Homogenisation techniques dedicated to paper industry: theory and applications.

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Paris, 30 septembre 2010

Outline

Part I –

Homogeneization theory applied to paper

Part II –

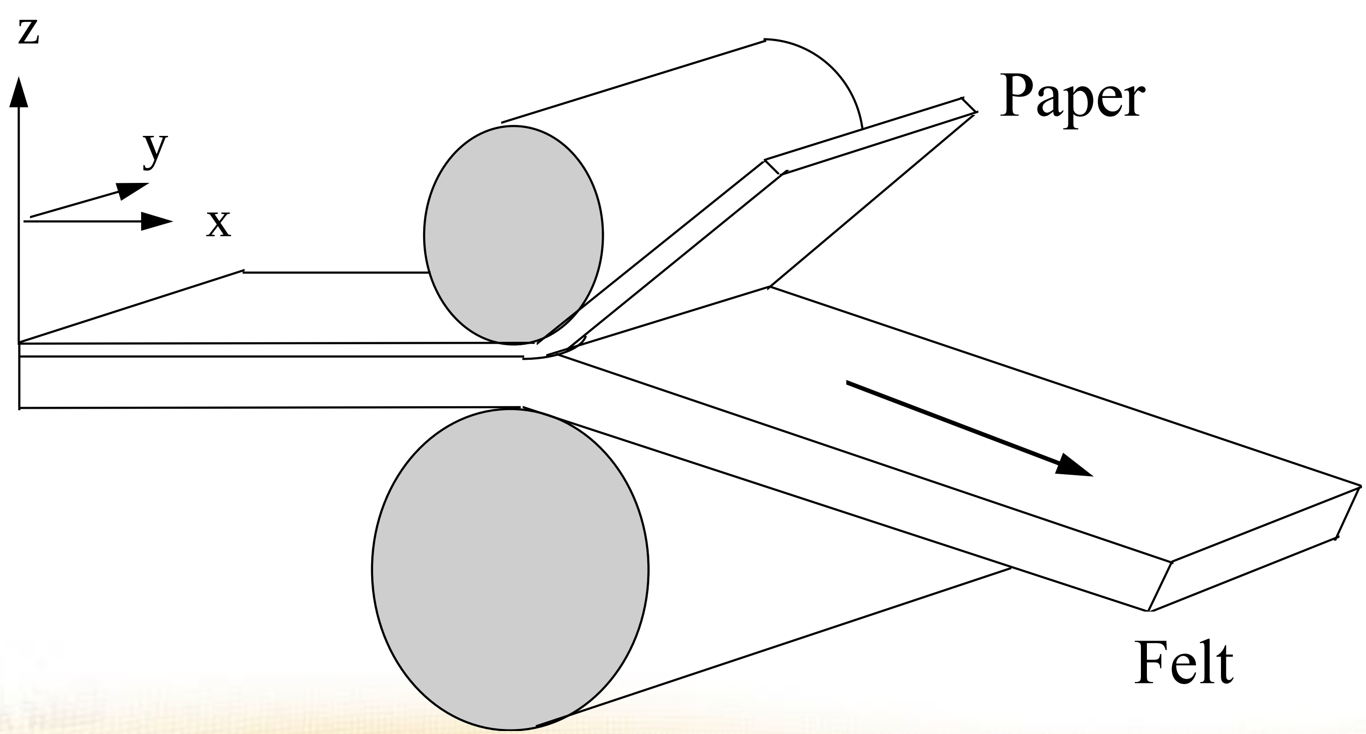
REV and X-Ray microtomography

Part I - CONTENT

I - INTRODUCTION

AIM :

Temperature field in paper during hot pressing



I - INTRODUCTION (2)

