

3D modeling of the ablation of fibrous materials in the Knudsen regime

Jean Lachaud, Nagi N. Mansour

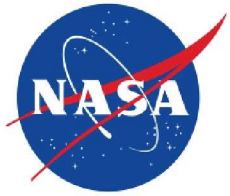
NASA ARC, Moffett Field, CA 94035, USA

ABSTRACT

During atmospheric entry of planetary probes, the thermal protection system (TPS) of the probe is exposed to high temperatures under low pressures. In these conditions, carbonous fibrous TPS materials may undergo oxidation leading to mass loss and wall recession called ablation. This work aims to improve the understanding of material/environment interactions through a study of the coupling between oxygen transport in the Knudsen regime, heterogeneous oxidation of carbon, and surface recession. A 3D Random Walk Monte Carlo simulation tool is used for this study. The fibrous architecture of a model material, consisting of high porosity random array of carbon fibers, is numerically represented on a 3D Cartesian grid. Mass transport in the Knudsen regime from the boundary layer to the surface, and inside this porous material is simulated by random walk. A reaction probability is used to simulate the heterogeneous oxidation reaction. The surface recession of the fibers is followed by front tracking using a simplified marching cube approach. The output data of the simulations are ablation velocity and dynamic evolution of the material porosity. A parametric study is carried out to analyze the material behavior as a function of Knudsen number for the porous media (length of the mean free path compared to the mean pore diameter) and the intrinsic reactivity of the carbon fibers. The model is applied to Stardust mission reentry conditions and explains the unexpected behavior of the TPS material that underwent mass loss in volume.

Key Words

3D fibrous architecture, Oxidation modeling, Random-walk, Knudsen regime, Front tracking



Multiscale modeling of Ablation and Pyrolysis in PICA-like materials

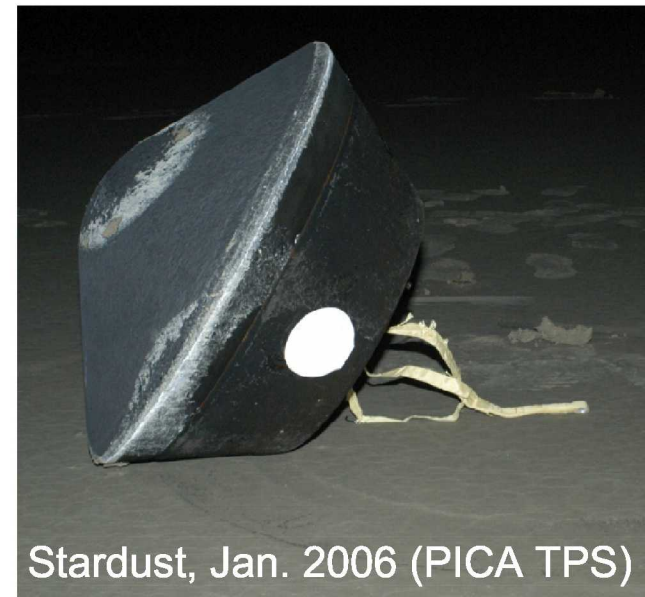
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Mairead Stackpoole and Ioana Cozmuta are acknowledged for providing results from their work:
M. Stackpoole *et al.*, Post-Flight Evaluation of Stardust Sample Return
Capsule Forebody Heatshield Material, AIAA 2008-1202.

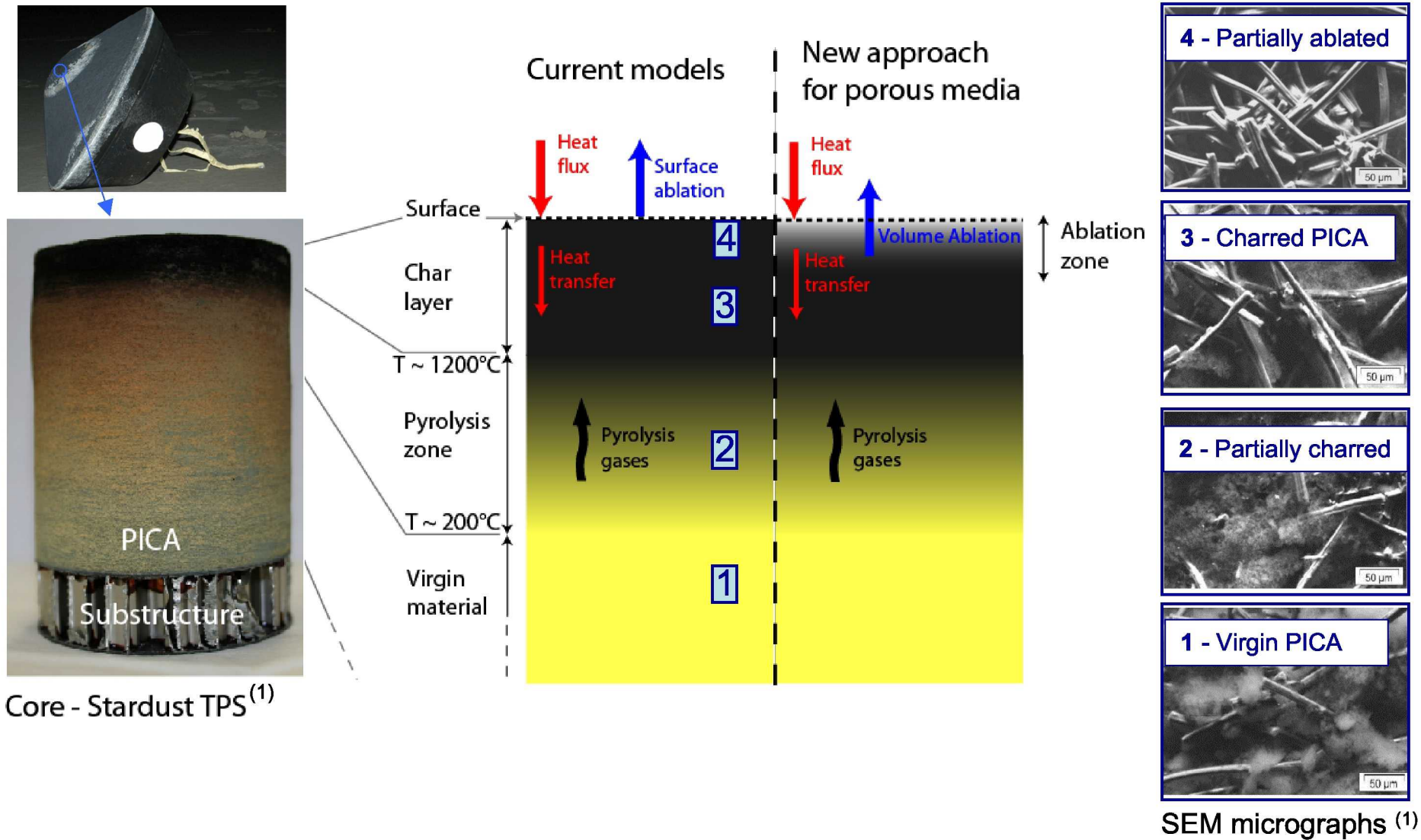
*Sponsored by NASA's Fundamental Aeronautics Program - Hypersonics Project





