# Microscopic scale simulation of the ablation of fibrous materials

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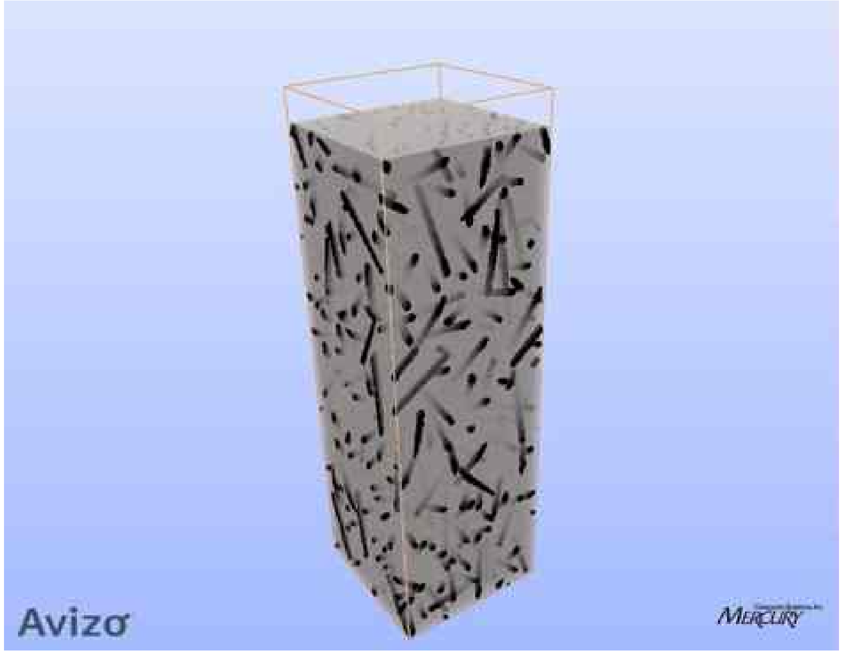

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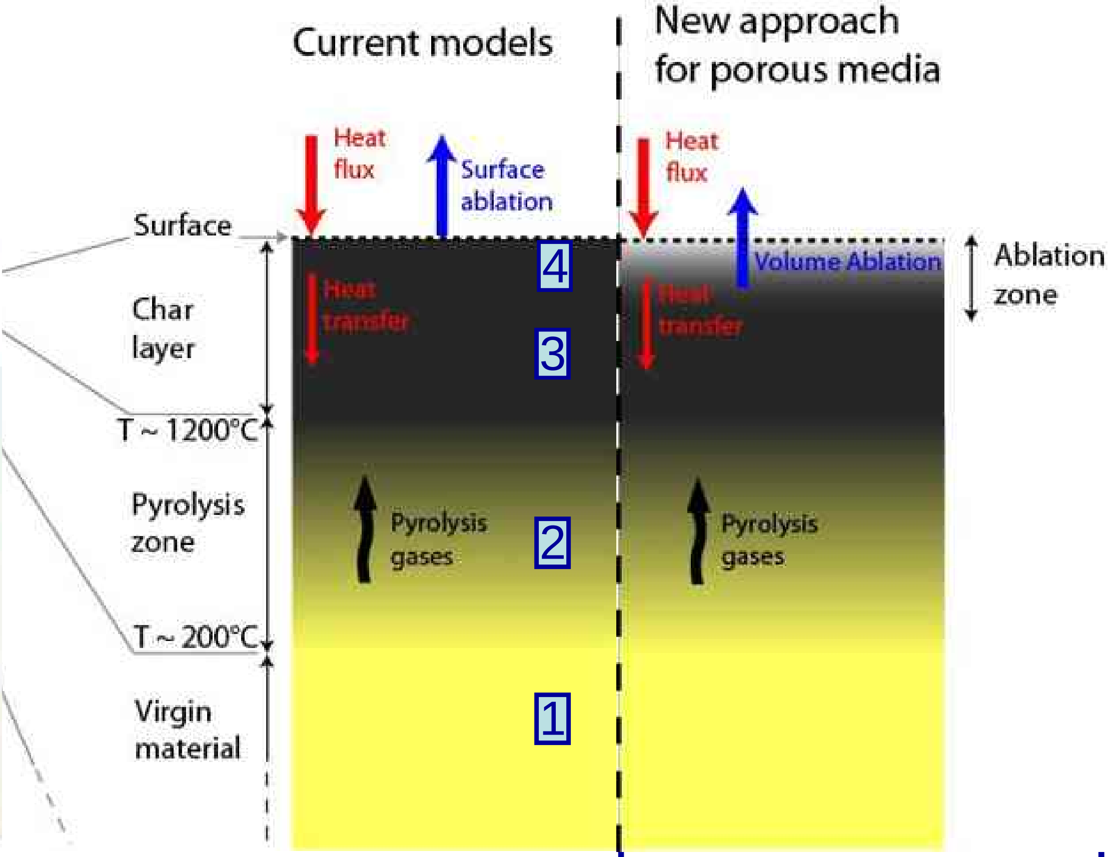
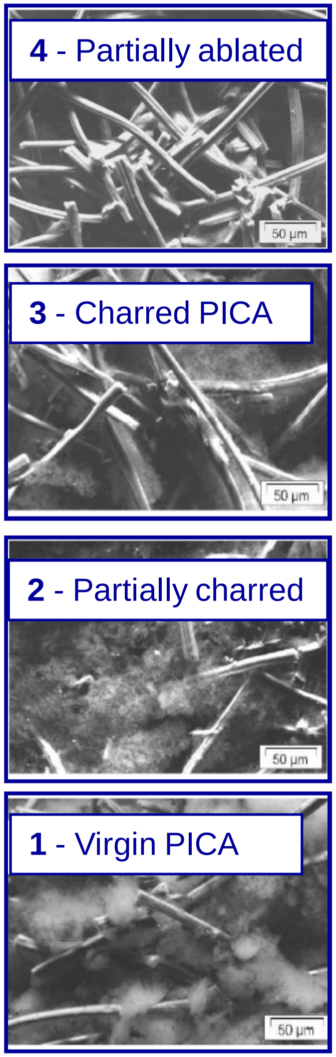
# . Introduction : (a) observation

## Fibrous Thermal Protection Systems (TPS); *e.g.* Stardust and PICA

Core - Stardust TPS(1)





**4** - Partially ablated

**3** - Charred PICA

**2** - Partially charred

**1** - Virgin PICA

SEM micrographs (1)

First step for the porous medium approach : oxidation

SEM 3 and 4 suggest the occurrence of some volume phenomena in the char layer:
- Oxidation (oxygen from the atmosphere)
- Sublimation
- Mechanical erosion of the matrix

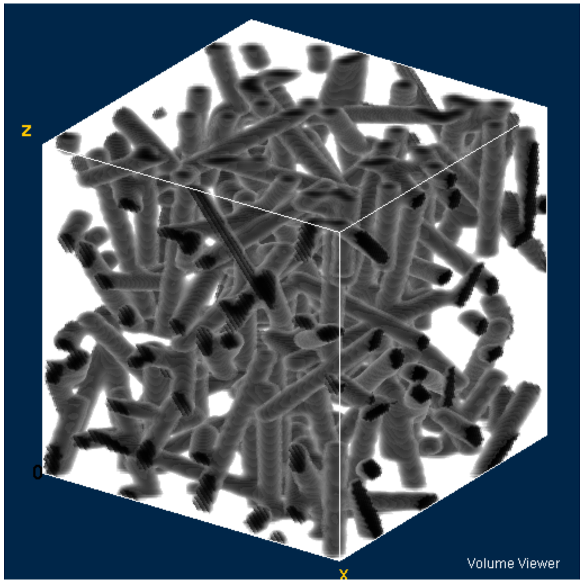
[1] M. Stackpoole *et al.,* Post-Flight Evaluation of Stardust Sample Return Capsule Forebody Heatshield Material, AIAA 2008-1202

# . Introduction : (b) comparison of 2 materials

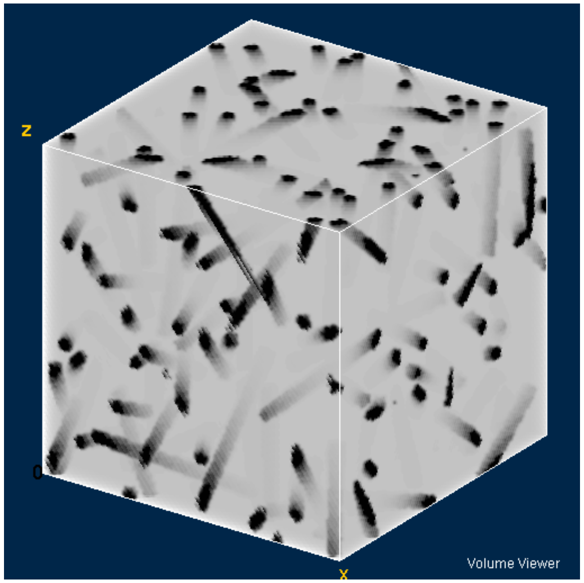
## Equilibrium chemistry vs. Finite-rate chemistry

Same fibrous preform, chemical composition, overall density

A : dense matrix layer around the fibers



B : Expanded, low density pore-filling matrix



- "Surface ablation" model (as described by *Kendall et al.,* NASA CR-1060, 1968)
  - Equilibrium chemistry → Only the chemical composition is important
  - model for A = model for B (in a control volume above the effective surface)
- "Ablation-zone model" model
  - Finite-rate chemistry → Material architecture is also important
  - model for A ≠ model for B (surface roughness and porosity are modeled)

# . Outline

## Microscopic scale simulation of the ablation of fibrous materials

### 1. Models and simulation tool

- Material models (A vs. B)
- Studied Problem
- Simulation tool : AMA

### 2. Simulation and analysis

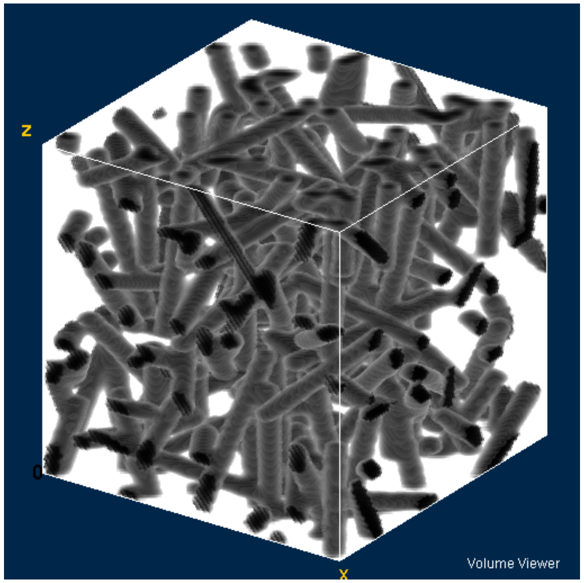
- Simulated Problem
- A vs. B: Moderate Thiele number
- A vs. B: Small Thiele number

### 3. Discussion

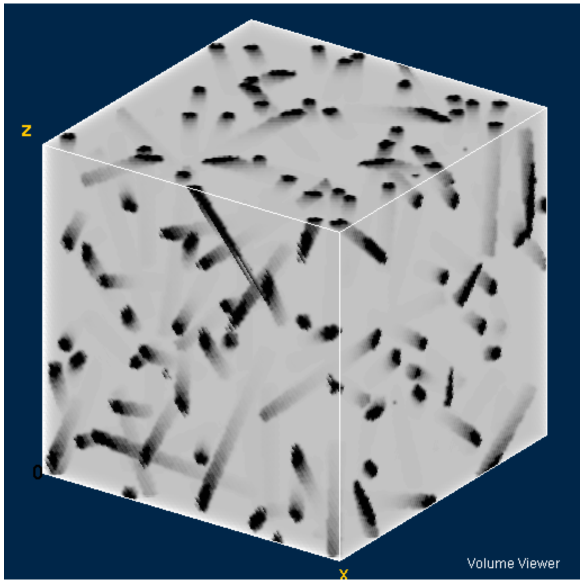
- Effective Reactive Surface Area
- Effective reactivity

