Approches analytiques pour la mise au point de nouvelles bornes de conductivité thermique effective dans les matériaux composites et pour le suivi de la corrosion en milieu marin.

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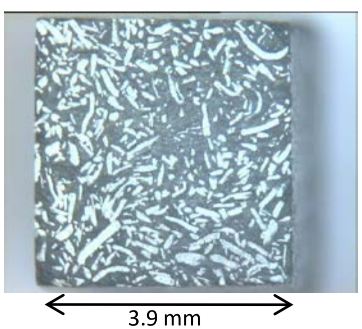
LTeN Nantes

✓ Context and objective : thermally conducting filled polymers

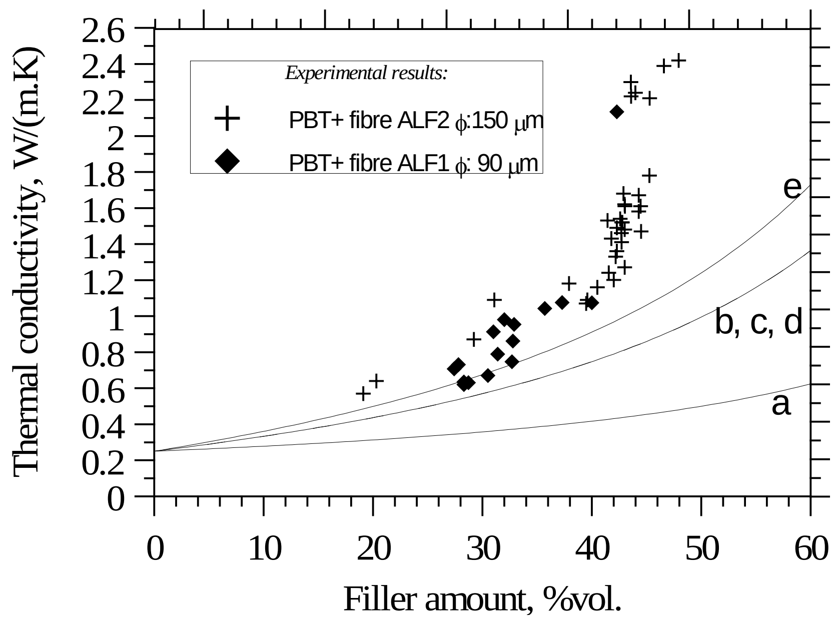
-heterogeneous materials with at least two phases (a continuous insulating one, disperse conducting phase)

- Comparison effective models/ experimental data

- Need for more accurate effective models



PBT+40%vol. al. Fiber
$\phi_{aver.}$=150µm [Dupuis 2003]



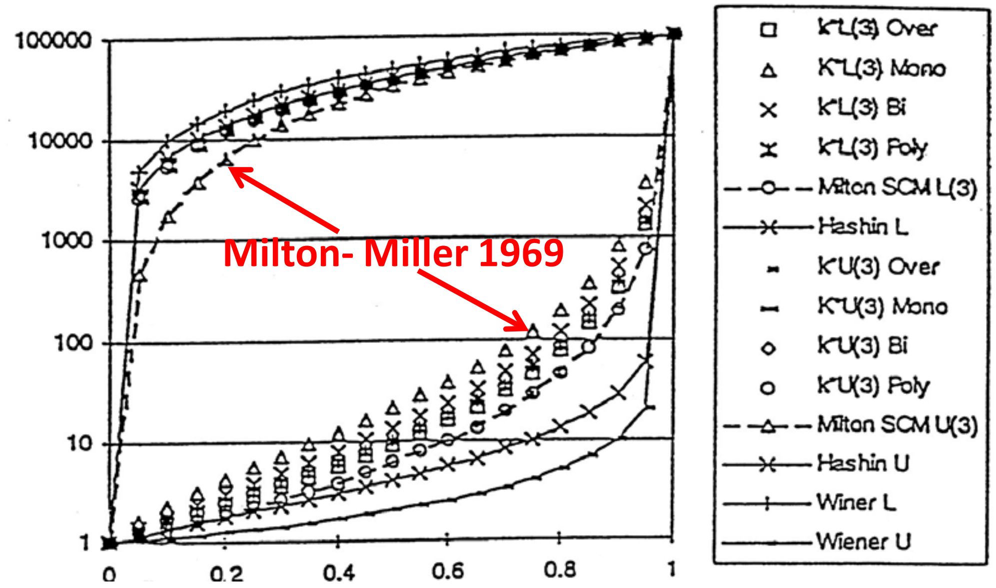
Models:

- a: Wiener 1912
- b: Hatta et Taya 1985
- c: Maxwell-Eucken 1932
- d: Nielsen 1974
- e: Hashin et Shtrikman 1962

→Use of analytical models with lower and upper bounds

$E = \lambda_{eff} / \lambda_m$

eff: effective
m: matrix



volumic filler amount

Figure 1 : Comparison between various Effective Thermal Conductivity models with lower and upper bounds (Decarlis 1998)

✓ Main features of the adopted models

- the stationary heat conduction equation

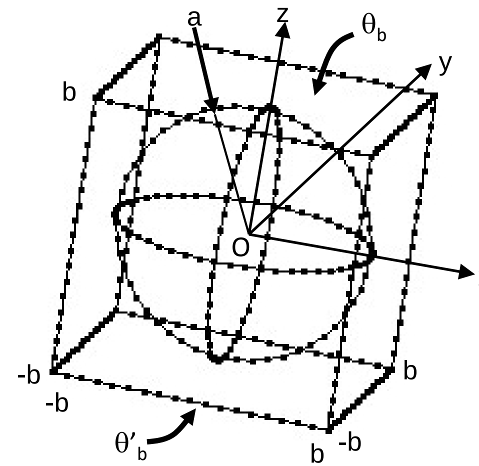
-a tetragonal lattice of spherical inclusions of equal size

- a thermal contact resistance between inclusion and matrix

- adiabatic conditions for all faces except the top and bottom ones (i.e. for z=-b and z=b)

- elementary cell:

sphere of radius *a* centered in
a tetragonal cell of dimensions: 2*b* x 2*b* x 2*b*



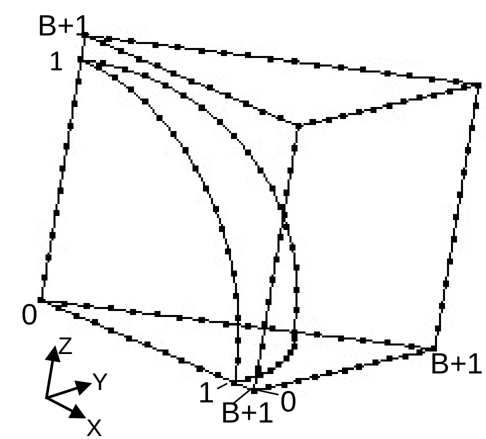
$E = \lambda_{eff} / \lambda_m$ with:

- $B = b/a - 1$
- $C = R_c \cdot \lambda_m / a$
- $D = \lambda_m / \lambda_f$

Vol. amount:

