WTNA102 - Diffusion of dissolved air (axi)

Summary:

One considers here a problem at temperature and saturation constants. By boundary conditions suitable one imposes a water pressure and a steam pressure constants. A gas pressure is imposed on an edge of the field (worthless flows on other side). Only the air pressures dryness and of dissolved air connected by the law 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 calculation DE Code_Aster.
1 Problem of reference

1.1 Geometry

```
  D---------C
     |
     X

With

A 0 0  C 1 0.5
B 1 0  D 0 0.5
```

Coordinates of the points (m):

1.2 Properties of material

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

<table>
<thead>
<tr>
<th>Material</th>
<th>Density (kg.m$^{-3}$)</th>
<th>Specific heat with constant pressure (J.K$^{-1}$)</th>
<th>Dynamic viscosity of liquid water (Pa.s)</th>
<th>Thermal dilation coefficient of the liquid (K$^{-1}$)</th>
<th>Permeability relating to water $kr_w(S) = 0.5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid water</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Vapor</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Gas</td>
<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dissolved air</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Initial state</td>
<td>Porosity</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Temperature (K)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Gas pressure (Pa)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Steam pressure (Pa)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Capillary pressure (Pa)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Initial saturation in liquid</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Constants</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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Coefficients homogenized

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Homogenized density ( kg m(^{-3}) )</td>
<td>2200</td>
</tr>
<tr>
<td>Isotherm of sorption</td>
<td></td>
</tr>
<tr>
<td>Coefficient of Biot</td>
<td>0</td>
</tr>
<tr>
<td>Fick Vapor ( m(^{2}) s(^{-1}) )</td>
<td></td>
</tr>
<tr>
<td>Fick dissolved air ( m(^{2}) s(^{-1}) )</td>
<td></td>
</tr>
<tr>
<td>Intrinsic permeability ( m(^{2}) )</td>
<td></td>
</tr>
</tbody>
</table>

### 1.3 Boundary conditions and loadings

On the whole of the field, one wants:

\[
p_w = cte = p_w^0
\]

\[
\frac{1}{K_w} = 0 \Rightarrow \rho_w = cte = \rho_w^0
\]

\[
p_{vp} = cte = p_{vp}^0
\]

\[
F_{vp} = 0
\]

\[
S(p_v) = cte = S_0
\]

\[
T = cte = T_0
\]

\[
\phi = 1
\]

\[
M_{as}^{vl} = M_{ad}^{vl} = M_{vp}^{vl}
\]

On all the edges: Hydraulic flows and worthless thermics.

One now will linearize \( p_{vp} \) according to \( p_w \).

**Writing of \( p_{vp} \), linear function of \( p_w \):**

Section 4.2.3 of the reference document *Code_Aster* [R7.01.11] the relation gives us:

\[
\frac{dp_{vp}}{p_{vp}} = \frac{M_{vp}^{vl}}{RT \rho_w^0} dp_w
\]

If this expression is linearized one obtains:

\[
p_{vp} = \frac{p_{vp}^0}{RT \rho_w^0} M_{vp}^{vl} p_w^0 + \left( p_{vp}^0 - \frac{p_{vp}^0}{RT \rho_w^0} M_{vp}^{vl} p_w^0 \right)
\]

that one can write in the form:

\[
p_{vp} = A p_w + B
\]

\[
eq 1.3-1
\]

with \( A = \frac{p_{vp}^0}{RT \rho_w^0} M_{vp}^{vl} \) and \( B = p_{vp}^0 - \frac{p_{vp}^0}{RT \rho_w^0} M_{vp}^{vl} p_w^0 \)

On the edge \( AB \):

\[
p_{vp} = A p_w + B
\]

\[
p_{gw} = 115000 \text{ and } p_v = 10^6
\]
2 Reference solution

2.1 Method of calculating

2.1.1 Calculation of the conservation of the mass of air

The conservation of the gas mass is written:

$$\frac{dm_{\text{air}}}{dt} + \text{div} (M_{\text{as}} + M_{\text{ad}}) = 0$$  \hspace{1cm} \text{éq 2.1.1-1}

It is written that the total water mass and the total mass of air are preserved (because there is no gas water flow nor at the edge) and one obtains:

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

thus

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

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

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

Calculation speeds:

$$\frac{M_{\text{as}}^{\text{ol}}}{\rho_{\text{as}}} = \lambda_g \left(-\nabla p_{\text{as}}\right)$$  \hspace{1cm} \text{éq 2.1.1-3}

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

and

$$M_{\text{ad}} = \rho_{\text{ad}} \lambda_{lq} \left(-\nabla p_{\text{lq}}\right) - F_{ad} \nabla C_{ad} \quad \text{with} \quad C_{ad} = \rho_{\text{ad}}$$

Like $$\nabla p_{\text{lq}} = \nabla p_{\text{w}} + \nabla p_{\text{ad}} = \nabla p_{\text{ad}} = \frac{RT}{K_H} \nabla p_{\text{as}}$$

$$M_{\text{ad}} = \rho_{\text{ad}} \lambda_{lq} \frac{RT}{K_H} \left(-\nabla p_{\text{as}}\right) - \frac{M_{\text{ad}}^{\text{ol}}}{K_H} F_{ad} \nabla p_{\text{as}}$$

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

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

with

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

and

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

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Equation of the heat whose one knows the result.

