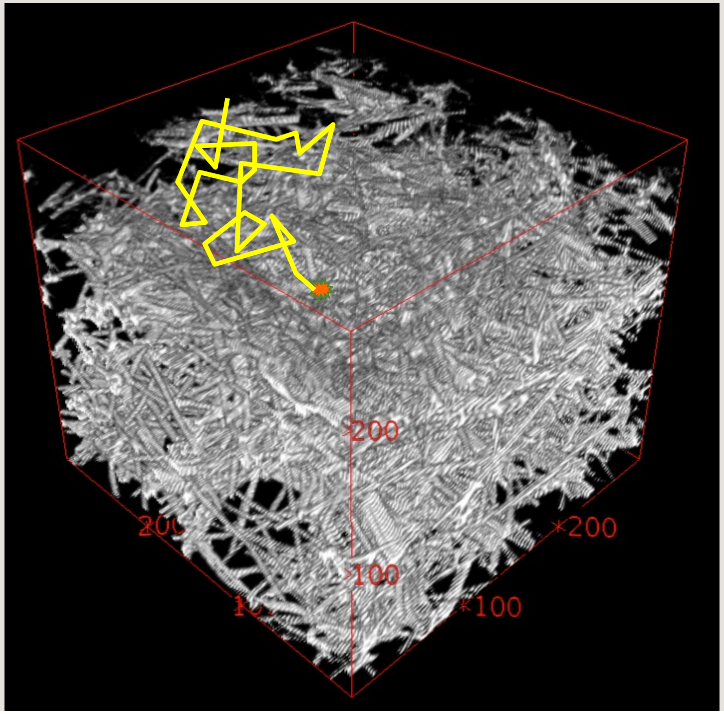
Intrinsic rate constants

DETAILED NUMERICAL MODEL FOR ABLATION

G. L. VIGNOLES et al., *Carbon* (2018), vol. **134**, pp. 376–390.

What does it solve ?

- Diffusion-reaction equation (1 species) (ablation + recomb.)
- + surface recession equation (solid)
- Single boundary condition : Fixed *C* at a given distance above surface
- Parameters: D, k_{nit}, k_{rec}



Random walk « engine » :

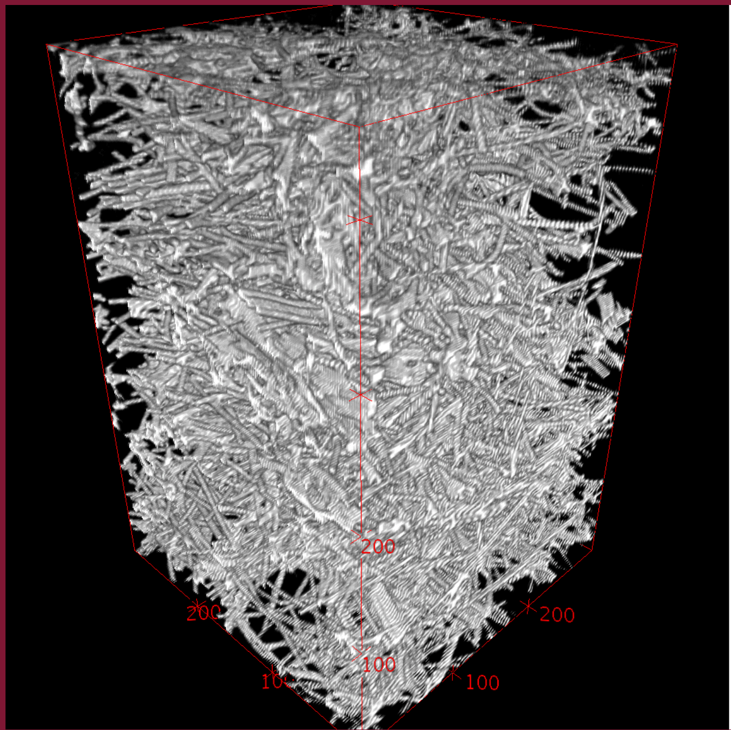
- Brownian walkers ➔ continuum diffusion
- Simplified Marching Cube

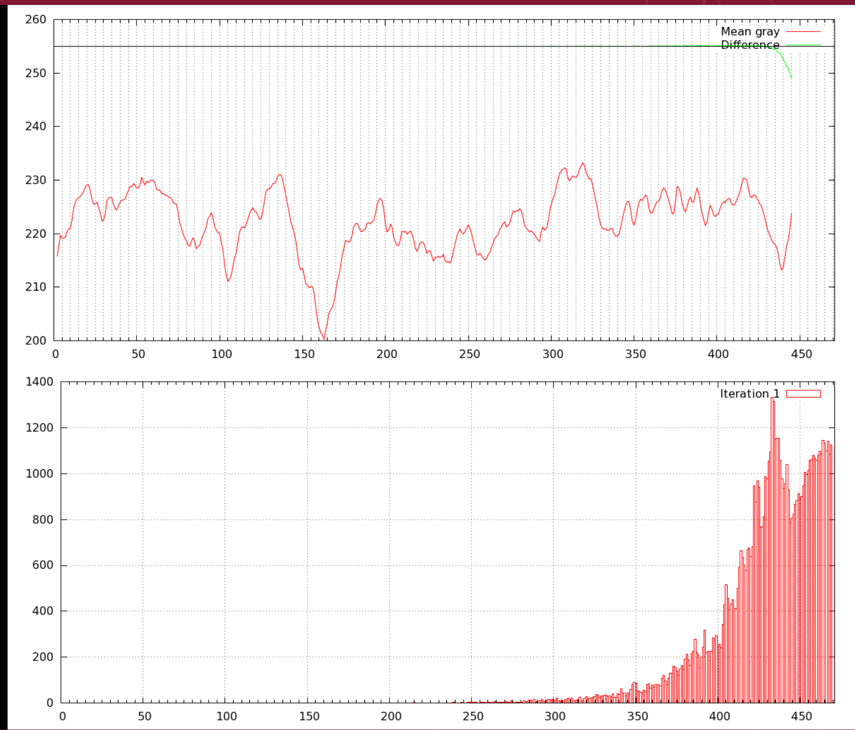
Output:

- Effective ablation depth
- Effective reaction rate = Impinging mole flux /surface concentration

