Finite Element Formulation and couplings

A.M. Habraken - F. Collin

- Introduction
- Mathematical formulation of HM problem
- Finite element formulation (CSOL2)
- Mathematical formulation of THM problem
- Mathematical formulation of C/B-THM problem
- Conclusion

The Lagamine code is able to tackle a wide variety of problem, from hot rolling of sheet piles to nuclear waste disposal. In this purpose, many finite elements were developed since 30 years.

- Non linear finite element formulation

  - Part 1 : Virtual work principal, definition of stress in large strain large displacement problem, formulation of a displacement finite element, thermo-mechanical coupled problem

  - Part 2 : Hydro-mechanical coupled problems, Thermo-hydro-mechanical problems, Chemo/Bio-Thermo-Hydro_mechanical problems, for soil and rock mechanics applications.

Most of these developments were initiated for the study of nuclear waste disposal, where many physical processes occur. They can be course used in other applications, like reservoir engineering, shale gas, underground projects …

In multi-physics problems, several physical processes occur simultaneously and interact each other. In the sequel, we will limit the presentation to (quasi-) static problems.

As for the mechanical problem, we will use the following balance equations:

- Momentum balance equation: it corresponds to the equilibrium equations (translation and rotation) of the considered body.

- Mass balance conservation: the mass of the system remains constant (open or closed system)

- Energy balance equation: we will express that the enthalpy of the system remains constant (open or closed system)

- Second thermodynamics law

Depending on the studied problem, we will used some of these latter balance equations. The remaining equations will be assumed more or less consciously.

In addition to these equations, we will need some state relationships (constitutive laws, thermodynamics relations …) that will be defined in order to close the system.

Non linearities in our problem come mainly from the constitutive behaviour of the geomaterials, the time-dependent physical processes (flows, heat transfer, chemical reaction) and the interactions between all the phenomena.

Focus on the coupling terms at the level of the finite element (monolithical approach)

Depending on the problem, a coupling effect might be more or less important and a numerical treatment is thus different.

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Solid mechanics

- Linear momentum balance equation (Quasi-static condition)

$$\frac{\partial \sigma_{ij}}{\partial x_j} - \rho g_i = 0$$

- Angular momentum balance equation (Quasi-static condition)

$$\sigma_{ij} = \sigma_{ji}$$

- Solid mass balance equation

$$\frac{\partial \rho}{\partial t} = 0$$

Flow problem

- Fluid mass balance equation

$$\frac{\partial M}{\partial t} + div(m_i) = Q$$

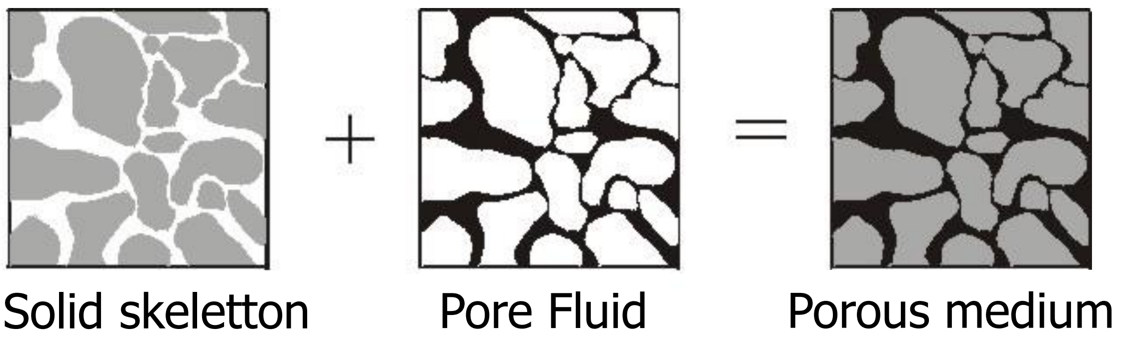
- Linear momentum balance equation (Quasi-static condition)

$$\frac{\partial p}{\partial x_i} + F_i^{S/W} + \rho_w g_i = 0$$

Where $F_i^{S/W}$ is the fluid drag force.

HM coupled problem

Saturated porous medium



The porous medium is considered as the superimposition of two continua, made of two chemical species (solid grain and water) and two phases (solid and fluid).

The balance equations can be alternatively written for each species or the mixture and one of the species.

HM coupled problem (saturated conditions)

- Linear momentum balance equation for the mixture (weak form)

$$\int_{\Omega} \sigma_{ij} \varepsilon_{ij}^{*} d\Omega = \int_{\Omega} \rho_{mix} g_i u_i^{*} d\Omega + \int_{\Gamma} \overline{t}_i u_i^{*} d\Gamma$$

Terzaghi's postulate $\sigma_{ij} = \sigma_{ij}^{'} - p\delta_{ij}$

Boundary condition $\sigma_{ij} n_j = \overline{t}_i$

Mixture density $\rho_{mix} = \rho_s.(1-\phi) + \phi.\rho_w$

HM coupled problem (saturated conditions)

- Fluid mass balance equation (weak form)

$$\int_{\Omega} \dot{M}\, p^{*} - m_i \frac{\partial p^{*}}{\partial x_i}\, d\Omega = \int_{\Omega} Q\, p^{*} d\Omega + \int_{\Gamma} \bar{q}\, p^{*} d\Gamma$$

Boundary condition $\bar{q} = m_i n_i$

Darcy's law $m_i = -\rho_w \frac{\kappa}{\mu}\left(\frac{\partial p}{\partial x_i} + \rho_w g_i\right)$

Storage law $\dot{M} = \rho_w \frac{\dot{p}}{k^w}\phi + \rho_w \frac{\dot{\Omega}}{\Omega}$

