# WTNA102 - Diffusion of dissolved air (axi)

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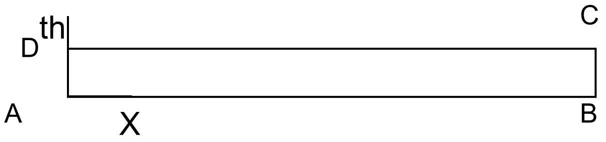
**Summarized:**

One considers here a problem with temperature and saturation constants. By suitable boundary conditions one imposes a water pressure and a steam pressure constants. A gas pressure is imposed on an edge of the field (null flux on other side). Only the air pressures dryness and of dissolved air connected by the model of Henry evolve. This problem is brought back in an equation for the air pressure dryness of type “equation of heat”. The reference solution will be then a thermal computation of Code_Aster.

# 1 Problem of reference

## 1.1 Geometry



Coordinated points ( $m$ ):

| | | | | | |
|---|---|---|---|---|---|
| $A$ | 0 | 0 | $C$ | 1 | 0,5 |
| $B$ | 1 | 0 | $D$ | 0 | 0,5 |

## 1.2 Properties of the material

One gives here only the properties whose solution depends, knowing that the command file contains other material characteristics (elasticity moduli, thermal conductivity…) who finally do not play any part in the solution of with the dealt problem.

| | | |
|---|---|---|
| Liquid water | Density ( $kg.m^{-3}$ ) | $10^3$ |
| | Specific heat with pressure constant ( $J.K^{-1}$ ) | 0 |
| | Dynamic viscosity of liquid water ( $Pa.s$ ) | 0.001 |
| | thermal coefficient of thermal expansion of the fluid ( $K^{-1}$ ) | 0 |
| | Permeability relating to water | $kr_w(S)=0.5$ |
| Vapor | Specific heat ( $J.K^{-1}$ ) | 0 |
| | Molar mass ( $kg.mol^{-1}$ ) | 0.01 |
| Gas | Specific heat ( $J.K^{-1}$ ) | 0 |
| | Molar mass ( $kg.mol^{-1}$ ) | 0.01 |
| | Permeability relating to the gas | $kr_{gz}(S)=0.5$ |
| | Viscosity of gas ( $kg.m^{-1}.s^{-1}$ ) | 0.001 |
| dissolved Air | Specific heat ( $J.K^{-1}$ ) | 0 |
| | Constant of Henry ( $\mathrm{Pa.m^3.mol^{-1}}$ ) | 50000 |
| State initial | Porosity | 1 |
| | Temperature ( $K$ ) | 300 |
| | Pressure of gas ( $Pa$ ) | $1.01\,10^5$ |
| | Steam pressure ( $Pa$ ) | 1000 |
| | capillary Pressure ( $Pa$ ) | $10^6$ |
| | initial Saturation out of fluid | 0.4 |
| Constants | Constant of perfect gases | 8.32 |

| | | |
|---|---|---|
| homogenized Coefficients | homogenized Density ( $kg.m^{-3}$ ) | $2200$ |
| | Isothermal of sorption | $S(p_c)=0.4$ |
| | Coefficient of Biot | $0$ |
| | Fick Vapor ( $m^{2.}s^{-1}$ ) | $0$ |
| | Fick dissolved air ( $m^{2.}s^{-1}$ ) | $FA=6^{-10}$ |
| | Intrinsic Permeability ( $m^2$ ) | $1^{-19}$ |

## 1.3 Boundary conditions and loadings

On the group of the field, one wants:

$$p_w=cte=p_w^0$$
$$\frac{1}{K_w}=0\Rightarrow\rho_w=cte=\rho_w^0$$
$$p_{vp}=cte=p_{vp}^0$$
$$F_{vp}=0$$
$$S(p_c)=cte=S_0$$
$$T=cte=T_0$$
$$\phi=1$$
$$M_{as}^{ol}=M_{ad}^{ol}=M_{vp}^{ol}$$

On all the edges: Hydraulic flux and null thermals.

One now will linearize $p_{vp}$ according to $p_w$.