$$\varphi = \frac{\pi}{6 \cdot (1+B)^3}$$

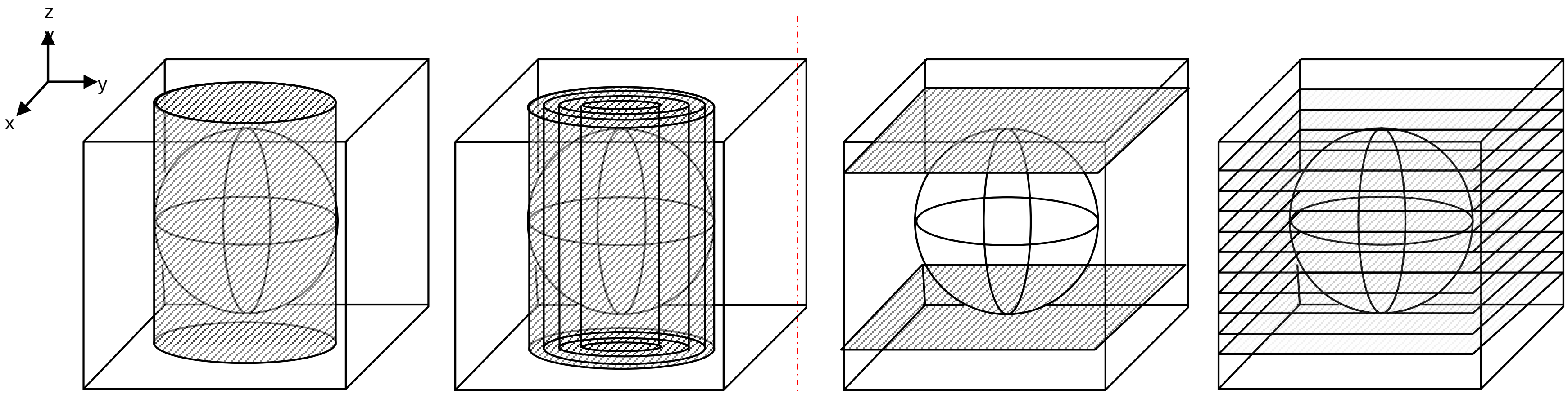
→ $E = E(B, C, D)$



eff: effective
m: matrix
f: filler

✓ New bounds by inserting insulating and equipotential surfaces

z is the main heat flux direction

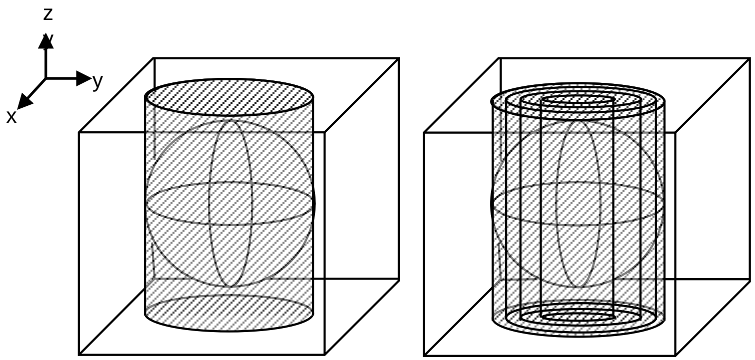


(1a) : E_{W1a} (1b) : $E_{W\infty a}$ (1c) : E_{W1b} (1d) : $E_{W\infty b}$

→ Lower bounds → Upper bounds

Fig. 1. Four geometric models with inserted adiabatic wall(s) (E_{W1a} and $E_{W\infty a}$) or isothermal plane (E_{W1b} and $E_{W\infty b}$)

✓ **New bounds by inserting insulating surfaces** → $E = \lambda_{eff} / \lambda_m$?



(1a) : E_{W1a} (1b) : $E_{W\infty a}$

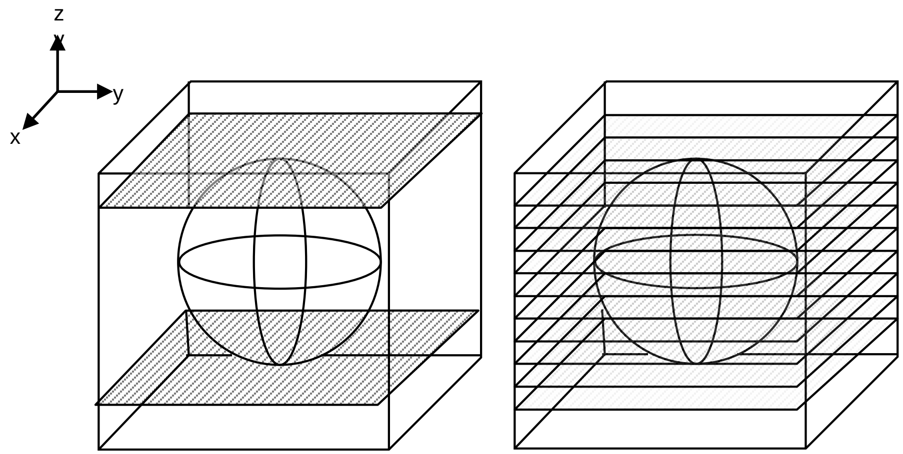
$$E_{w1a} = 1 + (\pi/4)\cdot(E_{II}\cdot - 1)/(1+B)^2$$