### 2.2 Results of reference

With the preceding digital values, one finds:

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

\[ \rho_{as}^0 = \frac{M_{as}^{ol}}{R} p_{as}^0 = 0.4 \text{ and } \rho_{ad}^0 = \frac{M_{ad}^{ol}}{R} p_{ad}^0 = 0.02 \]

\[ \rho_{vP} = \rho_{vP} = 4 \times 10^{-3} \]

The constants of the equation of heat are then:

\[ C = 2.48 \times 10^{-6} \]
\[ L = 1.4 \times 10^{-16} \]

### 2.3 Uncertainties

Uncertainties are rather large because the analytical solution is a solution approached because of linearization of the equations.
3 Modeling A

3.1 Characteristics of modeling A

Modeling $AXIS_{HH2D}$, 20 elements $QUAD8$.

Discretization in time: 100 pas de time of $5E7 s$ each one.

3.2 Sizes tested and results

<table>
<thead>
<tr>
<th>$X \ (m)$</th>
<th>Time (s)</th>
<th>$PRE2$ Aster</th>
<th>$PRE2$ thermal calculation</th>
<th>Tolerance (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>$3.10^9$</td>
<td>$8.1.10^3$</td>
<td>$7.9.10^3$</td>
<td>10.0</td>
</tr>
<tr>
<td>0.2</td>
<td>$5.10^9$</td>
<td>$9.7.10^3$</td>
<td>$9.5.10^3$</td>
<td>10.0</td>
</tr>
</tbody>
</table>

Values obtained by Code_Aster are tested in nonregression with a tolerance of 0.01%.

---

**Comparaison pression d'air sec, calcul thermique**

- Pas; $t=1E9$
- Pas; $t=1E10s$
- Pas; $t=2E10s$
- TEMP; $t=2E9s$
- TEMP; $t=1E10s$
- TEMP; $t=2E10s$
4 Modeling B

4.1 Characteristics of modeling B

Modeling AXIS_HH2S. 20 elements QUAD8.

Discretization in time: 100 pas de time of $5 \times 10^7$ s each one.

4.2 Sizes tested and results

<table>
<thead>
<tr>
<th>$X$ (m)</th>
<th>Time (s)</th>
<th>$PRE2$ Aster</th>
<th>$PRE2$ thermal calculation</th>
<th>Tolerance (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>$3 \times 10^9$</td>
<td>$8.1 \times 10^3$</td>
<td>$7.9 \times 10^3$</td>
<td>10.0</td>
</tr>
<tr>
<td>0.2</td>
<td>$5 \times 10^9$</td>
<td>$9.7 \times 10^3$</td>
<td>$9.5 \times 10^3$</td>
<td>10.0</td>
</tr>
</tbody>
</table>

Values obtained by Code_Aster are youstées in nonregression with a tolerance of $0.01\%$.
5 Modeling C

5.1 Characteristics of modeling C

Modeling 3D_HH_2S, 200 elements HEXA20. This test consists of a bar and cannot thus have the same analytical solution as previously. It is obtained same manner by a thermal calculation.

Discretization in time: 100 pas de time of 5E7s each one.

5.2 Sizes tested and results

<table>
<thead>
<tr>
<th>X (m)</th>
<th>Time (s)</th>
<th>PRE2 Aster</th>
<th>PRE2 thermal calculation</th>
<th>Relative error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>310⁹</td>
<td>14682</td>
<td>14617</td>
<td>0.45%</td>
</tr>
<tr>
<td>0.2</td>
<td>510⁹</td>
<td>14953</td>
<td>14935</td>
<td>0.12%</td>
</tr>
</tbody>
</table>

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6 Modeling D

6.1 Characteristics of modeling D

Modeling 3D__HH2D. 200 elements HEXA20.

Discretization in time: 100 pas de time of 5E-7 s each one.

6.2 Sizes tested and results

<table>
<thead>
<tr>
<th>X (m)</th>
<th>Time (s)</th>
<th>PRE2 Aster</th>
<th>PRE2 thermal calculation</th>
<th>Relative error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>3 \times 10^9</td>
<td>14687</td>
<td>14617</td>
<td>0.48%</td>
</tr>
<tr>
<td>0.2</td>
<td>5 \times 10^9</td>
<td>14954</td>
<td>14935</td>
<td>0.13%</td>
</tr>
</tbody>
</table>
7 Modeling E

7.1 Characteristics of modeling E

Axisymmetric modeling THHM2D with blocked temperatures and displacements. 20 elements QUAD8.

Discretization in time: 100 pas de time of $5\times10^7$ s each one.