**Linear writing $p_{vp}$ of function of $p_w$ :**

Section 4.2.3 of the reference document `Code_Aster` [`R7.01.11`] gives us the relation: $\frac{dp_{vp}}{p_{vp}}=\frac{M_{vp}^{ol}}{RT}\frac{dp_w}{\rho_w}$. If this statement is linearized one obtains: $p_{vp}=\frac{p_{vp}^0}{RT}\frac{M_{vp}^{ol}}{\rho_w^0}p_w+\left(p_{vp}^0-\frac{p_{vp}^0}{RT}\frac{M_{vp}^{ol}}{\rho_w^0}p_w^0\right)$ that one can write in the form:

$$p_{vp}=A\,p_w+B \qquad \text{éq 1.3-1}$$

with $A=\frac{p_{vp}^0}{RT}\frac{M_{vp}^{ol}}{\rho_w^0}$ and $B=p_{vp}^0-\frac{p_{vp}^0}{RT}\frac{M_{vp}^{ol}}{\rho_w^0}p_w^0$

On edge $AB$ : $p_{vp}=A\,p_w+B$
$p_{gz}=115000$ and $p_c=10^6$

# 2 Reference solution

## 2.1 Method of calculating

### 2.1.1 Computation of the conservation of the mass of air

the conservation of the mass of gas is written:

$$\frac{dm_{air}}{dt}+div\left(\boldsymbol{M}_{\boldsymbol{as}}+\boldsymbol{M}_{\boldsymbol{ad}}\right) \qquad \text{éq 2.1.1-1}$$

One writes that the total mass of water and the total mass of air are preserved (because there is no water flux nor of gas to edge) and one obtains:

$$m_{air}=m_{as}+m_{ad}=S_0(\rho_{ad}-\rho_{ad}^0)+(1-S_0)(\rho_{as}-\rho_{as}^0)$$

thus

$$d\,(m_{as}+m_{ad})=S_0\,d\,\rho_{ad}+(1-S_0)\,d\,\rho_{as} \qquad \text{éq 2.1.1-2}$$

$d\,\rho_{as}=\frac{M_{as}^{ol}}{RT}dp_{as}$ and $d\,\rho_{ad}=\frac{M_{ad}^{ol}}{K_H}dp_{as}$

$$\frac{dm_{air}}{dt}=div\left(\frac{M_{ad}^{ol}}{K_H}S_0+(1-S_0)\frac{M_{as}^{ol}}{RT}dp_{as}\right)$$

Calcul velocities:

$$\frac{\boldsymbol{M}_{\boldsymbol{as}}}{\rho_{as}}=\lambda_{gz}(-\nabla p_{as}) \qquad \text{éq 2.1.1-3}$$

since $F_{\boldsymbol{vp}}=0$ and $\nabla p_{\boldsymbol{vp}}=0$

$$\boldsymbol{M}_{\boldsymbol{ad}}=\rho_{ad}\lambda_{lq}(-\nabla p_{lq})-F_{ad}\nabla C_{ad} \quad \text{with} \quad C_{ad}=\rho_{ad}$$

As $\nabla p_{lq}=\nabla p_w+\nabla p_{ad}=\nabla p_{ad}=\frac{RT}{K_H}\nabla p_{as}$

$$\boldsymbol{M}_{\boldsymbol{ad}}=\rho_{ad}\lambda_{lq}\frac{RT}{K_H}(-\nabla p_{as})-\frac{M_{ad}^{ol}}{K_H}F_{ad}\nabla p_{as}$$

[éq 2.1.1-1] can then be simplified in the following form:

$$C\frac{dp_{as}}{dt}=L\,div(\nabla p_{as})$$

with

$$C=\frac{M_{ad}^{ol}}{K_H}S_0+(1-S_0)\frac{M_{as}^{ol}}{RT}$$

and

$$L=\rho_{as}^0\lambda_{gz}+\frac{RT}{K_H}\rho_{ad}^0\lambda_{lq}+\frac{M_{as}^{ol}}{K_H}F_{ad}$$

Equation of the heat which one knows result.

## 2.2 Results of reference

With the preceding numerical values, one finds:

$$p_{as}=10^5 \Rightarrow p_{ad}^0=\frac{RT}{K_H} p_{as}^0=4992$$

$\rho_{as}^0=\frac{M_{as}^{ol}}{RT} p_{as}^0=0.4$ and the $\rho_{ad}^0=\frac{M_{ad}^{ol}}{RT} p_{ad}^0=0.02$

$$\rho_{vp}^0=\rho_{vp}=4.10^{-3}$$

constant of the equation of heat are then:

$C=2.48 10^{-6}$

$L=1.4 10^{-16}$

## 2.3 Uncertainties

uncertainties are rather large because the analytical solution is a solution approached because of linearization of the equations.

