Capillary rise in demineralized dentin and more generally in a fibrous tissue

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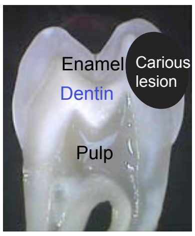
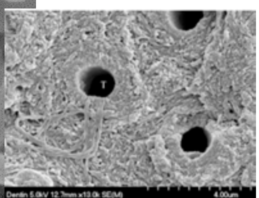
One of the biggest issue in restorative dentistry

- Composite based restorations of dentin are not sufficiently durable




Intact dentin

- Carious lesion removal
- Superficial demineralization : hydroxyapatite removal on a few microns

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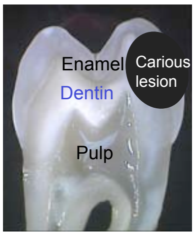

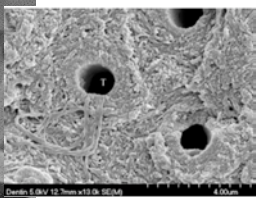

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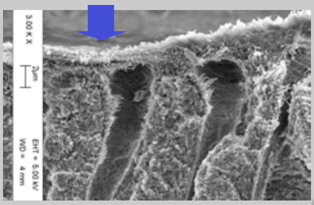
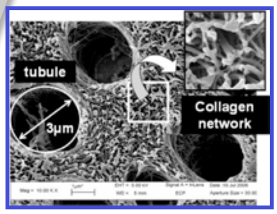


Dentin superficially demineralized



Demineralized dentin

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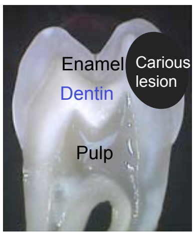

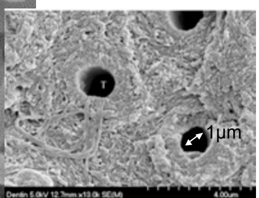

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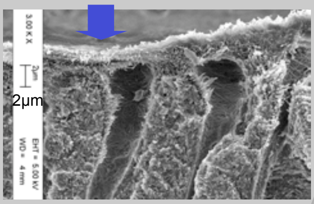

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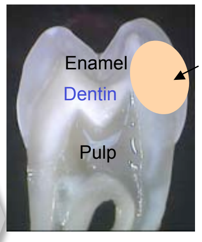
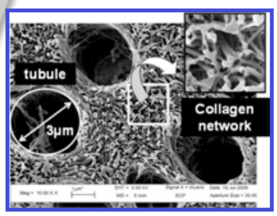




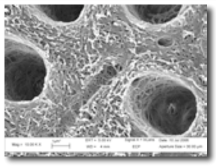
Demineralized dentin

Modeling the fibrous tissue infiltration

- Lack of durability -> due to insufficient impregnation of the fibrous tissue
- The fibrous tissue -> a collagen fiber network revealed by demineralization

2 Infiltration model:
- Vertical fibers
- General fibrous tissue

Data for the model



Model validation and porosimetry test better understanding

1 Porosimetry tests (MIP) and SEM observation

Comparison

3 Applications:
- Porosimetry test
- Demineralized dentin infiltration

1 Porosimetry tests

- MIP
  - Porosity quantification
  - Detection of pore sizes between 10nm and 100µm
- Principle
  - Dry sample
  - Sample chamber : filled with mercury
  - Incremental pressure p_{Hg} : applied to mercury
  - Measuring the mercury volume that entered the pores of the sample at each pressure increment p_{Hg}
  - Volume versus pore diameter D
  - Porosity, pores sizes and their distribution

$$p_{H_g} = 4\frac{\gamma_{H_g} \cos\theta_{H_g}}{D}$$

Jurin-Laplace

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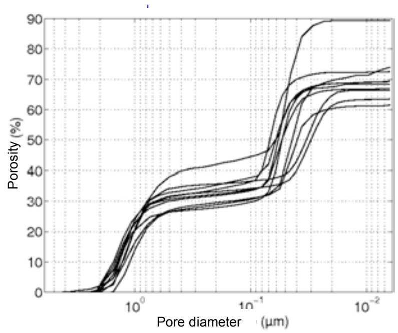
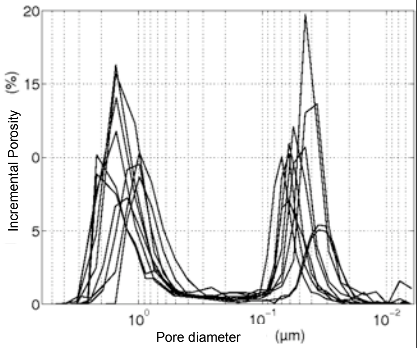
Porosimetry tests

- Demineralized and freeze dried dentin





Vennat et al. (2009)