### 4. Conclusion

A



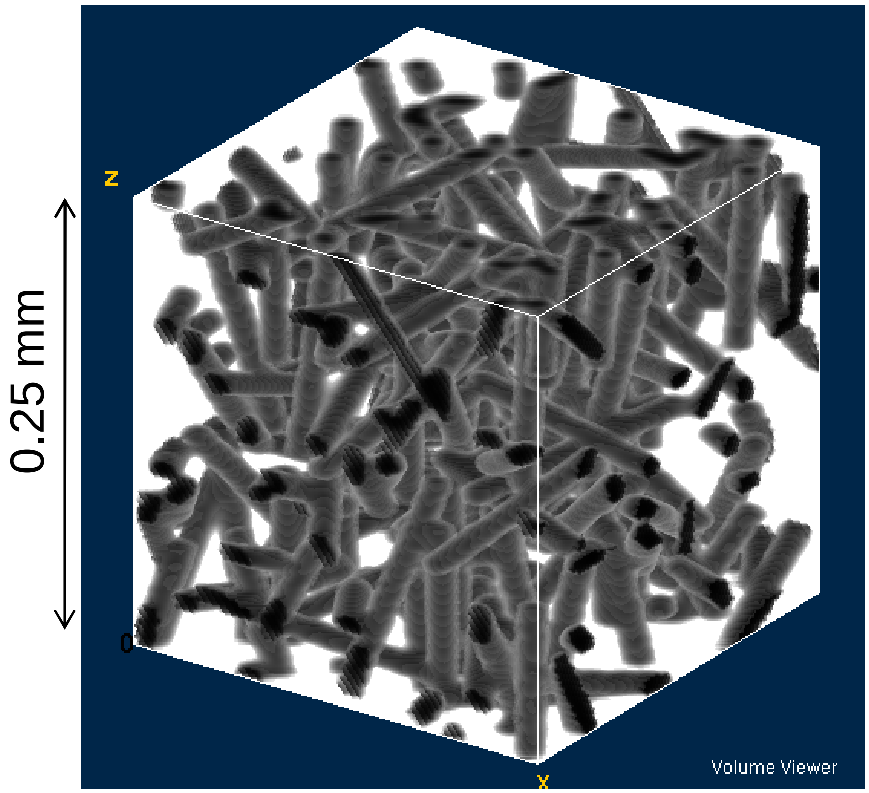
B



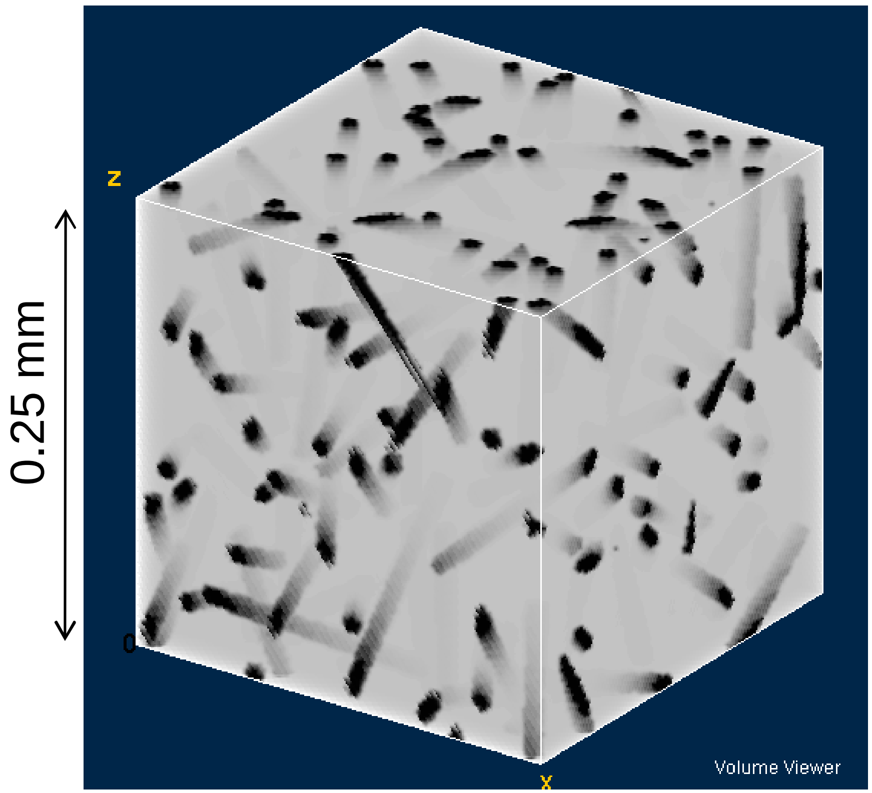
# 1. Models

## Materials: 2 ideal low density carbon/phenolic ablators

## A



## B



### Similarities

Preform: carbon fibers, random orientations
Fibers: diameter (10 µm), length (0.5 mm)
Virgin mass fractions: carbon fiber (65%), Phenolic resin (35%)
Overall density (Virgin : 280 kg/m$^3$; Pyrolyzed: 230 kg/m$^3$)

Preform: carbon fibers, random orientations
Fibers: diameter (10 µm), length (0.5 mm)
Virgin mass fractions: carbon fiber (65%), Phenolic resin (35%)
Overall density (Virgin : 280 kg/m$^3$; Pyrolyzed: 230 kg/m$^3$)

### Difference

**Dense phenolic resin surrounding the fibers: 1 µm**
Virgin phenolic resin density: 1200 kg/m$^3$
Pyrolyzed phenolic resin density: 600 kg/m$^3$
Overall porosity: 0.85

**Low density pore-filling matrix**
Virgin phenolic resin density: 100 kg/m$^3$
Pyrolyzed phenolic resin density: 50 kg/m$^3$
Overall accessible porosity: 0; **closed porosity**

# 1. Models and simulation tool

## Ablation model: Transport, Reaction, and Local Surface Recession

- **Problem studied:** Isothermal oxidation of materials A and B in their charred form
- **Model**

Starting point : differential recession of a heterogeneous surface ***S*** by gasification

$$\frac{\partial S}{\partial t} + \mathbf{v}.\nabla S = 0$$

Local recession velocity

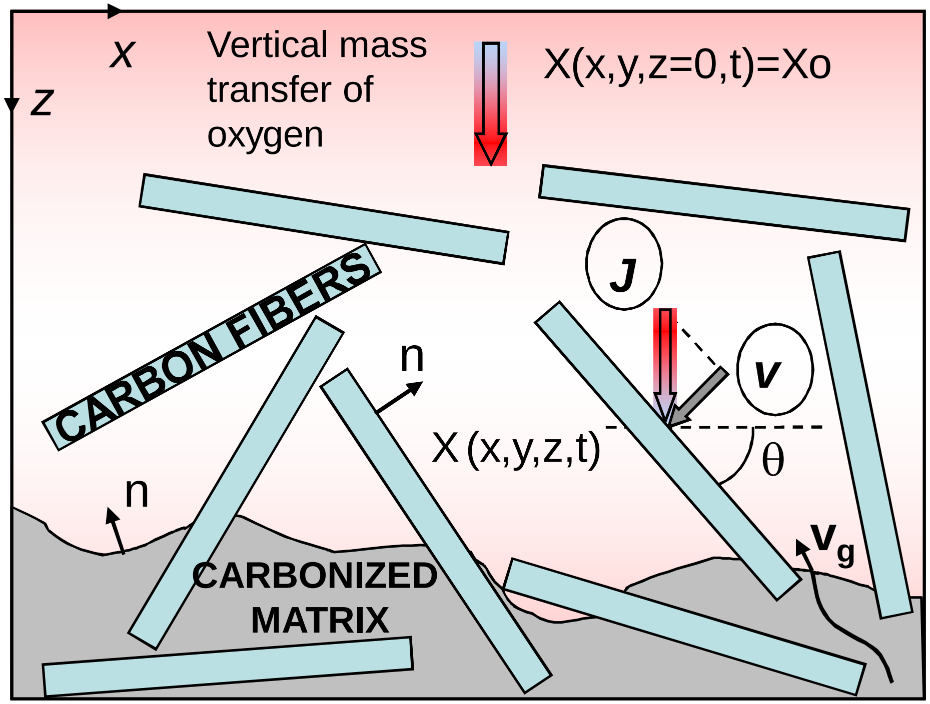
$$\mathbf{v} = -J\ \Omega_i\ \mathbf{n}\ ;\quad \mathrm{i = \{fiber\ ,\ matrix\}}$$

**Local ablation flux per surface unit**

$$\mathrm{J\ =\ k_i\ X\ \ ;\ \ i = \{fiber\ ,\ matrix\}}$$

**Oxygen transport**

$$\underbrace{\frac{\partial X}{\partial t}}_{\text{Local concentration}} + \underbrace{\nabla\cdot(-D\nabla X)}_{\text{Diffusion}} + \underbrace{\boldsymbol{v}_g\cdot\nabla X}_{\text{Convection (if any)}} = 0$$



***Nomenclature***

*X* = Oxygen concentration (mol m$^{-3}$)

D = Diffusion coefficient (m$^2$ s$^{-1}$)

*k* = Reactivity (m s$^{-1}$)

***n*** = Normal to the surface ( - )

$\boldsymbol{v_g}$ = Pyrolysis gas velocity (m s$^{-1}$)

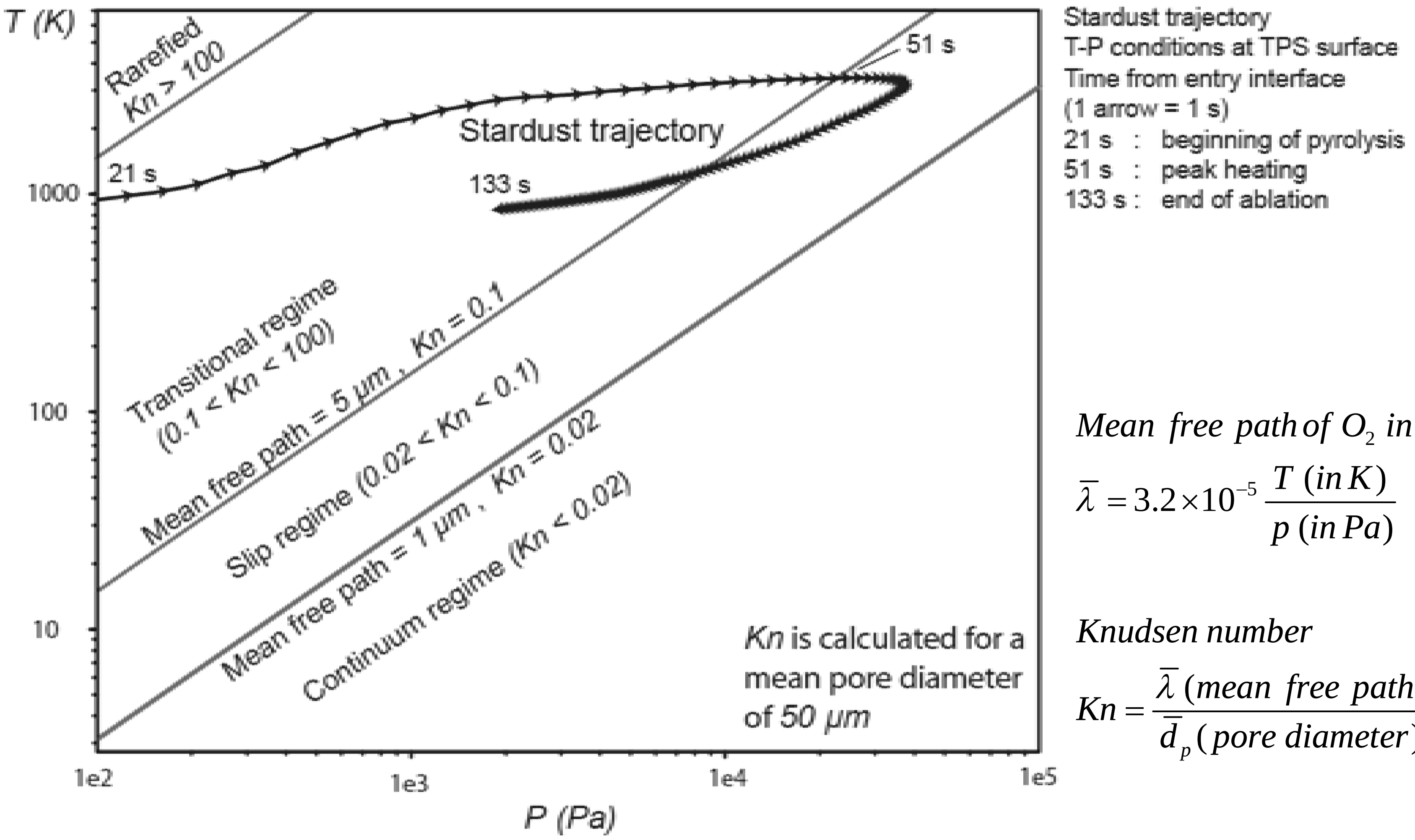
***Ω*** = Solid molar volume (m$^3$ mol$^{-1}$)