. Scientific context

Pyrolysis and ablation of PICA (Phenolic Impregnated Carbon Ablator)

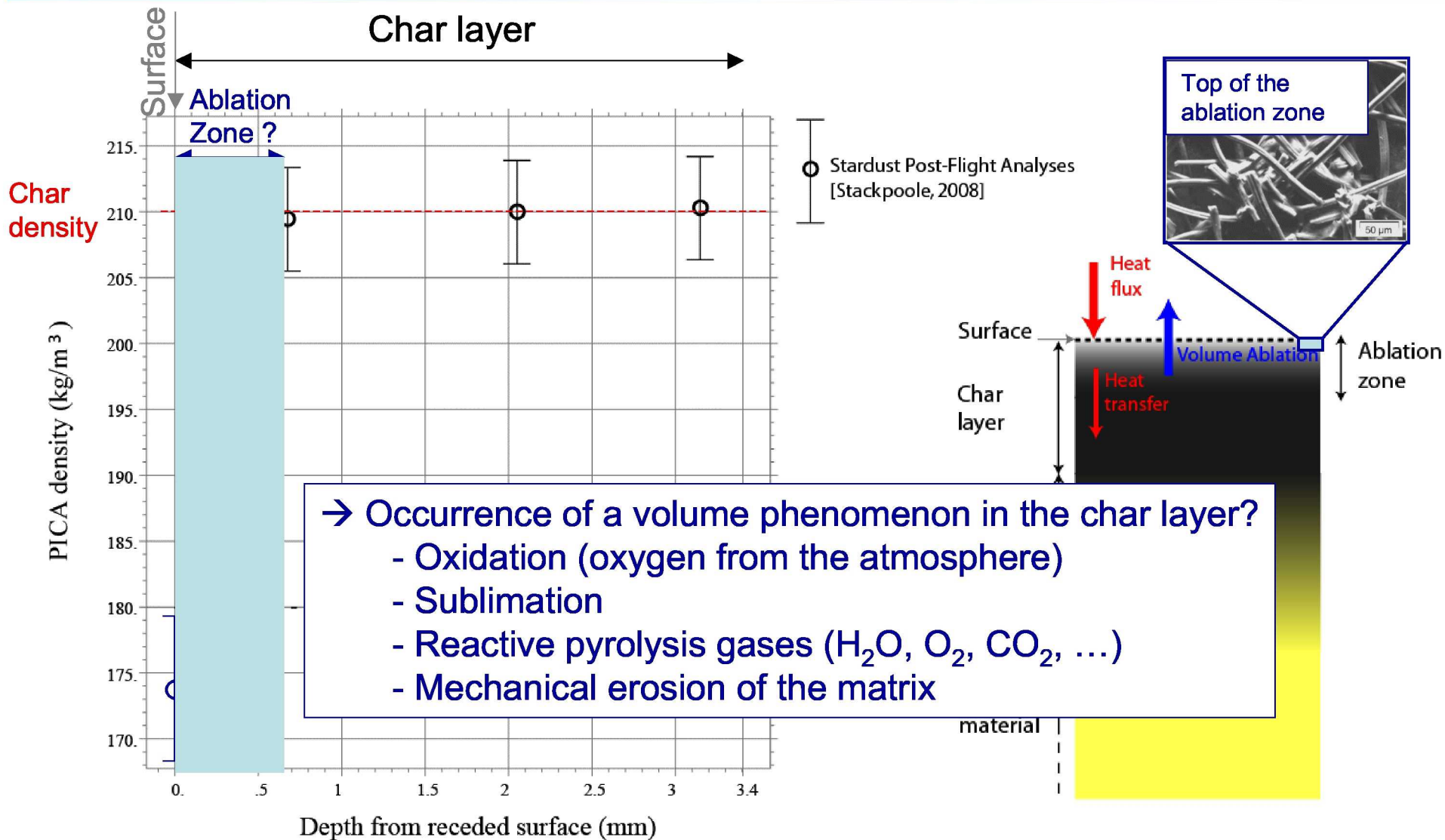


(1) M. Stackpoole *et al.*, Post-Flight Evaluation of Stardust Sample Return Capsule Forebody Heatshield Material, AIAA 2008-1202
October 15, 2008
Hypersonics Materials and Structures - Ablators Discussion
2



. Literature data

Stardust Post-flight Analyses (1)



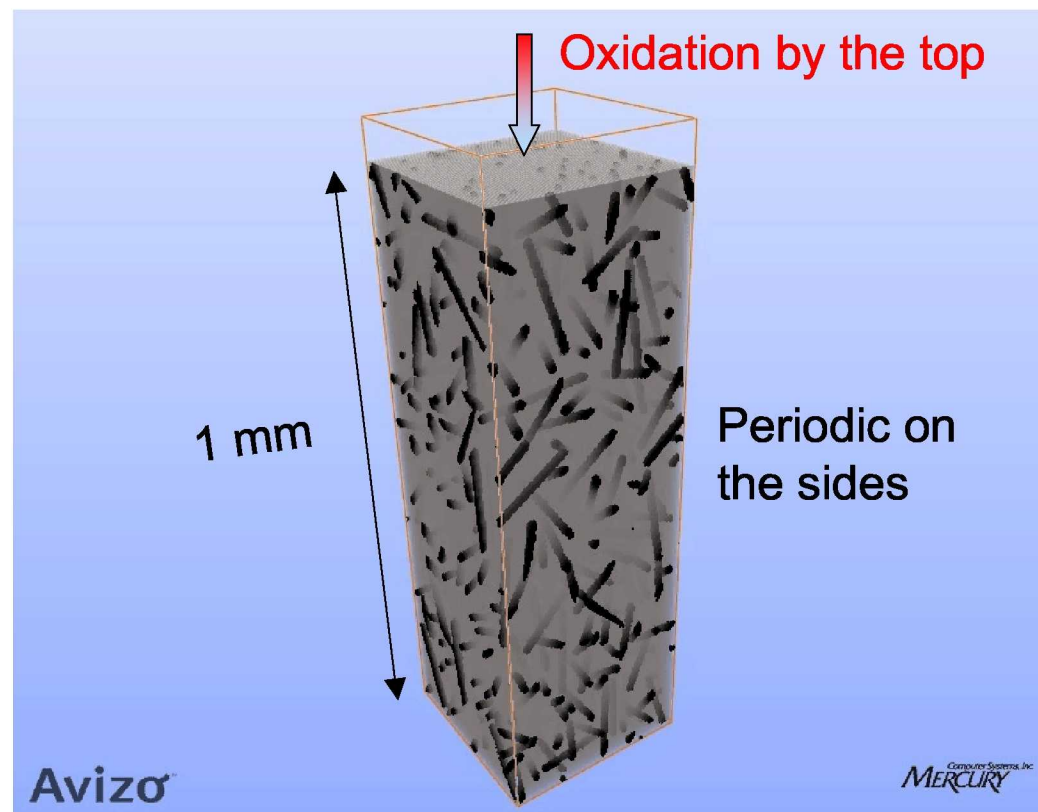


. Ablation model : multiscale approach

Microscopic simulation of the oxidation of a carbonized PICA

- **Hypotheses :**

- $T = 3360 \text{ K}$ (isothermal)
- $P = 0.26 \text{ Atm}$
- Air
- No pyrolysis gas blowing
- $\rho_f = 32 \rho_m = 1.8 \text{ g/cm}^3$
[Stackpoole *et al.*, 2008]
- $k_m = 10 k_f = 13.7 \text{ m/s}$
[Drawin 1992, Lachaud 2007]
- Simulation : 1.2 s