$$E_{w\infty a}(B, C, D) = 1 - \frac{\pi}{2\cdot(B+1)^2}\cdot\left[\frac{1}{2}+\frac{1}{1-G}+\frac{\ln G}{(1-G)^2}\right]$$

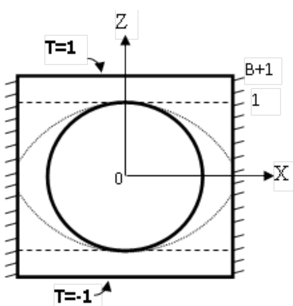
E_{II} : computed using FE

With : $G \equiv \frac{B+C+D}{B+1}$

✓ **New bounds by inserting isothermal surfaces** → $E = \lambda_{eff} / \lambda_m$?



(1c) : E_{W1b} (1d) : $E_{W\infty b}$



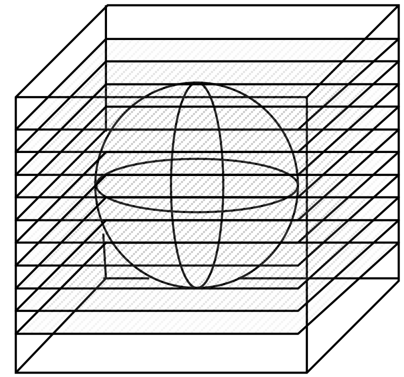
$E_{w1,b}(B, C, D) = (B + 1) / (B + 1 / E_{1,bot})$

ODE system ?

$E_{1,bot}(B, C, D)$ computed using FE
Sphere diam.: 2a
Cell: 2a(1+B) *2a(1+B) *2a

ODE system?

$\rightarrow E = \lambda_{eff} / \lambda_m$?

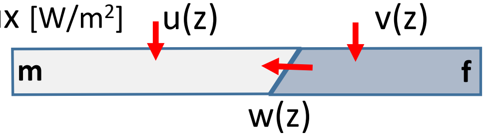


(1d) : $E_{W\infty b}$

Between z and z+dz

z

Temp. $\tau(z)$ Heat flux [W/m²] $u(z)$



Temp. $\sigma(z)$ Heat flux [W/m²] $v(z)$

[W] $dq_c = w\, d(2\cdot\pi\cdot a\cdot z) = [(\tau - \sigma)/ r_c]\cdot d(2\cdot\pi\cdot a\cdot z)$

$dq_f = [\pi\cdot(a^2 - z^2)]\cdot dv - v\cdot[2\cdot\pi\cdot z]\cdot dz$

$dq_m = [(4\cdot b^2 - \pi\cdot(a^2 - z^2)]\cdot du + u\cdot[2\cdot\pi\cdot z]\cdot dz$

Since : $-dq_c = dq_m$ and $dq_f = dq_c$

we have :

$$\begin{cases} [\pi\cdot(a^2 - z^2)]\cdot dv/ dz = v\cdot[2\cdot\pi\cdot z] + \dfrac{2\cdot\pi\cdot a\cdot(\tau-\sigma)}{r_c} \\ [4\cdot b^2 - \pi\cdot(a^2 - z^2)]\cdot du/ dz = -u\cdot[2\cdot\pi\cdot z] + \dfrac{2\cdot\pi\cdot a\cdot(\tau-\sigma)}{r_c} \end{cases}$$