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Porosimetry tests

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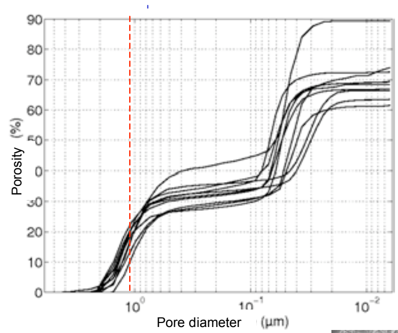

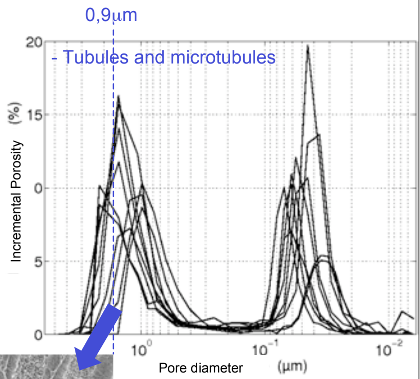

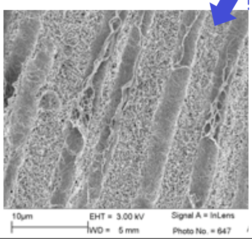

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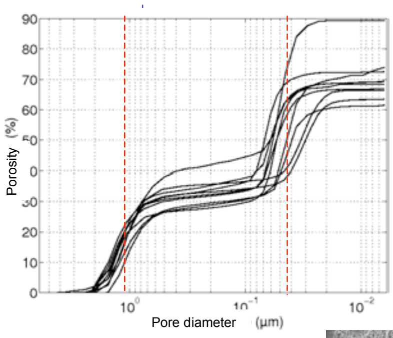

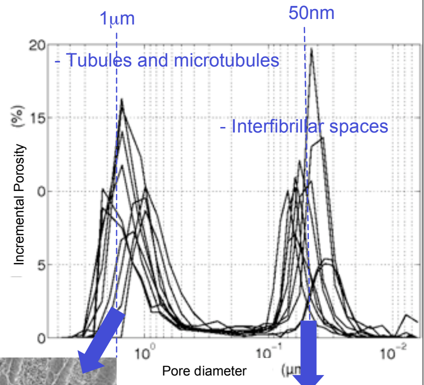

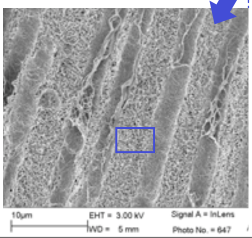

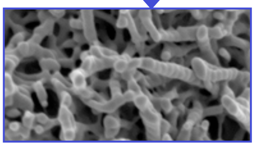

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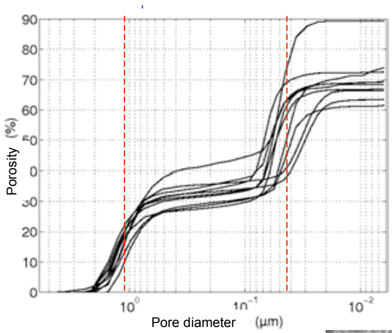
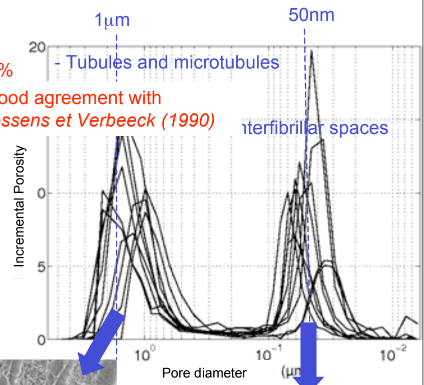
Porosimetry tests

- Demineralized and freeze dried dentin

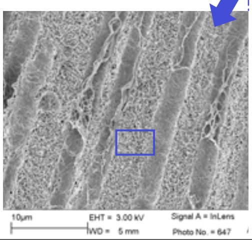


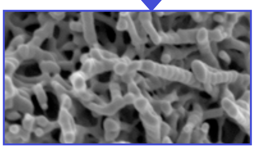
60-90%

In good agreement with *Driessens et Verbeeck (1990)*



Bimodal distribution :
- Tubules and microtubules
- Interfibrillar spaces



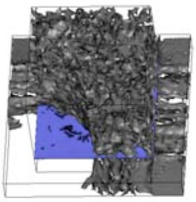


Vennat et al. (2009)

1 Porosimetry tests

- Data deduced from MIP
  - Demineralized dentin mean porosity : 70%
  - Fiber network porosity : 55%
  - Limitations : drying (artifacts), overestimation of small porosities, cylinder geometry hypothesis

2 Infiltration model in the fibrous network



- The question : how the resin is infiltrating the fibrous network?