Simulation
tool

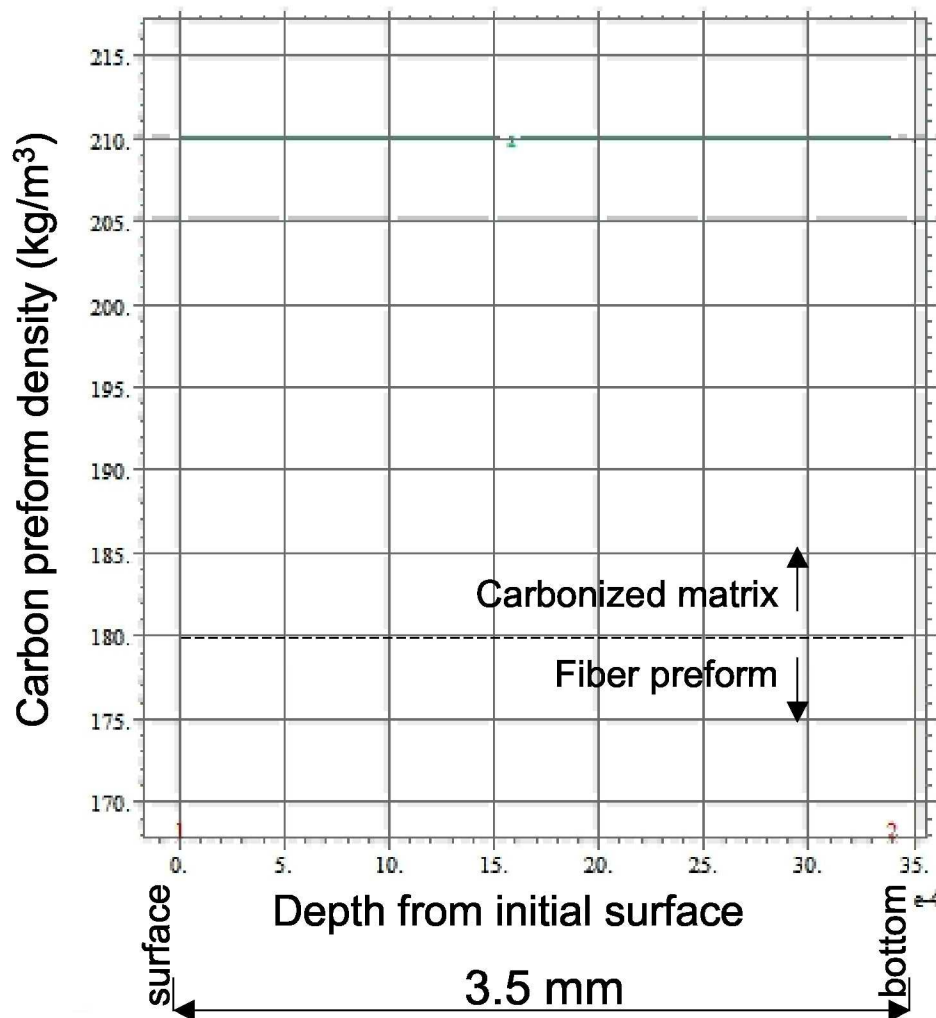




. Application : Stardust Reentry Conditions

End of the ablative part of Stardust trajectory : 90s ($T_{\text{wall}} = 1350 \text{ K} < T_{\text{sublim}}$) to 130s ($T_{\text{wall}} = 850 \text{ K} < T_{\text{oxi}}$)

- Pure oxidation of the char layer of a PICA



Loosely coupled with traditional tools:

- **data from FIAT inside the material**

- Temperature gradient
- Pyrolysis gas velocity

- **data from DPLR at the wall**

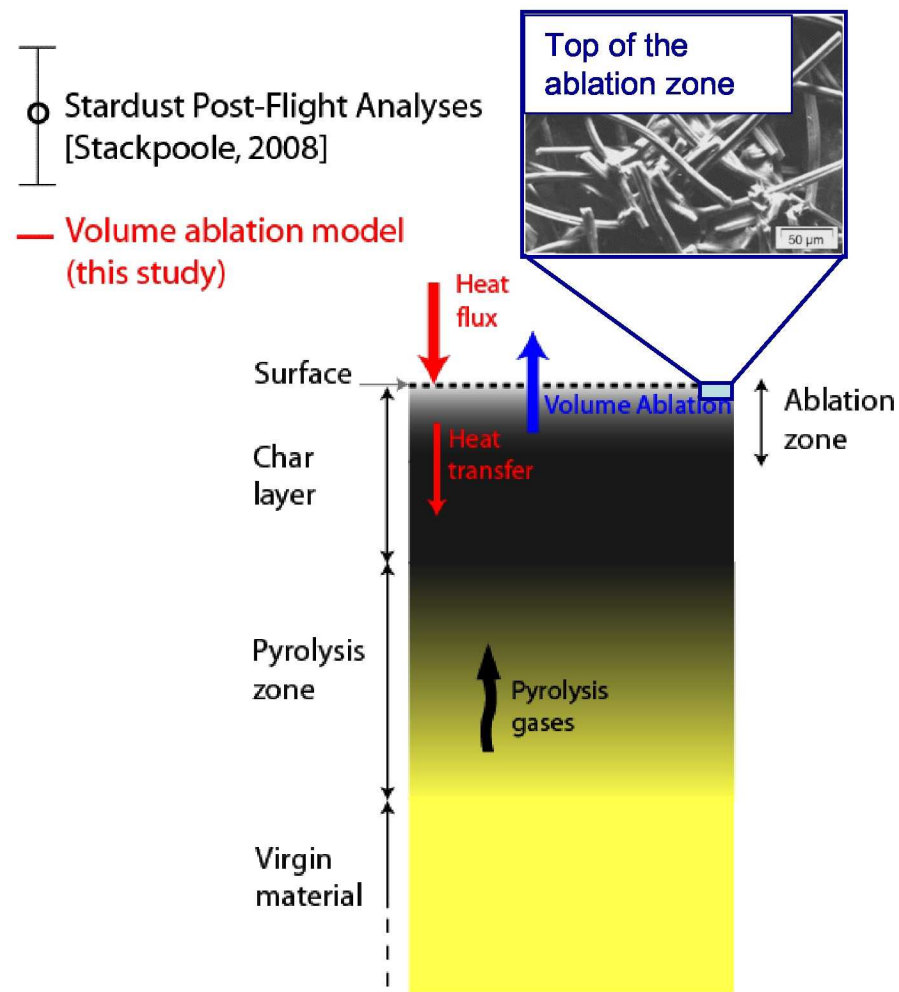
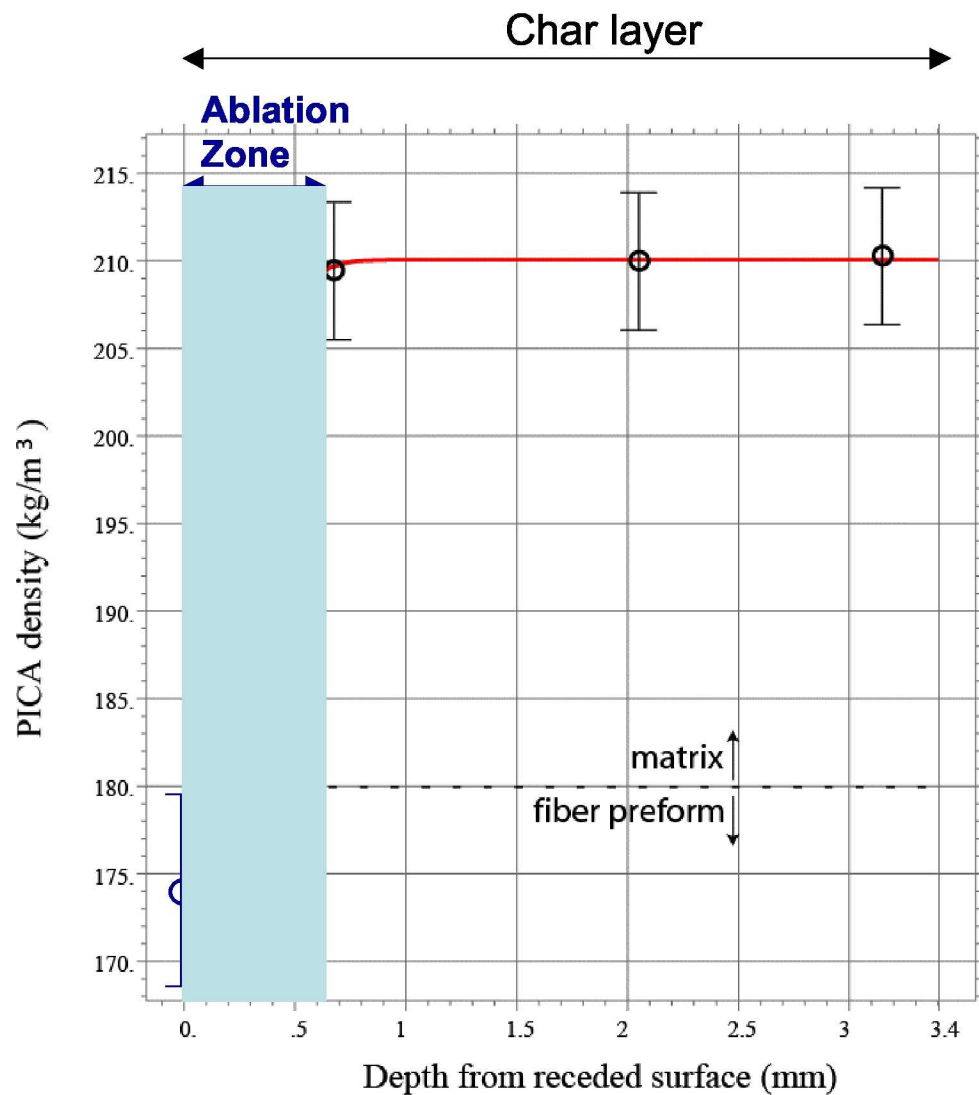
- Oxygen partial pressure
- Total pressure