Dimensionless system

$Z \equiv z/ a$

$S \equiv (\sigma - \theta_e)/ (\theta_b - \theta_e)$

$T \equiv (\tau - \theta_e)/ (\theta_b - \theta_e)$

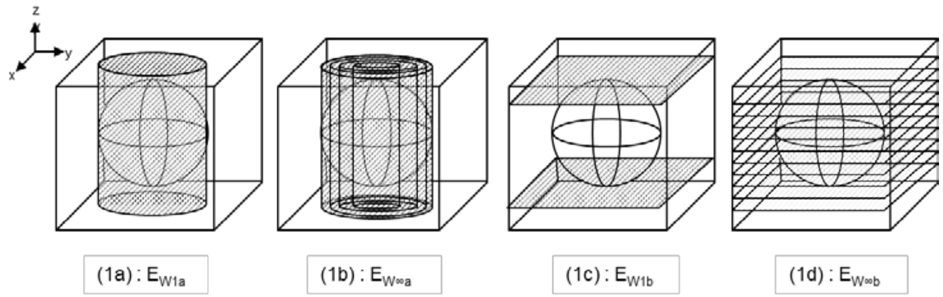
$V = (-v\cdot a\cdot B/\lambda_m\cdot - \tau + \theta_e)/ (\theta_b - \theta_e)$

$U = (-u\cdot a\cdot B/\lambda_m\cdot - \tau + \theta_e)/ (\theta_b - \theta_e)$

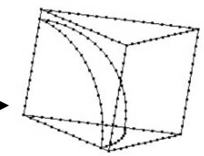
$$\begin{cases} B\cdot\left(\dfrac{2\cdot(1+B)^2}{\pi} - \dfrac{1-Z^2}{2}\right)\cdot\dfrac{dU}{dZ} = \left(\dfrac{2\cdot(1+B)^2}{\pi} - \dfrac{1-Z^2}{2} - B\cdot Z\right)\cdot(U - T) + B^2\cdot\dfrac{T-S}{C} \\ B\cdot\left(\dfrac{1-Z^2}{2}\right)\cdot\dfrac{dV}{dZ} = \left(\dfrac{1-Z^2}{2}\right)\cdot(U - T) + B\cdot Z\cdot(V - T) - B^2\cdot\dfrac{T-S}{C} \\ Z=0,\ S=0;\quad Z=0,\ T=0;\quad Z=1, U = 1;\quad Z=1,\ V = 1 \end{cases}$$