Paper and Felt: deformable porous media

Non saturated: (non /) wetting phases

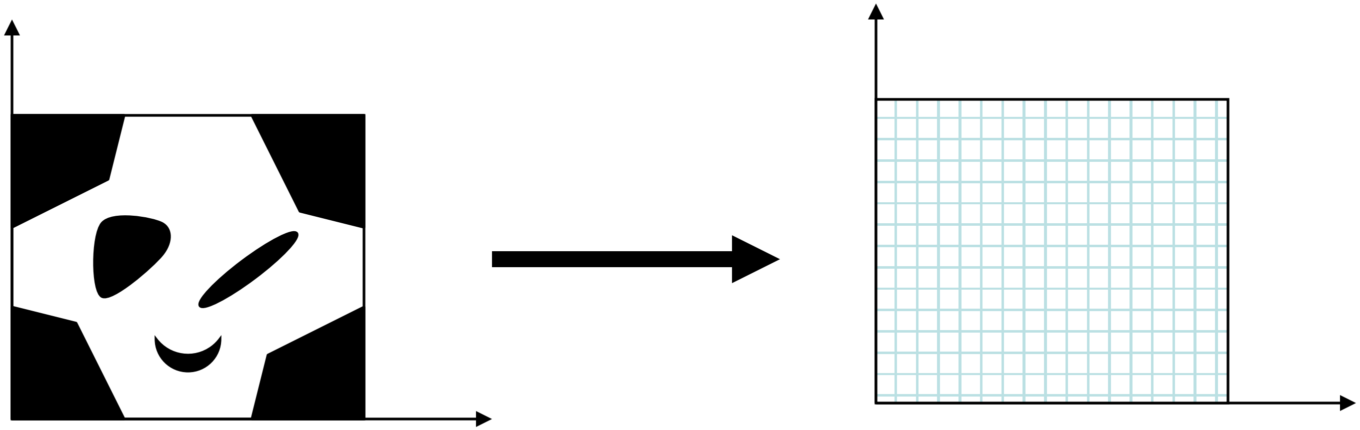
Complex structure at the pore scale

⇒ Macroscopic modelling:
Homogeneization

I - INTRODUCTION (3)

Homogeneization:

microscale to macroscale



EQUIVALENT POROUS MEDIUM

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II – METHOD PRESENTATION

The medium is assumed as periodic.

Random media yield similar macroscopic description modelling.

AURIAULT J.-L. (1991) ”Heterogeneous medium. Is an equivalent macroscopic description possible?”, Int. J. Engng. Sci., 29, 7, pages 785-795.

II – METHOD PRESENTATION:

Multiscale expansion method

- without macroscopic prerequisites,
- the macroscopic law,
- the effective parameters,
- the validity domain of the model.

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II – METHOD PRESENTATION: Multiscale expansion method

SCALE SEPARATION

pore dimension / sample size

$\Leftrightarrow$ model quality.

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II – METHOD PRESENTATION: Main steps

1 – Physical phenomena at the microscopic scale.

2 – Two different scales are defined (ε).

3 – Physical Equations at microscopic scale.

4 – The dimensionless parameters are expressed in function of ε.

II – METHOD PRESENTATION: Main steps (2)

5 – Asymptotic expansions in power of ε are introduced.

6 – Problems at different orders are solved to determine the successive approximations of the variables.

7 – Physical quantities are evaluated from the dimensionless ones.

II – METHOD PRESENTATION

- The scale ratio $\varepsilon = l / L$
- For a paper web, the characteristic lengths

$$l = 10\ \mu m \text{ and } L = 1\ mm$$

$$\Rightarrow \varepsilon = 10^{-2}$$

- Dimensionless parameters are evaluated in term of ε.

II – METHOD PRESENTATION

Energy balance for a domain (k = w, a, s):

$$\frac{\partial \rho_k C_{p_k} T_k}{\partial t} + v_k . \nabla (\rho_k C_{p_k} T_k) = \nabla . (\lambda_k \nabla T_k)$$

Flux conservation of heat on the interface:

$$\lambda_{k_{ij}} \left(\frac{\partial T_k}{\partial X_j} \right) N_i = \lambda_{l_{ij}} \left(\frac{\partial T_l}{\partial X_j} \right) N_i$$

Temperatures are continuous on each interface (no resistance) :

$$T_k = T_l$$

II – METHOD PRESENTATION

Dimensionless variables: $X = X^{*} . X^{R}$

Dimensionless parameters:

$$N_{\lambda_{aw}} = \frac{\lambda_a{}^R}{\lambda_w{}^R}$$

$$N_{\lambda_{sw}} = \frac{\lambda_s{}^R}{\lambda_w{}^R}$$

$$P = \frac{\left|\rho C_p \frac{\partial T}{\partial t}\right|^R}{\left|\frac{\partial}{\partial X_i} \lambda_{ij} \frac{\partial T}{\partial X_j}\right|^R}$$

$$Pe = \frac{\left|\rho C_p V_i \frac{\partial T}{\partial X_i}\right|^R}{\left|\frac{\partial}{\partial X_i} \lambda_{ij} \frac{\partial T}{\partial X_j}\right|^R}$$

(R)

- in Ω_k :

$$P \frac{\partial \rho_k C_k T_k}{\partial t} = \frac{\partial}{\partial y_i}\left(\lambda_{k_{ij}} \frac{\partial T_k}{\partial y_j}\right) - P_e V_{k_i} \frac{\partial \rho_k C_k T_k}{\partial y_i}$$

- in Γ_{kl}:

$$N_{\lambda_{kl}} \lambda_{k_{ij}} \left(\frac{\partial T_k}{\partial y_j}\right) N_i = \lambda_{l_{ij}} \left(\frac{\partial T_l}{\partial y_j}\right) N_i$$

(*)

