Morphological and non Beerian radiative characterization of a fibrous medium

Presented by : Mahé Souveton
Supervision : Franck Enguehard
Vital Le Dez

Summary

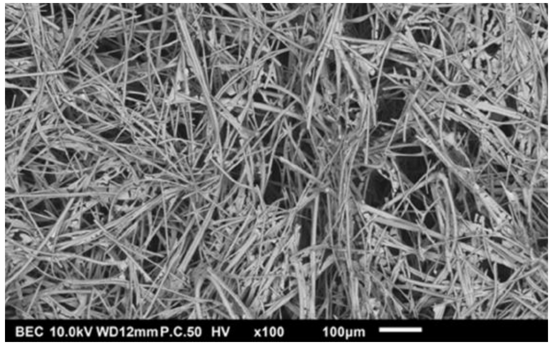
- **Introduction to the subject**
  - Context
  - Radiative characterization
  - Morphological results
- **Development of a non Beerian model**
  - Definitions
  - Practical application
  - Monte Carlo algorithm
  - Results and discussions
- **Conclusion and perspectives**

Introduction to the subject

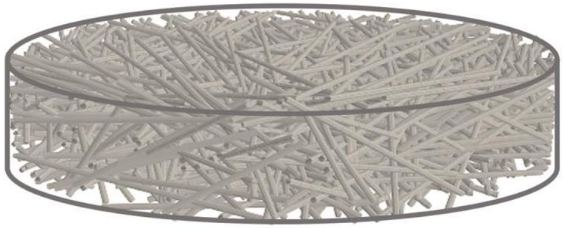
Introduction to the subject

Context

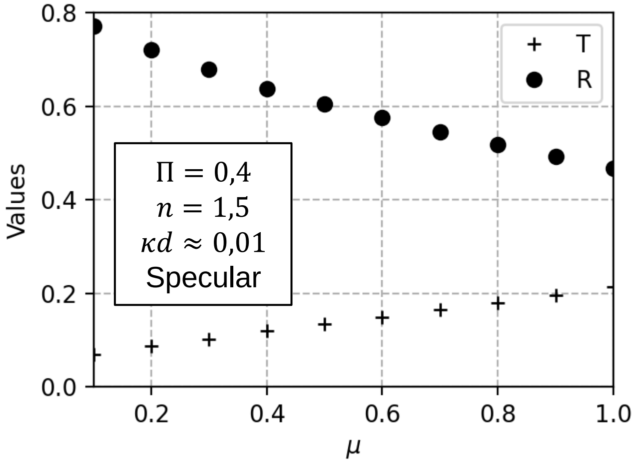
- **Industrial context:**
  - Thermal insulation at high temperatures often relies on highly porous materials.
  - The radiative transfer must be characterized at all scales.
- **Representative medium:**
  - Theoretical study of a virtual cold fibrous medium composed of overlapping cylinders (acting as an absorbing and scattering phase).
  - Morphological simplification: infinite cylinders, same shape and properties, randomly orientated ⇒ medium statistically homogeneous and isotropic.
  - Either specular or diffuse conditions imposed between void and fibers. No interface events on entrance and exit of the calculation box.
- **Radiative characterization:**
  - Directional-hemispherical transmittance T and reflectance R values.
  - Homogenization procedure: determining an equivalent continuous medium.



SEM of a zirconia felt



A computer-generated virtual fibrous medium



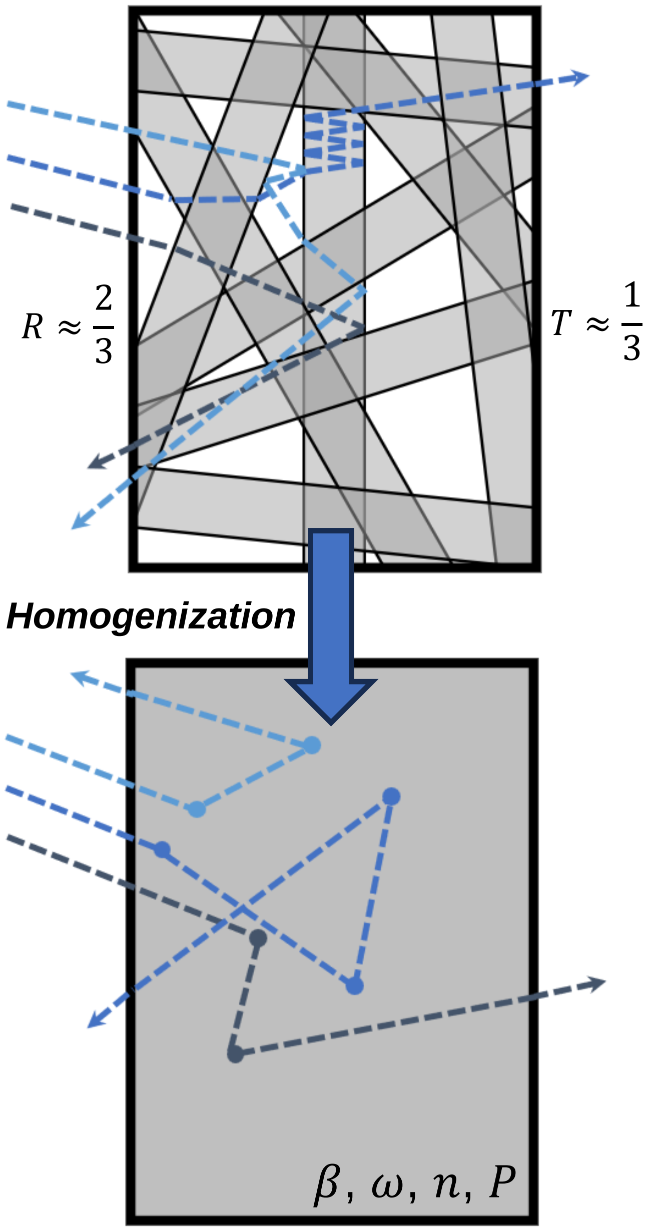
T and R values as a function of the angle of the incident radiation

