

## SSNP 160 – Hydrogen diffusion in an elastoplastic steel

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### Summary:

This test of nonlinear quasi-static mechanics simulates the hydrogen diffusion in a homogeneous volume of steel according to the plastic deformations.

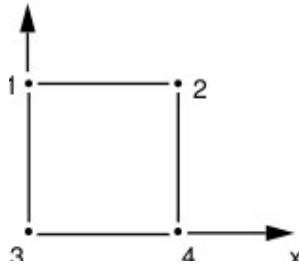
Modeling A is carried out with elements plans (mechanical modeling C\_PLAN, thermal modeling PLAN\_DIAG).

Modeling A is carried out with elements 3D (modeling mechanical 3D, thermal modeling 3D\_DIAG).

## 1 Problem of reference

### 1.1 Geometry

The homogeneous solution is obtained on an element of plan volume (square on side 1) or 3D (cubic on side 1). Dimensions are without influence on the solution.



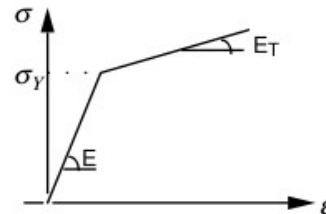
### 1.2 Properties of materials

$$E = 2.10^7 \text{ Pa}$$

$$\nu = 0.3$$

$$\sigma_y = 2.10^8 \text{ Pa}$$

$$E_T = 2.10^9 \text{ Pa}$$



For the diffusion, the coefficients material are, for a temperature of  $T = 293 \text{ K}$  :

$$D_L = 1.27 \cdot 10^{-8}$$

$$N_L = 5.1 \cdot 10^{29} \text{ m}^{-3}$$

$$K_T = e^{60000./RT}$$

$$a_1 = 23.26 \quad a_2 = -2.33 \quad a_3 = -5.5$$

$$V_h = 2.e-6 \quad R = 8.3144 \text{ J/mol/K}$$

### 1.3 Boundary conditions and loadings

Side 1-3 :  $F_x$  imposed

Side 2-4 :  $u_x = 0$ .

Not 2 :  $u_y = 0$ .

Loading by a force distributed  $F_x$  increasing according to time:

Moment ( s )	0	$10^7$	$2.10^7$
Force $F_x$	0	$\sigma_y$	$3\sigma_y$

Temporal discretization:

- 1 pas until  $t = 10^7$
- 100 pas until  $t = 2.10^7$  : for each step, a mechanical calculation then a calculation of diffusion.

Initial concentrations in H2 :

- In the crystal lattice ("lattice")  $C_L(0) = 2.08 \cdot 10^{21} \text{ m}^{-3}$

- In the traps ("traps")  $C_T(0) = 8.42 \cdot 10^{20} m^{-3}$

## 2 Reference solution

### 2.1 Method of calculating used for the reference solution

In the document [1], a model of diffusion of the hydrogen atoms in steels is proposed. He considers two types of concentration of the hydrogen atoms:

- $C_L$  is the concentration in the crystal lattice (Lattice)
- $C_T$  is the concentration in the "traps" or gaps (Traps)

Without taking again here all the approach followed by the authors of [1], the formulation suggested for the equation of diffusion of  $C_L$  is:

$$\frac{C_L + C_T(1 - \theta_T)}{C_L} \frac{\partial C_L}{\partial t} - \nabla \cdot (D_L \nabla C_L) + \nabla \cdot \left( \frac{D_L C_L V_H}{RT} \nabla \sigma_H \right) + \theta_T \frac{d N_T}{d \varepsilon_{eq}^p} \frac{d \varepsilon_{eq}^p}{dt} = 0 \quad \text{eq1}$$

It is thus noted that the equation of diffusion takes account of the local gradient of the trace of the constraints (forced hydrostatic  $\sigma_H = 1/3 \text{tr}(\sigma)$ ) and of the equivalent plastic deformation of Von Mises.