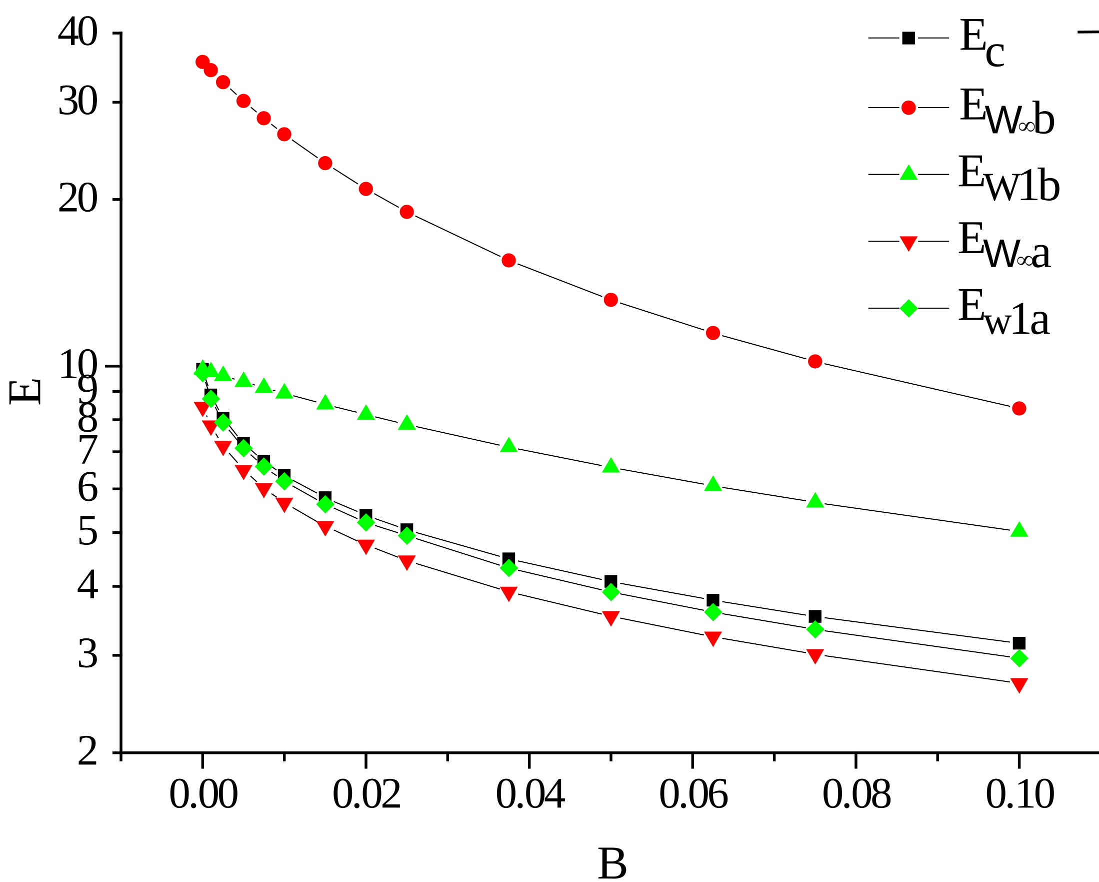
0/ 0 indetermination

$E = (1 + 1/ B)\cdot(1 - T_{Z=1})$ ← L. Shampine 2003, Singular boundary value problem for ODEs



Full FE





C =0.001 D = 0.001.

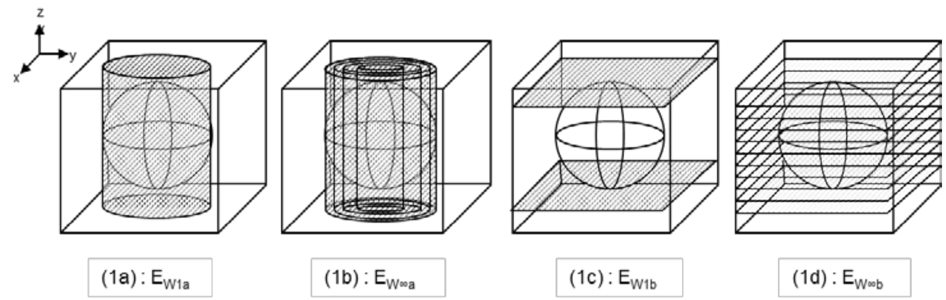


Table 1 Global features of the bound deviations

$$\varepsilon_{X/c} \equiv 100 \ln(E_X / E_c).$$

Bound model			logarithmic deviation ε,%		
Name	symbol	proposed by	average	min	max
Variational - 3rd order, lower	V3L	Torquato & Rintoul	–28	–127	–2
Wall insertion- infin. adiab.long.	W∞a	this work	–13	–45	–6
Wall insertion- single adiab. long.	W1a	this work	–3	–6	–1
Wall insertion- infin. isotherm. transv.	W∞b	this work	97	4	332
Variational - 3rd order, upper	V3U	Torquato & Rintoul	368	6	827

Torquato & Rintoul 1995:

$$E_{V3L} = \frac{1}{1-\varphi+\varphi\cdot(D+3\cdot C)-\dfrac{2\cdot\varphi\cdot\{(1-\varphi)\cdot(1-D-C)\cdot(1-D-3\cdot C)+3\cdot C\}^2}{(1-\varphi)\cdot(1-D-C)^2\cdot[3-(1-D)\cdot(2-2\cdot\varphi+\xi)]+3\cdot C\cdot\Phi}}$$