In the following
$\mathbf{v_g = 0}$

# 1. Models and simulation tool

## Flow regime **in the pores** of the material [1] : from Knudsen to continuum

Just as an illustration, Knudsen number in the pores along the Stardust trajectory



*Mean free path of* $O_2$ *in air*

$$\bar{\lambda} = 3.2 \times 10^{-5} \frac{T\ (in\, K)}{p\ (in\, Pa)}$$

*Knudsen number*

$$Kn = \frac{\bar{\lambda}\,(mean\ \ free\ \ path)}{\bar{d}_p\,(pore\ diameter)}$$

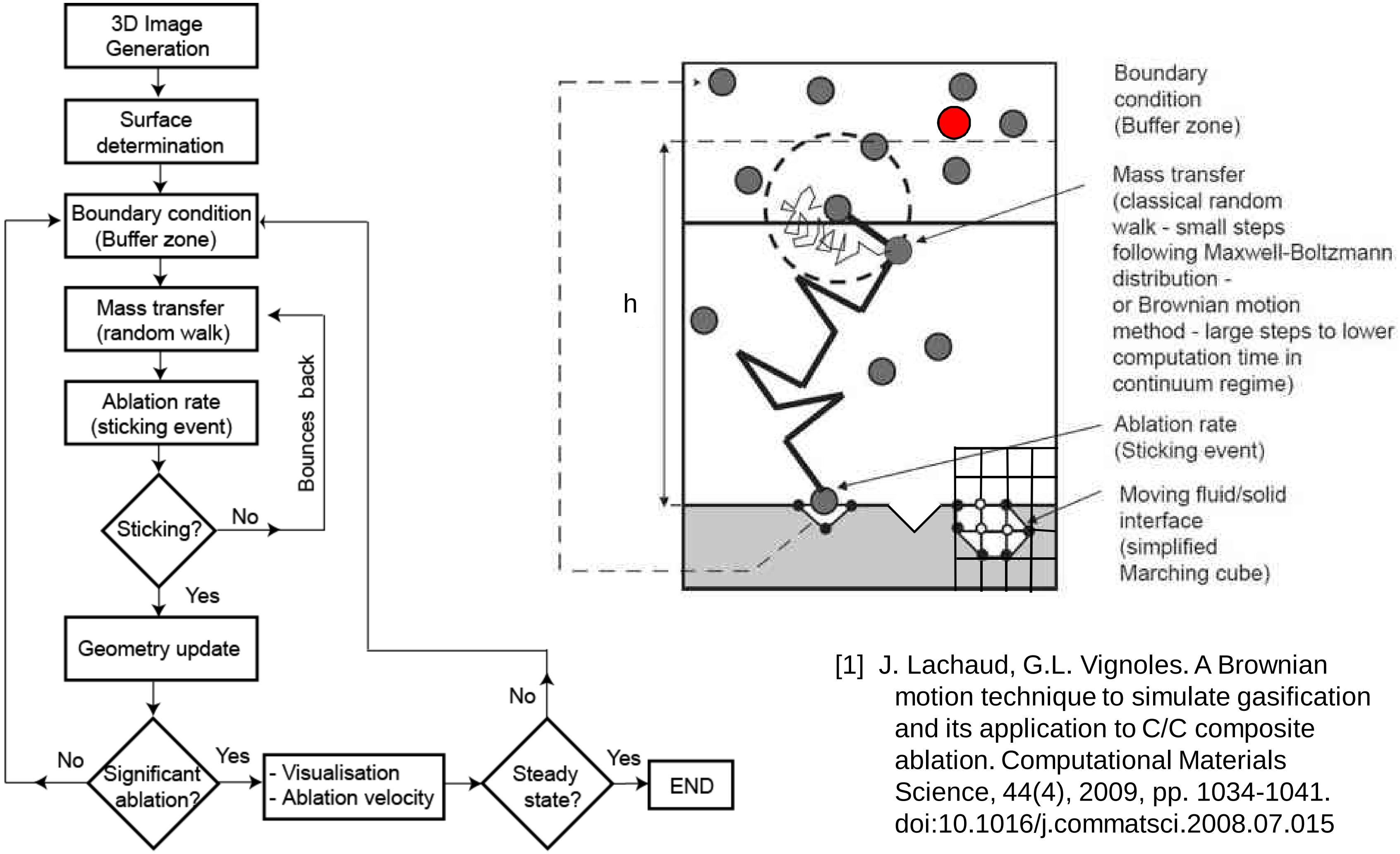
[1] J. Lachaud, I. Cozmuta, N. N. Mansour. Multiscale approach to ablation modeling of phenolic impregnated carbon ablators. Journal of Spacecraft and Rockets, accepted for publication.

# 1. Models and simulation tool

*Random Walk* for reaction/diffusion & *Triangle Marching Cube* for surface recession

*Random Walk :* Knudsen & Intermediate (classical) - Continuum regime (Brownian Motion)

## 3D simulation tool : AMA [1]

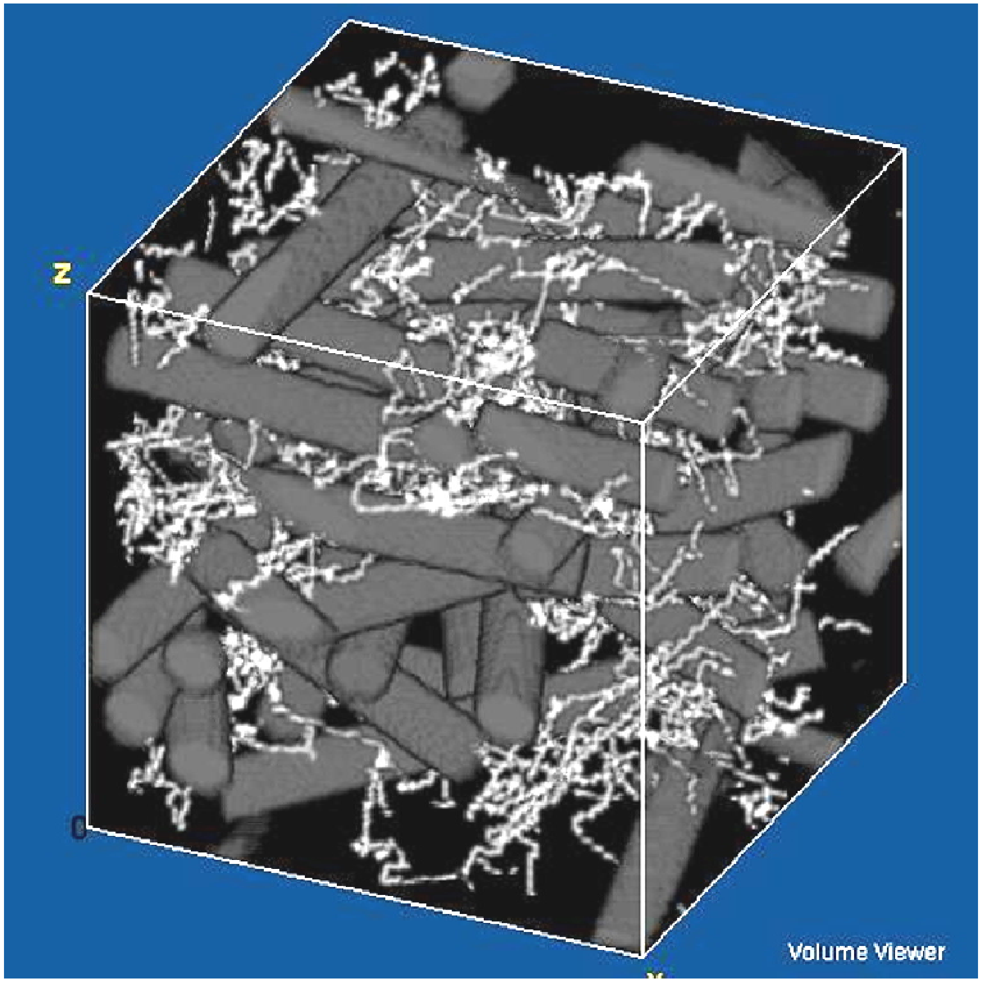


[1] J. Lachaud, G.L. Vignoles. A Brownian motion technique to simulate gasification and its application to C/C composite ablation. Computational Materials Science, 44(4), 2009, pp. 1034-1041. doi:10.1016/j.commatsci.2008.07.015

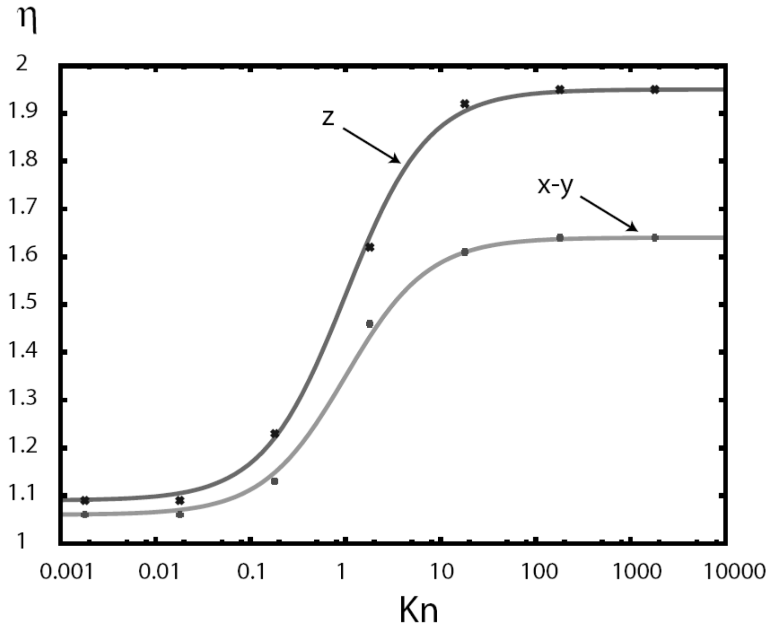
# 1. Models and simulation tool

## Determination of the effective diffusion coefficient from first principle

Illustration : path of a walker in a periodic cell (code **AMA**). The material in this illustration is anisotropic.



The fibrous media is tortuous. This slows the diffusion process (collisions on the walls). We can determine the tortuosity factor as a function of the mean free path of the molecules; that is, as a function of the Knudsen number.