Introduction to the subject

Radiative characterization

- **Direct Simulation Monte Carlo (DSMC):**
  - A Monte Carlo algorithm follows each ray through reflection and refraction events until its absorption or its exit of the calculation box.
- **Standard homogenization procedure:**
  - Scalar coefficients have to be determined (β, κ, σ, ω, n, …):

    - By inversion (requires to specify a phase function).
    - By direct identification (RDFI [1]).
- **Non Beerian approach:**
  - The statistics in our fibrous medium does not follow Beer-Lambert law !
  - A non Beerian model, integrated inside a Monte Carlo algorithm, could be constructed with the true statistics of absorption and scattering.



Monte Carlo in the fibrous medium (top) and in the continuous medium (bottom)

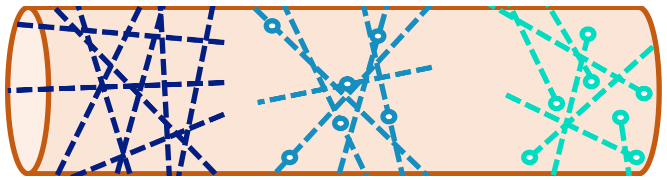
[1] Tancrez, M., & Taine, J. (2004). Direct identification of absorption and scattering coefficients and phase function of a porous medium by a Monte Carlo technique. *International Journal of Heat and Mass Transfer*, *47*(2), 373-383

Introduction to the subject

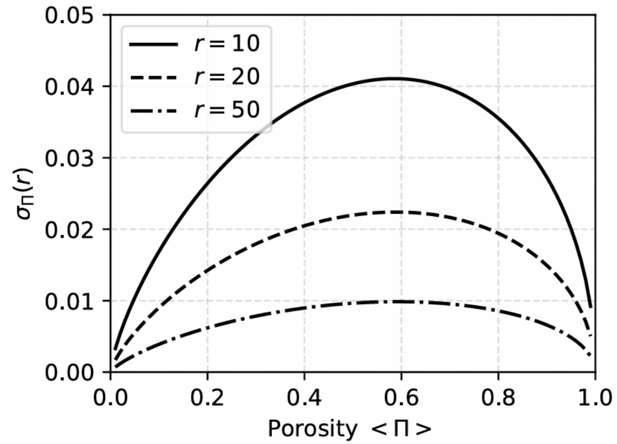
Morphological results [2]

- **Study of random chords**
  - μ-random, I-random, i-random chords, etc…
  - Provides an algorithm to construct an homogeneous and isotropic fibrous medium.
- **Analytical derivation for a stack of cylinders**
  - Porosity Π as a function of the number of fibers N.
  - REV (from the standard deviation of porosity σ_Π)
  - Autocorrelation function.
- **Final result**
  - CDF of i-random chord lengths in the fibrous phase :

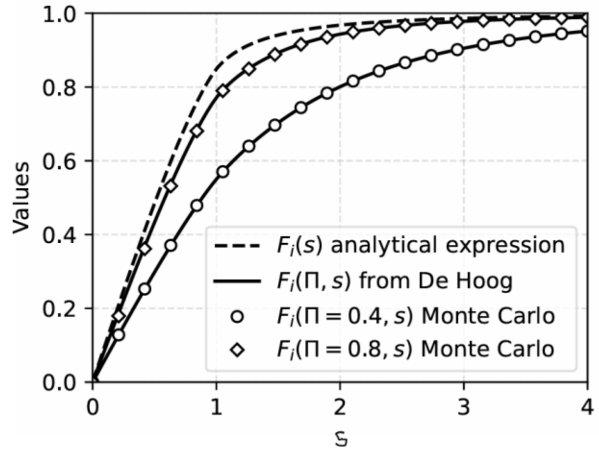
$$F_{i,f}(\Pi, s) = \frac{\Pi}{1-\Pi}\mathcal{L}^{-1}\left\{\frac{1}{p^2\mathcal{L}\{\Pi^{F_i}\}(p)} - \frac{1}{p}\right\}(s)$$



Chords in an isolated cylinder (μ, I and i)



σ_Π as a function of the porosity for circular observation subsurfaces of various radius r



$F_i(\Pi, s)$ analytical vs measurements

[2] Souveton M. et al. (2026). Morphological properties of random arrays of infinitely long overlapping cylinders for modeling statistically homogeneous and isotropic fibrous media. *Physical Review E*, *113, 024111.*