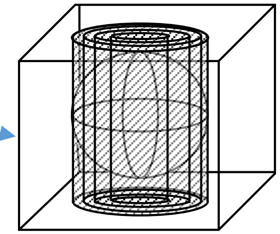
$$\Phi = 1+2\cdot(C+D)^2+\varphi\cdot(1-D-C)\cdot\left\{4\cdot(C+D)+(1-C-D)\cdot\left[\frac{8}{27}+\frac{\varphi\cdot(5+\varphi)}{2}\right]\right\}$$

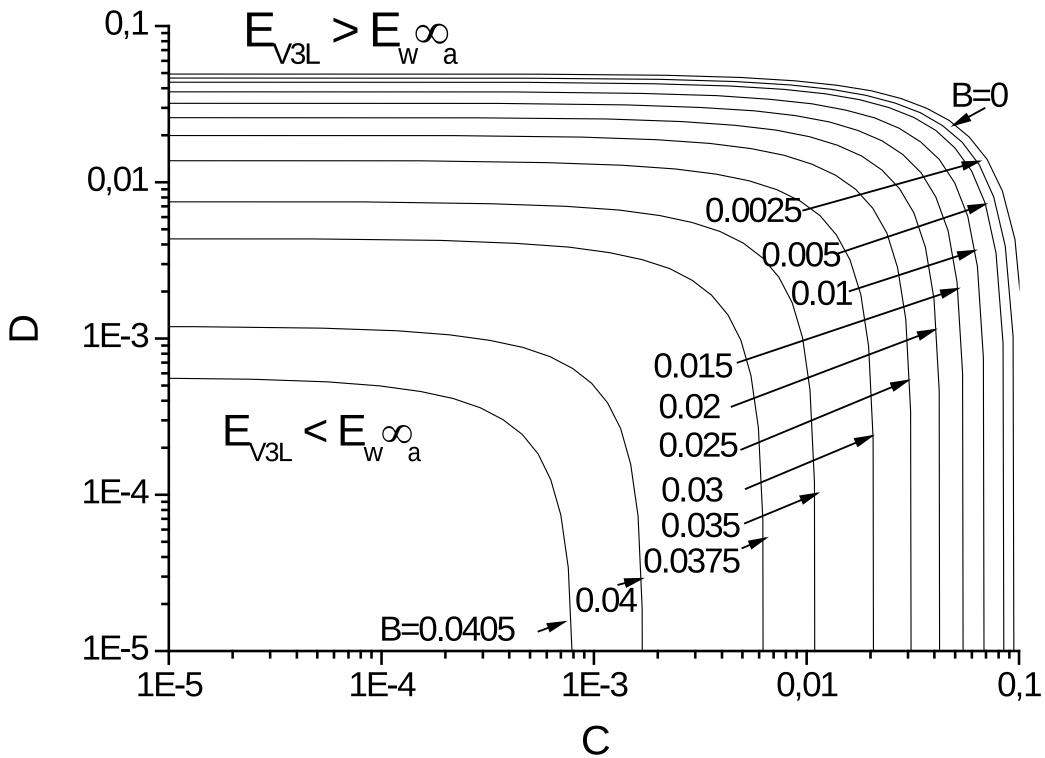
$$E_{V3U} = 1-\varphi+\frac{\varphi}{D}-\frac{\varphi\cdot[(1-\varphi)\cdot(1-D)\cdot(1-D-C)+3\cdot C]^2}{3\cdot(1-\varphi)\cdot D^2\cdot(1-D-C)\cdot(1-D+C)+9\cdot D^2\cdot C\cdot(1+C)+D\cdot(1-D)\cdot\Xi}$$

$$\Xi = [(1-\varphi)\cdot(1-D-C)+3\cdot C]^2+2\cdot(1-\varphi)\cdot\xi\cdot(1-D-C)^2$$

Preference map: V3L-model vs W∞a

Torquato &Rintoul





V3L-model tighter lower bound for

- for C≥0.1081 , whatever are the values of B and D; or,
- for D≥0.0496 , whatever are the values of B and C.