NUMERICAL SIMULATION OF ABLATION

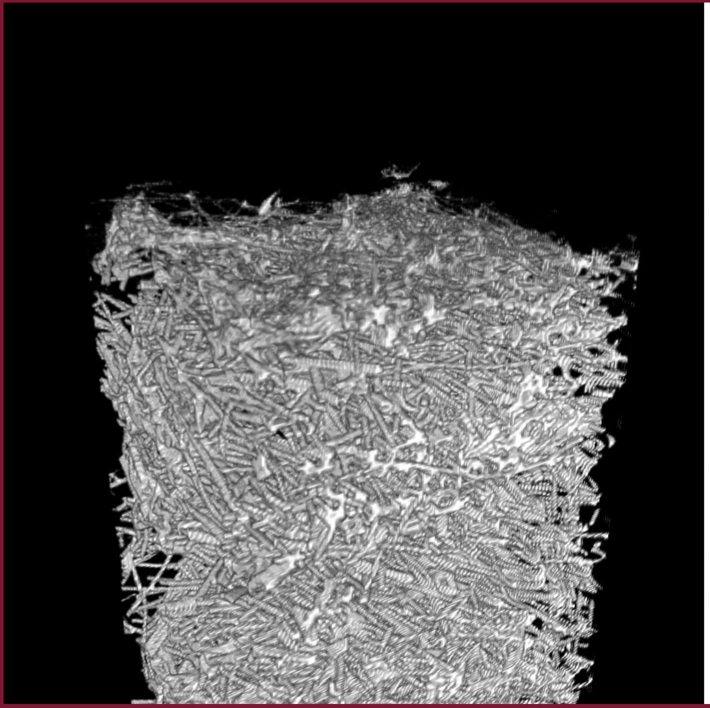
G. L. VIGNOLES et al., *Carbon* (2018), vol. **134**, pp. 376–390.

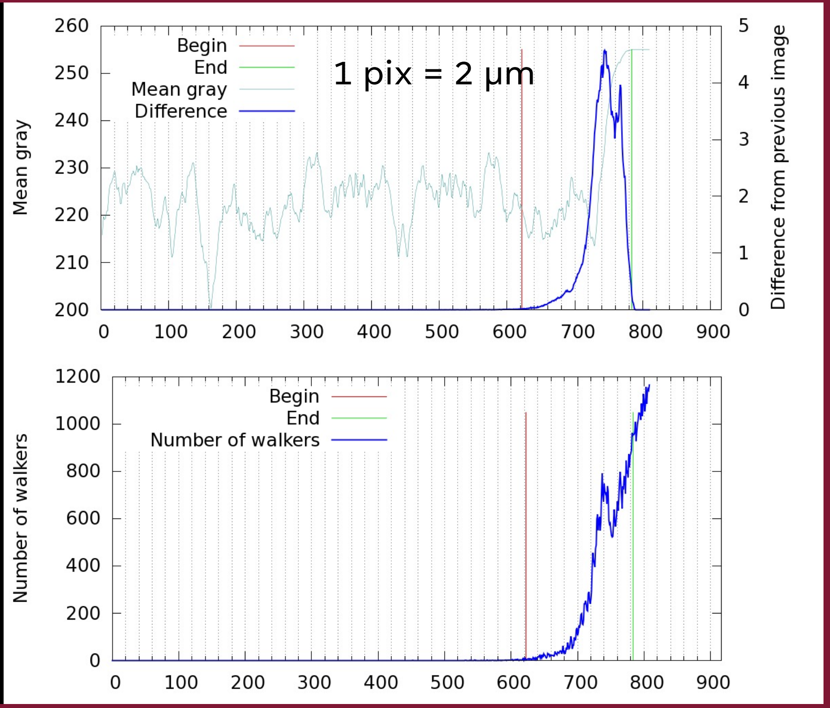




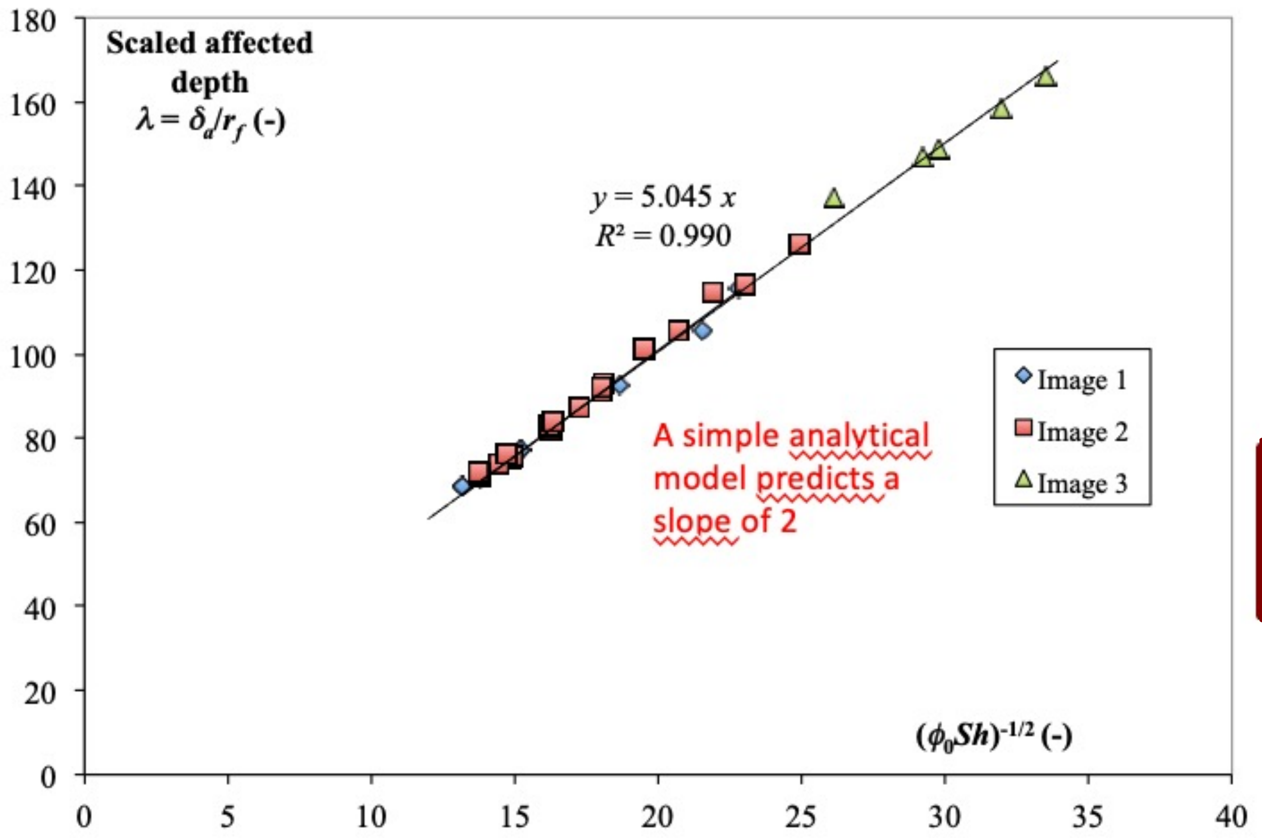
G. L. VIGNOLES et al., *Carbon* (2018), vol. **134**, pp. 376–390.

