# SSNP 160 – Hydrogen diffusion in an elastoplastic steel

**Summary:**

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

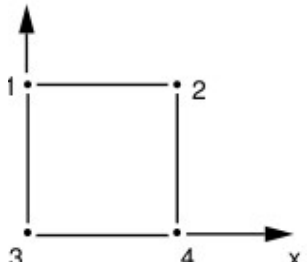
Modeling A is carried out with elements plans (mechanical modeling C_PLAN, thermal modeling PLAN_DIAG).

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

# 1 Problem of reference

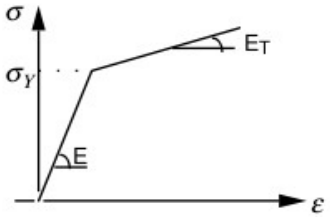
## 1.1 Geometry

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

$E=2.10^{7}\,Pa$
$\nu=0.3$
$\sigma_y=2.10^{8}\,Pa$
$E_T=2.10^{9}\,Pa$




For the diffusion, the coefficients material are, for a temperature of $T=293\,K$ :
$D_L=1.27\,10^{-8}$
$N_L=5.1\,10^{29}\,m^{-3}$
$K_T=e^{60000./RT}$
$a_1=23.26 \quad a_2=-2.33 \quad a_3=-5.5$
$V_h=2.e-6 \quad R=8.3144\,J/mol/K$

## 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”) $C_L(0)=2.08\,10^{21}\,m^{-3}$

- In the traps (“traps”) $C_T(0)=8.42\,10^{20}\,m^{-3}$

# 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:

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

It is thus noted that the equation of diffusion takes account of the local gradient of the trace of the constraints (forced hydrostatic $\sigma_H=1/3tr(\sigma)$ ) 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 $N_L=5{,}1\,10^{29}\,m^{-3}$ 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].

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

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

$C_T=\frac{N_T}{1+\frac{1}{K_T\theta_L}}$ , with $K_T=\exp(-\Delta E_T/RT)=4{,}9710^{10}$ with room temperature, following [1], while taking $\Delta E_T=-60\,KJ/mol$ .

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:

$$\begin{cases} C_L = C_L^d & \text{sur} \quad \Gamma_1 \\ \boldsymbol{J}.\boldsymbol{n} = \phi & \text{sur} \quad \Gamma_2 \end{cases} \qquad \textbf{éq 3}$$

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

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:

$$\int_\Omega D^*(C_L)\frac{dC_L}{dt} v\, d\Omega + \int_\Omega D_L \nabla C_L \cdot \nabla v\, d\Omega - \int_\Omega \nabla \boldsymbol{v} \cdot \left( \frac{D_L C_L V_H}{RT} \nabla \sigma_{\boldsymbol{H}} \right) d\Omega = \int_\Omega r_{vol} v\, d\Omega + \int_{\Gamma_2} \phi v\, d\Gamma_2 \qquad \textbf{éq 4}$$

with:

$D^*(C_L) = \frac{C_L + C_T(1-\theta_T)}{C_L}$ $\phi = \left( D_L \nabla \boldsymbol{C_L} - \frac{D_L V_H}{RT} C_L \nabla \sigma_{\boldsymbol{H}} \right).\boldsymbol{n}$ and

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

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 $\int_\Omega \nabla \boldsymbol{v} \cdot \left( \frac{D_L C_L V_H}{RT} \nabla \sigma_{\boldsymbol{H}} \right) d\Omega$ 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 $\int_\Omega \nabla \boldsymbol{v} \cdot \left( \frac{D_L C_L V_H}{RT} \nabla \sigma_{\boldsymbol{H}} \right) d\Omega$ require to apply a variation in temperature $\nabla \boldsymbol{T_{ini}}$ presumedly uniform in the element. The second calculated elementary member is: $\int_\Omega \nabla \boldsymbol{T_{ini}} K \nabla \boldsymbol{v}\, d\Omega$ 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:

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

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 $\bar{\Phi}=\left(-D_L \nabla \boldsymbol{c_L}+\frac{D_L V_H}{R T} c_L \nabla \boldsymbol{\sigma_H}\right).\boldsymbol{n}$