II – METHOD PRESENTATION

- Reference Values

$(J \,.\, m^{-1} \,.\, s^{-1} \,.\, K^{-1})$	$(J \,.\, kg^{-1} \,.\, K^{-1})$	$(kg.m^{-3})$
λ_s	C_{ps}	ρ_s
0.33	$1.33.10^{3}$	1.5.10
λ_w	C_{pw}	ρ_w
0.602	$4.18.10^{3}$	10^{3}
λ_a	C_{pa}	ρ_a
0.026	10^{3}	1.23

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II – METHOD PRESENTATION

$$N_{\lambda_{aw}} = 0.043 = O(\varepsilon) \quad N_{\lambda_{sw}} = 0.548 = O(1)$$

$$P_w = \frac{C_w l^2}{\lambda_w \tau} = O(\varepsilon^{-1} P_a)$$

$$P_s = \frac{C_s l^2}{\lambda_s \tau} = O(P_w)$$

II – METHOD PRESENTATION

Each physical quantity ϕ is then looked as:

$$\varphi = \varphi^{(0)} + \varepsilon.\varphi^{(1)} + \varepsilon^{2}.\varphi^{(2)} + \varepsilon^{3}.\varphi^{(3)} + \ldots$$

Homogenisation process

$\Rightarrow$ approximated macroscopic models.

Model accuracies = $O(\varepsilon)$

$\Rightarrow$ The larger the scale separation is, the better is the result (approximation).

III - MAIN RESULTS

A - Small Péclet number: diffusion - convection

A-1: Pe $\leq$ O (ε^2) P = O (ε^2)

$$< C >_{w,s} \frac{\partial T}{\partial t} = \frac{\partial}{\partial x_i}\left(\lambda_{ij}^{eff} \frac{\partial T}{\partial x_j} \right) + O(\varepsilon)$$

With :

$$\lambda_{ij}^{eff} = \frac{1}{|\Omega|} \int_{\Omega_w + \Omega_s} \lambda_{ij} \left(I_{kj} + \frac{\partial \chi_{Ik}}{\partial y_j} \right) d\Omega$$

$$< C >_{w,s} = \frac{1}{|\Omega|} \left(\int_{\Omega_w} C_w d\Omega + \int_{\Omega_s} C_s d\Omega \right)$$

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III – MAIN RESULTS (2)

A-2 : Pe $\leq O(\varepsilon^2)$ P $\leq O(\varepsilon^3)$

$$0 = \frac{\partial}{\partial x_i}\left(\lambda_{ij}^{eff}\frac{\partial T}{\partial x_j}\right) + O(\varepsilon)$$

A-3 : Pe $= O(\varepsilon)$ P $= O(\varepsilon^2)$

$$< C >_{w,s}\frac{\partial T}{\partial t} = \frac{\partial}{\partial x_i}\left(\lambda_{ij}^{eff}\frac{\partial T}{\partial x_j}\right) - < C V_i >_{\Omega}\frac{\partial T}{\partial x_i} + O(\varepsilon)$$

J.-F. BLOCH, J.-L. AURIAULT, (1998) 'Heat Transfer in Nonsaturated Porous Media: Modelling by Homogenisation', TiPM, 30: 301–321.

III - MAIN RESULTS (3)

A-4 : Pe = O (ε) P ≤ O (ε ³)

$$0 = \frac{\partial}{\partial x_i}\left(\lambda_{ij}^{eff}\frac{\partial T}{\partial x_j}\right) - \langle C\, V_i \rangle_{\Omega}\frac{\partial T}{\partial x_i} + O(\varepsilon)$$

A-5 : $\mathbf{Pe_{a,w}}$ = O (ε) $\mathbf{Pe_s}$ = O (ε²) P = O (ε ²)

$$\langle C \rangle_{w,s}\frac{\partial T}{\partial t} = \frac{\partial}{\partial x_i}\left(\lambda_{ij}^{eff}\frac{\partial T}{\partial x_j}\right) - \langle CV_i \rangle_{\Omega_a + \Omega_w}\frac{\partial T}{\partial x_i} + O(\varepsilon)$$

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III - MAIN RESULTS (4)

B - Higher Péclet number : dispersion

B - 3 : Pe = O (1) P ≤ O (ε ³)

$$0 = \varepsilon \frac{\partial}{\partial x_i}\left(\lambda_{ij}^{***\text{eff}} \frac{\partial T}{\partial x_j}\right) - \langle C V_i \rangle_\Omega \frac{\partial T}{\partial x_i} + O(\varepsilon^2)$$

$$\lambda_{ij}^{***\text{eff}} = \frac{1}{|\Omega|}\int_{\Omega_{w,s}} \left[\lambda_{ij}\left(I_{lj} + \frac{\partial \chi_{III\,j}}{\partial y_l}\right) - C\, V_i^{(0)} \chi_{III\,j}\right] d\Omega$$