NUMERICAL SIMULATION OF ABLATION





ABLATION : DIMENSIONLESS RESULTS

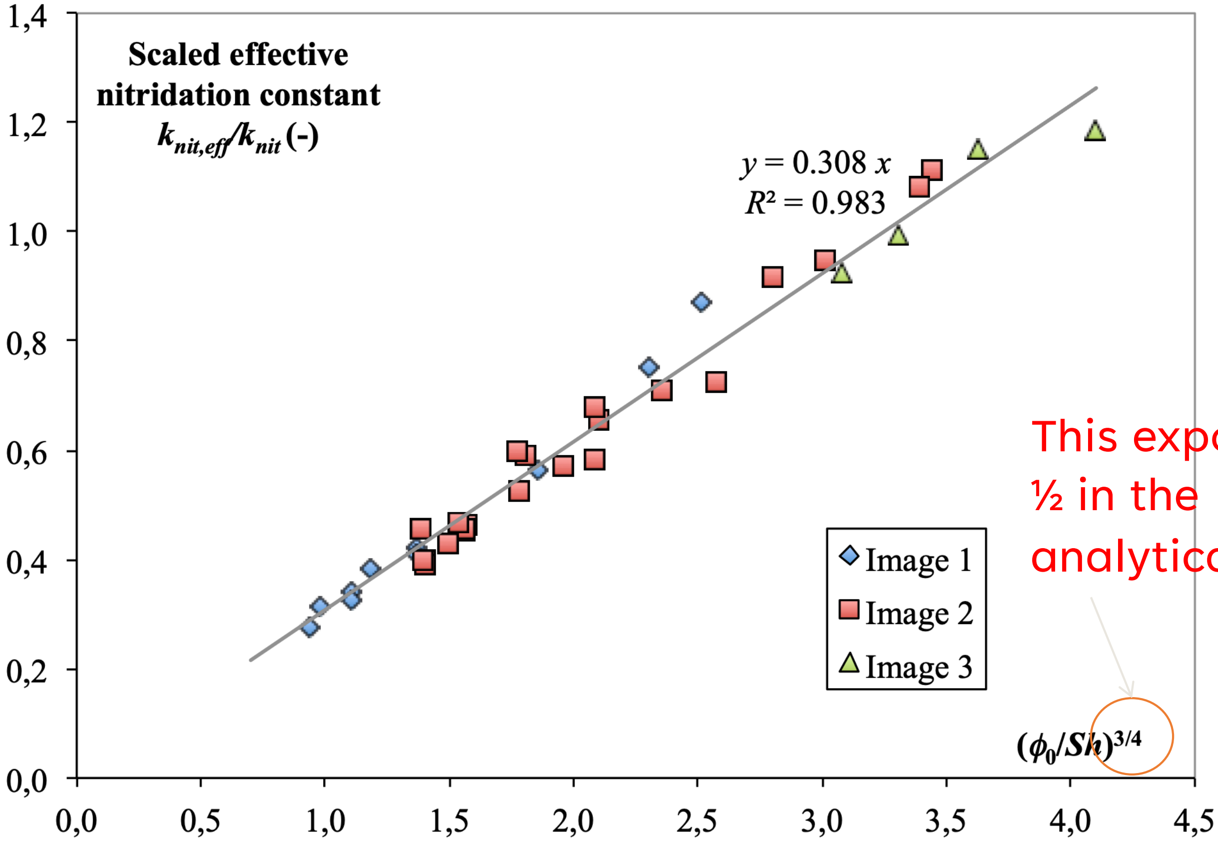


where

$$\mathrm{Sh} = \frac{r_0\left(k_{nit} + k_{rec}\right)}{D_0}$$

G. L. VIGNOLES et al., *Carbon* (2018), vol. **134**, pp. 376–390.

ABLATION : DIMENSIONLESS RESULTS



This exponent is ½ in the analytical model

G. L. VIGNOLES et al., *Carbon* (2018), vol. **134**, pp. 376–390.

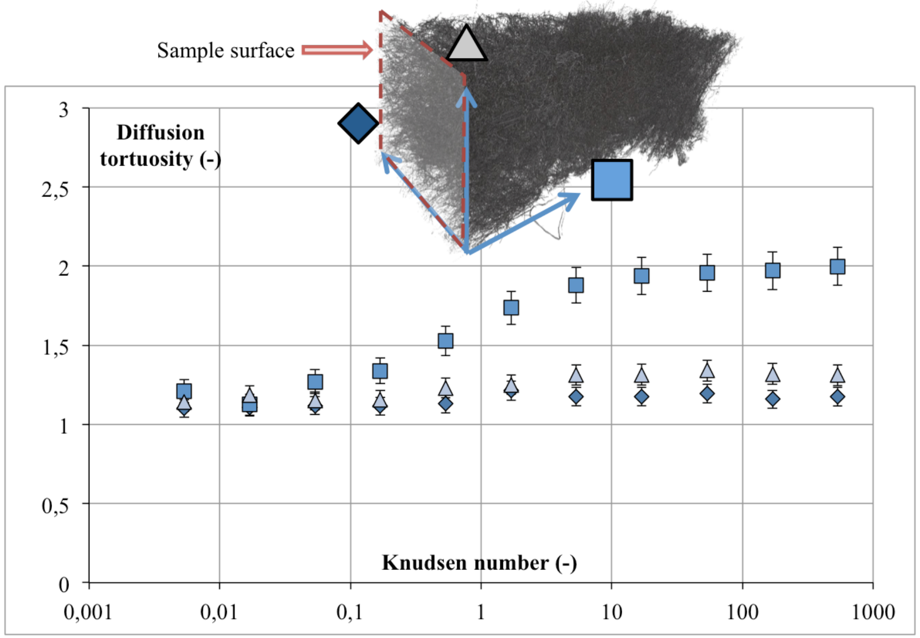
MODEL EXPLOITATION: NITRIDATION IN PLASMA

Diffusion coefficient is corrected by the Knudsen effect and tortuosity coefficient :