. Application : Stardust Reentry Conditions

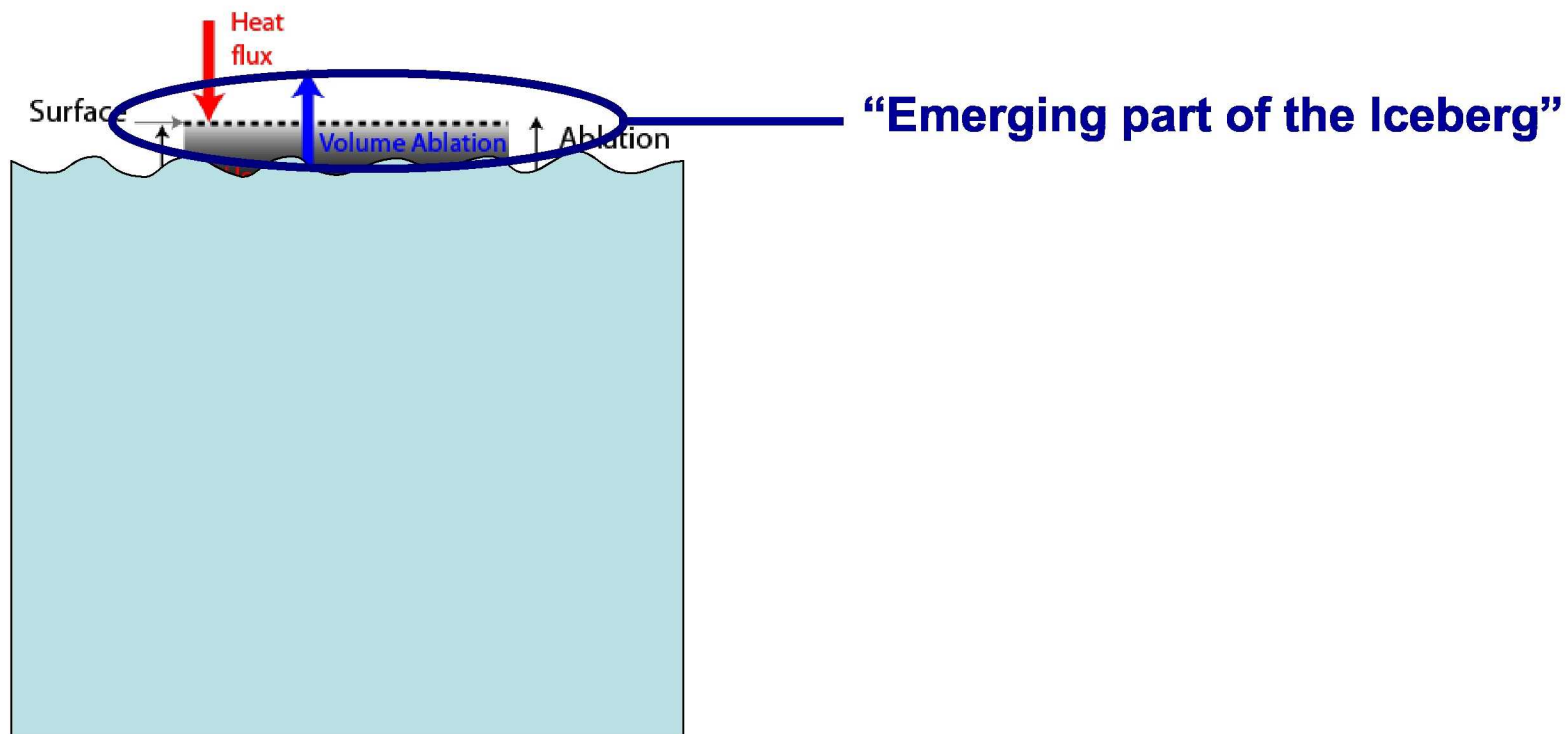
Fit of experimental data using the volume ablation model





. Conclusion

- Multi-scale model for the Ablation layer
 - Surface / Volume ? → depends on conditions
 - Transition criterion : Thiele Number $\gg 1$ → Surface
 - Stardust reentry conditions: Volume oxidation under the hypotheses of the model
 - First material response model accounting for volume ablation
 - capability to reproduce experimental data