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

porosity (<1)

tortuosity (>1)

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2. **Simulation and analysis**
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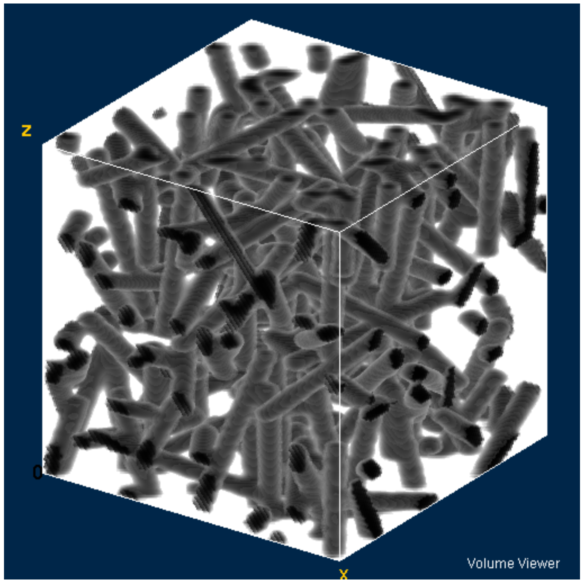
3. **Discussion**
   - Effective Reactive Surface Area
   - Effective reactivity
4. **Conclusion**

A



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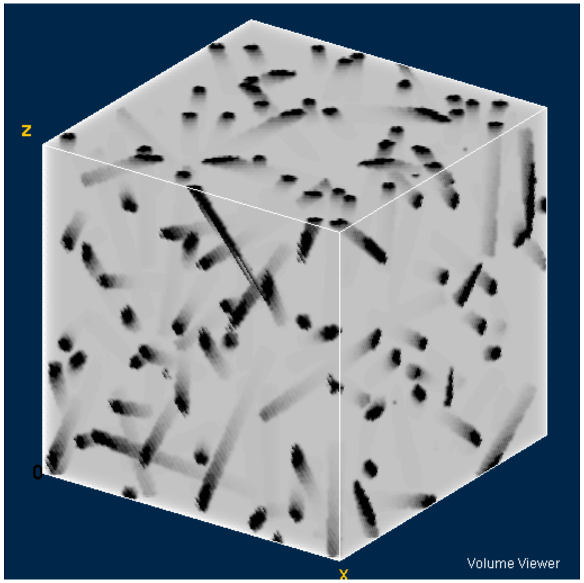


# 2. Simulation and analysis

## Fiber preform : 1D steady-state analysis (diffusion time << ablation time)

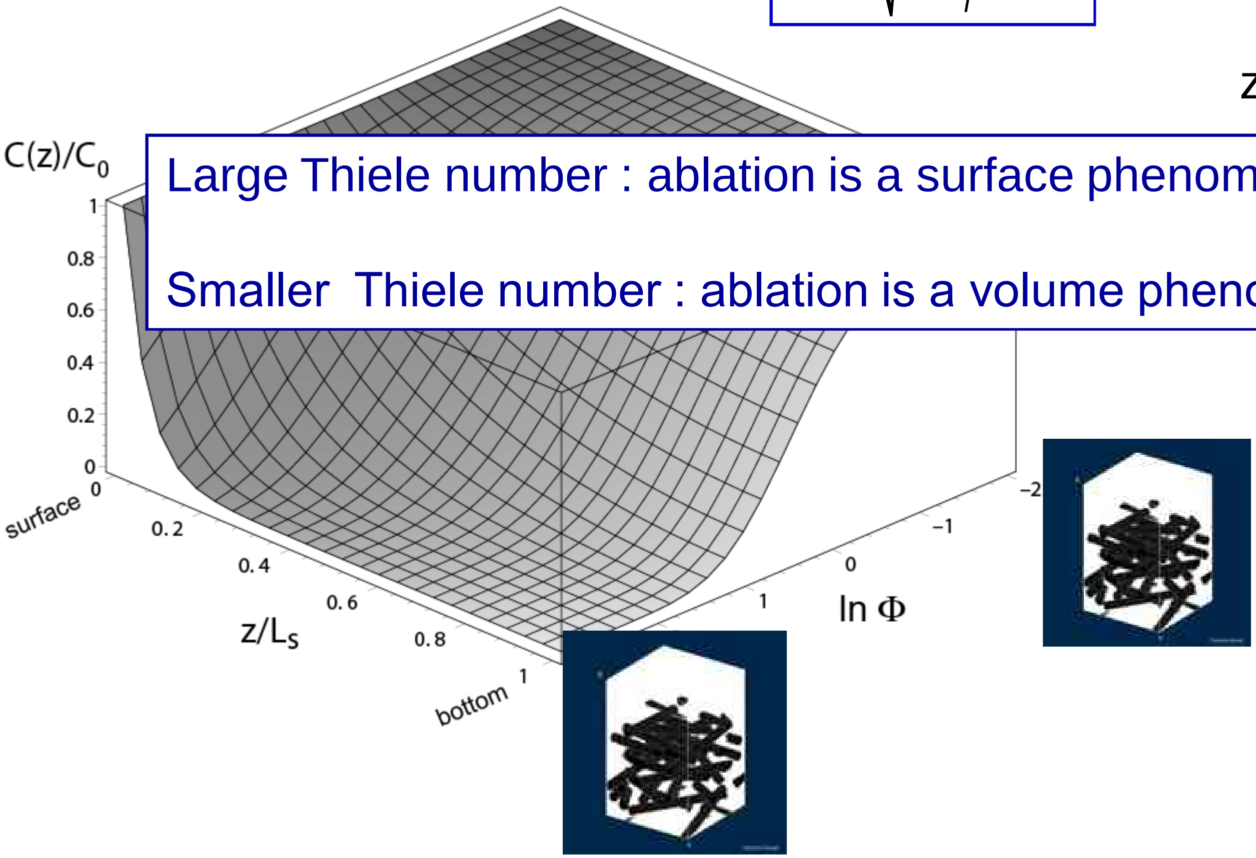
- **The concentration field is a function of the Thiele number**

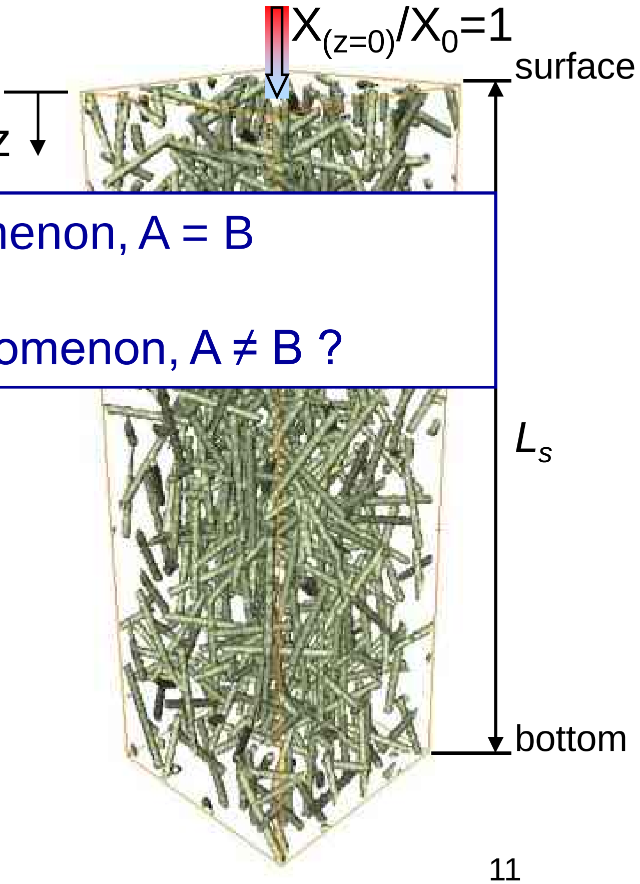
$$X(z) = X_0 \frac{\cosh\left[\Phi(z/L_s - 1)\right]}{\cosh\Phi}$$

Thiele number

$$\Phi = \frac{L_s}{\sqrt{\dfrac{D_{eff}}{sk_f}}}$$

*$L_s$: material depth (m)*
*$D_{eff}$: effective diffusivity (m²/s)*
*$k_f$: fiber reactivity (m/s)*
*s : specific surface (m²/m³)*





Large Thiele number : ablation is a surface phenomenon, A = B

Smaller Thiele number : ablation is a volume phenomenon, A ≠ B ?

# 2. Simulation and analysis

## Oxidation of B at moderate Thiele Number, Φ = 40

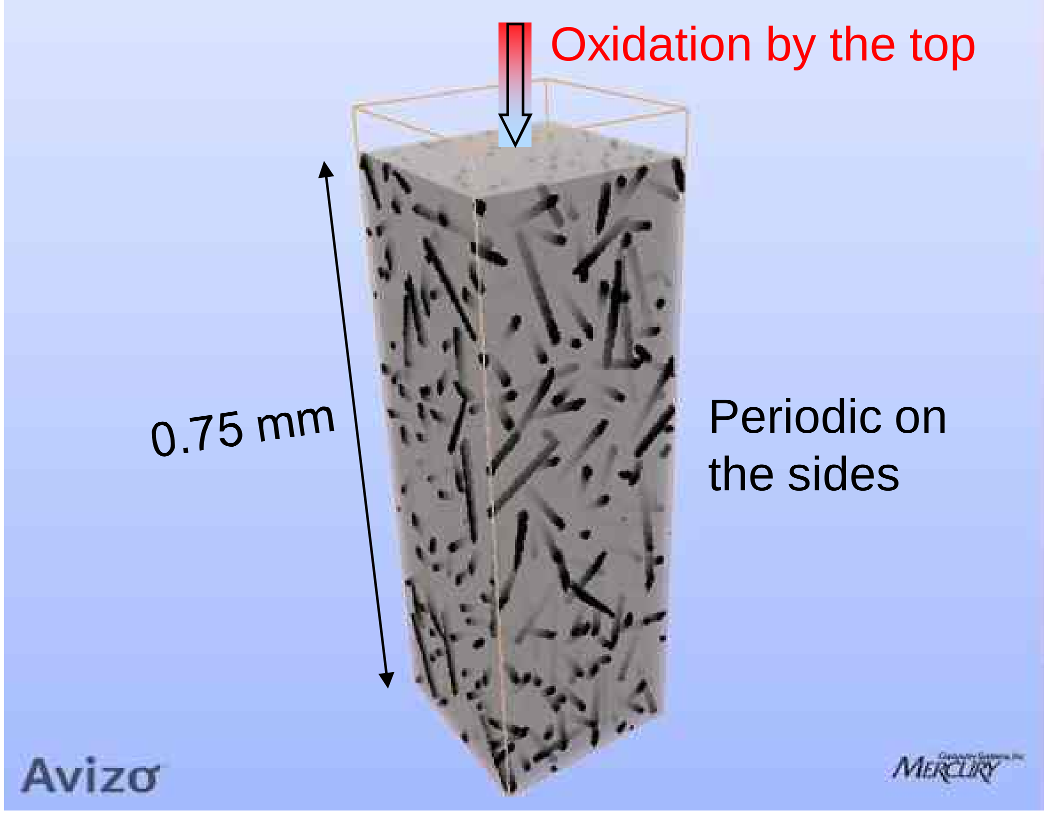
- **Hypotheses**
  - B is fully charred
  - No pyrolysis gas blowing
  - Air
  - **Φ = 40, e. g.**
    - T = 3360 K (isothermal)
    - P = 0.26 Atm
    - $\rho_f = 32\ \rho_m$
    - oxidation by $O_2$

    $k_m = 10\ k_f = 13.7$ m/s

    [Drawin 1992, Lachaud 2007]

    N.B.: oxidation by O

    $k_f = 100$ m/s [Park], Φ > 1000



- Diffusion/reaction DSMC simulation
  - Physical time: 1.2 s
  - Computational time : 2 days on a single core.