B - 2 : Pe = O (1) P = O (ε²)

$$\varepsilon \langle C \rangle_{w,s} \frac{\partial T}{\partial t} = \varepsilon \frac{\partial}{\partial x_i}\left(\lambda_{ij}^{***\text{eff}} \frac{\partial T}{\partial x_j}\right) - \langle C V_i \rangle_\Omega \frac{\partial T}{\partial x_i} + O(\varepsilon^2)$$

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III - MAIN RESULTS (5)

B - Higher Péclet number : dispersion

B - 1 : Pe = O (1) P = O (ε)

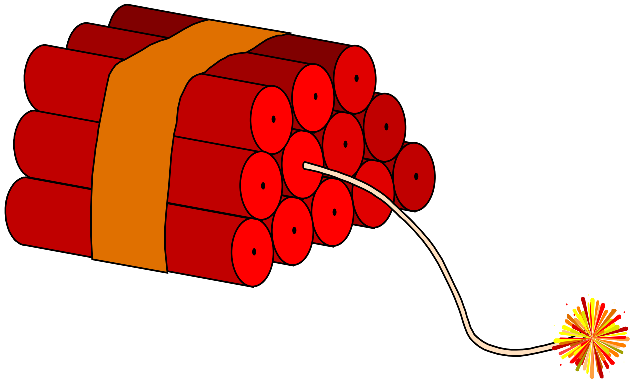
$$\left(< C >_{\Omega_w+\Omega_s} + \varepsilon < C >_{\Omega_a}\right)\frac{\partial T}{\partial t} + \varepsilon < C\chi_{II\,i} >_{\Omega_w+\Omega_s} \frac{\partial^2 T}{\partial t \partial x_i} =$$

$$\varepsilon \frac{\partial}{\partial x_i}\left(\lambda_{ij}^{**eff} \frac{\partial T}{\partial x_j}\right) - \left(< CV_i >_{\Omega} \frac{\partial T}{\partial x_i}\right) + O\left(\varepsilon^2\right)$$

$$\lambda_{ij}^{**eff} = \frac{1}{|\Omega|}\int_{\Omega w,s}\left[\lambda_{ij}\left(I_{lj} + \frac{\partial \chi_{II\,j}}{\partial y_l}\right) - C\left(V_i^{(0)}\chi_{II\,j}\right)\right] d\Omega$$

III - MAIN RESULTS (6)

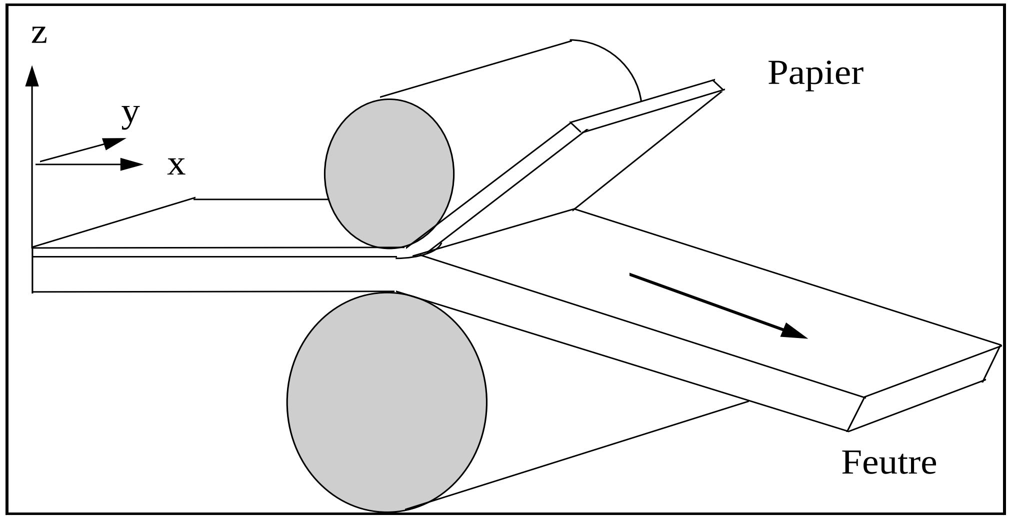
$$\mathbf{Pe \geq O(\varepsilon^{-1})}$$



This case is NOT homogeneizable

$\Leftrightarrow$ no equivalent medium exists !