Development of a non Beerian model

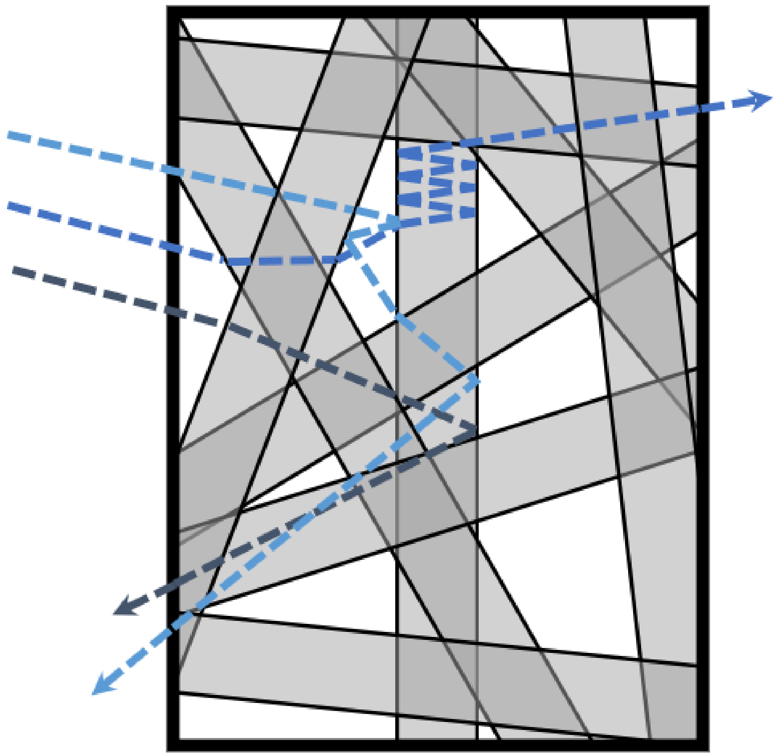
Development of a non Beerian model

Definitions and hypothesis [3]

- **Generalized radiative functions:**
  - Extinction CDF: $\boldsymbol{G^{(n)}_{ext,i}(s)}$ → β
  - Absorption and scattering PCF: $\boldsymbol{P^{(n)}_{abs,i}(s)}$ and $\boldsymbol{P^{(n)}_{sca,i}(s)}$ → κ, σ
  - Conditional probability of scattering: $\mathbb{P}^{(n)}_{sca,i}(\boldsymbol{s})$ → ω
  - Probability to be in the void phase: $\boldsymbol{\lambda_n}$ → Π

  Where n means « after the n^{th} scattering event » and $i = v$, f or h is the phase in which the ray is travelling.

- **First trajectories are i-chords, the next are μ-chords.**
- **Scattering phase function:**
  - Following Snell-Descartes's law (specular)
  - Following Lambert's law (diffuse) with $\rho = 1/2$



DSMC with a Monte Carlo raytracing algorithm in the fibrous medium

[3] Several works on a non Beerian approach by Dauvoix, Seyer, Enguehard, Taine, etc…

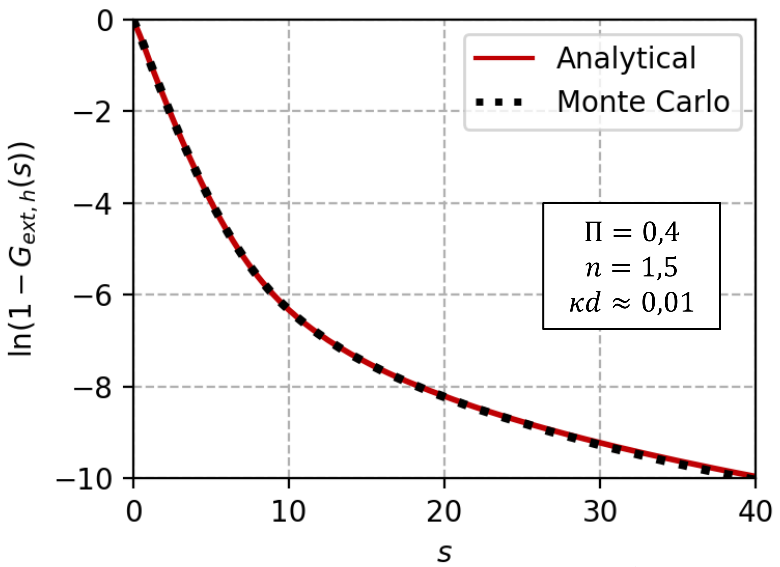
Development of a non Beerian model

Practical application

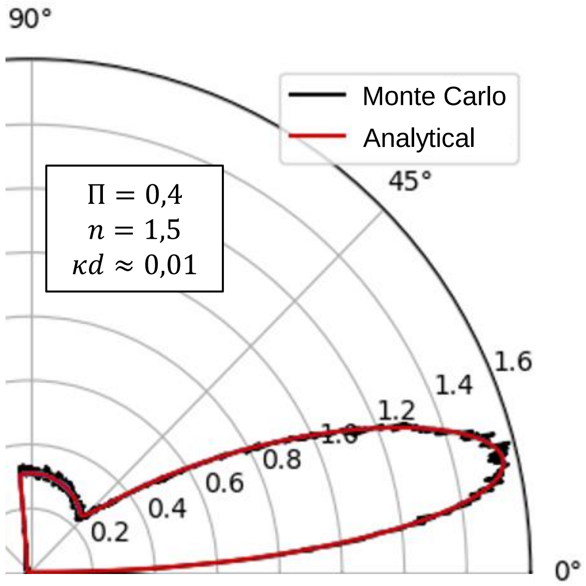
- **Example**:
  - $G_{ext,h}^{(n)}(s) = \lambda_n(1-\Pi^s) + (1-\lambda_n)(1-\exp(-\kappa s)(1-F_{X,f}(\Pi,s)))$
  - $\mathbb{P}_{sca,h}^{(n)}(s) = 1 - \frac{\kappa}{\kappa + \frac{f_{X,f}(\Pi,s)}{1-F_{X,f}(\Pi,s)} - \frac{\lambda_n}{1-\lambda_n}\ln\Pi\frac{\exp((\kappa+\ln\Pi)s)}{1-F_{X,f}(\Pi,s)}}$
  - $\lambda_0 = \Pi$ and:

    - Diffuse reflection: $\lambda_{n>0} = \rho = 1/2$
    - Specular reflection: $\lambda_1 = \Pi A + (1-\Pi)P_{sca,f}^{(0)}(+\infty)B$ and $\lambda_n \to cste$

- **Scattering phase function:**
  - Analytical expression derived for the specular case.
  - Expression obtained by a curve fitting for the diffuse case.



Extinction CDF ($\ln(1-G_{ext,h}^{(0)})$)



Scattering phase function indicatrix in the fibrous medium with specular conditions

Development of a non Beerian model

Monte Carlo algorithm for the model

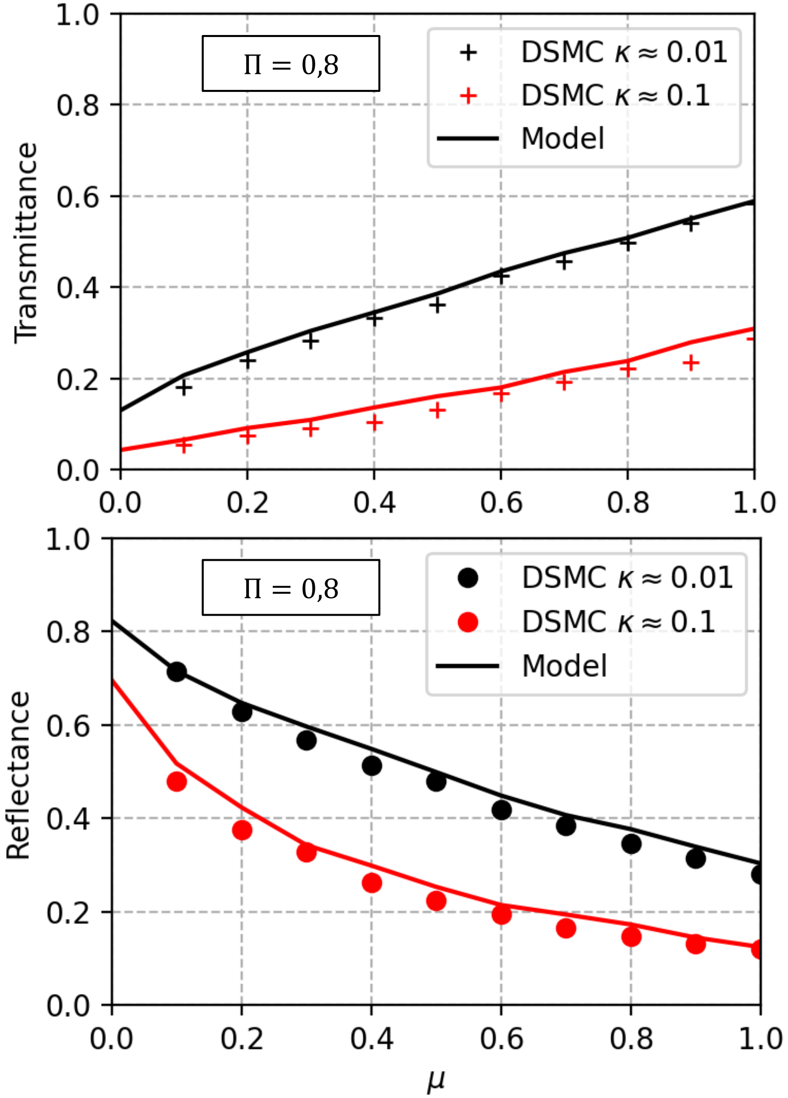
- **For each ray impinging the calculation box:**
  - A random distance s before extinction is drawn according to $G_{ext,h}^{(n)}$.
  - A uniform number on [0, 1] is drawn and compared to $\mathbb{P}_{\boldsymbol{sca,h}}^{(\boldsymbol{n})}(\boldsymbol{s})$.

    - If absorbed, a new ray is fired.
    - If scattered, a new direction is chosen in accordance with the scattering phase function.
  - The algorithm continues until the ray is out of the calculation box (or absorbed).