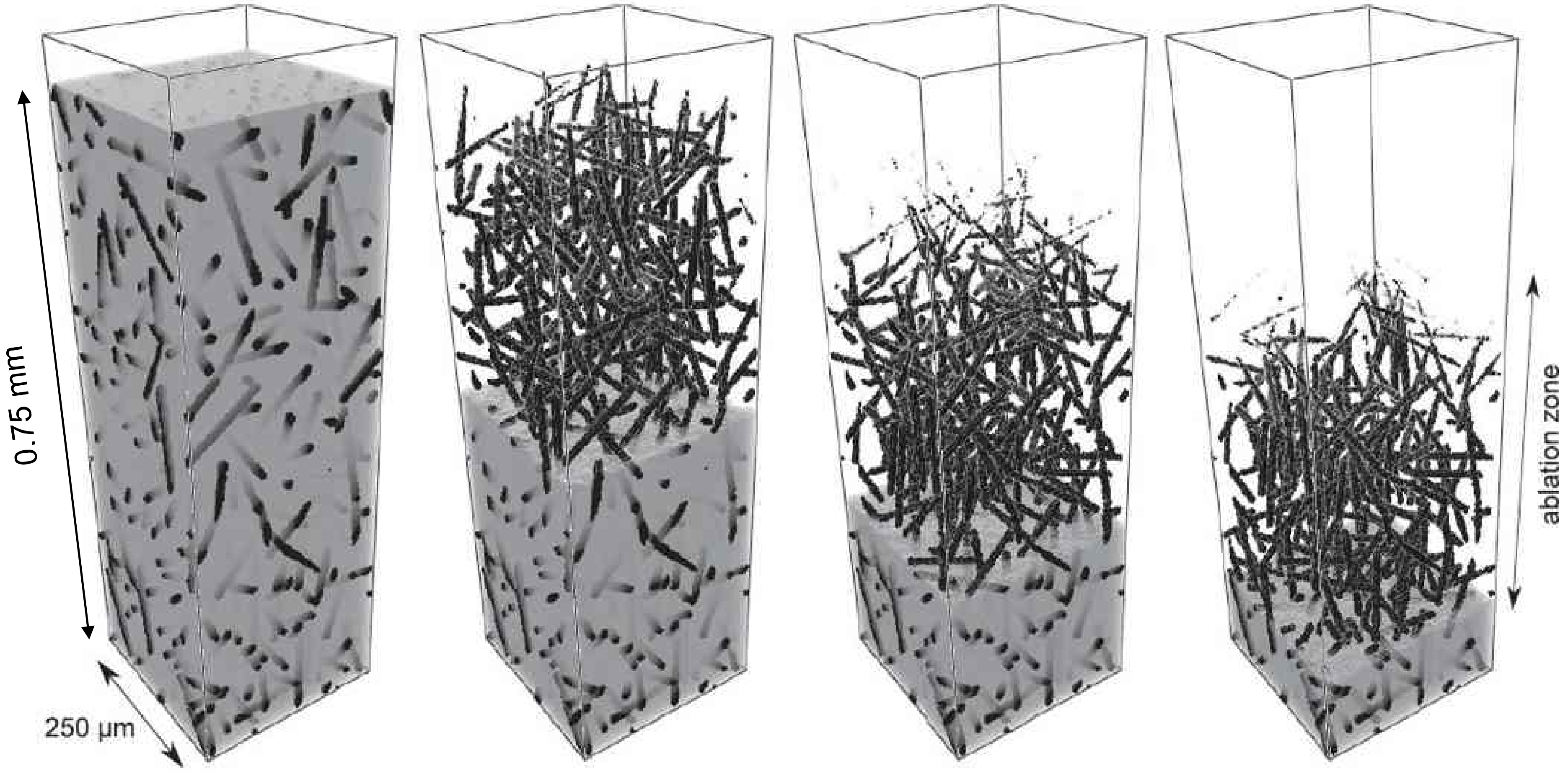
# 2. Simulation and analysis

## Oxidation of B at moderate Thiele number (Φ = 40): 3 stages

1) Matrix is removed first

2) Fiber diameter decreases

3) Overall surface recession



t = 0.0 s

0.4 s

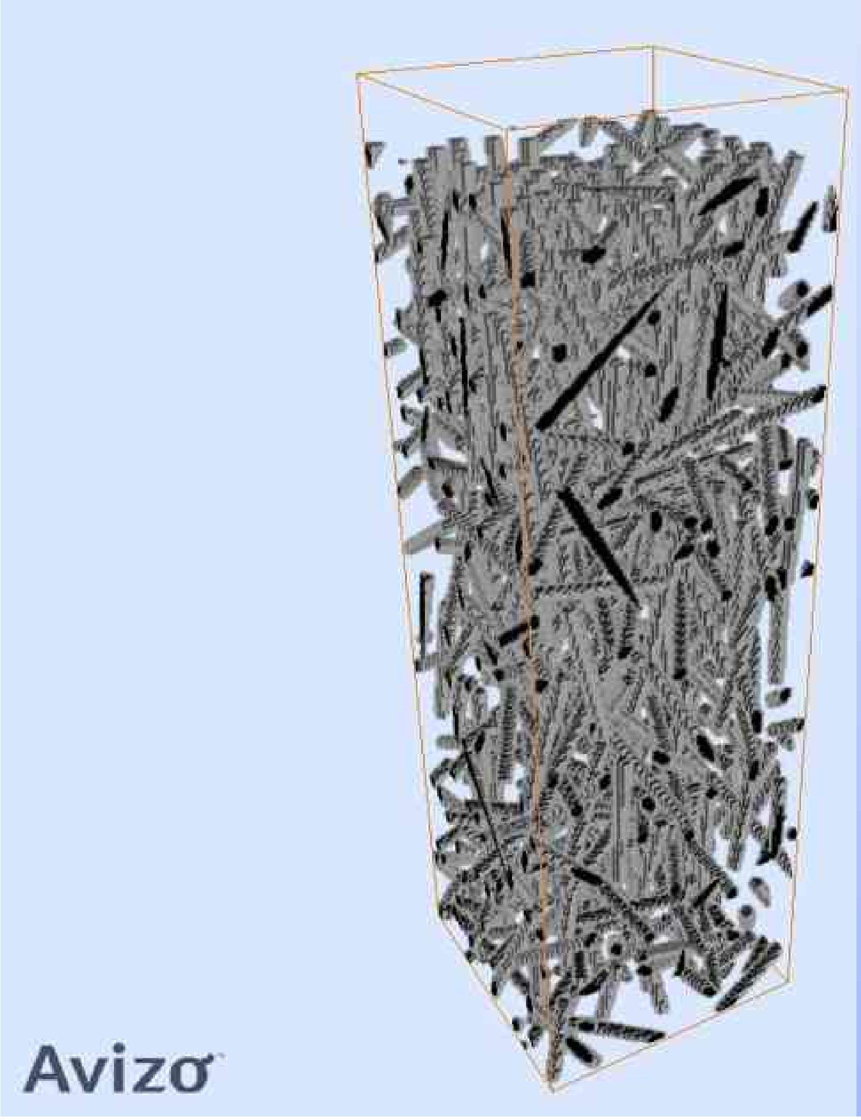
0.8 s

1.2 s

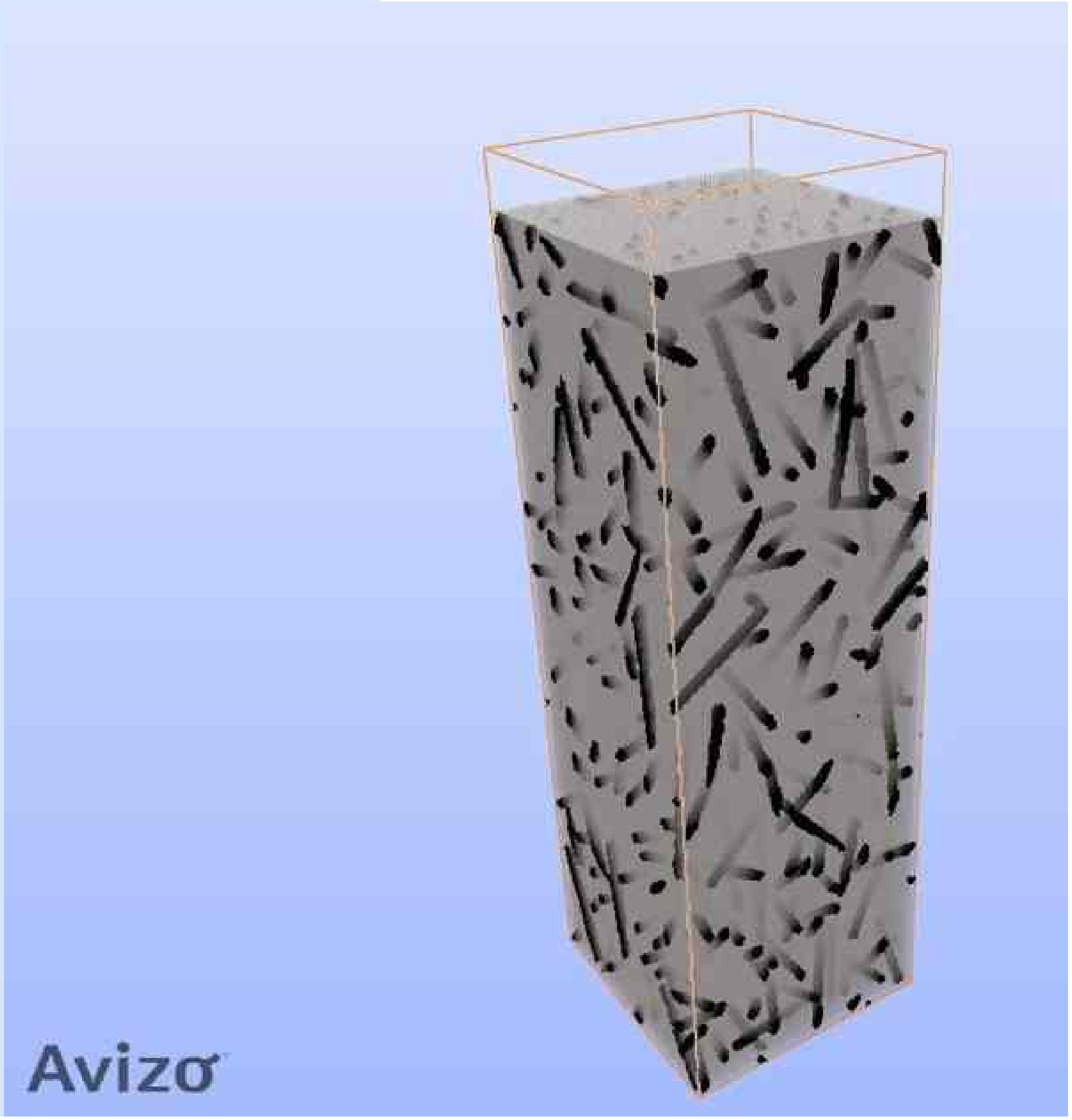
## 2. Simulation and analysis

Same conditions (Φ = 40): Comparison of A & B

**A**

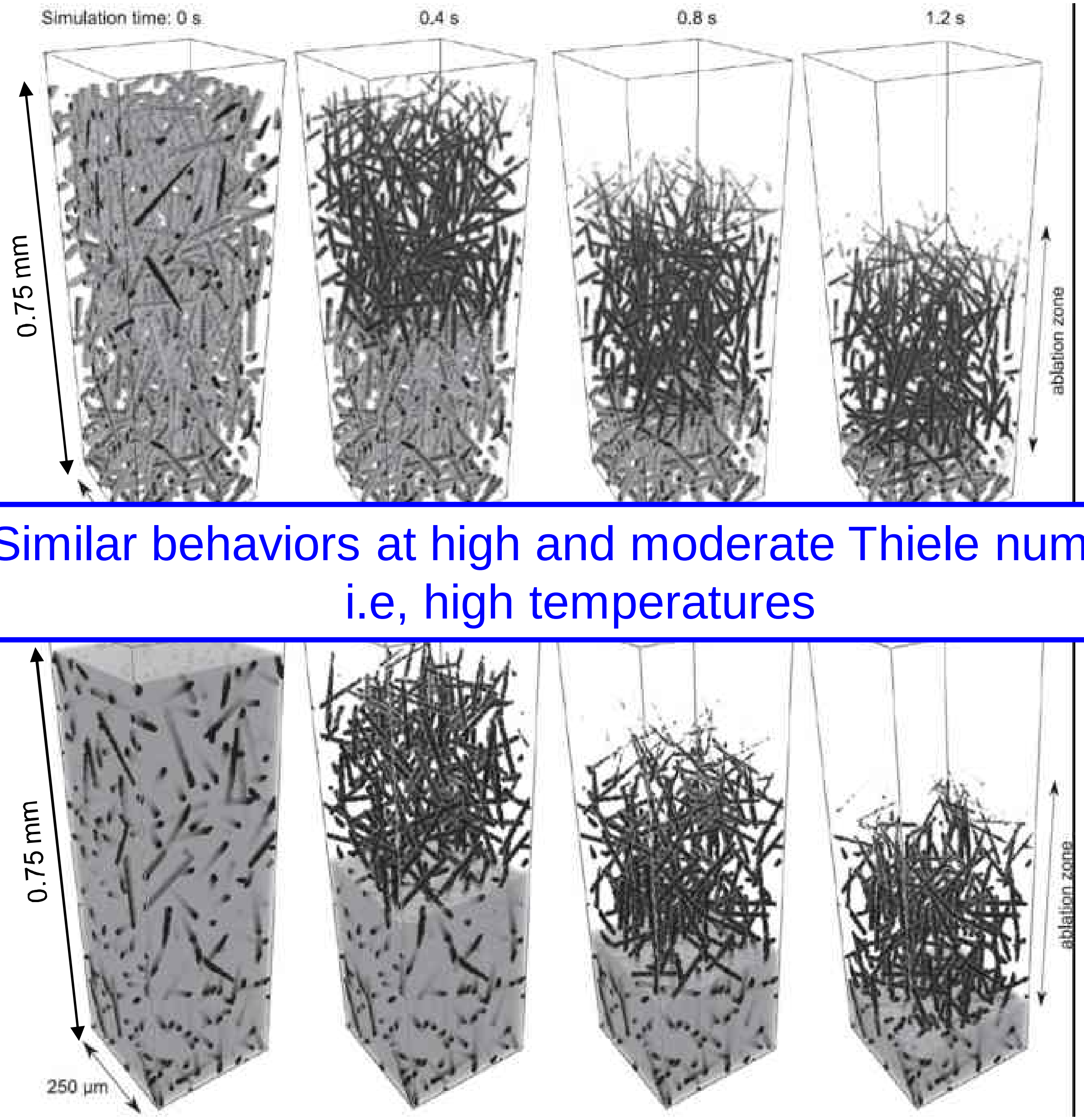


**B**



# 2. Simulation and analysis

## Same conditions (Φ = 40): Comparison of A & B



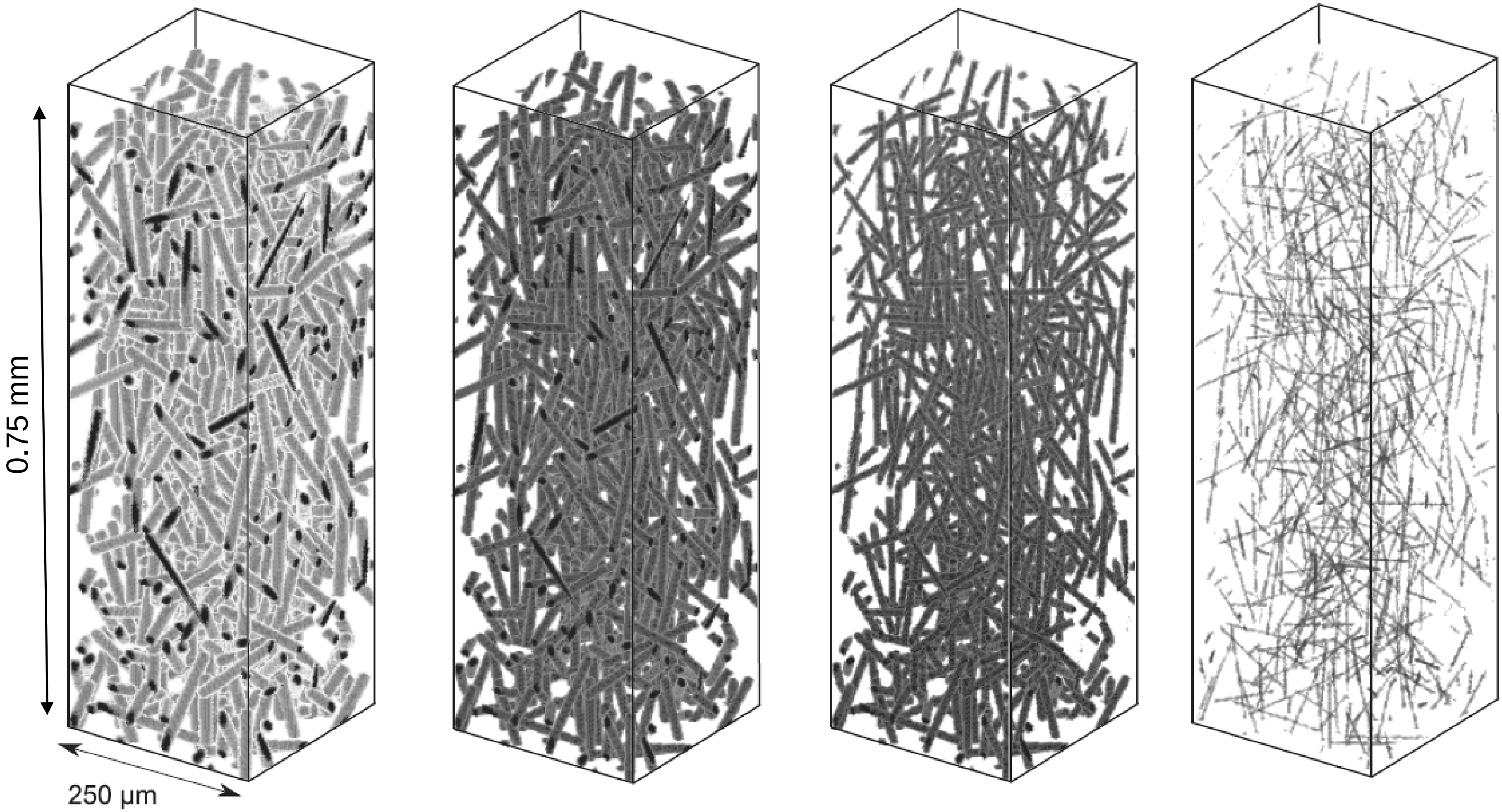
Material A

Similar behaviors at high and moderate Thiele number
i.e, high temperatures

Material B

# 2. Simulation and analysis

## Small Thiele number (Φ < 0.01); Material A

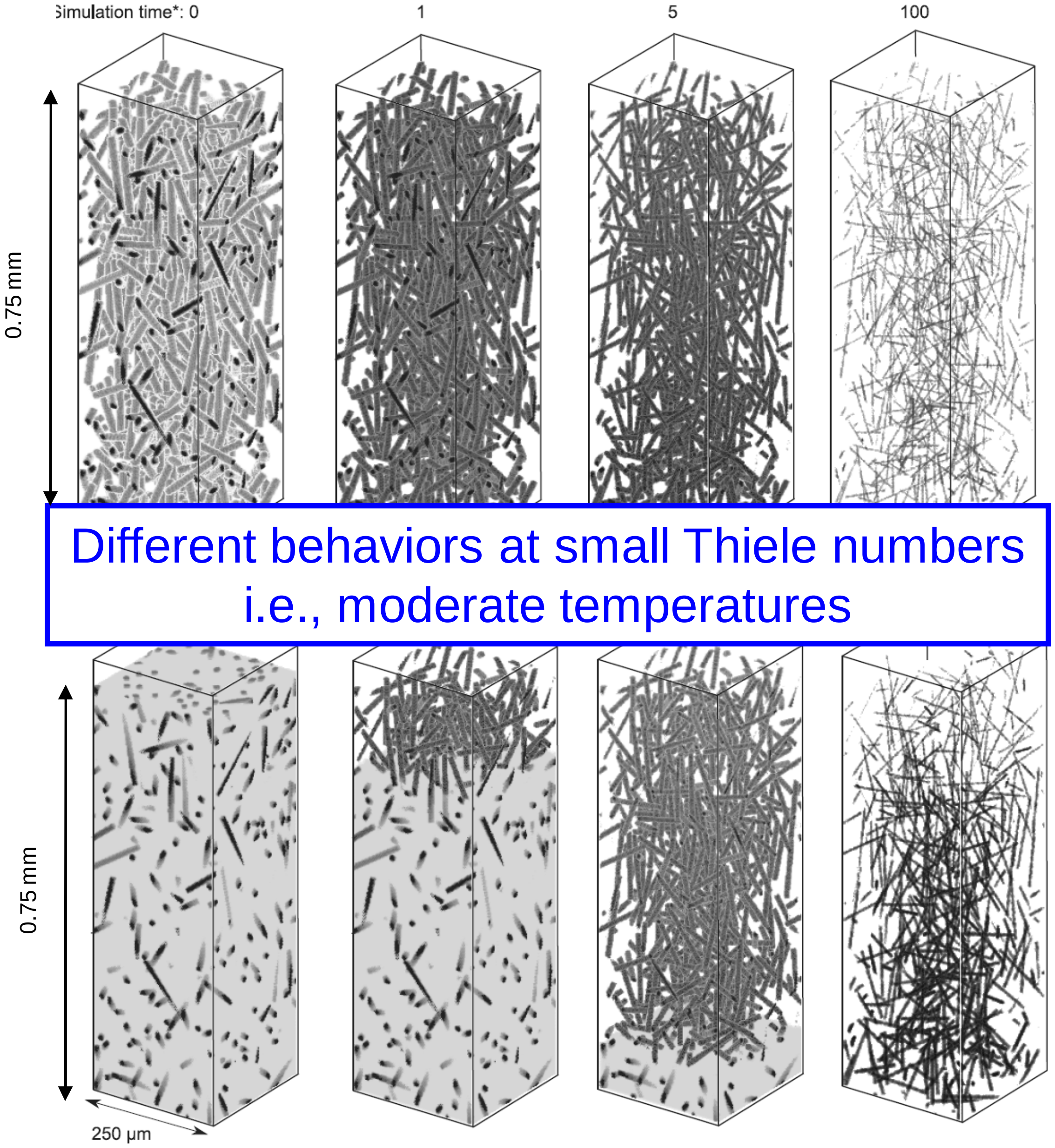


t = 0.0 t.u. 5 t.u. 10 t.u. 100 t.u.