# 3 Modelization A

## 3.1 Characteristic of the modelization A

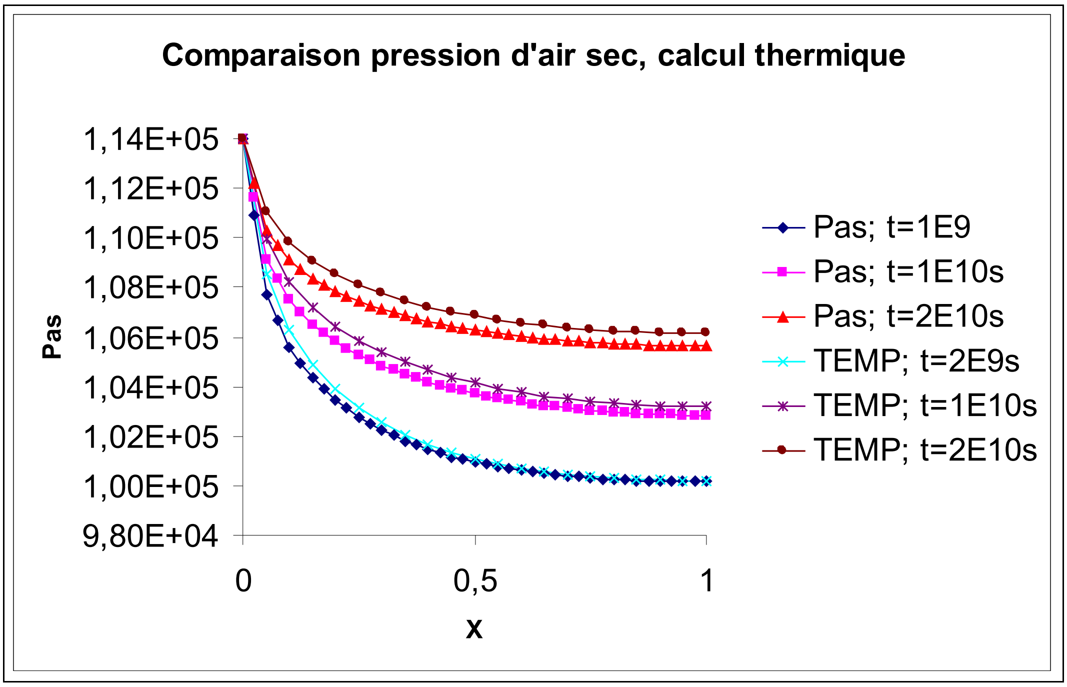
Modelization `AXIS_HH2D`. 20 elements `QUAD8`.

Discretization in time: 100 time step of $5E7\,s$ each one.

## 3.2 Quantities tested and results

| $X$ ( $m$ ) | Time ( $s$ ) | $PRE2$ Aster | $PRE2$ thermal computation | Tolerance ( $\%$ ) |
|---|---|---|---|---|
| 0.2 | $3\,10^{9}$ | $8.1\,10^{3}$ | $7.9\,10^{3}$ | 10.0 |
| 0.2 | $5\,10^{9}$ | $9.7\,10^{3}$ | $9.5\,10^{3}$ | 10.0 |

the values obtained by Code_Aster are tested into non regression with a tolerance of $0.01\%$ .



# 4 Modelization B

## 4.1 Characteristic of the modelization B

Modelization `AXIS_HH2S`. 20 elements `QUAD8`.

Discretization in time: 100 time step of $5\,10^{7}s$ each one.

## 4.2 Quantities tested and results

| $X$ ( $m$ ) | Time ( $s$ ) | $PRE2$ **Aster** | $PRE2$ **thermal computation** | **Tolerance ( $\%$ )** |
|---|---|---|---|---|
| $0.2$ | $3\,10^{9}$ | $8.1\,10^{3}$ | $7.9\,10^{3}$ | $10.0$ |
| $0.2$ | $5\,10^{9}$ | $9.7\,10^{3}$ | $9.5\,10^{3}$ | $10.0$ |

the values obtained by Code_Aster are tested into non regression with a tolerance of $0.01\%$.