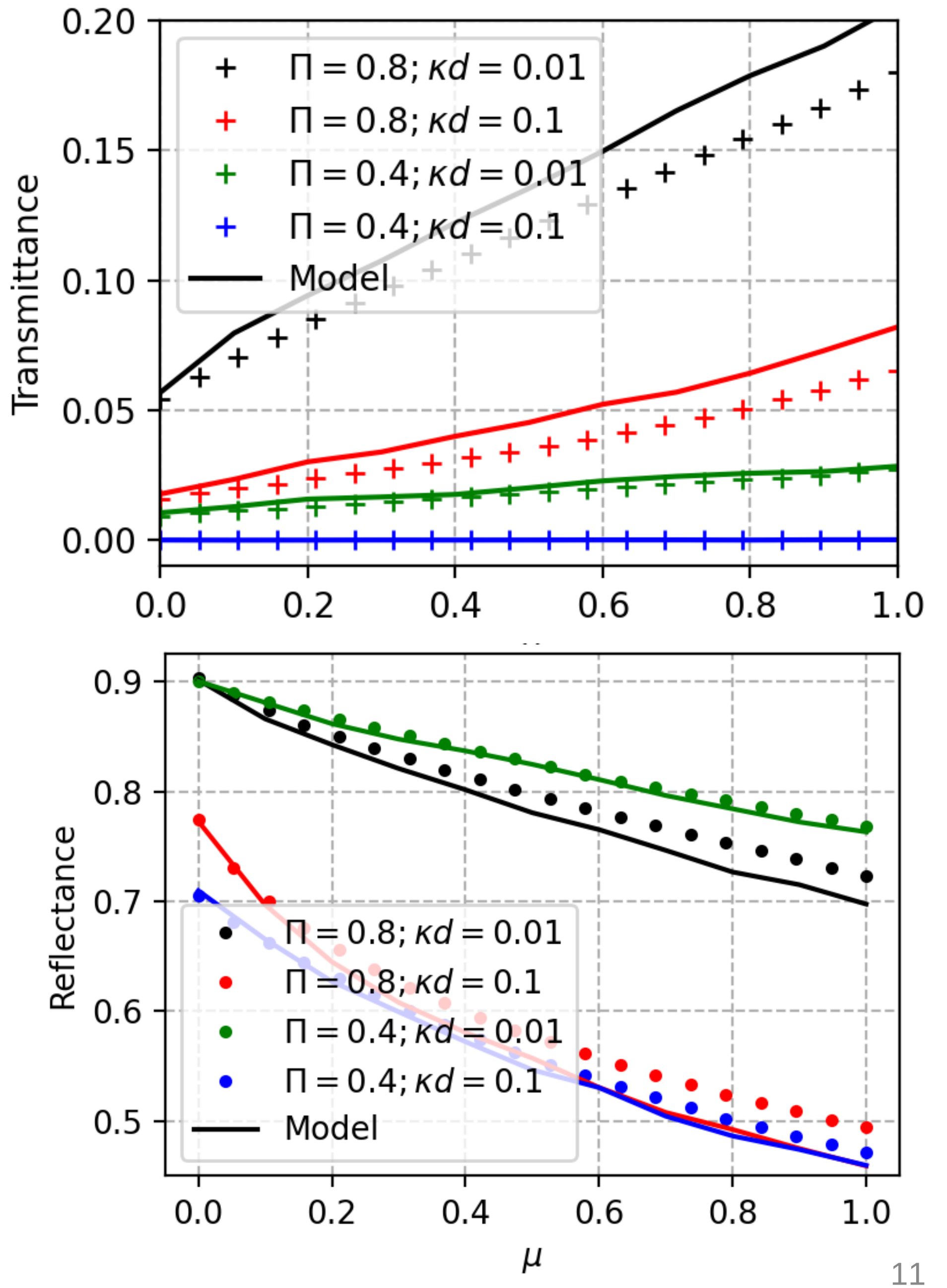
Development of a non Beerian model

Results and discussions

- **Specular interface:**



- **Diffuse interface:**



Development of a non Beerian model

Results and discussions

- **Highlighting the role of the variable $-\ln(\Pi)$**:
  - In the void phase: $G_{ext,v}^{(n)}(s) = 1 - \Pi^s = 1 - \exp(\ln(\Pi)s)$
  - At the optically thin limit: $\beta_{OT} = \frac{dG_{ext,h}^{(n)}}{ds}(s = 0) = \frac{\kappa - \ln \Pi}{2}$
  - Otherwise: $\beta = \frac{1}{\int_0^{+\infty}\left(1 - G_{ext,h}(s)\right)ds} = -2\kappa \ln \Pi \int_0^{+\infty} \exp(-\kappa s)\, \Pi^{F_i(s)} ds$
  - The asymptotic behavior of the conditional scattering probability:

$$\mathbb{P}_{sca,h}^{(n)}(+\infty) = 0 \qquad \text{if } \kappa < -\ln \Pi$$
$$\mathbb{P}_{sca,h}^{(n)}(+\infty) = 1 \qquad \text{if } \kappa \geq -\ln \Pi$$

Conclusion and Perspectives

- **Several morphological properties of statistically homogeneous and isotropic cylinder stacks have been determined analytically.**

- **The generalized non Beerian radiative properties of the equivalent homogeneous medium have also been determined analytically, especially:**
  - Extinction CDF
  - Scattering and absorption CPF
  - Specular scattering phase function

- **They have been used in a non Beerian radiative transfer model, and we are currently in the process of analyzing the results.**