$$D_g^{corr} = D_g (1 + Kn)^{-1}\, \eta(Kn)^{-1}$$

$$Kn = \frac{\lambda}{d_p}$$

$$d_p = 4\,(1 - \phi_0)\,/\sigma_{v0}$$



Effective nitridation rate is corrected by the blowing effect

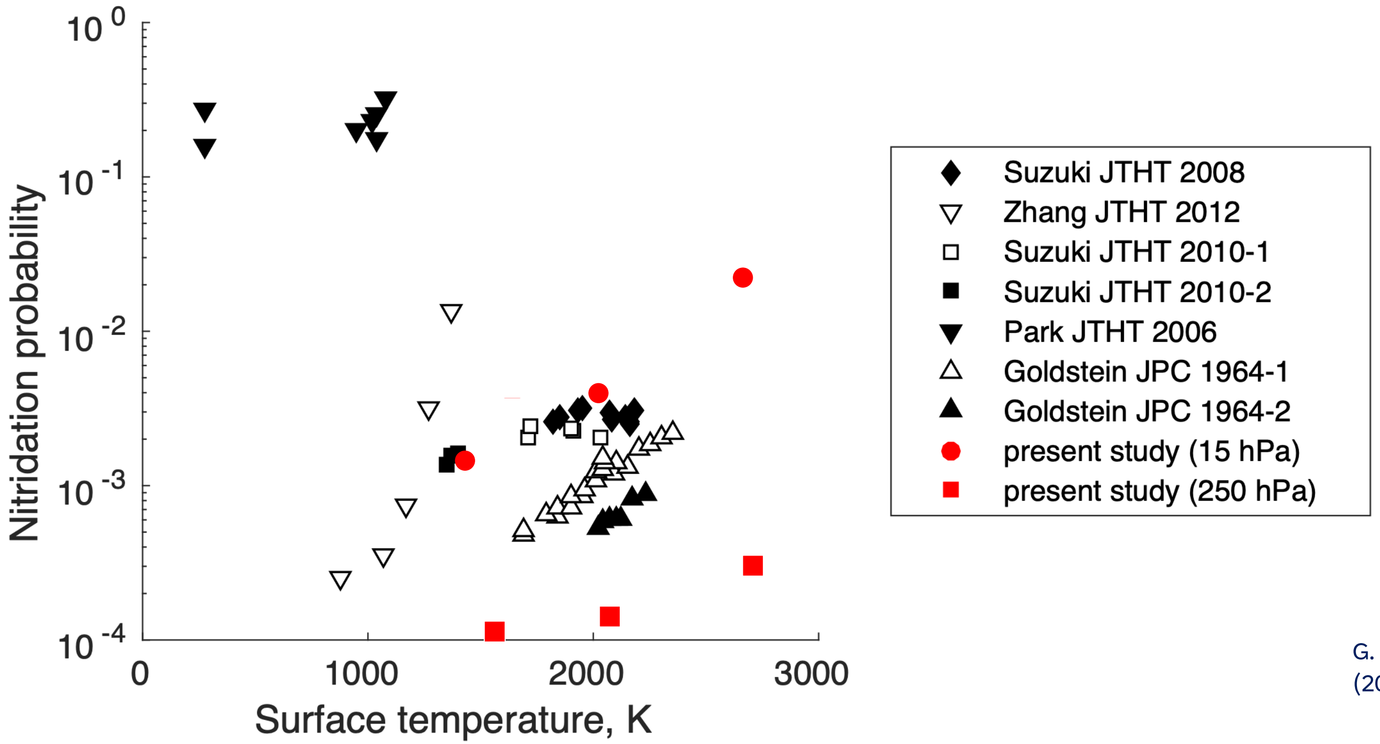
$$k_{nit}^{eff,app} = k_{nit}^{eff}(T)\left\{1 + \left(\frac{M_{CN}}{M_N} - 1\right) y_N\right\}$$

G. L. VIGNOLES et al., *Carbon* (2018), vol. **134**, pp. 376–390.

Rate constants are scaled wrt ¼ molecular velocity

$$k_{i,eff} = \frac{1}{4}\sqrt{\frac{8\mathcal{R}T}{\pi M_i}}\,\underbrace{\gamma_i^0 \exp\left(\frac{E_i}{\mathcal{R}T}\right)}_{\gamma_i}$$

IDENTIFIED NITRIDATION PROBABILITY



G. L. VIGNOLES et al., *Carbon* (2018), vol. **134**, pp. 376–390.

G. L. VIGNOLES et al., *Carbon* (2018), vol. **134**, pp. 376–390.

ABLATION – SUMMARY & OUTLOOK

Interest of the numerical model

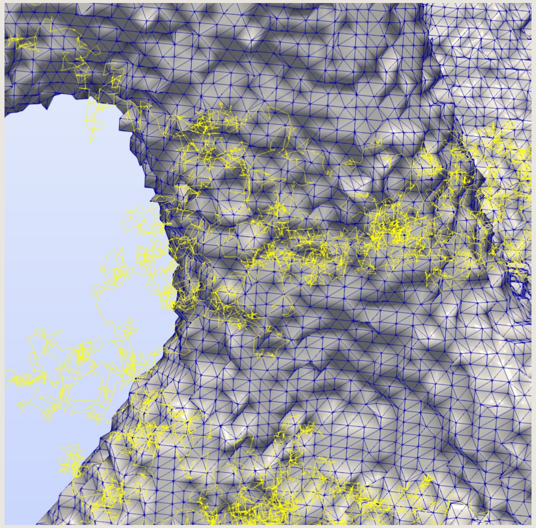
- Results are similar to predictions of a simple analytical model
- The differences are due to the complex porous structure

A complete strategy to interpret ablation tests

- Effective reaction constants can be recovered from CFD analysis + image analysis
- The method can be used the other way to obtain the influence of structural parameters on ablation rate
- ➔ It becomes a design tool