  2.1 Capillary rise in vertical cylinder arrays

  2.2 Capillary rise in the demineralized dentin collagen fiber network

  Finite element modeling with special care of surface tension effects

  Level set method to track the front

3 Applications

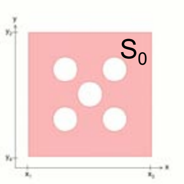
2.1 Capillary rise in a vertical cylinder array

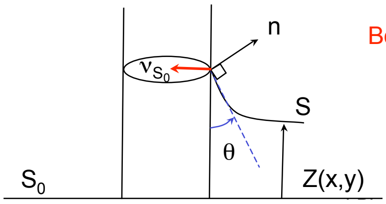
- Generalized Laplace's equation (Vennat *et al.*, 2010 and Finn, 2001)

$$\frac{\rho g Z}{\gamma_m} = div_S n(Z)$$

$$\int_{S_0} \left(\frac{\rho g}{\gamma_m} Z w - \frac{1}{a}(\nabla_{S_0} w, \nabla_{S_0} Z)\right) dS_0 = \int_{\partial S_0} w(n, \nu_{S_0}) dl_0$$

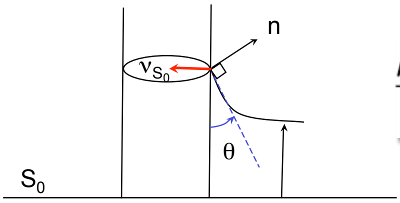
Boundary conditions



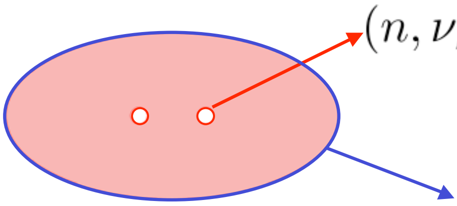


2.1 Capillary rise in a vertical cylinder array

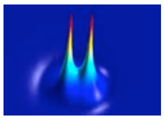
- Boundary conditions



$$\frac{\rho g Z}{\gamma m} = div_S n(Z)$$



$$(n, \nu_{S_0}) = -cos\theta$$



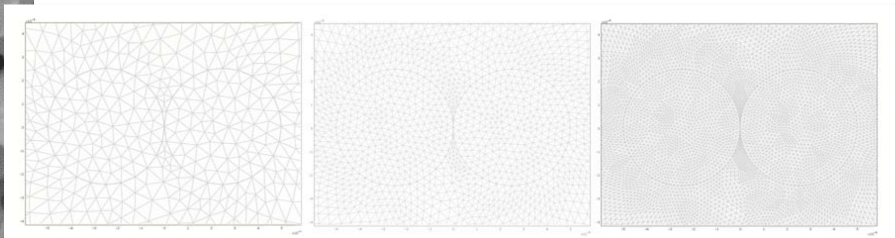
$$(n, \nu_{S_0}) = 0$$

This external boundary is chosen to be sufficiently far from the cylinders to have no influence on the height of rise

2.1 Capillary rise in a vertical cylinder array

- Generalized Laplace's equation
- Two touching cylinders
  - Theoretical height of rise h : « infinity »

$$\frac{\rho g Z}{\gamma m} = div_S n(Z)$$



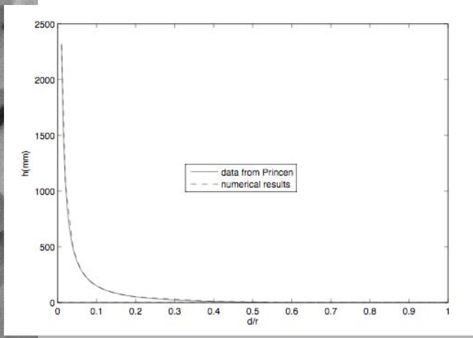
h=6m h=29m h=127m

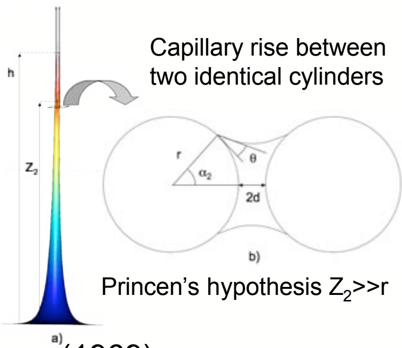
- Diverging computational height of rise h : OK

2.1 Capillary rise in a vertical cylinder array

$$\frac{\rho g Z}{\gamma_m} = div_S n(Z)$$

- Generalized Laplace's equation
- Comparison with the theoretical study of Princen (1969)



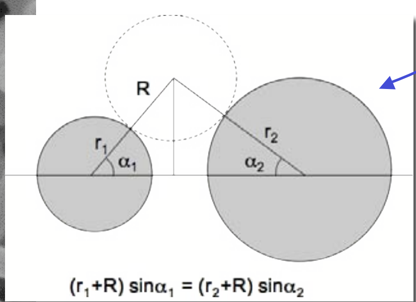


- In agreement with Princen (1969)
- No hypothesis on Z_2

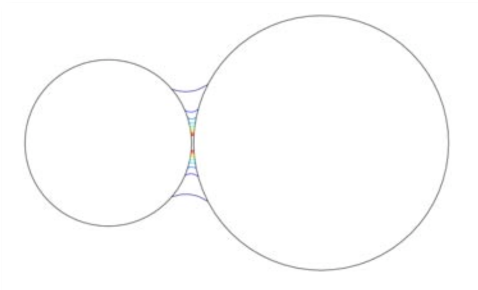
2.1 Capillary rise in a vertical cylinder array

$$\frac{\rho g Z}{\gamma_m} = div_S n(Z)$$

- Generalized Laplace's equation
- Comparison with the study of Liu et al. (2007)
  - No agreement because of a doubtful geometrical hypothesis
  - Agreement between numerical and theoretical study if this hypothesis is replaced by