IV - EXAMPLE:
Hot pressing of a paper web



$$Pe = \frac{\rho . C_p . V . l}{\lambda} \# \frac{10^3 . 10^3 . 10^{-2} . 10^{-6}}{0.5} = O\left(10^{-2}\right) = O(\ldots)$$

$$0 = \frac{\partial}{\partial x_i}\left(\lambda_{ij}^{eff} \frac{\partial T}{\partial x_j}\right) - \langle CV_i \rangle_{\Omega} \frac{\partial T}{\partial x_i}$$

IV – EXAMPLE: Assumptions

$$0 = \frac{\partial}{\partial x_i}\left(\lambda_{ij}^{eff}\,\frac{\partial T}{\partial x_j}\right) - \langle CV_i \rangle_\Omega \frac{\partial T}{\partial x_i}$$

$$\lambda_w = O(\lambda_s)$$

$$0 = \frac{\partial}{\partial x_i}\left(\lambda_w (n_w + n_s) I_{ij}\,\frac{\partial T}{\partial x_j}\right) - \langle C\ V_i \rangle_\Omega \frac{\partial T}{\partial x_i}$$

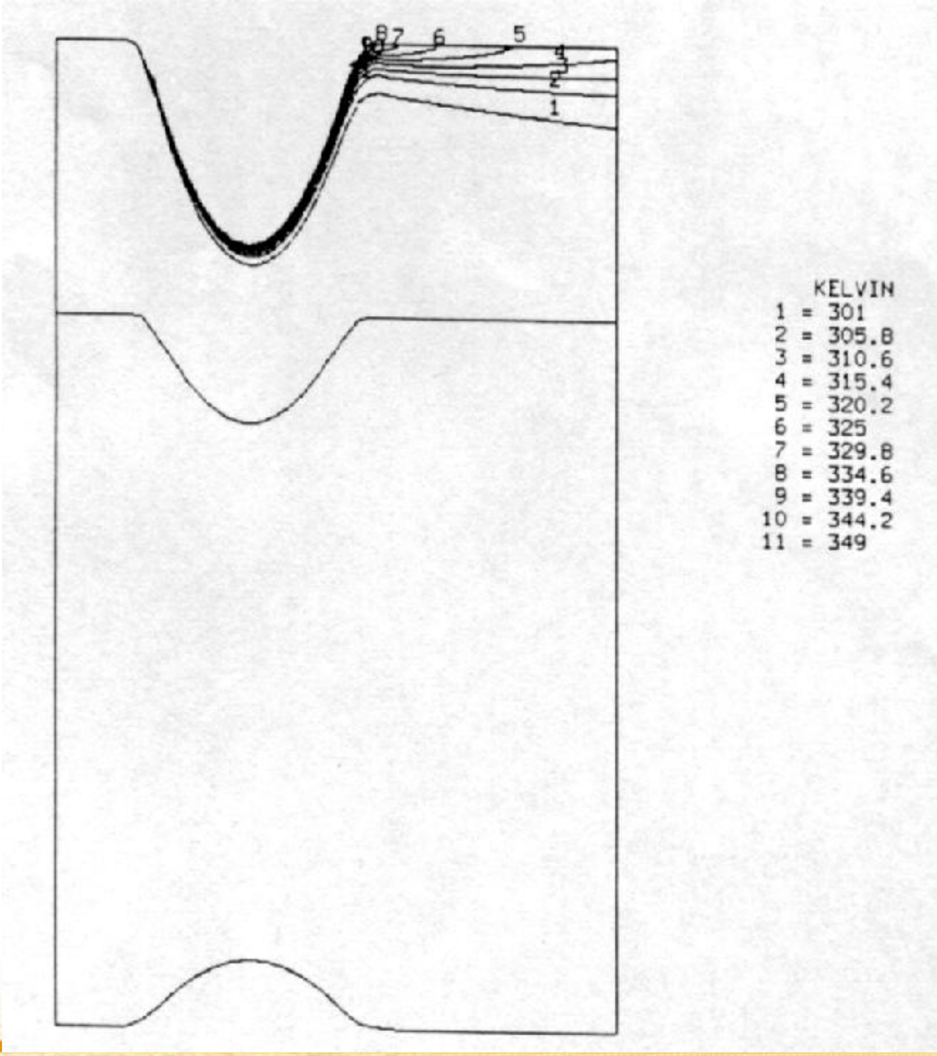
$$n_s + n_w \# 1.$$

$$0 = \frac{\partial}{\partial x_i}\left(\lambda_w\, I_{ij}\,\frac{\partial T}{\partial x_j}\right) - \langle CV_i \rangle_\Omega \frac{\partial T}{\partial x_i}$$

$$\rho_a C_{pa} V_a \ll \rho_w C_{pw} V_w$$

$$0 = \frac{\partial}{\partial x_i}\left(\lambda_w\, I_{ij}\,\frac{\partial T}{\partial x_j}\right) - \langle CV_i \rangle_{\Omega_s + \Omega_w} \frac{\partial T}{\partial x_i}$$

IV - EXAMPLE:
Temperature field in paper and felt



$T_{roll} = 50\ °C$

Mach. Speed:10 m.s^{-1},

Paper thick.: 320 µm,

Felt thick.: 2.5 mm,

Nip Length: 2.5 cm.