. Perspectives

Integration of volume ablation in the pyrolysis model

Energy balance

$$(\varepsilon \rho_g c_g + \varepsilon_f \rho_f c_f + \varepsilon_m \rho_m c_m) \frac{\partial T}{\partial t} = \overline{\nabla \cdot (k \cdot \nabla T)} - \varepsilon \rho_g c_g \vec{v}_g \cdot \nabla T + \delta h_p \frac{\partial \varepsilon_m \rho_m}{\partial t} + \delta h_f \frac{\partial \varepsilon_f \rho_f}{\partial t} + \delta h_m \frac{\partial \varepsilon_m \rho_m}{\partial t}$$

Pyrolysis law

$$\rho_m = \rho_v - \sum_{i=1}^n \text{laws} (\rho_{v,i} - \rho_{p,i}) \xi_i \quad \text{with} \quad \frac{\partial \xi_i}{\partial t} = (1 - \xi_i)^{n_i} A_i \exp\left(-\frac{E_{A_i}}{RT}\right)$$

Ablation laws (heterogeneous chemistry)

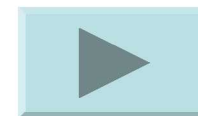
$$\text{Fibers : } \frac{\partial \varepsilon_f}{\partial t} = -\Omega_f S_f \sum_{i=1}^{\text{species}} k_{f,i} C_i^n \quad \text{Carbonized matrix : } \frac{\partial \varepsilon_{m,abla}}{\partial t} = -\Omega_m S_m \sum_{i=1}^{\text{species}} k_{m,i} C_i^n$$

Transport and chemistry (heterogeneous & homogeneous : oxygen from the air + pyrolysis gases + sublimated carbon)

$$\frac{\partial \langle C_i \rangle}{\partial t} + \nabla \cdot (\overline{-D_{i,eff} \nabla \langle C_i \rangle}) + \nabla \cdot (\langle \vec{v}_g \rangle \langle C_i \rangle) = \omega_f + \omega_{m,abla} + \omega_i$$

Momentum balance

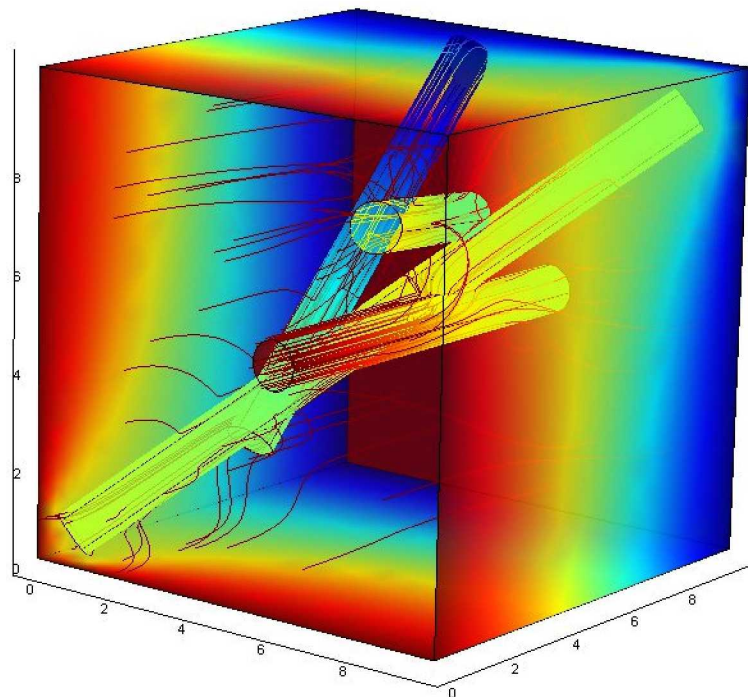
$$\varepsilon \vec{v}_g = -\frac{\overline{K}}{\mu} \cdot \nabla p$$





. Modeling conduction in porous media

Illustration



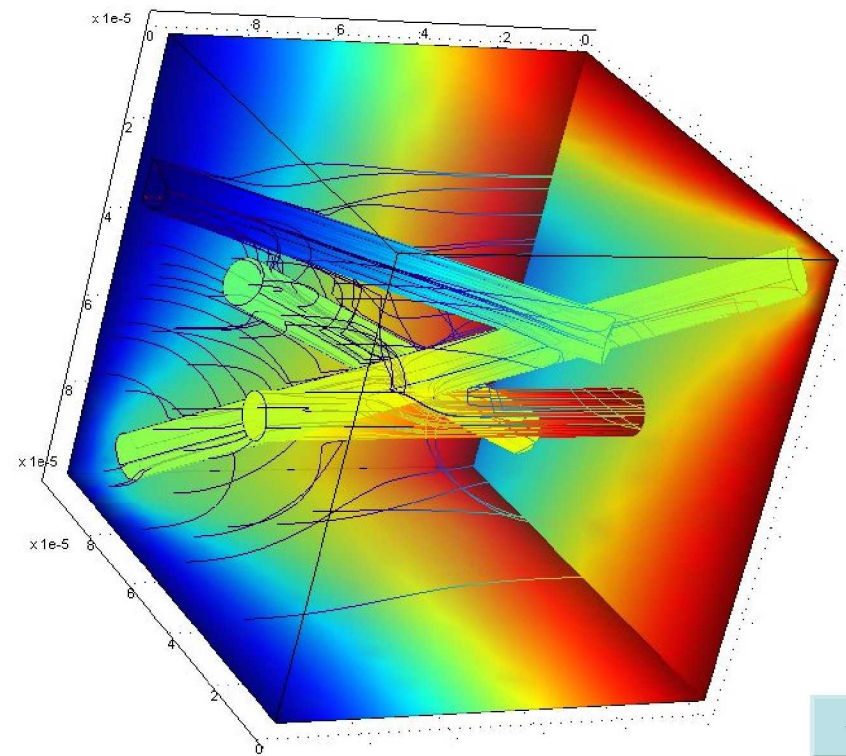
4 random fibers

$$\varepsilon = 0.97$$

$$k_{air} = 0.025 \text{ } W.m^{-1}.K^{-1}$$

$$k_{fiber} = 10 \text{ } W.m^{-1}.K^{-1}$$

$$k_{eff_simulation} = 0.1 \text{ } W.m^{-1}.K^{-1}$$





. Determination of the effective diffusion coefficient

Direct Simulation Monte Carlo (DSMC)

- **Monte Carlo Simulation :**

- Random Walk rules :

- (T,P) fixed = $(\bar{\lambda}, D)$ fixed
 - λ : Maxwell-Boltzmann distribution
 - constant velocity norm ($D = 1/3 \bar{v} \bar{\lambda}$)
 - 3D random direction drawing

1) Displacement ξ of 10000 walkers followed during τ (chosen for convergence)