For more: **Danes F., Garnier B. IJHMT 2011**

Et pour la corrosion….

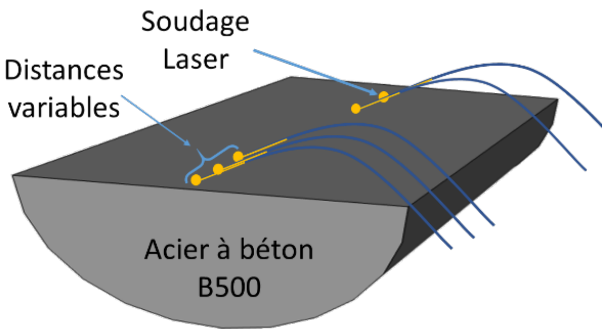
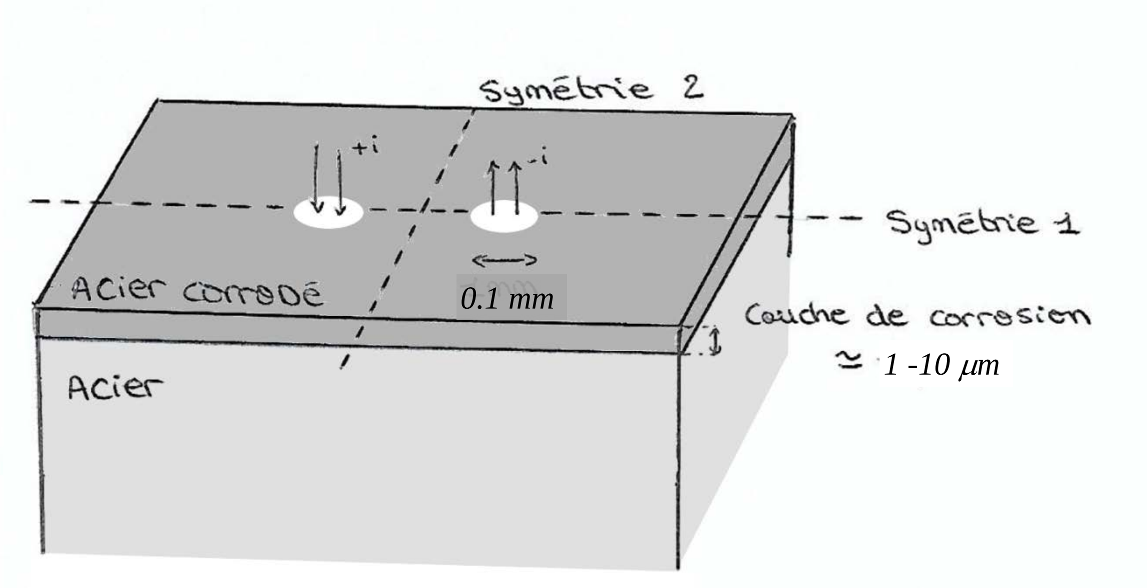
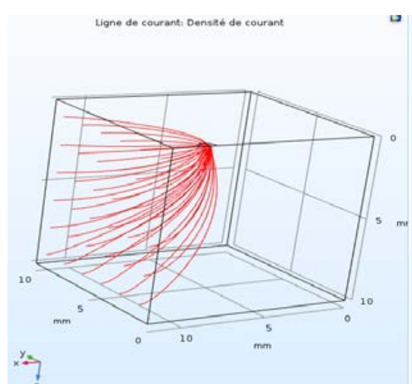


Fig. 1. Echantillon instrumenté

Fig. 2. Banc thermique 3ω et échantillon SYSCORR

Fig. 3. a) Système de marnage accéléré du GeM, (b) des échantillons avant et (c) après un mois d'exposition


Symétrie 2
+i
-i
Symétrie 1
Acier corrodé
0.1 mm
Couche de corrosion
≃ 1 -10 μm
Acier


Ligne de courant: Densité de courant
mm