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

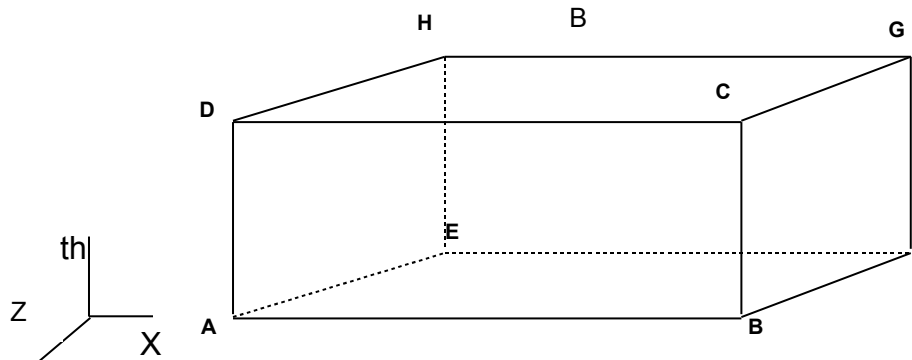
Summarized:

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 of the other with dimensions). Only the air pressures dryness and of dissolved air connected by the model 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 computation ASTER. This case test is the extension 3D of the case test WTNP103.

1 Problem of reference

1.1 Geometry

One considers a bar length 1m and section $0.1\text{m} \times 0.1\text{m}$.



Coordinated 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	0	0	-0,1	H	0.0,1		-0,1

1.2 Properties of the material

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

Liquid water	Density ($kg.m^{-3}$)	103
	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})	$kr_w(S) = 0.5$
	Permeability relating to water	
Vapor	Specific heat ($J.K^{-1}$)	0.
	Molar mass ($kg.mol^{-1}$)	0,01
Gases	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 ($Pa.m^3.mol^{-1}$)	50000
initial State	Porosity	fluids

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	Temperature (K)	
	Pressure of gas (Pa)	1.300
	Steam pressure (Pa)	1.01E5
	capillary Pressure (Pa)	1000
	initial Saturation out of Constant	1.E6
0,4	Constant of perfect gases	8,32
homogenized Coefficients	Density homogenized ($kg.m^{-3}$)	2200
	Isothermal of sorption	$S(P_c) = 0.4$
	Coefficient of Biot	0
	Fick Vapor ($m^2.s^{-1}$)	$FV = 0$
	Fick dissolved air ($m^2.s^{-1}$)	$FA = 6 .E - 10$
	intrinsic Permeability (m^2)	$Kint = 1.E - 19$

1.3 Boundary conditions and loadings

On the group field, one wants:

$$p_w = cte = p_w^0$$

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

$$p_{vp} = cte = p_{vp}^0$$

$$F_{vp} = 0$$

$$S(p_c) = cte = S_0$$

$$T = cte = T^0$$

$$\varphi = 1$$

$$M_{as}^{ol} = M_{vp}^{ol} = M_{ad}^{ol}$$

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 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: $p_{vp} = \frac{p_{vp}^0}{RT} \frac{M_{vp}^{ol}}{\rho_w} p_w + \left(p_{vp}^0 - \frac{p_{vp}^0}{RT} \frac{M_{vp}^{ol}}{\rho_w} p_w^0 \right)$

that one can write in the form:

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

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

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

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:

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

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

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

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

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

Calcul velocities:

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

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

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

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

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

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

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

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

2.2 Results of reference

With the preceding numerical values, one finds:

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

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

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

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 since the quasi-analytical solution (fruit of a thermal computation) is a solution approached because of linearization of the equations.

3 Modelization A

3.1 Characteristic of the modelization A

Modelization in 3D : 3D_THH2D 203 Tetra10 elements.

3.2 Quantities tested and results

It is pointed out that the temperature resulting from thermal computation corresponds to the air pressure dryness of our computation 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 Aster	PRE2 thermal computation	relative Error (%)
0,2	3E9s	1.127E4	1.120E4	0.7%
0,2	5E9s	1.227E4	1.223E3	0.31%
0,5	3E9s	6617	6570	0.72%
0,5	5E9s	8743	8685	0.67%

4 Modelization B

4.1 Characteristic of the modelization B

Even thing that the modelization A but in selective modelization: 3D_THH2S.

4.2 Quantities tested and results

It is pointed out that the temperature resulting from thermal computation corresponds to the air pressure dryness of our computation 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 Aster	PRE2 thermal computation	relative Error (%)
0,2	3E9s	1.127E4	1.120	0.59%
0,2	5E9s	1.227E4	1.223E3	0.43%
0,5	3E9s	6617	6570E3	3%.0,5
	5E9s	8743	8685	2.2%

5 Summary of the results

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