# 5 Modelization C

## 5.1 Characteristic of the modelization C

Modelization `3D_HH2S`. 200 elements `HEXA20`. This test consists of a bar and cannot thus have the same analytical solution as previously. It is obtained same way by a thermal computation.

Discretization in time: 100 time step of $5\mathrm{E}7\,s$ each one.

## 5.2 Quantities tested and results

| $X$ ( $m$ ) | **Time ( $s$ )** | $PRE2$ **Aster** | $PRE2$ **thermal computation** | **relative Error** |
|---|---|---|---|---|
| 0.2 | $3\,10^{9}$ | 14682 | 14617 | $0.45\%$ |
| 0.2 | $5\,10^{9}$ | 14953 | 14935 | $0.12\%$ |

# 6 Modelization D

## 6.1 Characteristic of the modelization D

Modelization `3D_HH2D`. 200 elements `HEXA20`.

Discretization in time: 100 time step of $5\mathrm{E}7\,s$ each one.

## 6.2 Quantities tested and results

| $X$ ( $m$ ) | Time ( $s$ ) | $PRE2$ Aster | $PRE2$ thermal computation | relative Error |
|---|---|---|---|---|
| 0.2 | $3\,10^{9}$ | 14687 | 14617 | $0.48\%$ |
| 0.2 | $5\,10^{9}$ | 14954 | 14935 | $0.13\%$ |

# 7 Modelization E

## 7.1 Characteristic of the axisymmetric modelization

E blocked `Modelization` THHM2D with temperatures and displacements. 20 elements `QUAD8`.

Discretization in time: 100 time step of $5\mathrm{E}7\,s$ each one.

## 7.2 Quantities tested and results

| $X$ ( $m$ ) | Time ( $s$ ) | $PRE2$ Aster | $PRE2$ thermal computation | Tolerance |
|---|---|---|---|---|
| 0.2 | $3\,10^9$ | 7944 | 7900 | $1\%$ |
| 0.2 | $5\,10^9$ | 9557 | 9500 | $1\%$ |

the values obtained by `Code_Aster` are tested into non regression with a tolerance of $0.01\%$.

# 8 Modelization F

## 8.1 Characteristic of the axisymmetric modelization

F blocked `Modelization` THHM2S with temperatures and displacements. 20 elements `QUAD8`.

Discretization in time: 100 time step of $5E7\,s$ each one.

## 8.2 Quantities tested and results

| $X$ ( $m$ ) | **Time ( $s$ )** | $PRE2$ **Aster** | $PRE2$ **thermal computation** | **Tolerance** |
|---|---|---|---|---|
| 0.2 | $3\,10^9$ | 7954 | 7900 | $1\%$ |
| 0.2 | $5\,10^9$ | 9566 | 9500 | $1\%$ |

the values obtained by `Code_Aster` are tested into non regression with a tolerance of $0.01\%$.

# 9 Modelization G

## 9.1 Characteristic of the axisymmetric modelization

G Modelization `THH2D` with blocked temperatures. 20 elements `QUAD8`.

Discretization in time: 100 time step of $5\mathrm{E}7\,s$ each one.

## 9.2 Quantities tested and results

| $X$ ( $m$ ) | Time ( $s$ ) | $PRE2$ Aster | $PRE2$ thermal computation | Tolerance |
|---|---|---|---|---|
| 0.2 | $3\,10^9$ | 7945 | 7900 | $10\%$ |
| 0.2 | $5\,10^9$ | 9557 | 9500 | $10\%$ |

the values obtained by `Code_Aster` are tested into non regression with a tolerance of $0.01\%$.

# 10 Modelization H

## 10.1 Characteristic of the axisymmetric modelization

H Modelization `THH2S` with blocked temperatures. 20 elements `QUAD8`.

Discretization in time: 100 time step of $5E7\,s$ each one.

## 10.2 Quantities tested and results

| $X$ ( $m$ ) | Time ( $s$ ) | $PRE2$ Aster | $PRE2$ thermal computation | Tolerance |
|---|---|---|---|---|
| 0.2 | $3\,10^9$ | 7948 | 7900 | $10\,\%$ |
| 0.2 | $5\,10^9$ | 9560 | 9500 | $10\,\%$ |

the values obtained by `Code_Aster` are tested into non regression with a tolerance of $0.01\,\%$.

# 11 Summary of the results

the results of Code_Aster are in very good agreement with the analytical solution.