2) Einstein relation on diffusion process :

$$D_{ej} = \frac{\langle \xi_j^2 \rangle}{2\tau}$$

- **Tortuosity as a function of Kn for the fibrous preform of this study**

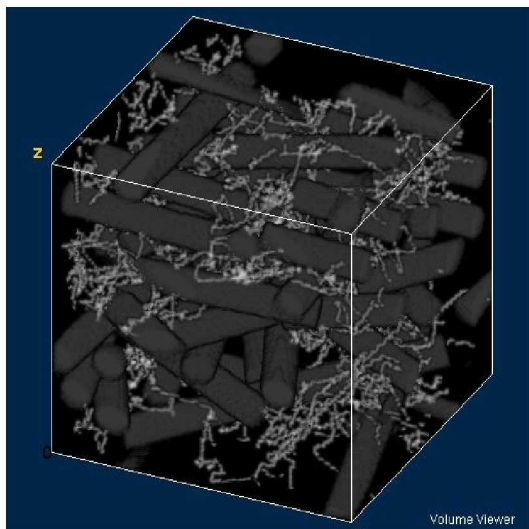
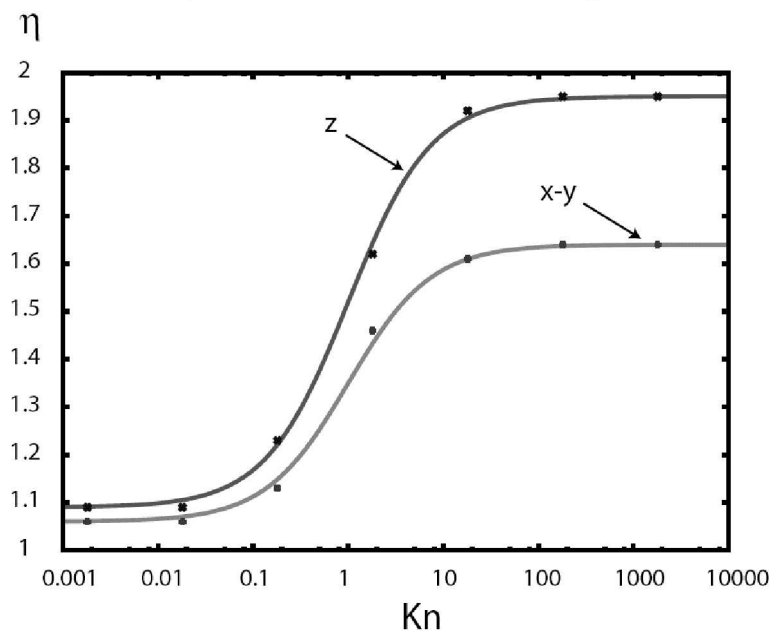


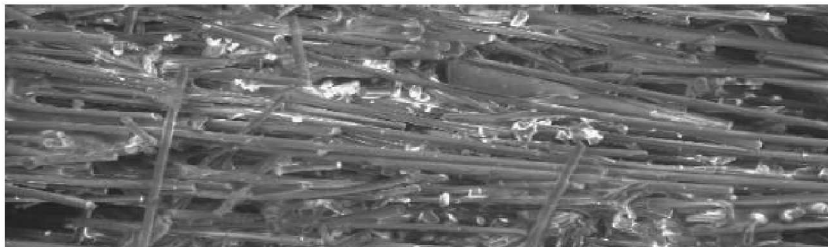
Illustration : path of a walker in a periodic cell



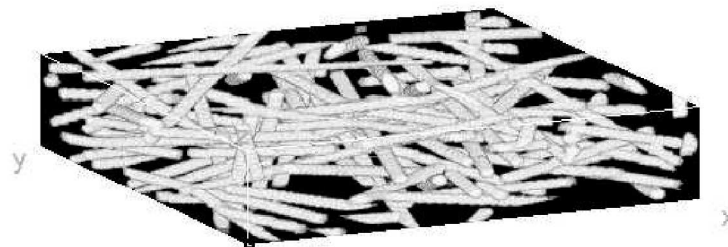


. Modeling advection in porous media

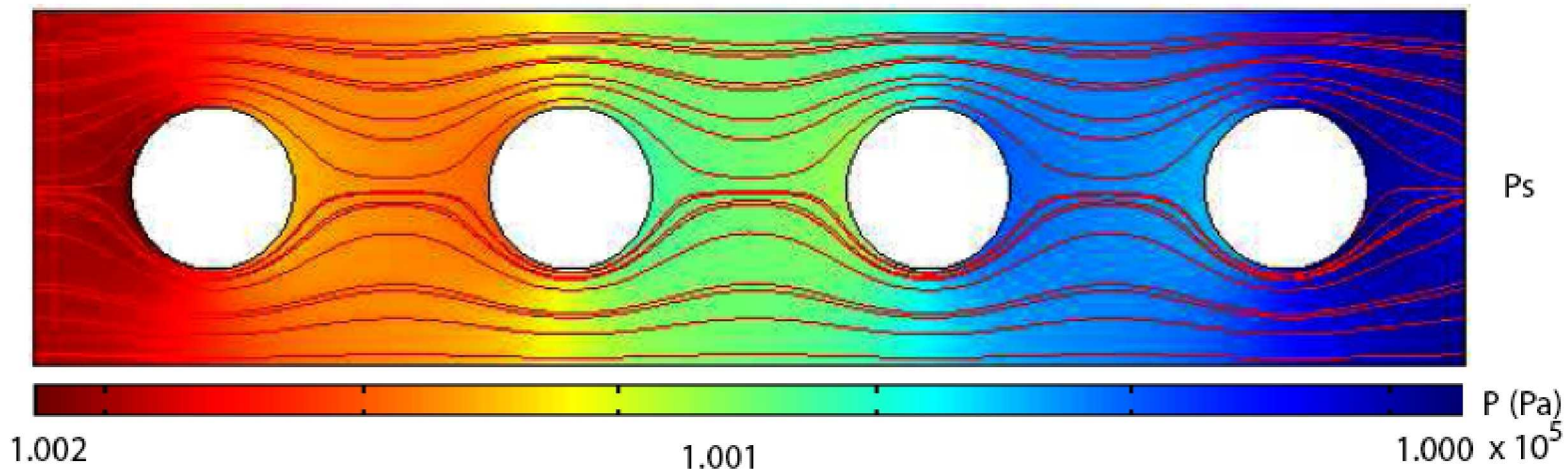
Traditional CFD method - DSMC to be used for Knudsen regime