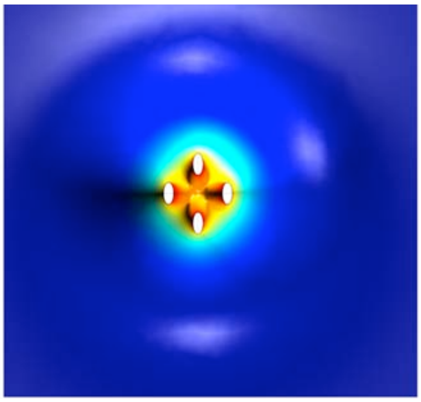
Additional geometrical condition to the theoretical study



Z Isovalues between cylinders of different diameters obtained numerically

2.1 Capillary rise in a vertical cylinder array

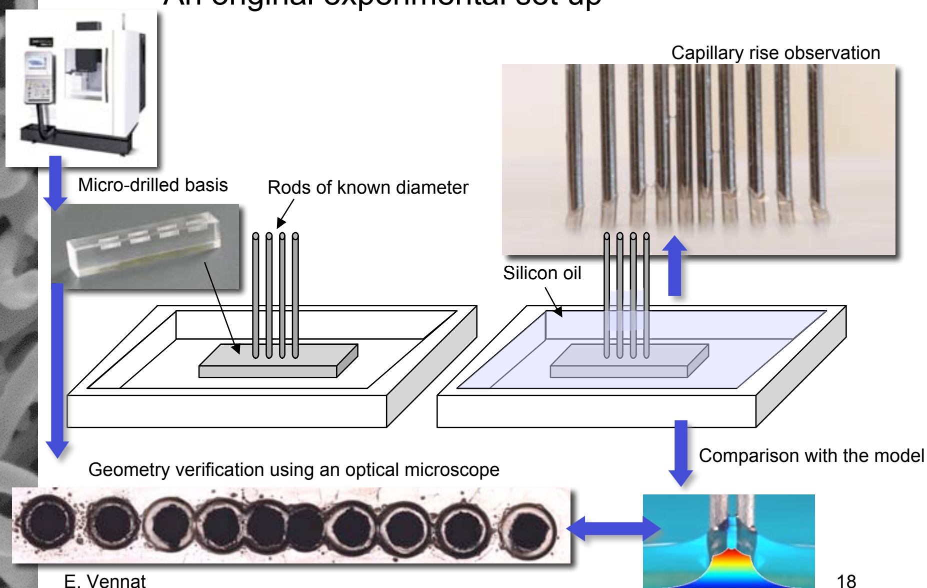
- Solving the generalized Laplace's equation allows:
  - To overcome the limitation $Z_2 >> r$
  - To consider any cylinder cross section (not only circular)



Example of capillary rise in a ellipse based cylinder array

2.1 Capillary rise in a vertical cylinder array

- An original experimental set up



2.2 Capillary front in a more complex geometry

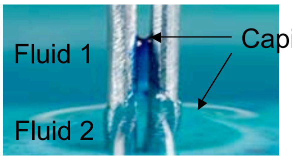
- Modified Navier-Stokes equations and Level Set Method coupling

Navier Stokes equation

Capillarity give rise to a new term

$$\rho a = Div\sigma + f_v + F_{cap}$$

Surface tension term

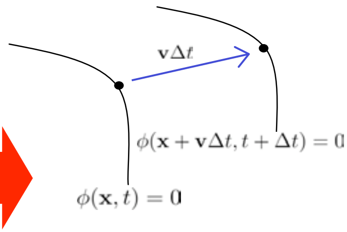


Brackbill (1992)

Coupling through v

Level Set Method to track the front defined as an isovalue of ϕ

$$\begin{cases} \frac{\partial \phi}{\partial t} + (\mathbf{v}.\nabla)\phi = 0 \\ \phi(\mathbf{x}, t) = 0 \end{cases}$$



Sethian (1996)

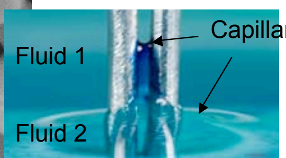
2.2 Capillary front in a more complex geometry

- Virtual power principle

Surface term taking into account capillary effects

$$\int_V (\rho(a-g), u)dV + \int_V Tr(\sigma Du)dV = \int_S (Div_S \sigma_m, u)dS$$

hypothesis $\sigma_m = \gamma_m I_S$



$$= -\int_S \gamma_m (div_S n, u_n)dS$$

$$= -\int_S \gamma_m (div u - (Du(n), n))dS - \int_{\partial S} \gamma_m (u, \nu)dl$$