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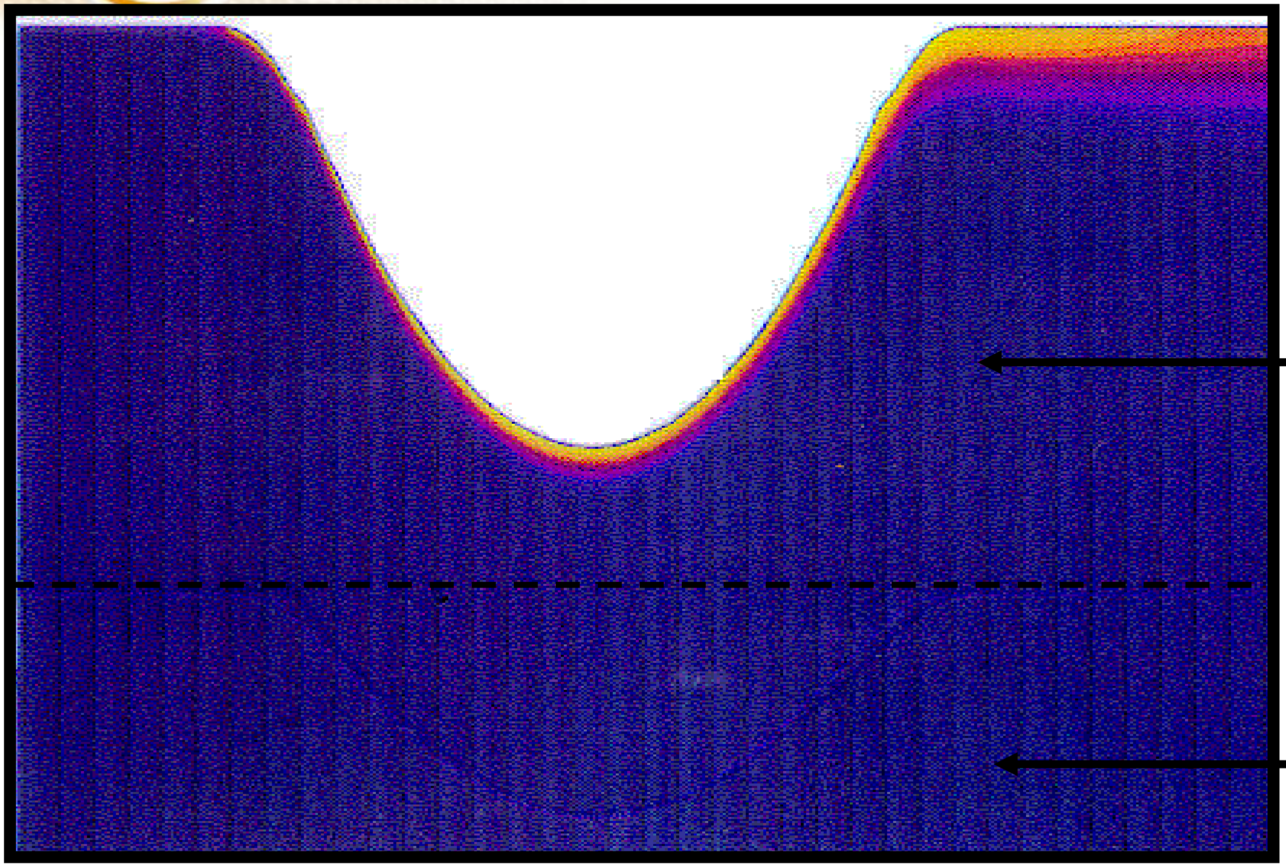
IV - EXAMPLE



T_{roll} = 50 °C

PAPER

FELT

Detail of temperature field in paper during hot pressing.

V – CONCLUSIONS / Part I

- Same microscopic physics, different law structures, with different effective coefficients.

- Evaluating dimensionless numbers (ε) :

  macroscopic model catalogue, their effective parameters and their validity domains are obtained.

- Physical characteristic values dedicated to the studied process.

V - CONCLUSION / Part I (2)

- The equivalent description corresponds to a medium that reacts globally to the considered physical excitation like the microscopic medium studied.

- If the medium cannot be homogenised, macroscopic properties are not intrinsic to the media.

- Applicable to any porous medium that satisfies the microscopic hypotheses in use here.

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Part II

3D structure of Papers

/ VER (X-Ray Microtomography)

Estimation of paper physical properties based on synchrotron X-ray microtomography.