Next step : application to oxidation of C_f/C composites

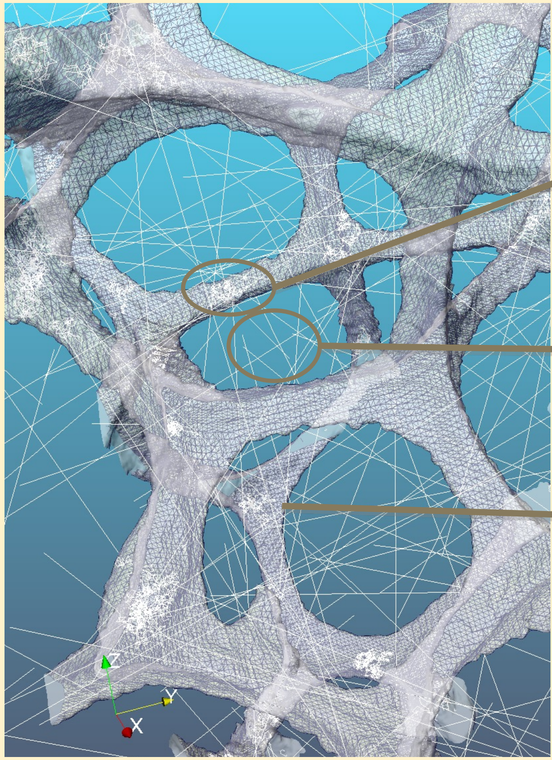
RESULTS - PART 2



HEAT TRANSFER
BY CONDUCTION AND RADIATION

HYBRID RANDOM WALK

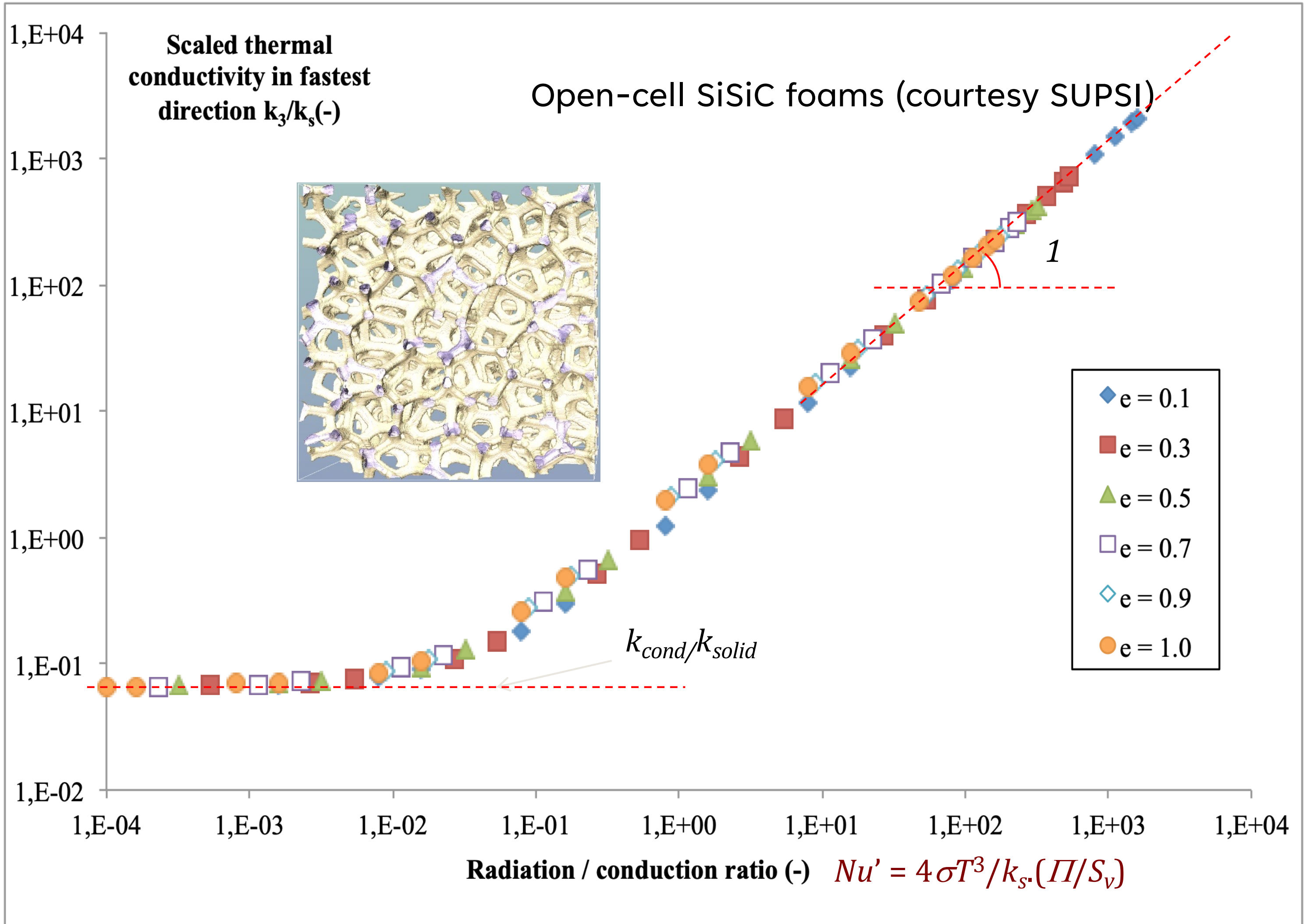
G. L. VIGNOLES, *Int. J. of Heat & Mass Transfer* **93**, 707–719 (2016)