Vennat et al. (2010)

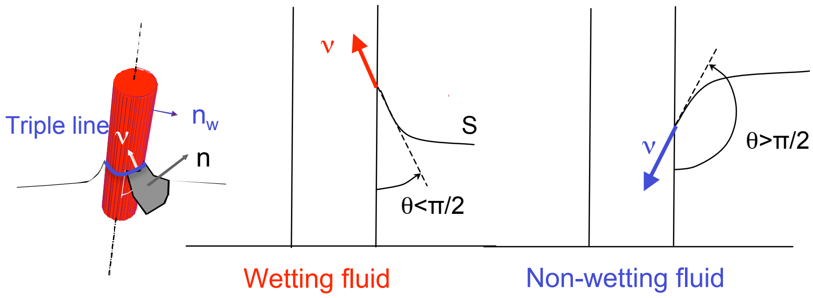
2.2 Capillary front in a more complex geometry

- Boundary condition on the triple line
  - Fixed contact angle θ

$$\int_{\partial S} \gamma m(\nu, u) dl = \int_{\partial S} \gamma m\left(\frac{n_w - n\cos\theta}{|n_w - n\cos\theta|}, u\right) dl$$

$|\sin\theta|$

  - Thus the capillary membrane is pulled down or up depending on ν



Wetting fluid
example: dental resin

Non-wetting fluid
example: mercury

Vennat et al. (2010)

2.2 Capillary front in a more complex geometry

- Previous equations allow to compute the capillary front:
  - In any complex geometry
  - Capillarity is taken into account (additional term in Navier Stokes equations)
  - Either wetting or non-wetting fluid can be considered

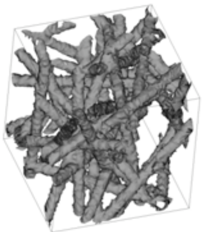
3

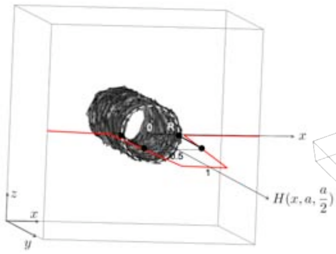
- Equations solved using FE method (Comsol)
  - 3.1 Validation through porosimetry test modeling
  - 3.2 Practical conclusion in the restorative dentistry field

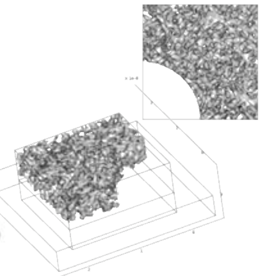
3

Demineralized dentin modeling

- FE modeling using COMSOL
- Geometrical modeling of demineralized dentin
  - Collagen fibers: cylinders (diameter 100nm)
  - Isotropic fiber distribution
  - Fiber network porosity: 55%
  - Materialization of the fibers using their characteristic function H and specific boundary conditions on the triple line







3

Demineralized dentin modeling

- FE modeling using COMSOL
- Geometrical modeling of demineralized dentin
  - Materialization of the fibers using their characteristic function H and the boundary conditions on the triple line

$$= -\int_S \gamma_m(\xcancel{div\, u} - (Du(n),n))\,dS - \int_{\partial S} \gamma_m(u,\nu)\,dl$$

Second part of weak formulation presented slide 15

Capillary membrane surface defined by the isovalue of ϕ

$$\int_{R^3} \gamma_m(Du(n),n)\delta(\phi)\,|\nabla\phi|\,dV$$

Osher. (2004)

Triple line

$$\int_{R^3} \gamma_m(u,\nu)\,|\nabla\phi \wedge \nabla H|\,\delta(\phi)\delta(H)dV$$

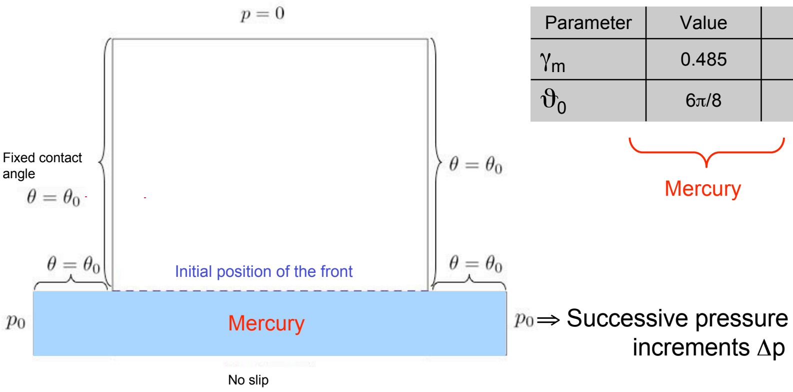
Burchard et al. (2001)