- **We need to compare the previous results with a Beerian approach.**

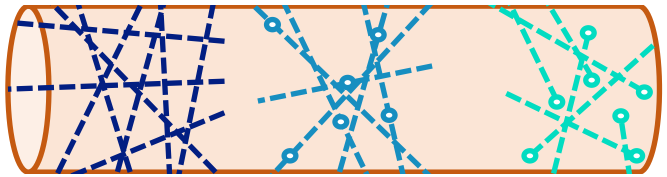
Appendix

Morphological study

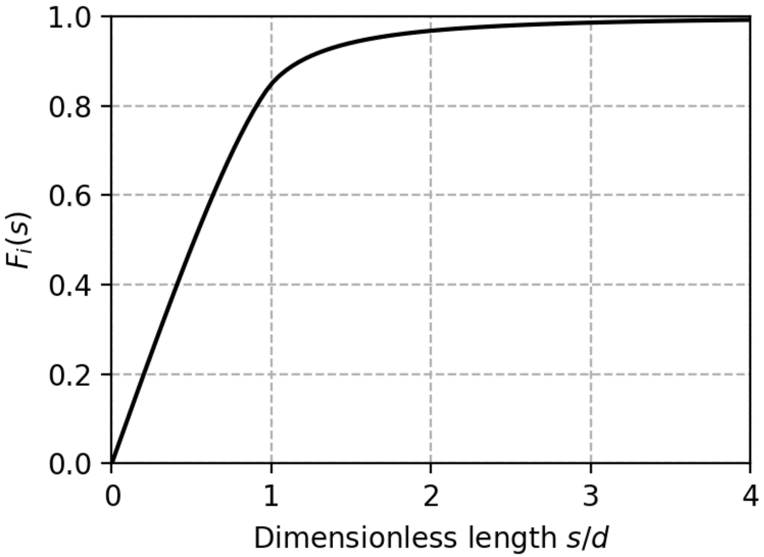
Definitions

- **Classic chords distributions:**
  - μ-random chords
  - I-random chords
  - i-random chords
- **Let us focus on i-random chords**
- **Probability density function (PDF) and cumulative distribution function (CDF) of i-random chord lengths in an isolated cylinder [2]:**
  - $f_i(s) = \frac{1-F_\mu(s)}{\overline{s_\mu}}$
  - $F_i(s) = \frac{4}{\pi} \int_0^s \int_a^{\frac{\pi}{2}} \cos^2(\theta) \sqrt{1 - x^2 \cos^2(\theta)} \, d\theta \, dx$

(results are scaled with respect to the diameter d of the fibers)



Chords in an isolated cylinder (μ, I and i)



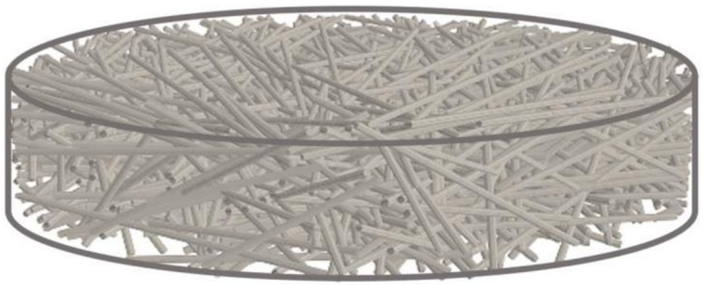
Probability that an i-random chord length in an isolated cylinder is less than s

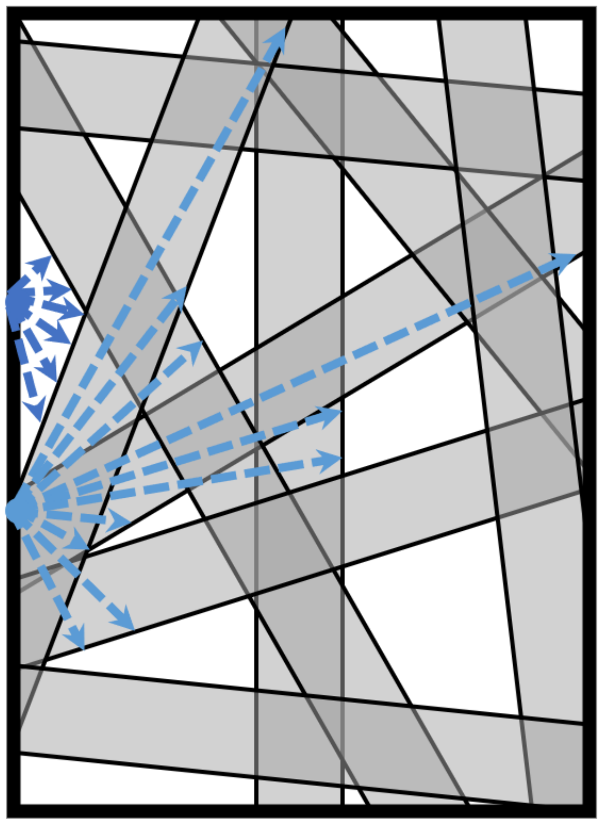
[2] Tomadakis, M. M., & Sotirchos, S. V. (1993). Random paths in random arrays of cylinders. *Radiation research*, *135*(3), 302-311.

