WTNV131 - Diffusion of air dissolved in water (3D)

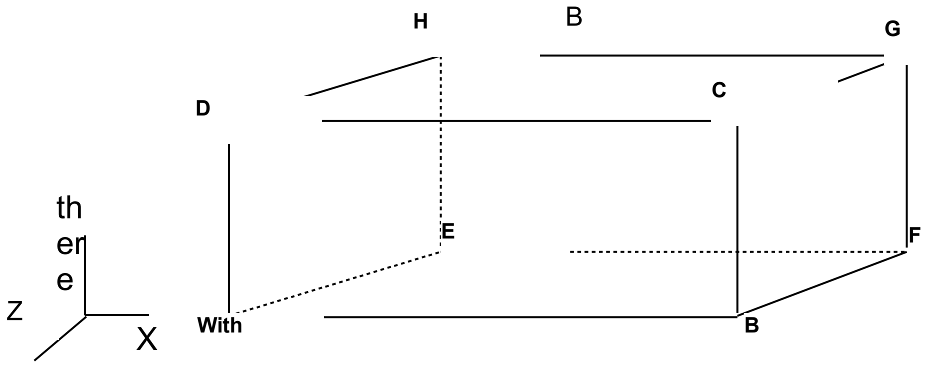
Summary:

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 of the other with dimensions). Only the air pressures dryness and of dissolved air connected by the law of Henry evolve. This problem is brought back to an equation for the air pressure dryness of type "equation of heat". The reference solution will be then a thermal calculation ASTER. This case test is the extension $3D$ case test WTNP103.

1 Problem of reference

1.1 Geometry

A bar length is considered $1\mathrm{m}$ and of section $0.1\mathrm{m}\times0.1\mathrm{m}$.



Coordinates of the points (m) :

	X	Y	Z		X	Y	Z
A	0	0	0	C	1	0.1	0
B	1	0	0	D	0	0.1	0
E	0	0	-0.1	G	1	0.1	-0.1
F	1	0	-0.1	H	0	0.1	-0.1

1.2 Properties of material

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

Liquid water	Density ($kg.m^{-3}$)	10^3
	Specific heat with constant pressure ($J.K^{-1}$)	0.
	Dynamic viscosity of liquid water ($Pa.s$)	0,001
	thermal dilation coefficient of the liquid (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 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 ($Pa.m^{3.}mol^{-1}$)	50000
Initial state	Porosity	1

	Temperature (K) Gas pressure (Pa) Steam pressure (Pa) Capillary pressure (Pa) Initial saturation in liquid	300 1.01E5 1000 1.E6 0.4
Constants	Constant of perfect gases	8.32
Homogenized coefficients	Homogenized density ($kg.m^{-3}$) Isotherm of sorption Coefficient of Biot Fick Vapor ($m^{2.}s^{-1}$) Fick dissolved air ($m^{2.}s^{-1}$) Intrinsic permeability (m^2)	2200 $S(P_c)=0.4$ 0 $FV=0$ $FA=6\ .E-10$ $Kint=1.E-19$

1.3 Boundary conditions and loadings

On the whole of the field, one wants:

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

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 *Aster* [R7.01.11] the relation gives us: $\frac{dp_{vp}}{p_{vp}} = \frac{M_{vp}^{ol}}{RT}\frac{dp_w}{\rho_w}$.

If this expression 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:

$$p_{vp} = Ap_w + B \quad \text{éq 1.3-1}$$

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 the left edge of the bar ($AEHD$) one imposes $\begin{cases} p_{gz} = 115000 \quad Pa \\ pc = 10^{6} \quad Pa \end{cases}$

2 Reference solution

2.1 Method of calculating

Calculation of the conservation of the mass of air

The conservation of the gas mass is written:

$$\frac{dm_{air}}{dt} + div(\mathbf{M}_{as} + \mathbf{M}_{ad}) = 0 \qquad \text{éq 2.1.1-1}$$

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:

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

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 $d\rho_{ad} = \frac{M_{ad}^{ol}}{K_H} dP_{as}$

$$\frac{dm_{air}}{dt} = \left(S_{0.} \frac{M_{as}^{ol}}{K_H} + (1 - S_0) \frac{M_{as}^{ol}}{RT} \right) \frac{dP_{as}}{dt}$$

Calculation speeds:

$$\frac{\mathbf{M_{as}}}{\rho_{as}} = \lambda_{gz} (-\nabla P_{as}) \qquad \text{éq 2.1.1-3}$$

since $F_{vp} = 0$ and $\nabla P_{vp} = 0$ and $\mathbf{M}_{\mathbf{a}d} = \rho_{ad} \lambda_{lq} (-\nabla P_{lq}) - F_{ad} \nabla C_{ad}$ with $C_{ad} = \rho_{ad}$.