ν: $\frac{n_w - n cos\theta}{|sin\theta|}$ $|\nabla\phi \wedge \nabla H|$: $|\nabla\phi|\,|\nabla H|\,|sin\theta|$

$$\int_{R^3} \gamma_m(u, n_w - n cos\theta)\delta(\phi)\delta(H)\,|\nabla\phi|\,|\nabla H|\,dV$$

3.1 Porosimetry test modeling

- Qualitative simulation of the porosimetry test
  - Thin 3D model

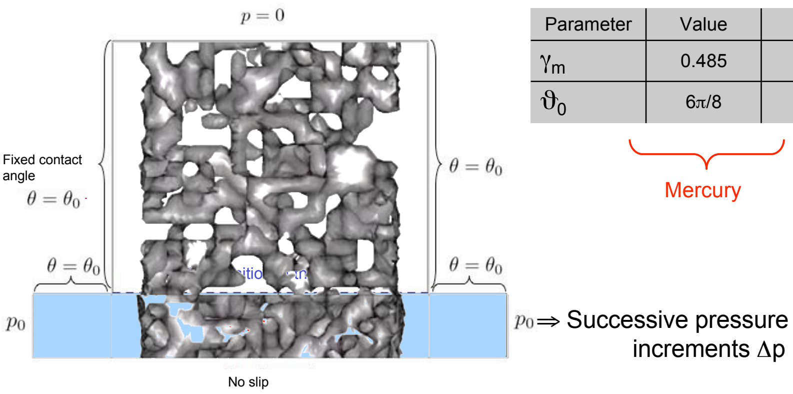


Parameter	Value	Unity
γ_m	0.485	N/m
ϑ_0	6π/8	rad

Mercury

3.1 Porosimetry test modeling

- Qualitative simulation of the porosimetry test
  - Thin 3D model



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Mercury

3.1

Porosimetry test modeling

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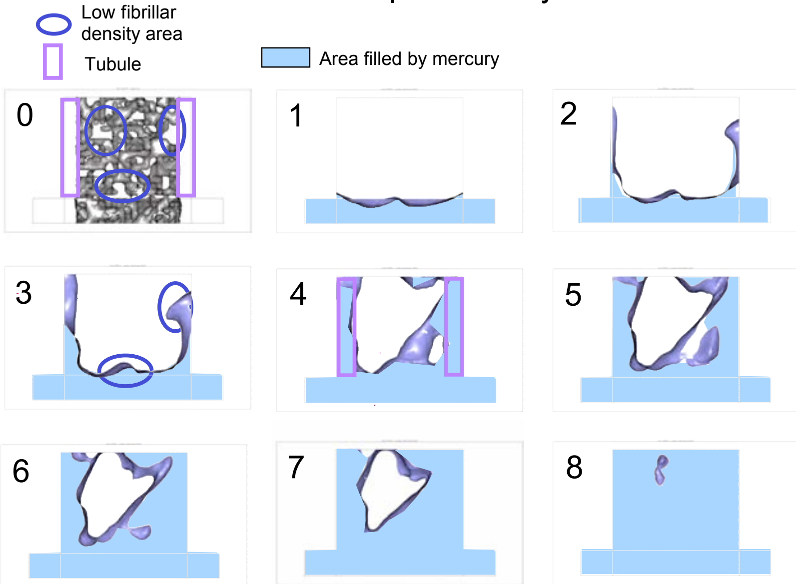
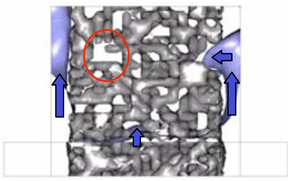


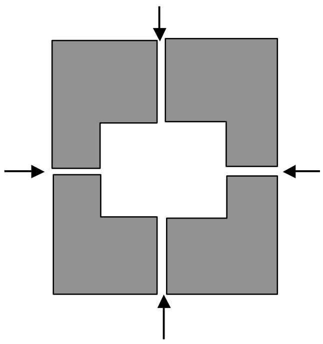
Vennat et al., accepted in CMBBE

3.1

Porosimetry test modeling

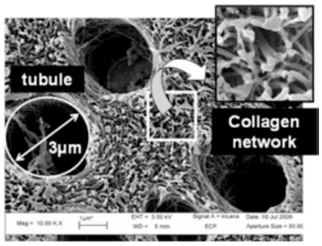
- Relevant qualitative simulation
  - Large pores are infiltrated first:
    - Tubules
    - Large interfibrillar spaces non-separated by a throat
  - Porosimetry limitation illustrated :
    - Small pores are overestimated