Solid phase: Brownian motion, simulates diffusion linked to heat conduction

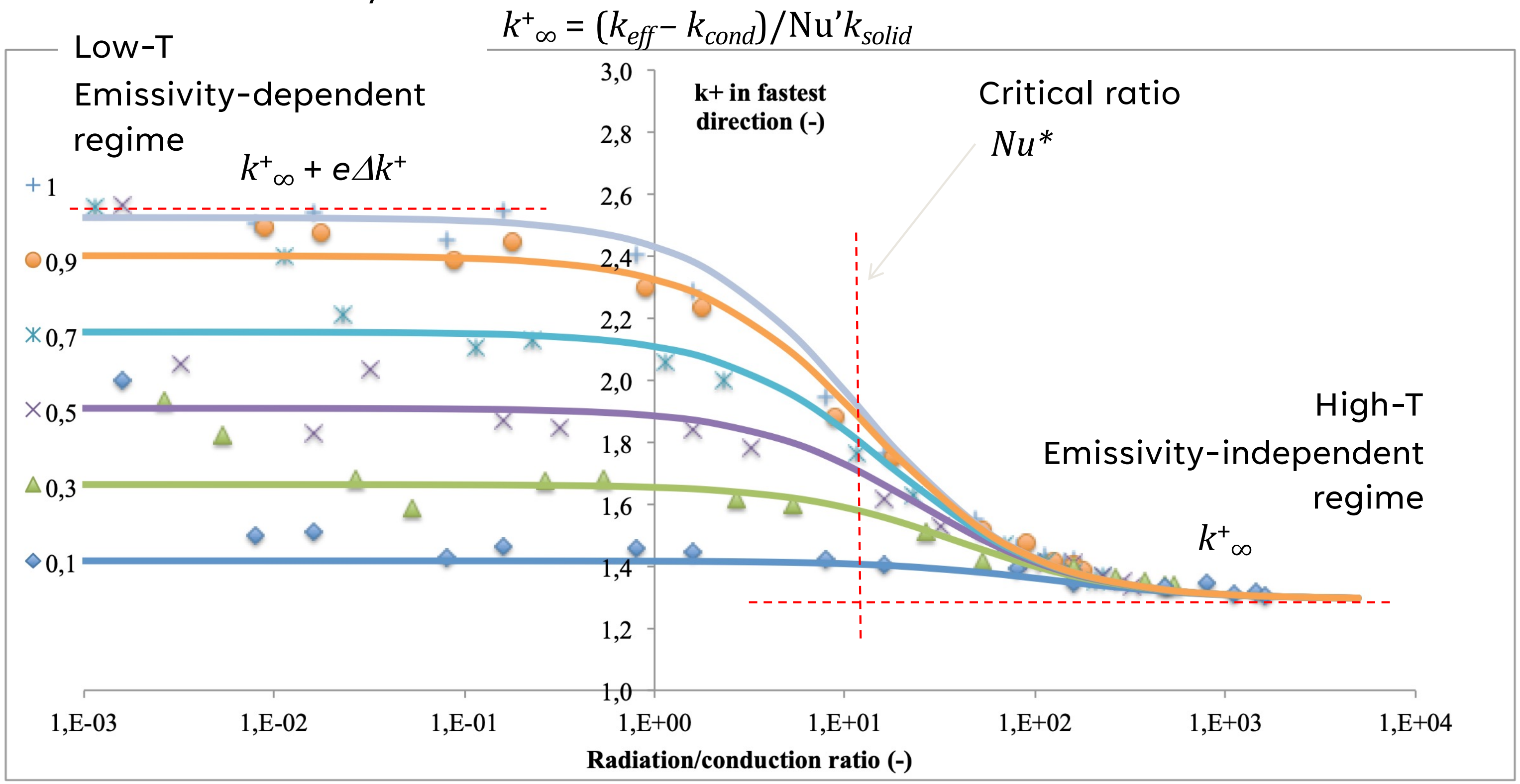
Fluid phase: ray-tracing or kinetic RW

Interface: « flux matching » condition



Vignoles - Interpore 2026, Nantes

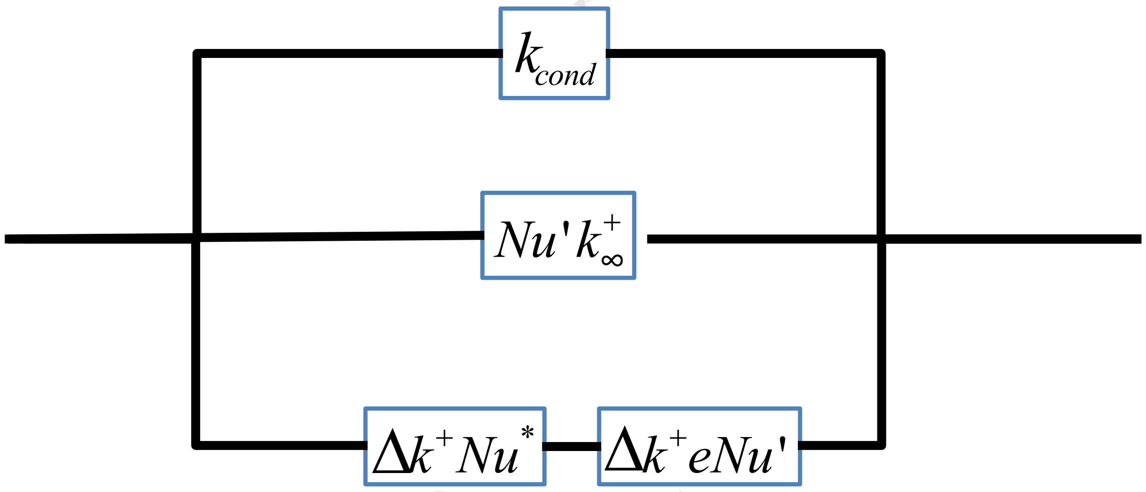
RADIATIVE ETC EXCESS *VS.* RADIATION/CONDUCTION RATIO



G. L. VIGNOLES & A. ORTONA, *Int. J. Therm. Sci.* (2016), vol. **109**, pp. 270–278

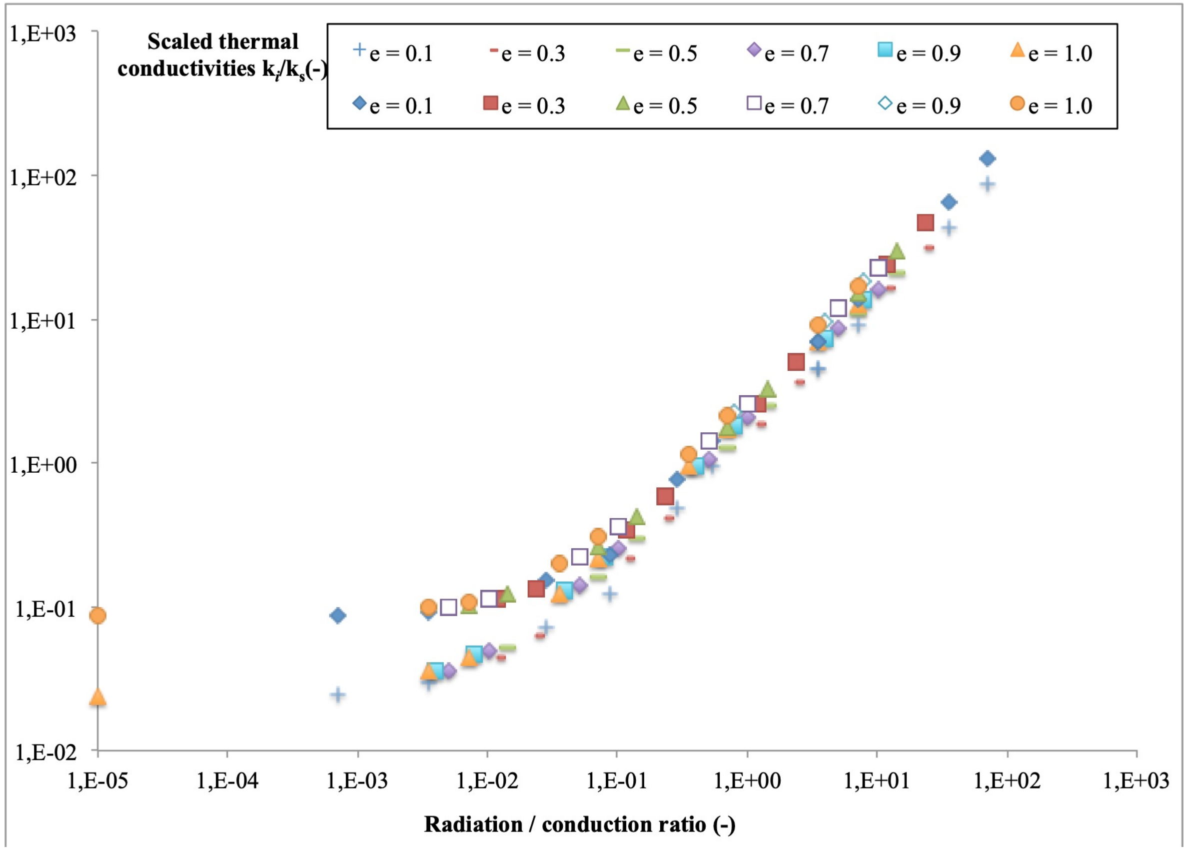
EQUIVALENT CIRCUIT

Pure conduction fully in //
with radiation : OPEN-CELL medium



When radiation fully dominates (Nu’ > Nu*), the emissivity-dependent part does not contribute any more