Jean-Francis Bloch

Sabine Rolland du Roscoat
Maxime Decain, Christian Geindreau

Content (Partie Non présentée)

I. Context
II. Materials and Methods
III. Estimation of paper structure / VER
    Deterministic approach
    Statistical approach
I. Estimation of paper properties
II. Conclusions and perspectives

I. Context

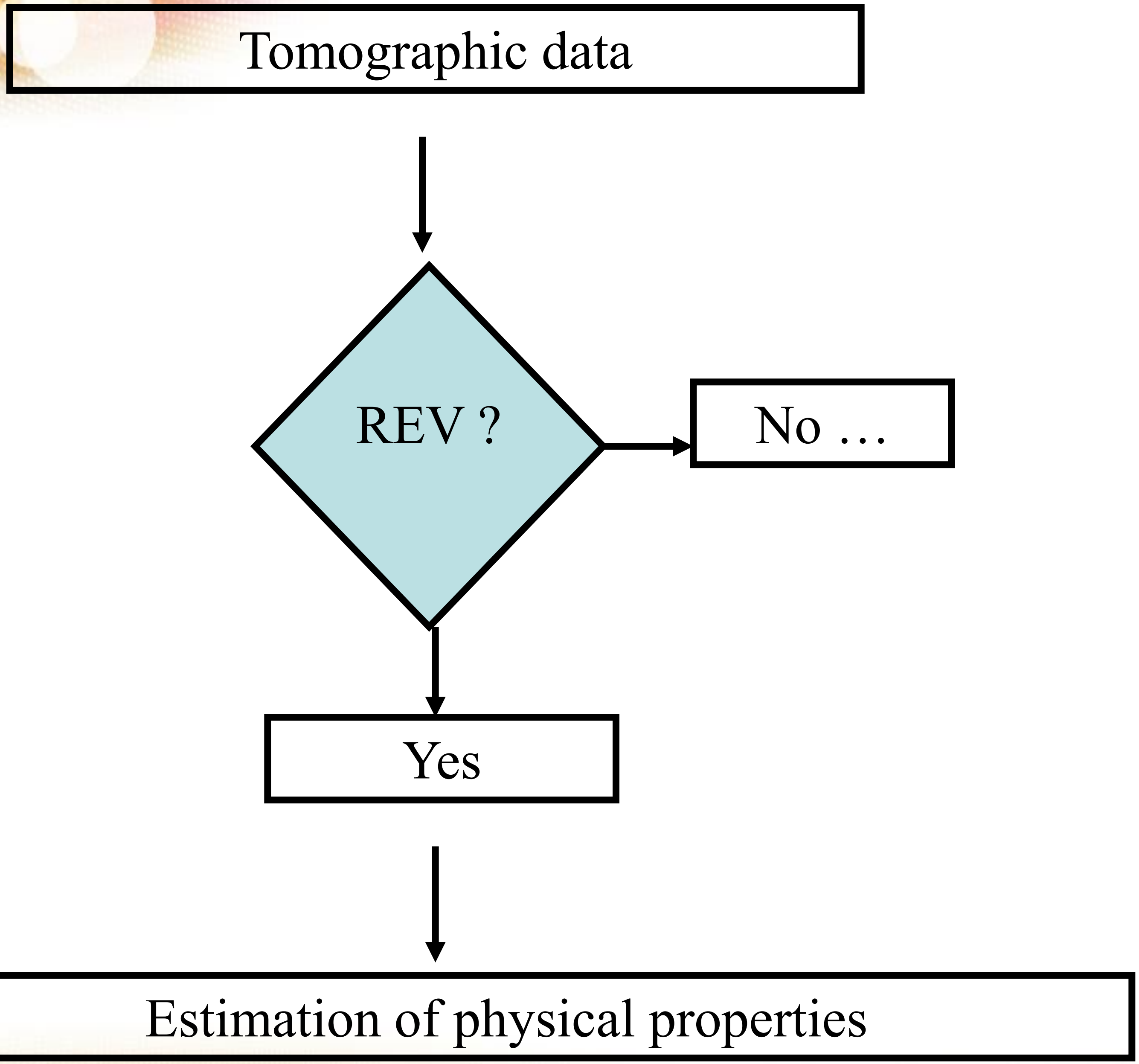
- Synchrotron X-ray microtomography gives access to the inner structure of samples at a micrometric scale
  - Quantification of the structure
  - Estimation of physical properties
- Comparison to experimental data

I. Position of the problem

- May Physical properties be simulated from X-Ray microtomography?
- Analysed volume is much smaller than the characteristic lengths / physical properties?