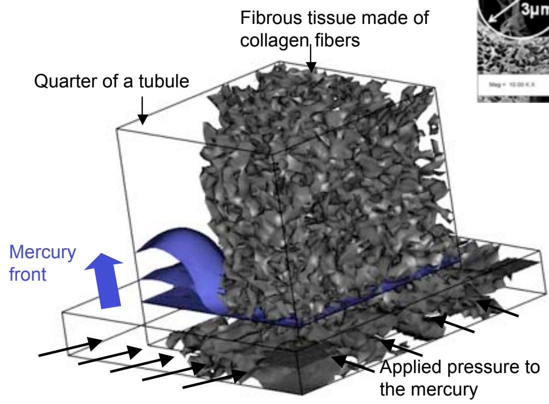




3.1 Porosimetry test modeling

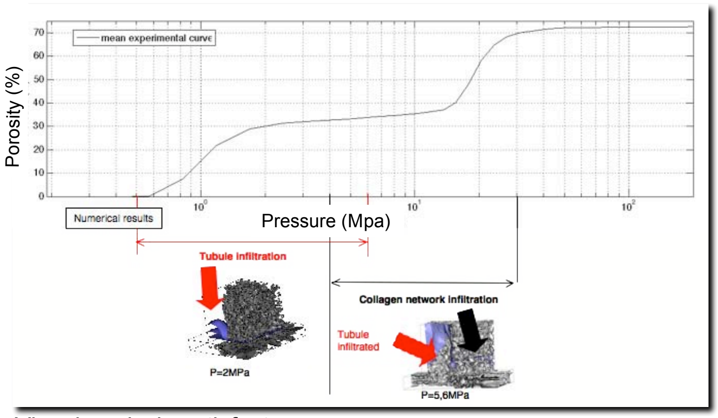
- Three dimensional modeling





3.1 Porosimetry test modeling

- Three dimension modeling
  - 0,3MPa (D=2microns) : tubule penetration
  - 3MPa (200nm) - 10MPa (70nm) : fibrous tissue penetration



Vennat et al., accepted in CMBBE

- Visual analysis satisfactory
- Pore sizes not so easy to distinguish

3.2

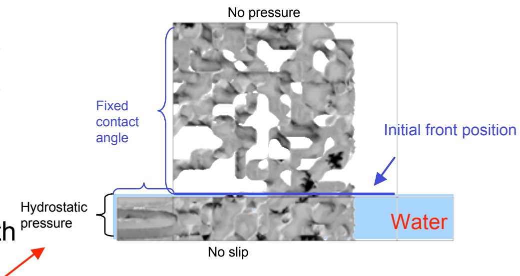
Wetting fluid infiltration

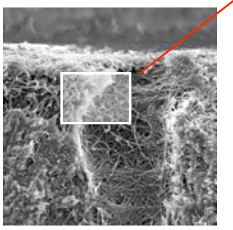
- Wetting liquid penetration in demineralized dentin

Parameter	Value	Unity
γ_m	0.073	N/m
ϑ_0	$3\pi/8$	rad

≈ Water

- Geometry in accordance with SEM images





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Wetting fluid infiltration

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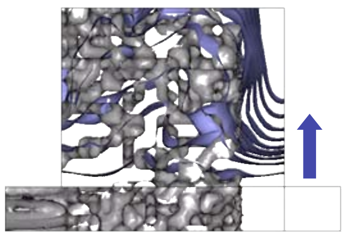
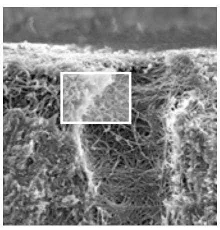


- interfibrillar spaces infiltration
- **Then** tubule penetration



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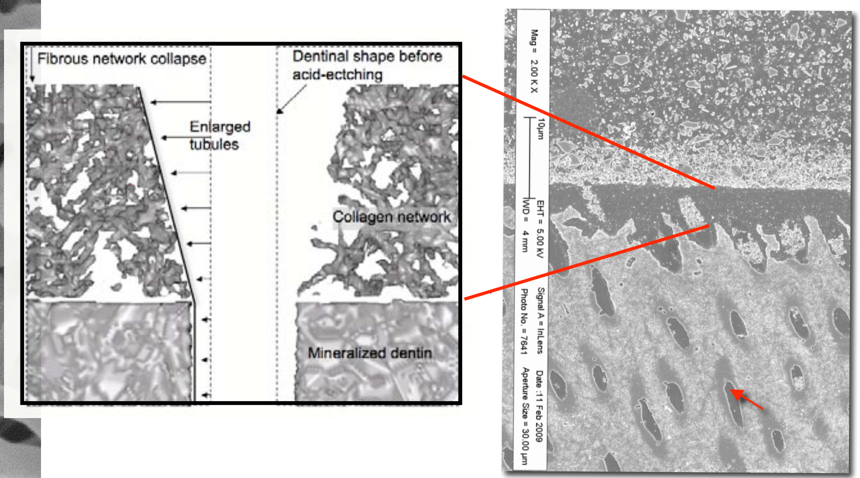
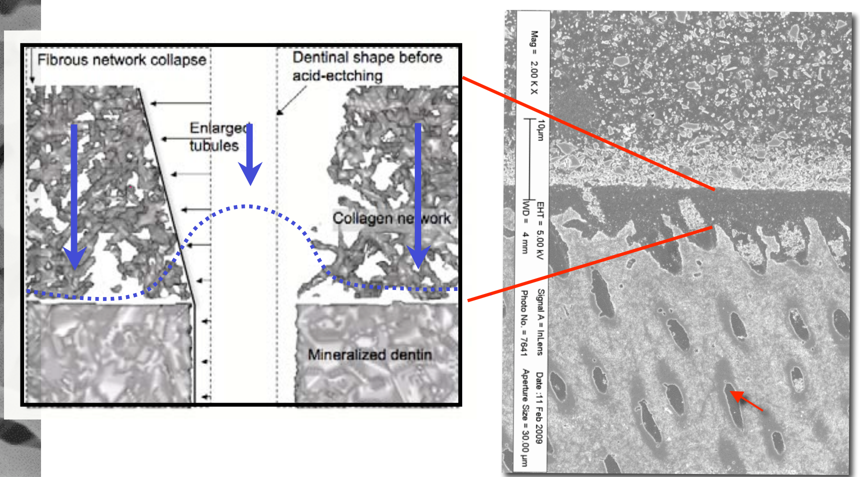
- Wetting liquid penetration in demineralized dentin