The relations defining the various quantities are:

$\theta_L = \frac{C_L}{N_L}$  is the occupancy rate of the sites of the crystal lattice, with  $N_T$  the number of sites per unit of volume.  $N_L$  is a constant estimated at  $N_L = 5,1 \cdot 10^{29} \text{ m}^{-3}$  for iron  $\alpha$  in [1].

$\theta_T = \frac{C_T}{N_T}$  is the occupancy rate of the sites of the traps, with  $N_T$  density of the traps, i.e. the number of sites corresponding to traps per unit of volume.

Contrary to  $N_L$  who is a constant,  $N_T$  is function of the plastic deformation according to the expression:  $\log_{10}(N_T) = a_1 - a_2 \exp(-a_3 \varepsilon_{eq}^p)$ , with:  $a_1 = 23.26$ ,  $a_2 = 2,33$ ,  $a_3 = -5,5$  [1].

$D_L = 1,2710^{-8} \text{ m}^2/\text{s}$   $V_H = 210^{-6} \text{ m}^3$  for iron  $\alpha$  with room temperature,  $R = 8,3144 \text{ J/mol/K}$  is the constant of perfect gases, and  $T$  the temperature in  $^\circ \text{K}$ .

It remains to define  $C_T$  according to  $C_L$ : according to [1] with balance, which is the case for the CSC:

$$C_T = \frac{N_T}{1 + \frac{1}{K_T \theta_L}}, \text{ with } K_T = \exp(-\Delta E_T / RT) = 4,9710^{10} \text{ with room temperature, following [1],}$$

while taking  $\Delta E_T = -60 \text{ KJ/mol}$ .

In a way similar to nonlinear thermics, the variational formulation is written then:

That is to say  $\Omega$  open of  $R^3$ , of border  $\Gamma = \Gamma_1 \cup \Gamma_2$ .

One must solve the equation [eq. 1] in  $C_L$  on  $\Omega \times ]0, t[$  with the boundary conditions:

$$\begin{cases} C_L = C_L^d & \text{sur } \Gamma_1 \\ \mathbf{J} \cdot \mathbf{n} = \phi & \text{sur } \Gamma_2 \end{cases} \quad \text{éq 3}$$

with  $\mathbf{J} = -D_L \nabla C_L + \frac{D_L V_H}{RT} C_L \nabla \sigma_H$

and with initial conditions  $C_L(t=0)$  (and  $C_T(t=0)$ ).

That is to say  $v$  a sufficiently regular function cancelling itself on  $\Gamma_1$ , the variational formulation of the problem is written:

$$\int_{\Omega} D^*(C_L) \frac{dC_L}{dt} v d\Omega + \int_{\Omega} D_L \nabla C_L \cdot \nabla v d\Omega - \int_{\Omega} \nabla \mathbf{v} \cdot \left( \frac{D_L C_L V_H}{RT} \nabla \sigma_H \right) d\Omega = \int_{\Omega} r_{vol} v d\Omega + \int_{\Gamma_2} \phi v d\Gamma_2 \quad \text{éq 4}$$

with:

$$D^*(C_L) = \frac{C_L + C_T(1 - \theta_T)}{C_L} \quad \phi = \left( D_L \nabla C_L - \frac{D_L V_H}{RT} C_L \nabla \sigma_H \right) \cdot \mathbf{n} \quad \text{and}$$

$$r_{vol} = -\theta_T \frac{dN_T}{d\varepsilon_{eq}^p} \frac{d\varepsilon_{eq}^p}{dt} = 0$$

The digital resolution by finite elements is thus similar to that of nonlinear thermics, and rests on one  $\theta$  - method, modulo two characteristics:

- the source term  $r_{vol}$  is nonlinear, as in the modeling of drying [R7.01.12], and will be integrated explicitly;
- the term  $\int_{\Omega} \nabla \mathbf{v} \cdot \left( \frac{D_L C_L V_H}{RT} \nabla \sigma_H \right) d\Omega$  is nonsymmetrical, and will be also deferred to the second member, as in [1] and will be integrated explicitly.