At T=1000 K, 1 t.u. ≈ 4 minutes, oxidation by molecular oxygen.

# 2. Simulation and analysis

## Small Thiele number ($\Phi < 0.01$): comparison of A and B



Material A

Material B

Different behaviors at small Thiele numbers
i.e., moderate temperatures

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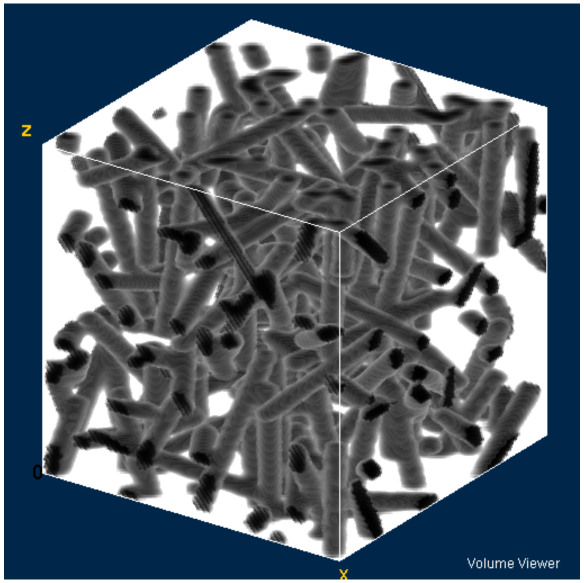
3. **Discussion**
   - Effective Reactive Surface Area
   - Effective reactivity model

4. **Conclusion**

A



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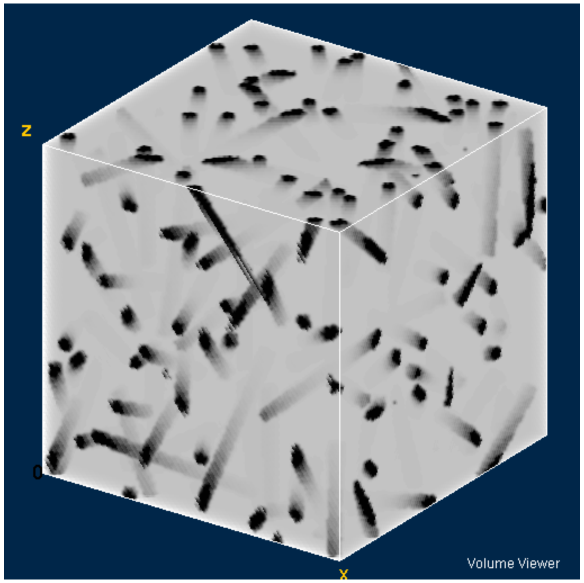


# 3. Discussion

## Effective Reactive Surface Area (ERSA). Illustration: fiber preform [1].

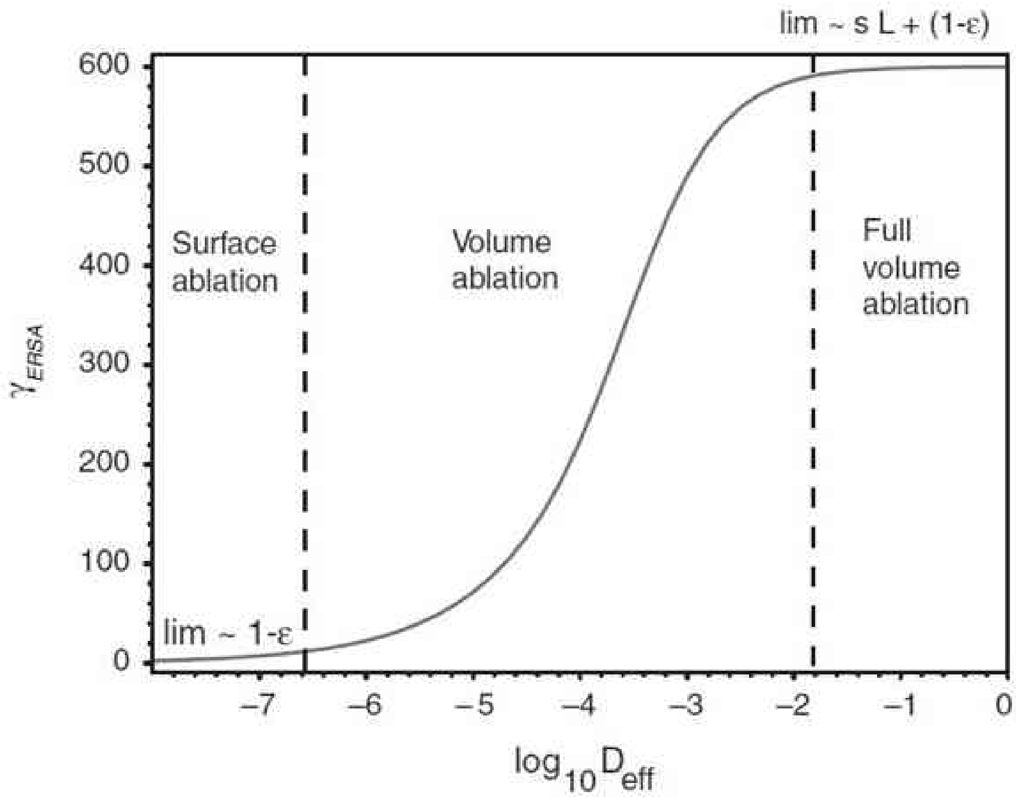
For a fiber preform, the effective reactivity is $k_{eff} = \gamma_{ERSA}\, k_f(T)$

$$\gamma_{ERSA} = \frac{ERSA}{GSA} = \int_{z=0}^{L} s_f\, X(z)/X_0\, dz = \left[ sL \frac{\tanh\phi}{\phi} + (1-\varepsilon) \right]$$