Like $\nabla P_{lq} = \nabla P_w + \nabla P_{ad} = \nabla P_{ad} = \frac{RT}{K_H} \nabla P_{as}$

$$\mathbf{M}_{\mathbf{a}d} = \rho_{ad} \lambda_{lq} \frac{RT}{K_H} (-\nabla P_{as}) - .\frac{M_{ad}^{ol}}{K_H} .F_{ad} \nabla P_{as}$$

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

$$C \frac{dP_{as}}{dt} = L div(\nabla P_{as})$$

$$\text{with} \begin{cases} C = S_{0.} \frac{M_{as}^{ol}}{K_H} + (1 - S_0) \frac{M_{as}^{ol}}{RT} \\ L = \rho_{as}^0 \lambda_{gz} + \frac{RT}{K_H} \rho_{ad}^0 \lambda_{lq} + \frac{M_{as}^{ol}}{K_H} .F_{ad} \end{cases}$$

Equation of the classical heat which one treats by a thermal calculation.

2.2 Results of reference

With the preceding digital values, one finds:

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

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

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

The constants of the equation of heat are then:

$$C=2{,}48.10^{-6}$$
$$L=1{,}4.10^{-16}$$

2.3 Uncertainties on the solution

Uncertainties are rather large since the quasi-analytical solution (fruit of a thermal calculation) is a solution approached because of linearization of the equations.

3 Modeling A

3.1 Characteristics of modeling

Modeling in 3D : 3D_HH2MD.

3.2 Characteristics of modeling

203 elements TETRA10.

3.3 Sizes tested and results

It is pointed out that the temperature resulting from thermal calculation corresponds to the air pressure dryness of our calculation thermo-hydro-mechanics. The steam pressure being constant one a:

$$P_{gz} = PRE2^{DDL} + PRE2^{init} = P_{vp}^0 + P_{as}$$

$X(m)$	**Time** (s)	$PRE2$	**Tolerance (** $\%$ **)**
0.2	3E9	1.120E4	1%
0.2	5E9	1.223E3	1%
0.5	3E9	6570	1%
0.5	5E9	8685	1%

In addition, two tests of not-regression are carried out on the constraint of Von Mises (VMIS) and of Tresca (TRESCA).

4 Modeling B

4.1 Characteristics of modeling B

Even thing that modeling A but in modeling selective: `3D_HH2MS`.

4.2 Sizes tested and results

It is pointed out that the temperature resulting from thermal calculation corresponds to the air pressure dryness of our calculation thermo-hydro-mechanics. The steam pressure being constant one a:

$$P_{gz} = PRE2^{DDL} + PRE2^{init} = P_{vp}^{0} + P_{as}$$

$X(m)$	Time (s)	$PRE2$	Tolerance ($\%$)
0.2	3E9	1.120E4	1%
0.2	5E9	1.223E3	1%
0.5	3E9	6570	1%
0.5	5E9	8685	1%

In addition, two tests of not-regression are carried out on the constraint of Von Mises (`VMIS`) and of Tresca (`TRESCA`).

5 Modeling C

5.1 Characteristics of modeling C

Even thing that modeling A but in selective modeling: `3D_HH2M_SI`.

5.2 Sizes tested and results

It is pointed out that the temperature resulting from thermal calculation corresponds to the air pressure dryness of our calculation thermo-hydro-mechanics. The steam pressure being constant one a:

$$P_{gz} = PRE2^{DDL} + PRE2^{init} = P_{vp}^{0} + P_{as}$$

$X(m)$	**Time** (s)	$PRE2$	**Tolerance (** $\%$ **)**
0.2	3E9	1.120E4	1%
0.2	5E9	1.223E3	1%
0.5	3E9	6570	1%
0.5	5E9	8685	1%

In addition, two tests of not-regression are carried out on the constraint of Von Mises (`VMIS`) and of Tresca (`TRESCA`).

6 Summary of the results

The results are in very good agreement with the semi-analytical solution.

For modelings A and C, the convergence criteria are fixed at `RESI_GLOB_RELA = 1E-14` in order to minimize the error on the solution (tests of not-regression) related to the mixed formulation of the problem.