3.2 Wetting fluid infiltration

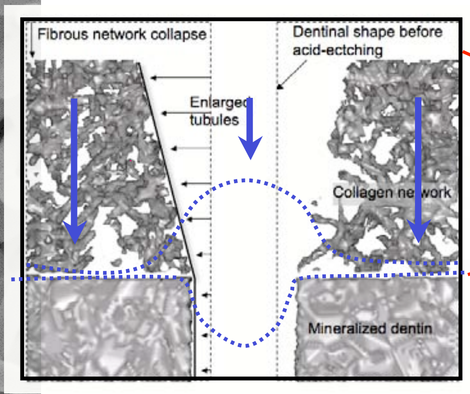
- Wetting liquid penetration in demineralized dentin

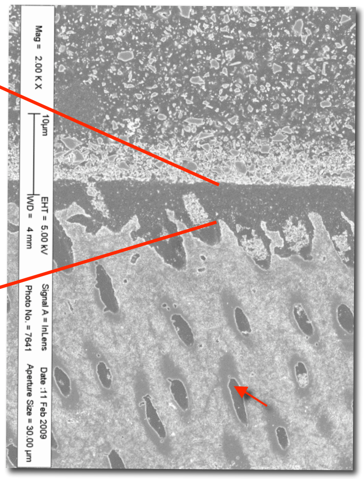


3.2

Wetting fluid infiltration

- Wetting liquid penetration in demineralized dentin



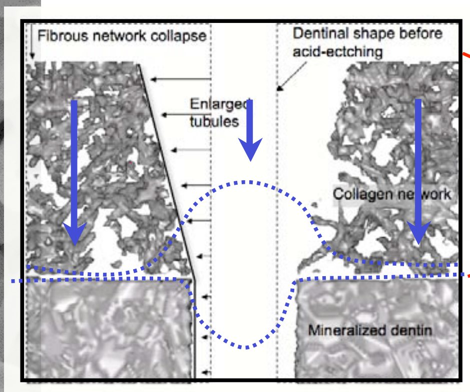


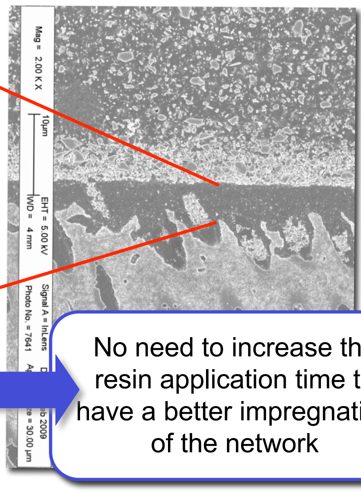
Vennat et al., accepted in CMBBE

3.2

Wetting fluid infiltration

- Wetting liquid penetration in demineralized dentin





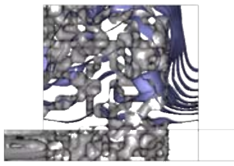
No need to increase the resin application time to have a better impregnation of the network

Conclusion

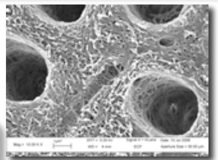
Data for the model :
Total porosity 70%
Fiber network porosity 55%
Two distinct pore sizes

1 Porosimetry tests and SEM observation

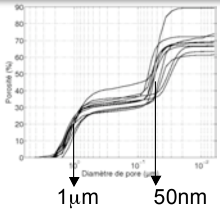
2 Infiltration model:
- vertical fibers
- general fibrous tissue



Model validation and porosimetry test better understanding



3 Applications:
- Porosimetry test
- Demineralized dentin infiltration



Comparison
Pore sizes OK
But hard to distinguish on a graph

Contribution:
Educational tool
3D simulation

Future work

- Taking into account fiber deformation : elasto-capillarity
  - Experimental and computational studies