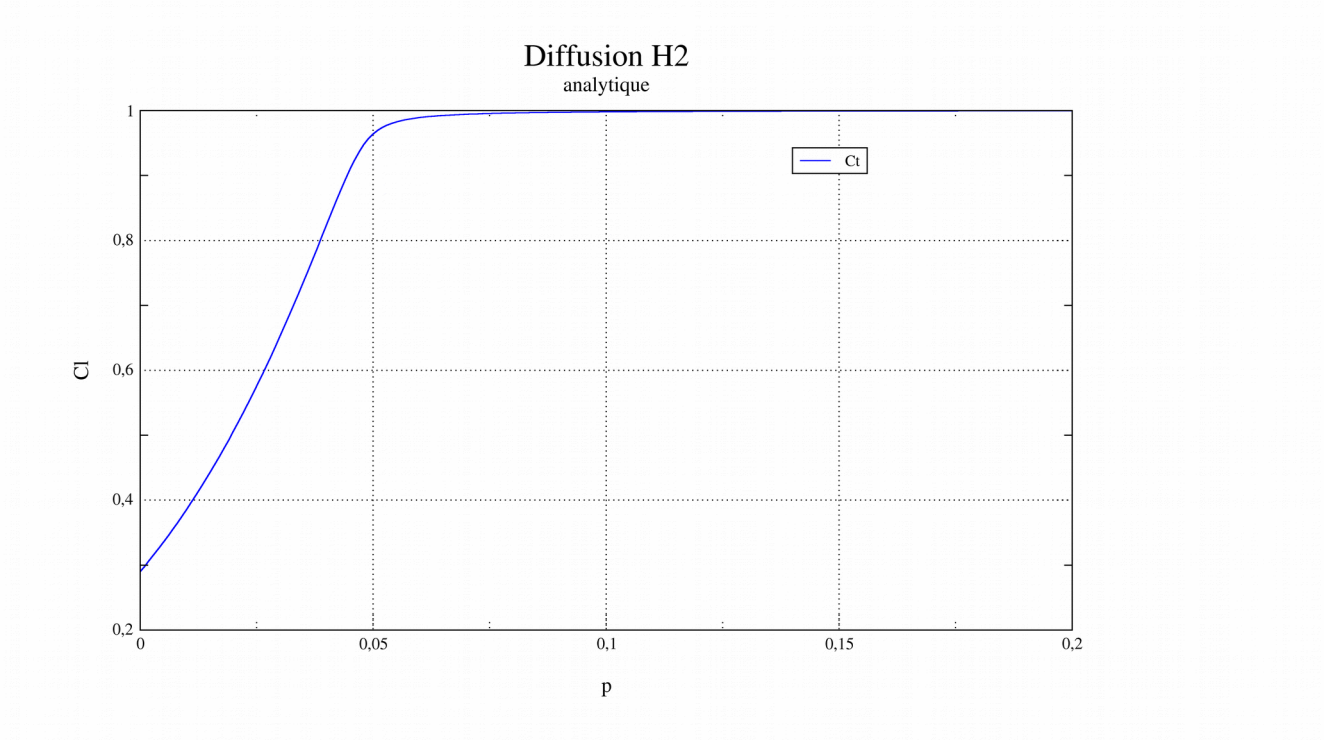
The coefficient of heat capacity $D^*$ is a field represented by a variable of order (NEUT1) .

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 $C_{tot}=C_l+C_t$ 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