SEM observation



Fibrous media geometry model



$$\epsilon_g \mathbf{v}_g = -\frac{K_g}{\mu_g} \cdot \nabla p_g$$

$$K_g (\text{virgin}) = 1.6 \cdot 10^{-11} \text{ m}^2$$

$$K_g (\text{pyrolysed}) = 2.0 \cdot 10^{-11} \text{ m}^2$$

Same order of magnitude as the Kozeny-Carman law



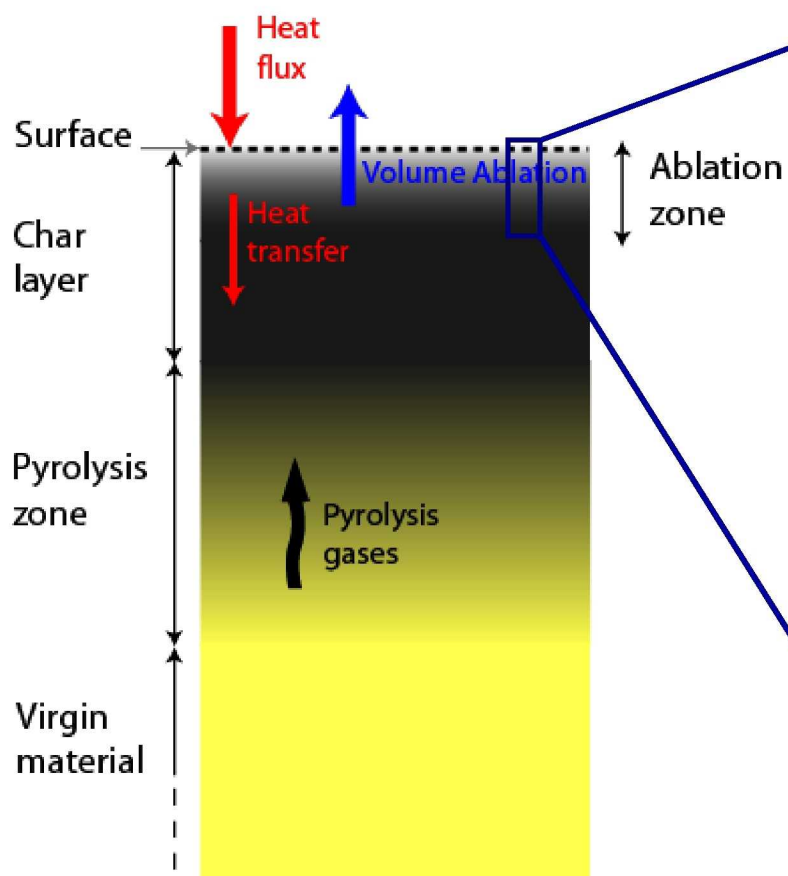


. Perspectives : Summary

Multiscale modeling strategy

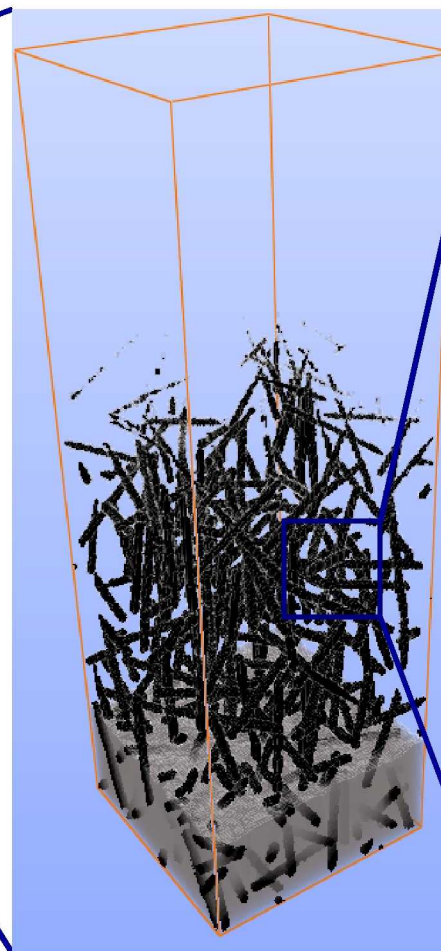
Macroscopic model : Ablation & Pyrolysis