This explicit discretization of these two terms is not constraining: indeed the resolution of the equation [eq. 4] is carried out with each step of time, chained with a mechanical resolution.

On the other hand the term  $\int_{\Omega} \nabla \mathbf{v} \cdot \left( \frac{D_L C_L V_H}{RT} \nabla \sigma_H \right) d\Omega$  require to apply a variation in

temperature  $\nabla T_{ini}$  presumed uniform in the element. The second calculated elementary member is:  $\int_{\Omega} \nabla T_{ini} K \nabla v d\Omega$  where  $K$  is the tensor of thermal conductivities.

Knowing the initial conditions  $C_L^0 = C_L(t=0)$  and  $C_T^0 = C_T(t=0)$ , one calculates  $C_{tot}^0 = C_L^0 + C_T^0$ .

and one adimensionne the unknown factor (concentration); the variational formulation is then:

$$\int_{\Omega} D^* \frac{dc_L}{dt} v d\Omega + \int_{\Omega} D_L \nabla c_L \cdot \nabla v d\Omega = \int_{\Omega} \nabla \mathbf{v} \cdot \left( \frac{D_L V_H}{RT} c_L \nabla \sigma_H \right) d\Omega + \int_{\Omega} \bar{r}_{vol} v d\Omega + \int_{\Gamma_2} \bar{\phi} v d\Gamma_2$$

with:  $c_L = \frac{C_L}{C_{tot}^0}$   $\bar{r}_{vol} = \frac{-\theta_T}{C_{tot}^0} \frac{d N_T}{d \varepsilon_{eq}^p} \frac{d \varepsilon_{eq}^p}{dt}$  and  $\bar{\phi} = \left( -D_L \nabla c_L + \frac{D_L V_H}{RT} c_L \nabla \sigma_H \right) \cdot \mathbf{n}$

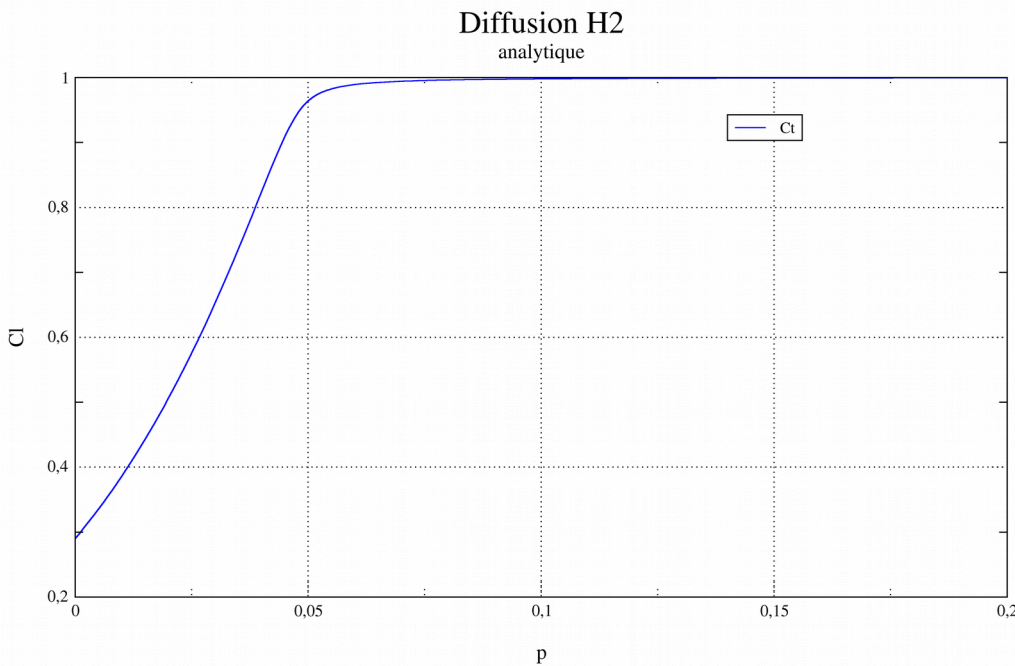
The coefficient of heat capacity  $D^*$  is a field represented by a variable of order (NEUT1) .