Morphological study

i-random chords in a random stack of cylinders

- **We study now a random stack of overlapping infinite cylinders. The medium is statistically homogeneous and isotropic. Let us denote the porosity (void volume fraction) Π. What is $F_i(\Pi, s)$?**
- **In the void phase, the behaviour is known:**
  - $F_i(\Pi, s) = 1 - \Pi^s$: Beerian phase [2]
- **In the fiber phase:**
  - $F_i(\Pi \to 1, s) = F_i(s)$
  - $F_i(\Pi \to 0, s) = 1 - \exp\left(s \frac{\Pi \ln \Pi}{1-\Pi}\right)$ [2]
  - In the Laplace domain [3]: $\widehat{F_i}(\Pi, \hat{s}) = \frac{\Pi}{1-\Pi}\left(\frac{\Pi}{\hat{s}^2 \widehat{S_v}(\hat{s})} - \frac{1}{\hat{s}}\right)$ with $S_v(s)$ the autocorrelation function of the void phase
- **Knowing $S_v(s)$ will allow the numerical evaluation of $F_i(\Pi, s)$**





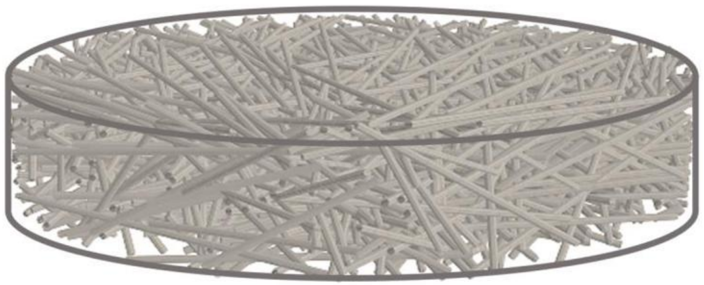
Visual representation of chords emitted in volume in the void phase (dark blue) and in the fiber phase (light blue)

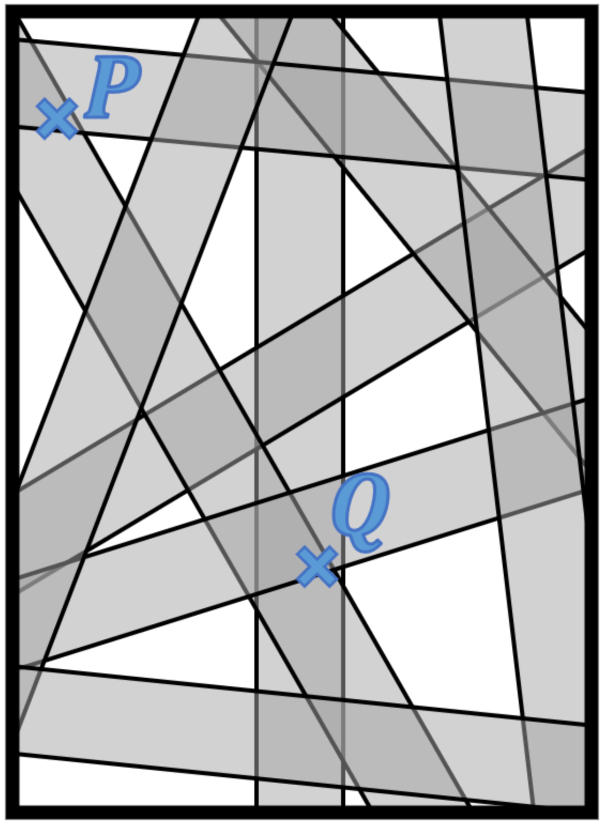
[3] Roberts, A. P., & Torquato, S. (1999). Chord-distribution functions of three-dimensional random media: approximate first-passage times of Gaussian processes. *Physical Review E*, *59*(5), 4953.

Morphological study

Statistics of overlapping fibers

- **Let P and Q be two random points, s their distance, and X_P, X_Q two random variables counting the number of cylinders covering P and Q.**
- **The covering theory says:**
  - $\mathbb{P}(X_P = p) = \frac{\lambda^p}{p!}\exp(-\lambda)$ [4]
  - Therefore : $\mathbb{P}(X_P = 0) = \Pi = \exp(-\lambda)$ and $\mathbb{P}(X_P = p) = \Pi\,(-\ln \Pi)^p / p!$
  - Overlapping ratio : $\tau = \mathbb{P}(X_P \geq 2) = 1 - \Pi + \Pi \ln \Pi$
- **With more calculations, we can deduce:**
  - $\mathbb{P}\left(X_P = p \cap X_Q = q\right) = \Pi^{1+F_i(s)} \frac{(-Fi(s)\ln \Pi)^{p+q}}{p!q!} \sum_{k=0}^{\min(p,q)} \binom{p}{k}\binom{q}{k} \frac{k!}{\left(-\frac{F_i(s)^2}{1-F_i(s)}\ln \Pi\right)^k}$





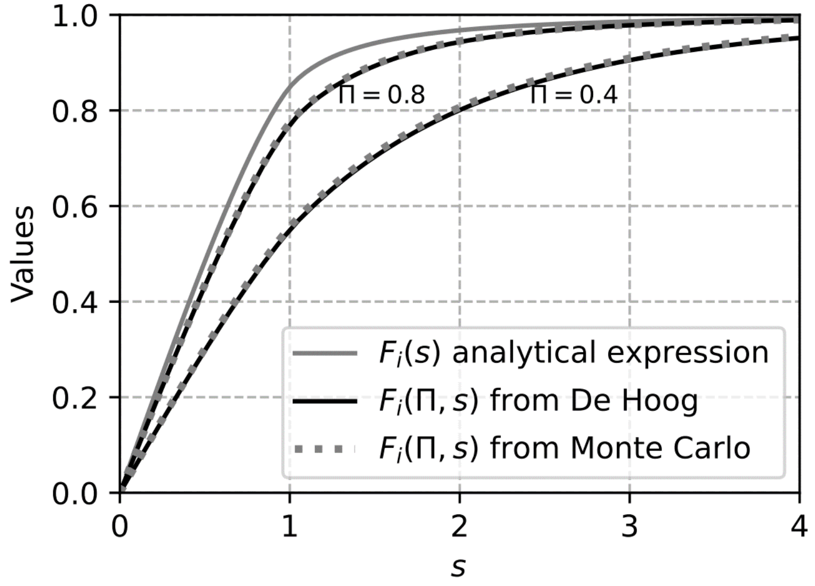
Visual representation of two random points within the medium

[4] Sampson, W. W. (2008). *Modelling stochastic fibrous materials with mathematica®*. Springer Science & Business Media.