Problem of the representativity for:

- Porosity and specific surface area
- Effective thermal conductivity and permeability


Tomographic data
REV ?
No …
Yes
Estimation of physical properties

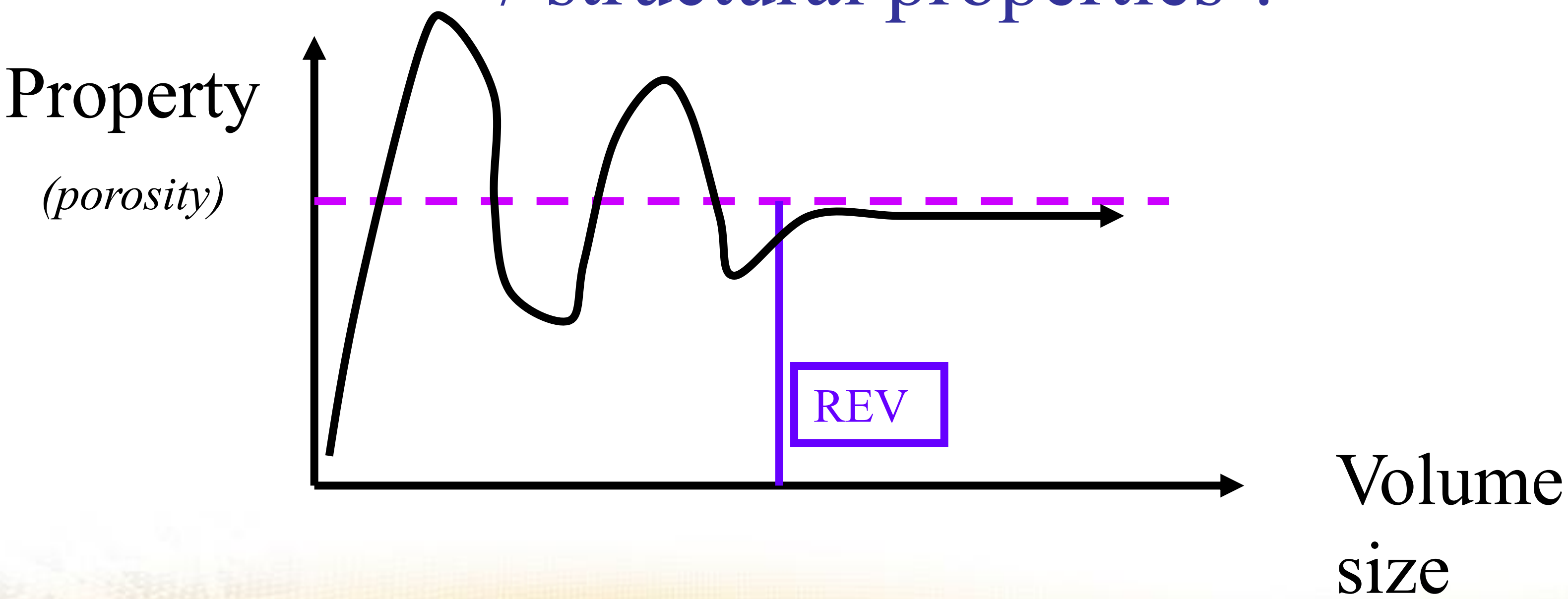
II.4. Representative Elementary Volume

REV

- Definition

Small samples (mm) !?

How Long is Long enough / structural properties ?



II.4. Applied methods

- Two approaches
  - Deterministic (classical)[1]
  - Statistical[2]

[1] W.J. Drugan, J.R. Willis, "A micromecanics-based nonlocal constitutive equation and estimates of representative volume element size for elastic composites.", J. Mech, Phys Solids, Vol. 44, No 4, 1996, pp 497-524.

[2] T. Kanit, S. Forest, I. Galliet, V. Mounoury, D. Jeulin, "Determination of the size of the representative volume element for random composites: statistical and numerical approach", International Journal of Solids and Structures 40, 2003, pp 3647-3679.

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III.5. Conclusions / Statistical REV

- Estimation of properties on volumes smaller than the deterministic REV

saving computing time in the case of the estimation of physical properties

Rolland du Roscoat, S., Decain, M., Thibault, X., Geindreau, C., Bloch J.-F. *Estimation of microstructural properties from synchrotron X-Ray microtomography and determination of the REV size in paper materials*. Acta Materiala, 55(8), 2007, 2841-2850

Content

IV.1. Estimation of permeability

- Estimation of tensor of permeability
  - No penetration of fluid into fibres
  - Pressure gradient is imposed at the interface
  - Estimation of the local fluid velocity
  - Deducing the permeability

  from Darcy Law

Koivu, V., Geindreau, C., Decain, M., Mattila, K., Bloch, J.-F., Kataja, M., *Transport properties of heterogeneous materials combining computerized x-ray micro-tomography and direct numerical simulations*, International Journal of Computational Fluid Dynamics, 23(10), 2010, 713-721