In an element of isolated volume ( $\nabla C_L = 0$  on the border) and charged so that the stress and strain state is uniform, total concentration  $C_{tot} = C_l + C_i$  is constant.

The analytical solution described in [1] is obtained directly in the form of the quadratic equation:  $C_T^2 - B C_T + N_T C_{tot} = 0$ , with  $B = N_L / K_T + C_{tot} + N_T$  : one of the two solutions would lead to negative values of  $C_L$ , the solution is thus.  $C_T = 1/2 (B - \sqrt{B^2 - 4 N_T C_{tot}})$

The representation of  $C_T(\varepsilon_{eq}^p)$  and  $C_L(\varepsilon_{eq}^p)$  obtained analytically and numerically in [1] is:

## 2.2 Results of reference



## 2.3 Uncertainty on the solution

Uncertainty lower than 1 % .

## 2.4 Bibliographical references

- 1) "Hydrogen near transport has blunting ace tip" A.H.M. Krom, R.W.J.Koers, A.Bakker in "Newspaper of the Mechanics and Physics of Solids" 45 (1999) 971-992

## 3 Modeling A

### 3.1 Characteristics of modeling A

Mechanics: modeling C\_PLAN  
Thermics: modeling PLAN\_DIAG

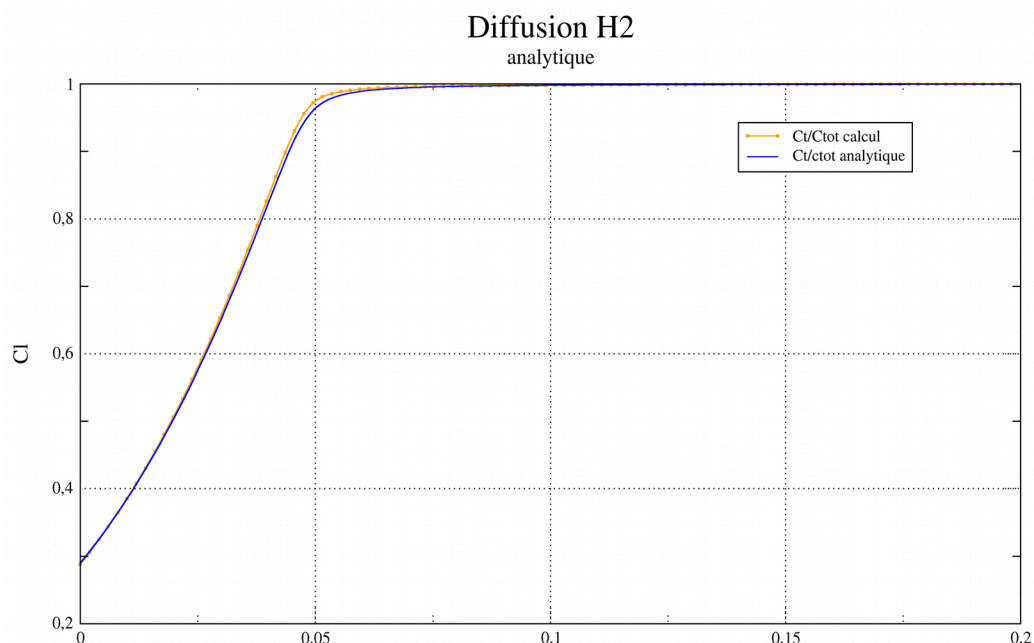
### 3.2 Characteristics of the grid

An element QUAD4 . Many nodes: 4

### 3.3 Sizes tested and results

The analytical solution being obtained according to the plastic deformation, one tests initially this value according to time, then the hydrogen concentration according to time:

Identification	Moment	Reference	Tolerance %
P1	11000000.0	0.0198	0,10%
P1	11500000.0	0.0297	0,10%
P1	12000000.0	0.0396	0,10%
P1	12500000.0	0.0495	0,10%
P1	13000000.0	0.0594	0,10%
P1	15100000.0	0.100980	0,10%
P1	20000000.0	0.1980	0,10%
CT2	11000000.0	0.5058	0,10%
CT2	11500000.0	0.6522	0.3%
CT2	12000000.0	0.8239	0.4%
CT2	12500000.0	0,964	1.0%
CT2	13000000.0	0,989	0.4%
CT2	15100000.0	0.99807	0,10%
CT2	20000000.0	0.999628	0,10%



## 4 Modeling B

### 4.1 Characteristics of modeling B

Mechanics: modeling 3D  
Thermics: modeling 3D\_DIAG

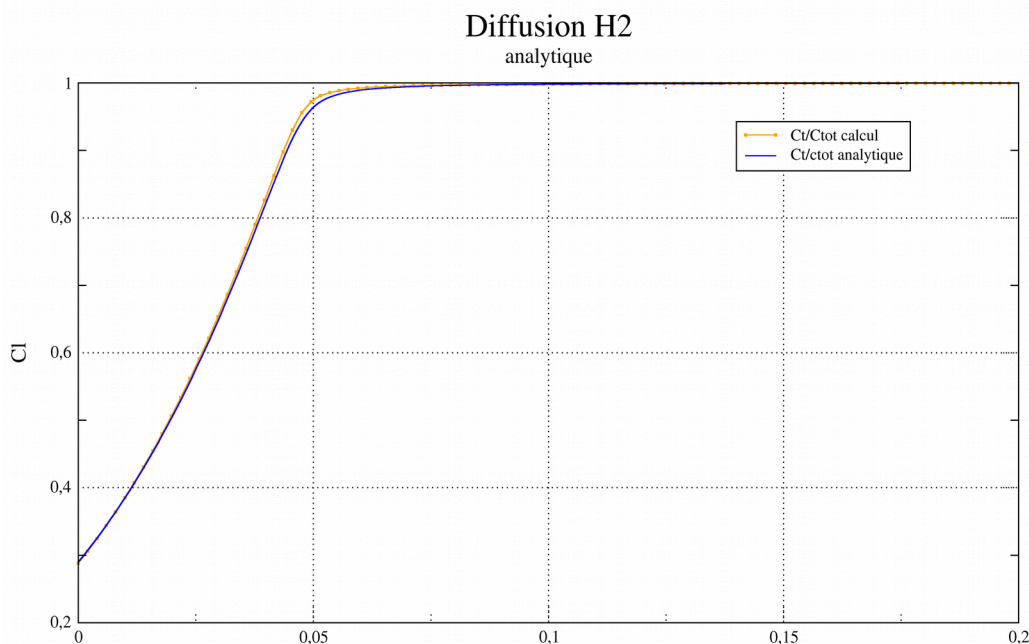
### 4.2 Characteristics of the grid

An element HEXA8. Many nodes: 8

### 4.3 Sizes tested and results

The analytical solution being obtained according to the plastic deformation, one tests initially this value according to time, then the hydrogen concentration according to time:

Identification	Moment	Reference	Tolerance %
P1	11000000.0	0.0198	0,10%
P1	11500000.0	0.0297	0,10%
P1	12000000.0	0.0396	0,10%
P1	12500000.0	0.0495	0,10%
P1	13000000.0	0.0594	0,10%
P1	15100000.0	0.100980	0,10%
P1	20000000.0	0.1980	0,10%
CT2	11000000.0	0.5058	0,10%
CT2	11500000.0	0.6522	0.3%
CT2	12000000.0	0.8239	0.4%
CT2	12500000.0	0,964	1.0%
CT2	13000000.0	0,989	0.4%
CT2	15100000.0	0.99807	0,10%
CT2	20000000.0	0.999628	0,10%





## 5 Summary of the results

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The calculated solution is very close to the analytical and valid solution the methodology of simulation of the hydrogen diffusion in a steel.