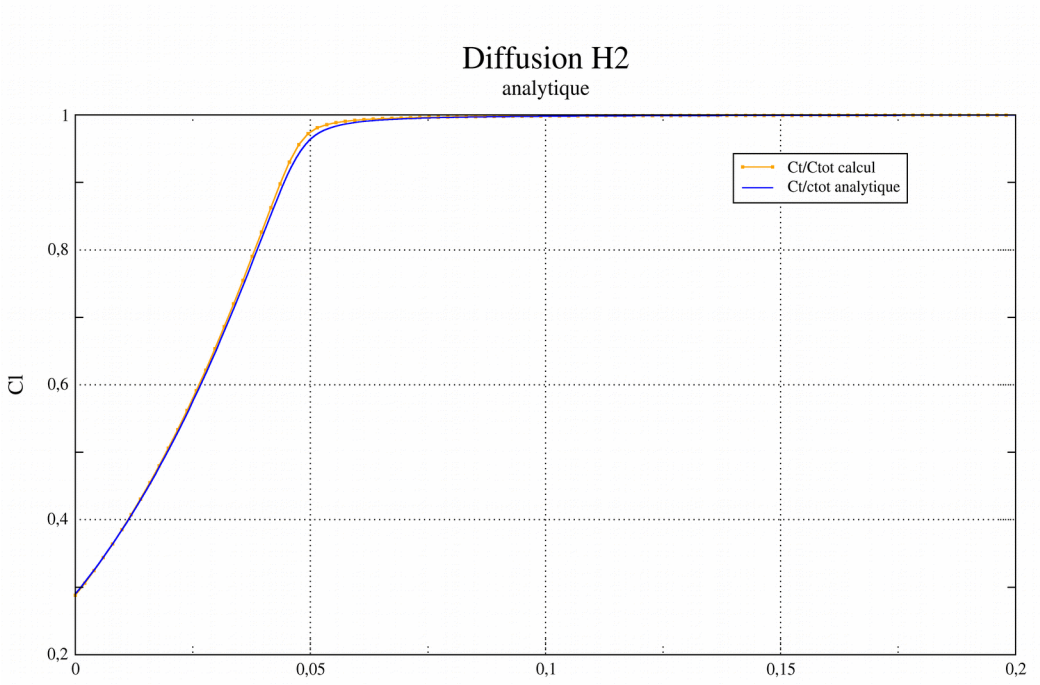
## 3.2 Characteristics of the grid

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

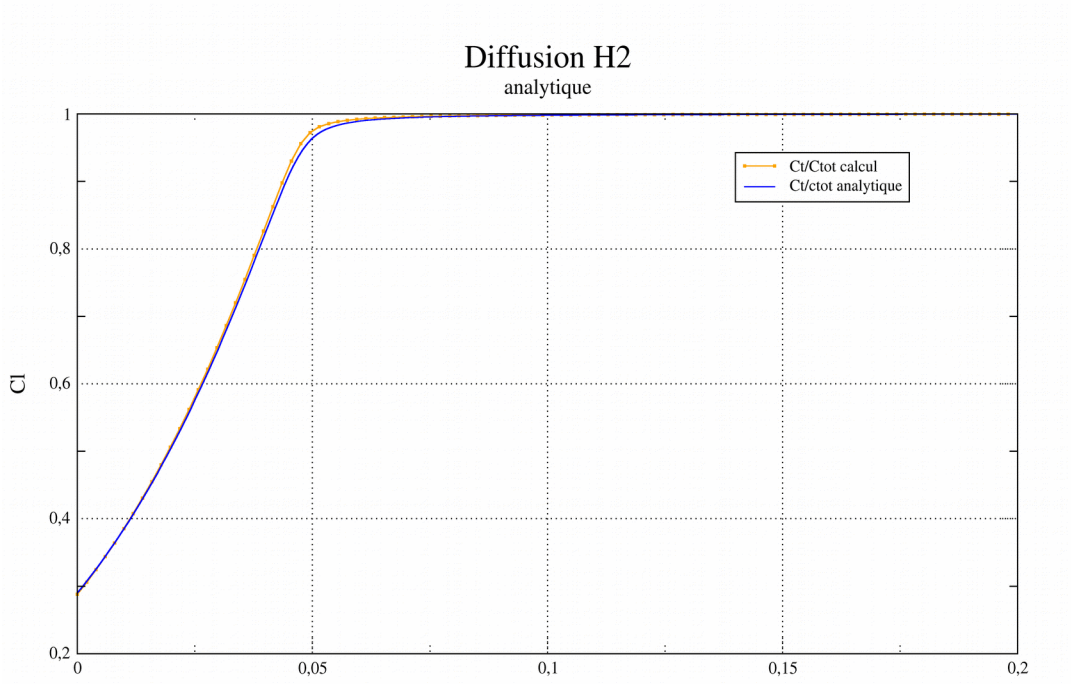
## 4.2 Characteristics of the grid

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

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