FIBROUS PREFORM



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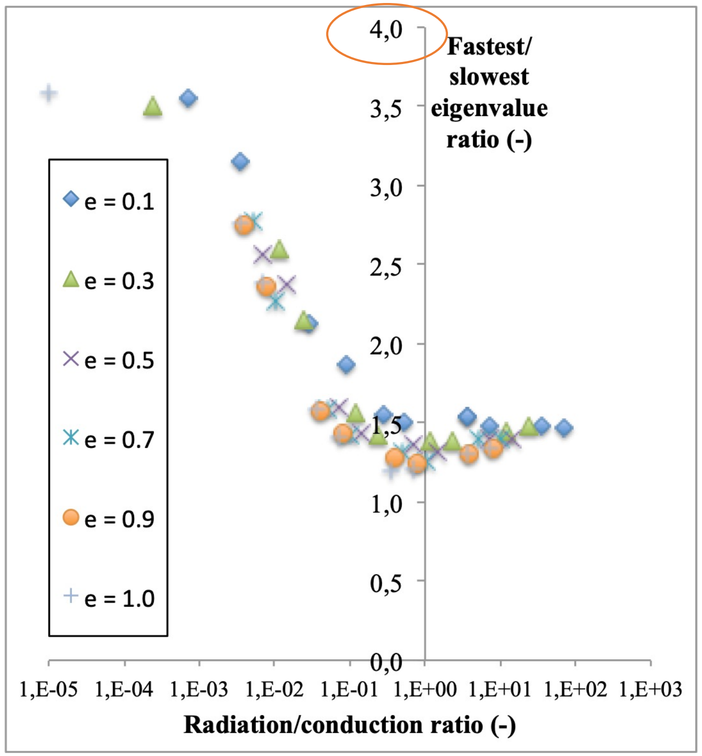
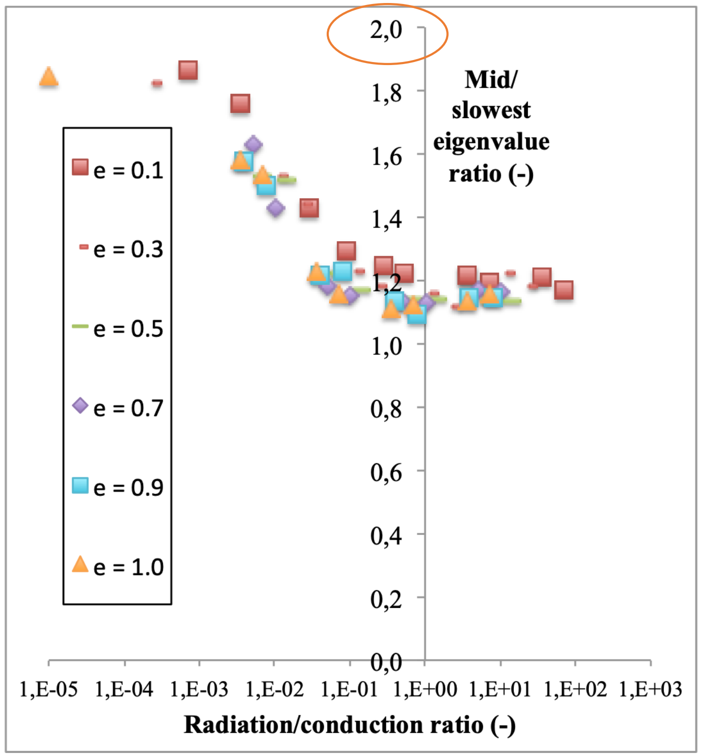
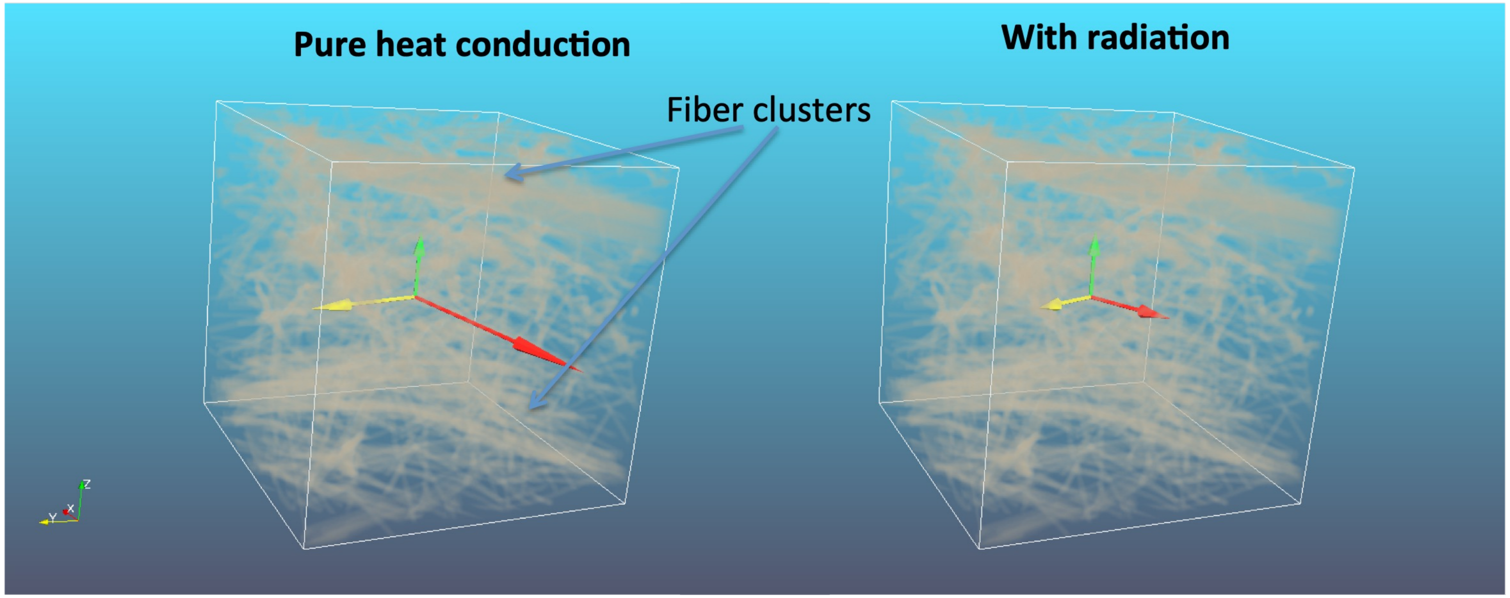




FIBROUS PREFORM



FIBROUS PREFORM

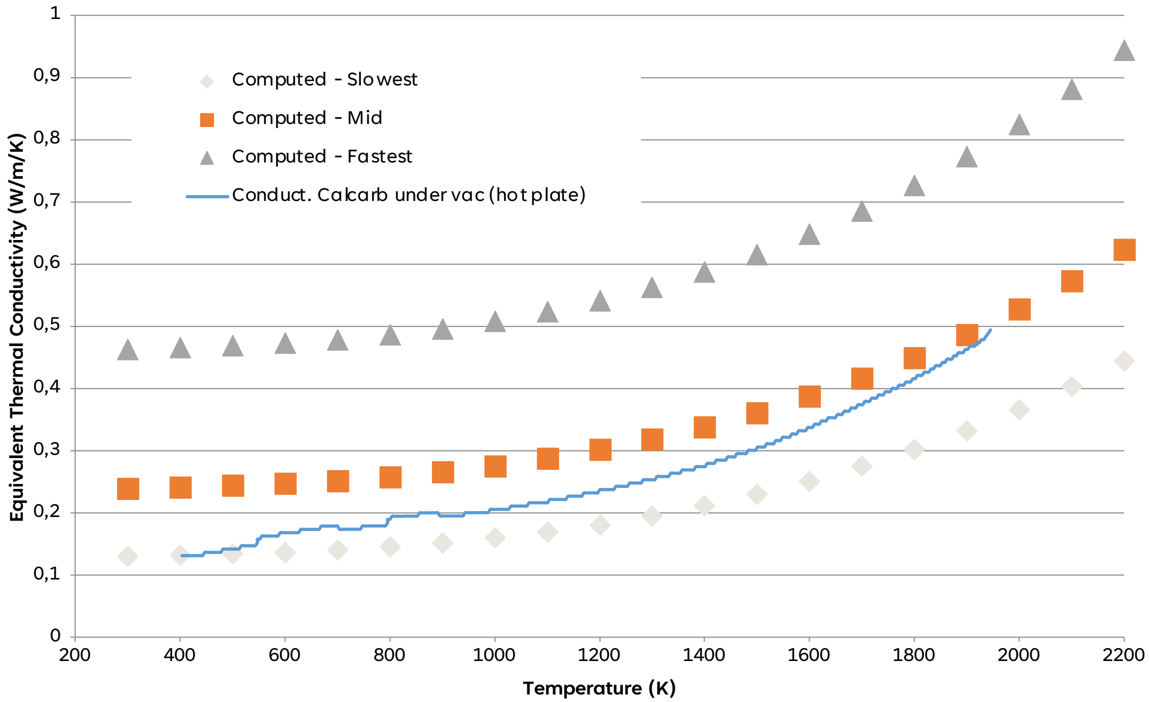
Pure conduction $k_{cond}/(k_s\phi)$	Slowest (X) Intermediate (Y) Fastest (Z) *Fast/slow ratio*	1.09 2.10 3.79 *3.48*
Pure radiation (slope) k^+_∞	Slowest (X) Intermediate (Y) Fastest (Z) *Fast/slow ratio*	1.10 1.35 1.70 *1.55*
Low radiation additional slope contribution Δk^+	Slowest (X) Intermediate (Y) Fastest (Z)	1.45 1.45 1.45
Critical rad/cond ratio	$Nu^* = D_h/\widetilde{d_f} = \varepsilon/(1-\varepsilon)$	5.67