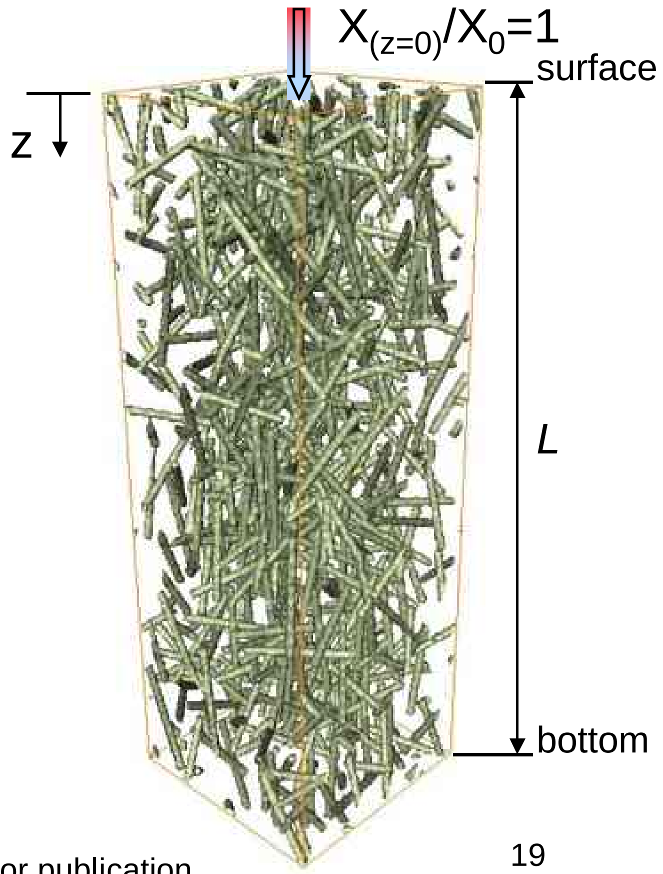
$L_s$: *material depth (m)*
$D_{eff}$: *effective diffusivity (m²/s)*
$k_f$: *fiber reactivity (m/s)*
*s : specific surface (m²/m³)*
*GSA: geometric surface area (m²)*

Thiele number

$$\Phi = \frac{L_s}{\sqrt{\dfrac{D_{eff}}{s k_f}}}$$



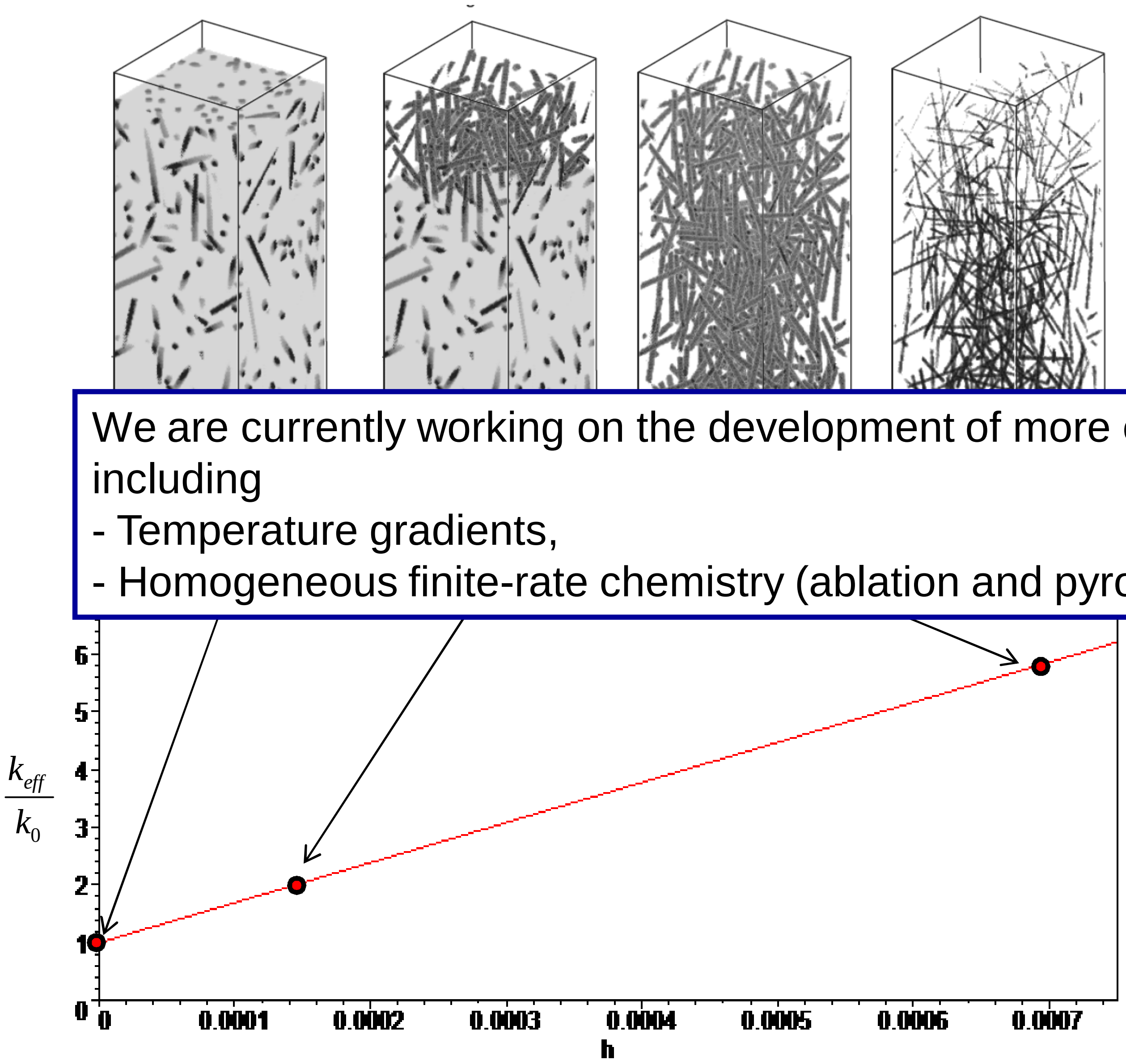
*Plotted for:* $k_f$*=1 m/s; L=1cm;* $s=6\times10^5$ *m²/m³*



[1] J. Lachaud, I. Cozmuta, N. N. Mansour. Multiscale approach to ablation modeling of phenolic impregnated carbon ablators. Journal of Spacecraft and Rockets, accepted for publication.

# 3. Discussion

## Effective reactivity of material B at small Thiele number (Φ < 0.01)



In this case, the effective reactivity can be estimated analytically under the following hypotheses:

- No temperature gradient
- No pyrolysis gas flux
- The fiber diameter reduction is small

age)

We are currently working on the development of more elaborated models including

- Temperature gradients,
- Homogeneous finite-rate chemistry (ablation and pyrolysis gases)

$$k_{eff} = k_0 \left[ 1 + \frac{\quad}{(\varepsilon_m k_m / k_f + \varepsilon_f)} \right]$$

*$k_0$: reactivity at t=0 (m/s)*
*s : specific surface ($m^2/m^3$)*
*h: matrix depth (m)*
*$\varepsilon_f$: fiber volume fraction*
*$k_f$: fiber reactivity (m/s)*
*$\varepsilon_m$ : matrix volume fraction*
*$k_m$: matrix reactivity (m/s)*

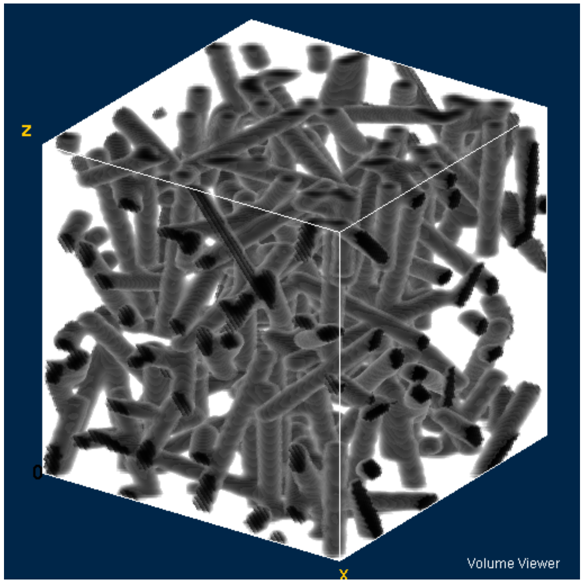
## . Conclusion and perspectives

✓ New volume ablation model (oxidation only)
  - o Large Thiele number : A ≈ B (usually high temperatures)
  - o Smaller Thiele number : A ≠ B (usually moderate and low temperatures)

✓ Finite-rate chemistry
  - o **The effective reactivity of a material is not only a function of the temperature**. It is also a function of the ERSA; that is, of:
    - the geometric surface area available (depends on the ablation history);
    - the Thiele number;
    - the temperature gradient;
    - homogeneous reactions occurring with pyrolysis gases.

✓ Perspective: Application to real re-entry conditions
  - o Thermal gradients
  - o Pyrolysis-ablation coupling (pyrolysis gases)