Morphological study

Autocorrelation function and $F_i(\Pi, s)$:

- **The autocorrelation function of the void phase is easily obtained:**
  - $S_v(s) = \mathbb{P}\left(X_P = 0 \cap X_Q = 0\right) = \Pi^{1+F_i(s)}$
- **Therefore we conclude:**
  - $\widehat{F_i}(\Pi, \hat{s}) = \frac{\Pi}{1-\Pi}\left(\frac{1}{\hat{s}^2 \mathcal{L}\left(\Pi^{F_i(s)}\right)} - \frac{1}{\hat{s}}\right)$
- **Numerical inversion of the Laplace expression:**
  - For a very fast inversion with precision up to 2 digits: Wilcox's algorithm.
  - A slower approach with precision up to 8 digits: De Hoog's algorithm.
- **Asymptotic expansion:**
  - $F_i(\Pi, s \to +\infty) \sim 1 + \frac{\ln \Pi}{8(1-\Pi)s^2}$

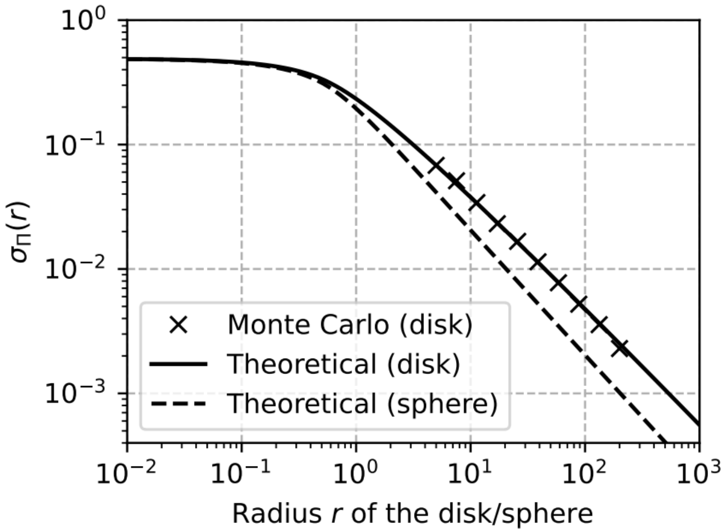


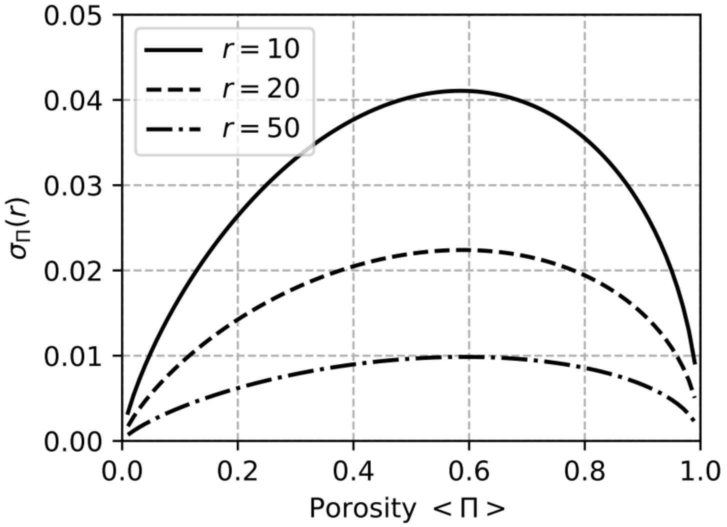
Probability that an i-random chord length is less than s in the fiber phase for different porosities

Morphological study

Representative Elementary Volume for porosity:

- **In a representative box, the effective porosity of a subarea or a subvolume v is not Π, but fluctuates.**
- **Let us note $\sigma_\Pi(v)$ the standard deviation of the effective porosity when v is moved around.**
- **Analytical expressions [5]:**
  - $\sigma_\Pi^2(v = \pi r^2) = \frac{4}{\pi r^2} \int_0^{2r} (S_v(r) - \Pi^2) \left(\arccos \frac{x}{2r} - \frac{x}{2r} \sqrt{1 - \frac{x^2}{4r^2}} \right) x dx$
  - $\sigma_\Pi^2 \left(v = \frac{4\pi r^3}{3} \right) = \frac{3}{r^3} \int_0^{2r} (S_v(r) - \Pi^2) \left(1 - \frac{3x}{4r} + \frac{x^3}{16r^3} \right) x^2 dx$
- **Asymptotic behaviors for large r:**
  - $\sigma_\Pi(v = \pi r^2) \propto \frac{1}{r}$
  - $\sigma_\Pi \left(v = \frac{4\pi r^3}{3} \right) \propto \frac{1}{r^{3/2}}$





Standard deviation of the effective porosity in an observation domain as a function of its dimension r and the mean porosity

[5] Torquato, S. (2002). *Random heterogeneous materials: microstructure and macroscopic properties* (Vol. 16). New York: Springer.