Much more than foams (~0.4) !!

Large decrease of anisotropy when going from low T (conduction) to high T (radiation)

Isotropic, again !

COMPARISON WITH EXP. DATA



Data published by Mersen on Calcarb CBCF 15-2000

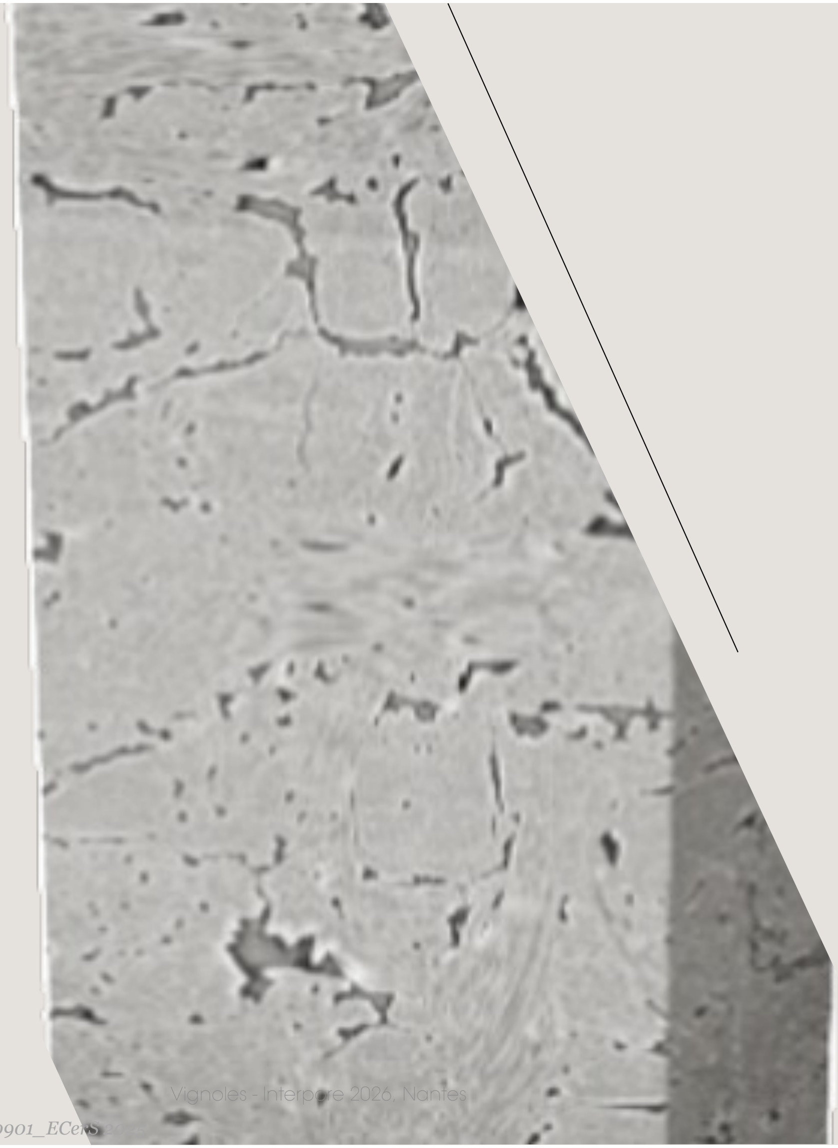
HYBRID RANDOM WALKS: SUMMARY

Numerical tool

- Fast convergence to effective behavior (although detailed field is not converged)
- Effective conducto-radiative conductivity described with few dimensionless parameters
- Nonlinearity successfully introduced (see talk by Penazzi et al.)

Perspectives

- Study semi-transparent media, e.g. ox/ox CMCs
- Development of other numerical methods (« moments » methods)



CONCLUSION

SUMMARY
OUTLOOK

PROS & CONS OF MC/RW METHODS

Pros

- Low memory requirements
- Easily parallelizable
- Easy handling of non-standard boundary conditions
- Fast « pre-convergence » to effective properties

Cons

- Actual convergence rate is only $N^{-1/2}$
- Some physical problems are more difficult to « translate » into MC/RW

MAIN RESULTS

Monte-Carlo Random Walks are well adapted to image-based modeling :

- Effective gas diffusivity in rarefied regime
- Ablation simulations (also, infiltration)
- Effective conducto-radiative heat conductivity

Applications relevant to space technology problems :

- Ablation
- Thermal protection systems modeling
- … but also Chemical Vapor Infiltration

OUTLOOK

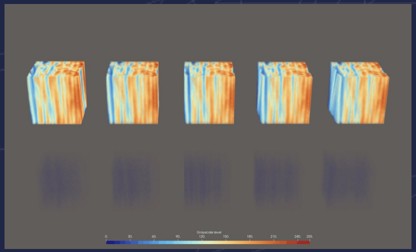
It has been proved that a Brownian walk can be replaced by a more efficient « kinetic-like » walk

Poëtte, G., De La Vauvre, A., Vignoles, G.,
Int. J. Heat Mass Transf. **239** (2025) 126603

- ➔ **Modified solver for ablation**
- ➔ **Modified solver for CVI**
- ➔ **Modified solver for conducto-radiative media**

Possibility to address convective flow

- ➔ **Specific algorithm to solve Stokes' equation and get the velocity field**
- ➔ **Then, convection is easy to include in the algorithm**



Still more projects on Chemical Vapor Infiltration

- ➔ **Incorporation of thermal gradients**

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THANK YOU !
QUESTIONS ?

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