- 3D Cartesian code (Finite Volume / 3D Level set)
- Experiments

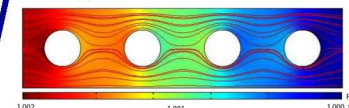


Microscopic approach : multi-physics

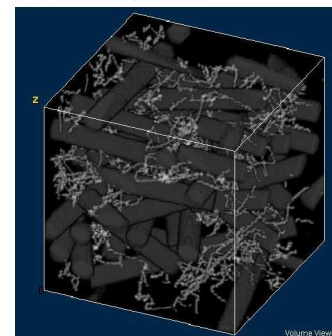
- Analytic, CFD & DSMC
- Experiments



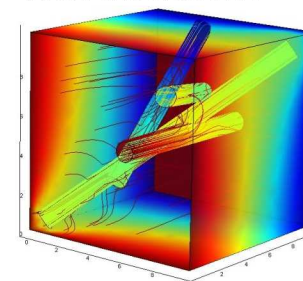
Flow



Diffusion



Conduction



Chemistry

$$\omega_f + \omega_{m,abla} + \omega_i$$

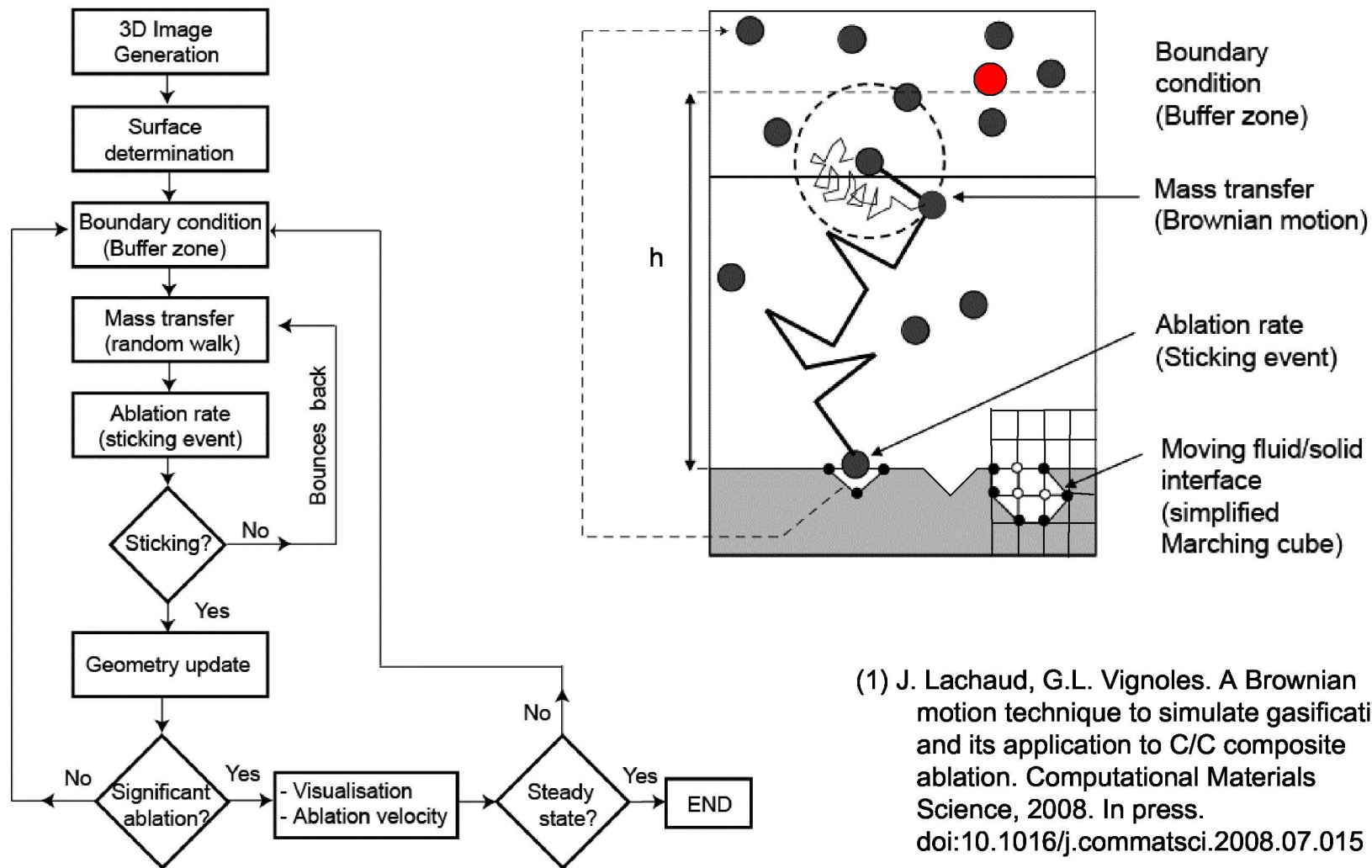


Appendix



. 3D simulation tool : AMA⁽¹⁾

Random walk algorithm / 3D Marching Cube front tracking





. Ablation model : multiscale approach

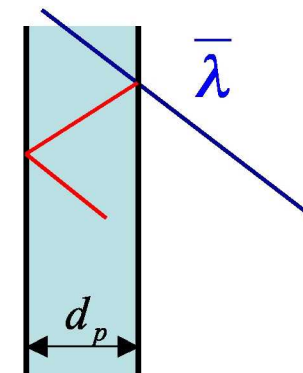
Effective diffusion coefficient

- **Knudsen effects**

Bosanquet model

$$\frac{1}{D_{ref}} = \frac{1}{D_B} + \frac{1}{D_K} = \frac{1}{\frac{1}{3}v\bar{\lambda}} + \frac{1}{\frac{1}{3}vd_p} \quad (\text{harmonic average})$$

E.g. Stardust peak heating $Kn \approx 0.1$, i.e. $\bar{\lambda} \approx 10 d_p$

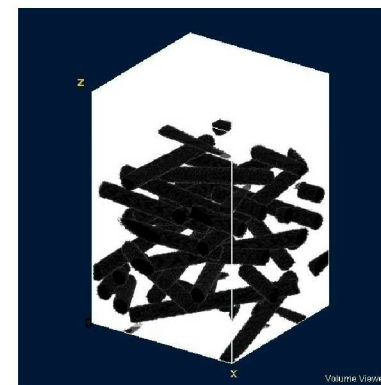
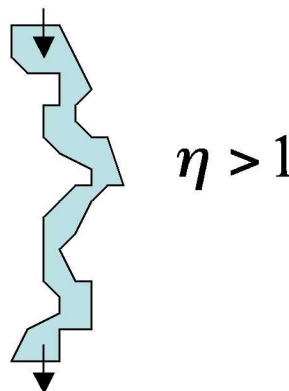


- **Tortuosity effects**

Averaging method

$$D_{eff} = \frac{\epsilon}{\eta} D_{ref}$$

Tortuosity has to be assessed by numerical simulation





. Ablation model : multiscale approach

Determination of the effective diffusion coefficient D_{eff}

- **Monte Carlo Simulation :**

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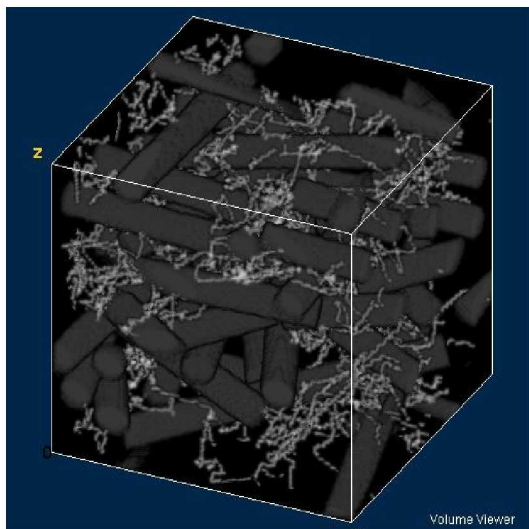
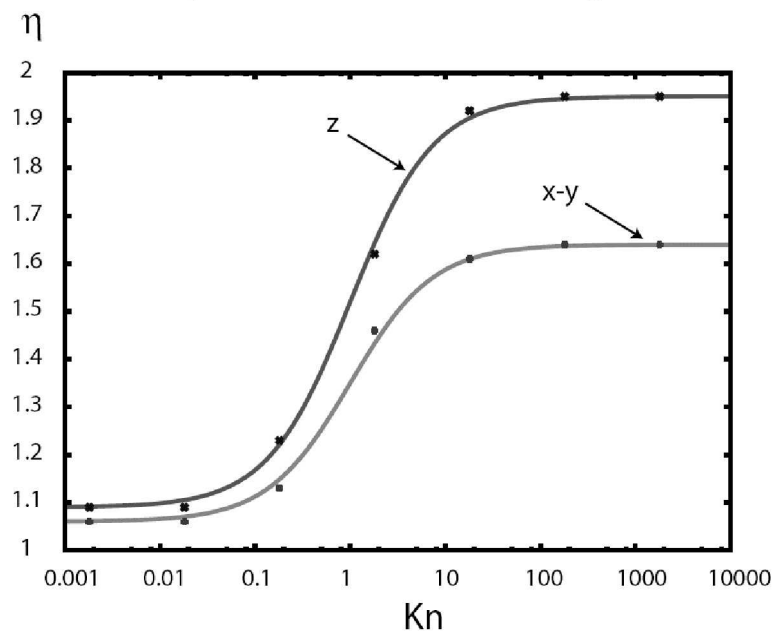


Illustration : path of a walker in a periodic cell





3 kinds of Experiments

Improvement & Validation of the models

Device	Measured data	Dimension & scale	Time scale	Difficulty	Interest	Other comments
SEM* Scanning Electron Microscopy)	Architecture (intuitive) resolution: 100 nm	2D surface micro to macro	1 month	Image analysis	Help into architecture modeling at all scales	Relatively low cost for fast preliminary results
Microstructure XOMO** X-ray scanning micro-tomography)	Architecture (accurate) resolution : 1µm	3D micro	1+ year	- prepare samples - image segmentation	Enable an accurate direct numerical simulation	Key results -> master or PhD student in Bordeaux? +10kEuros
Physico-chemistry TGA** Thermo Gravimetric Analysis) + mass spectrometer	Chemistry Pyrolysis gas analysis Carbon fibers reactivity to these gas	1D micro	1+ year	- data analysis	Understanding of heterogeneous and homogeneous chemistry	- No rush - Data from 1970 - Useful again for porous TPS
Physico-chemistry Short ramp PR tests* 0-2500K	Effective conductivity $k=f(T)$	3D macro	6 month	-thermocouple position -data analysis	Useful for radiation analysis	Needed ASAP
Validation Long steady state PR tests** + tangential blowing)	Thermal gradient Density profile Recession	3D micro 2D ortho macro	1-2 years	-thermocouple position -quantify spallation= f(shear stress)	Ablation/pyrolysis coupling Spallation Model validation	Parametrical study on blowing and grad(T)
Validation Plasma tests**	idem	3D micro 2D ortho macro	2-3 years	-test conditions -data analysis	Global validation fluid + mater	Parametrical study on P, T, v

* : to be done in priority with available funding / ** : to plan now and begin in 1 year