7.2 Sizes tested and results

<table>
<thead>
<tr>
<th>$X$ (m)</th>
<th>Time (s)</th>
<th>PRE2 Aster</th>
<th>PRE2 thermal calculation</th>
<th>Tolerance</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>$3\times10^9$</td>
<td>7944</td>
<td>7900</td>
<td>1%</td>
</tr>
<tr>
<td>0.2</td>
<td>$5\times10^9$</td>
<td>9557</td>
<td>9500</td>
<td>1%</td>
</tr>
</tbody>
</table>

Values obtained by Code_Aster are tested in nonregression with a tolerance of 0.01%.
8 Modeling F

8.1 Characteristics of modeling F

Axisymmetric modeling THRM2S with blocked temperatures and displacements. 20 elements QUAD8.

Discretization in time: 100 pas de time of 5E7 s each one.

8.2 Sizes tested and results

<table>
<thead>
<tr>
<th>$X$ (m)</th>
<th>Time (s)</th>
<th>PRE2 Aster</th>
<th>PRE2 thermal calculation</th>
<th>Tolerance</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>$3 \times 10^9$</td>
<td>7954</td>
<td>7900</td>
<td>1%</td>
</tr>
<tr>
<td>0.2</td>
<td>$5 \times 10^9$</td>
<td>9566</td>
<td>9500</td>
<td>1%</td>
</tr>
</tbody>
</table>

Values obtained by Code_Aster are tested in nonregression with a tolerance of 0.01%.
9 Modeling G

9.1 Characteristics of modeling G

Axisymmetric modeling $\text{THH2D}$ with blocked temperatures. 20 elements $\text{QUAD8}$.

Discretization in time: 100 pas de time of $5\times 10^7$ s each one.

9.2 Sizes tested and results

<table>
<thead>
<tr>
<th>$X$ (m)</th>
<th>Time (s)</th>
<th>$\text{PRE2 Aster}$</th>
<th>$\text{PRE2 thermal calculation}$</th>
<th>Tolerance</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>$3 \times 10^9$</td>
<td>7945</td>
<td>7900</td>
<td>10%</td>
</tr>
<tr>
<td>0.2</td>
<td>$5 \times 10^9$</td>
<td>9557</td>
<td>9500</td>
<td>10%</td>
</tr>
</tbody>
</table>

Values obtained by $\text{Code_Aster}$ are tested in nonregression with a tolerance of 0.01%.
10 Modeling H

10.1 Characteristics of modeling H

Axisymmetric modeling THH2S with blocked temperatures. 20 elements QUAD8.

Discretization in time: 100 pas de time of $5E7$ s each one.

10.2 Sizes tested and results

<table>
<thead>
<tr>
<th>$X$ (m)</th>
<th>Time (s)</th>
<th>PRE2 Aster</th>
<th>PRE2 thermal calculation</th>
<th>Tolerance</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>$3 \times 10^9$</td>
<td>7944</td>
<td>7900</td>
<td>10%</td>
</tr>
<tr>
<td>0.2</td>
<td>$5 \times 10^9$</td>
<td>9560</td>
<td>9500</td>
<td>10%</td>
</tr>
</tbody>
</table>

Values obtained by Code_Aster are tested in nonregression with a tolerance of 0.01%. Modeling H...
11 Modeling I

11.1 Characteristics of modeling I

Axisymmetric modeling HH2MD with blocked displacements. 20 elements QUAD8.

Discretization in time: 100 pas de time of 5E7 s each one.

11.2 Sizes tested and results

<table>
<thead>
<tr>
<th>( X ) (m)</th>
<th>Time (s)</th>
<th>( PRE2 ) Aster</th>
<th>( PRE2 ) thermal calculation</th>
<th>Tolerance</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>3 ( 10^9 )</td>
<td>7944</td>
<td>7900</td>
<td>1%</td>
</tr>
<tr>
<td>0.2</td>
<td>5 ( 10^9 )</td>
<td>9557</td>
<td>9500</td>
<td>1%</td>
</tr>
</tbody>
</table>

Values obtained by Code_Aster are tested in nonregression with a tolerance of 0.01%.
12 Modeling J

12.1 Characteristics of modeling J

Axisymmetric modeling HH2MD with blocked displacements. 20 elements QUAD8.

Discretization in time: 100 pas de time of $5 \times 10^7$ s each one.

12.2 Sizes tested and results

<table>
<thead>
<tr>
<th>$X$ (m)</th>
<th>Time (s)</th>
<th>PRE2 Aster</th>
<th>PRE2 thermal calculation</th>
<th>Tolerance</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>$3 \times 10^9$</td>
<td>7948</td>
<td>7900</td>
<td>1%</td>
</tr>
<tr>
<td>0.2</td>
<td>$5 \times 10^9$</td>
<td>9560</td>
<td>9500</td>
<td>1%</td>
</tr>
</tbody>
</table>

Values obtained by Code_Aster are tested in nonregression with a tolerance of 0.01%.
13 Summary of the results

The resultS of Code_Aster soNT in very good agreement with the analytical solution.