A



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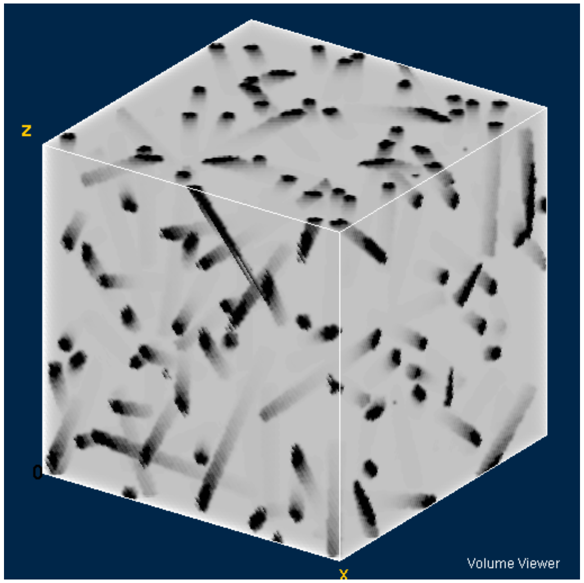
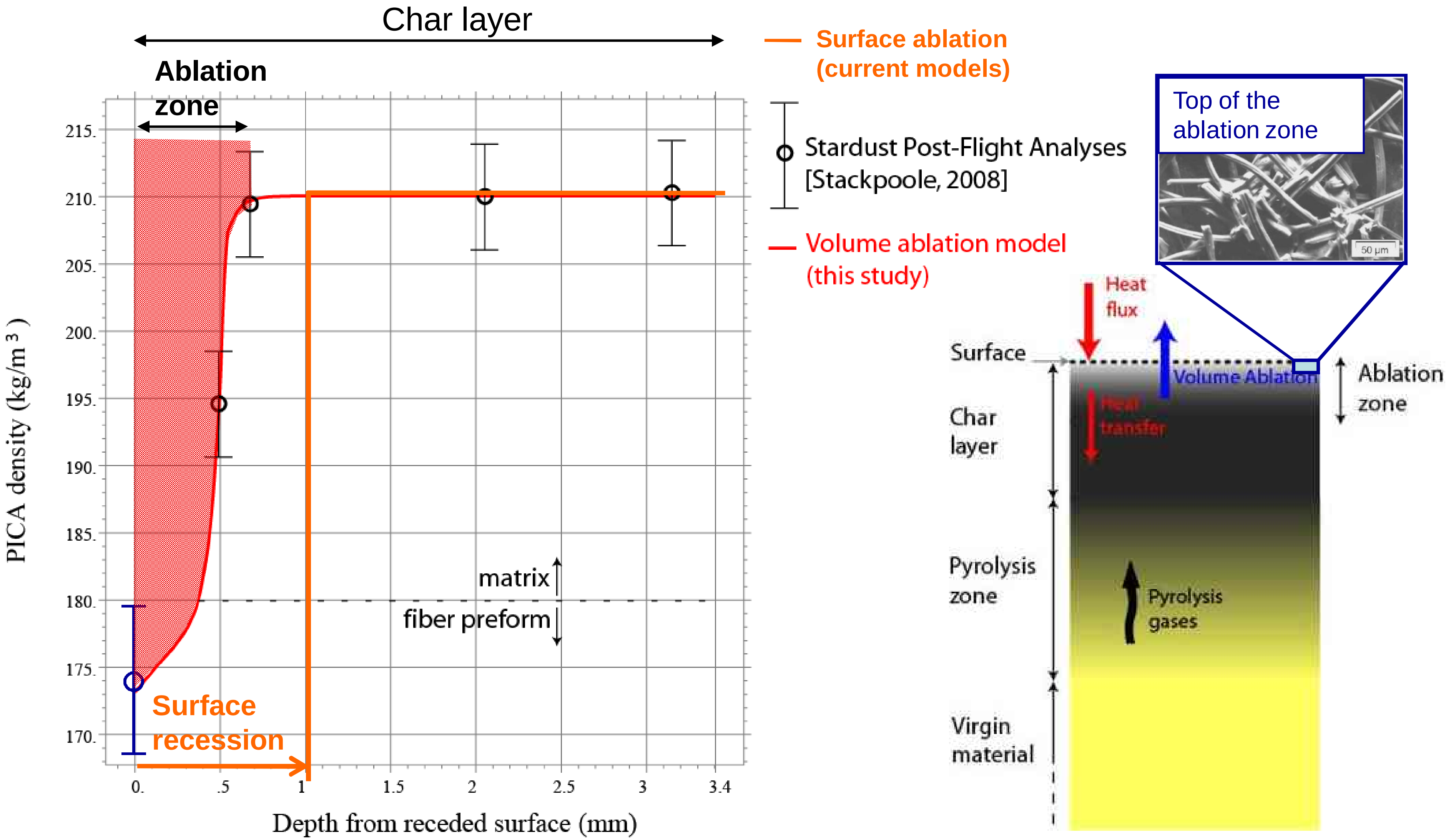


# Appendix

# . Application to Stardust conditions

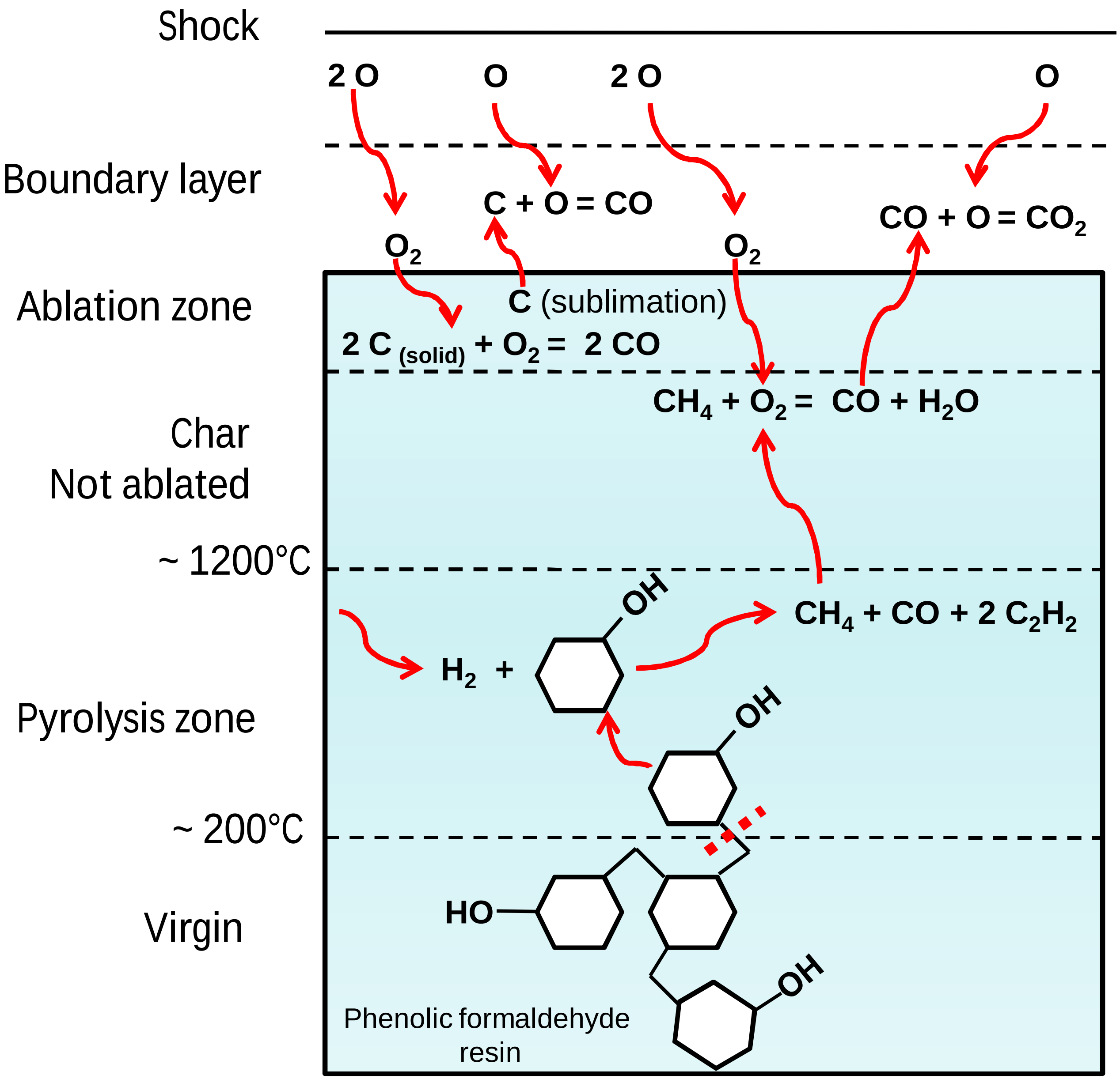
## Material B : Fit of post-flight density profile [1]



[1] J. Lachaud, I. Cozmuta, N. N. Mansour. Multiscale approach to ablation modeling of phenolic impregnated carbon ablators. Journal of Spacecraft and Rockets, accepted for publication.

# . Current developments: chemistry

## Pyrolysis-ablation coupling. Main problem : Finite-rate chemistry.



Shock

Boundary layer

Ablation zone

Char
Not ablated

~ 1200°C

Pyrolysis zone

~ 200°C

Virgin

2 O  O  2 O  O

$O_2$

$C + O = CO$

$O_2$

$CO + O = CO_2$

C (sublimation)

$2\,C_{(solid)} + O_2 = 2\,CO$

$CH_4 + O_2 = CO + H_2O$

$CH_4 + CO + 2\,C_2H_2$

$H_2$ +

OH

OH

HO

OH

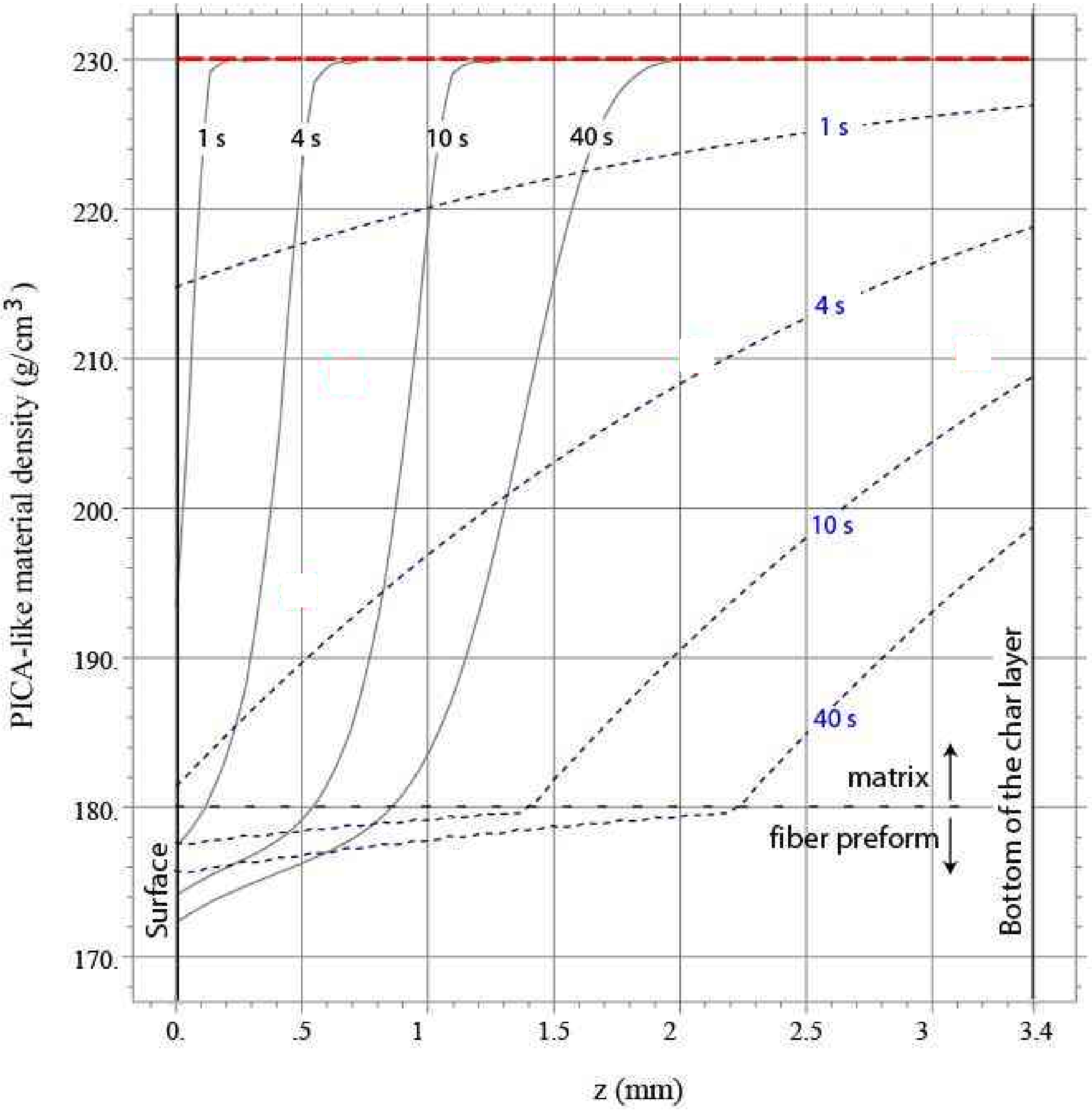
Phenolic formaldehyde resin

CFD :
- finite rate chemistry (homogeneous only)
- diffusion
- convection

Material code :
- ablation + pyrolysis →finite rate chemistry (homogeneous and heterogeneous)
- pyrolysis : multi-laws
- diffusion
- convection

# . Current developments: macroscopic scale model

## Comparison of A & B for the end of Stardust re-entry



– – Surface ablation models

— Material B + Volume ablation model

---- Material A + Volume ablation model

1D simulation of the evolution of the density profile of the char layer of A &B in the conditions encountered during the end of the reentry of Stardust

Trajectory time
90s < t < 130s
Wall temperature
1300 K > T > 850 K

Temperatures provided by the TPS-ADP / Stardust post-flight analysis team.

Hypothesis
Thermal Conductivity
$k_A=k_B= k_{PICA}$