HM coupled problem (saturated conditions)

- Fluid Linear momentum balance equation (strong form)

$$\frac{\partial p}{\partial x_i} + F_i^{S/W} + \rho_w g_i = 0$$

Viscous drag force : $F_i^{S/W} = \frac{\rho_w . \phi . g}{K} V_i^{W/S}$

- Solid mass balance equation (strong form)

$$\frac{\partial\left(\rho_s (1-\phi)\Omega\right)}{\partial t} = 0$$

HM coupled problem (saturated conditions)

- System of equations to be solved:

$$\int_{\Omega} \sigma_{ij} \varepsilon_{ij}^{*} d\Omega = \int_{\Omega} \rho_{mix} g_i u_i^{*} d\Omega + \int_{\Gamma} \bar{t}_i u_i^{*} d\Gamma$$

$$\int_{\Omega} \dot{M}\, p^{*} - m_i \frac{\partial p^{*}}{\partial x_i} d\Omega = \int_{\Omega} Q\, p^{*} d\Omega + \int_{\Gamma} \bar{q}\, p^{*} d\Gamma$$

HM coupled problem (saturated conditions)

- Terzaghi postulate: $\sigma_{ij}^{t} = \sigma_{ij}^{\prime t} - p^{t}\delta_{ij}$
- Viscous drag forces $F_{i}^{S/W,t} = \frac{\varrho^{w,t}\phi^{t} g}{K} V_{i}^{W/S,t}$
- Relative velocity of the fluid: $m_{i}^{t} = -\frac{K}{g}\left(\frac{\partial p^{t}}{\partial x_{i}^{t}} + \varrho^{w,t} g_{i}\right) = -\varrho^{w,t}\frac{\kappa}{\mu}\left(\frac{\partial p^{t}}{\partial x_{i}^{t}} + \varrho^{w,t} g_{i}\right)$
- Rate of fluid mass: $\dot{M}^{t} = \varrho^{w,t}\left[\frac{\dot{p}^{t}}{k^{w}}\phi^{t} + \frac{\dot{\Omega}^{t}}{\Omega^{t}}\right]$
- Boundary conditions: total stresses
- Boundary conditions: fluxes $\overline{q}^{t} = m_{i}^{t} n_{i}^{t}$

Auxiliary linear problem

The out-of-balance forces are usually different from zero and an iterative procedure is necessary to find a new configuration in equilibrium (where the out-of-balance forces vanish). Let's consider a first configuration $\tau 1$ which is not in equilibrium:

$$\int_{\Omega^{\tau 1}} \sigma_{ij}^{\tau 1} \frac{\partial u_i^\star}{\partial x_j^{\tau 1}} d\Omega^{\tau 1} - \int_{\Omega^{\tau 1}} (\varrho^{s,\tau 1}(1-\phi^{\tau 1}) + \varrho^{w,\tau 1}\phi^{\tau 1}) g_i u_i^\star d\Omega^{\tau 1} - \int_{\Gamma_\sigma^{\tau 1}} \bar{t}_i^{\tau 1} u_i^\star d\Gamma^{\tau 1} = \int_{\Omega^{\tau 1}} F_i^{\mathrm{HE}} u_i^\star \, d\Omega^{\tau 1}$$

$$\int_{\Omega^{\tau 1}} (\dot{M}^{\tau 1} p^\star - m_i^{\tau 1} \frac{\partial p^\star}{\partial x_i^{\tau 1}}) d\Omega^{\tau 1} - \int_{\Omega^{\tau 1}} Q^{\tau 1} p^\star d\Omega^{\tau 1} + \int_{\Gamma_q^{\tau 1}} \bar{q}^{\tau 1} p^\star d\Gamma^{\tau 1} = \int_{\Omega^{\tau 1}} F_p^{\mathrm{HE}} p^\star \, d\Omega^{\tau 1}$$

Our goal is to find a new configuration $\tau 2$ for which the out-of-balance forces vanish:

$$\int_{\Omega^{\tau 2}} \sigma_{ij}^{\tau 2} \frac{\partial u_i^\star}{\partial x_j^{\tau 2}} d\Omega^{\tau 2} - \int_{\Omega^{\tau 2}} (\varrho^{s,\tau 2}(1-\phi^{\tau 2}) + \varrho^{w,\tau 2}\phi^{\tau 2}) g_i u_i^\star d\Omega^{\tau 2} - \int_{\Gamma_\sigma^{\tau 2}} \bar{t}_i^{\tau 2} u_i^\star d\Gamma^{\tau 2} = 0$$

$$\int_{\Omega^{\tau 2}} (\dot{M}^{\tau 2} p^\star - m_i^{\tau 2} \frac{\partial p^\star}{\partial x_i^{\tau 2}}) d\Omega^{\tau 2} - \int_{\Omega^{\tau 2}} Q^{\tau 2} p^\star d\Omega^{\tau 2} + \int_{\Gamma_q^{\tau 2}} \bar{q}^{\tau 2} p^\star d\Gamma^{\tau 2} = 0$$

In order to find this better approximation $\tau 2$, we rewrite these latter equations in the configuration $\tau 1$ and the resulting equations are substracted from the initial equations. This yields first for the momentum balance equation:

$$\int_{\Omega^{\tau 1}} \frac{\partial u_i^\star}{\partial x_k^{\tau 1}} (\sigma_{ij}^{\tau 2} \frac{\partial x_k^{\tau 1}}{\partial x_j^{\tau 2}} \det F - \sigma_{ik}^{\tau 1}) d\Omega^{\tau 1} = \int_{\Omega^{\tau 1}} F_i^{\mathrm{HE}} u_i^\star d\Gamma^{\tau 1}$$

In a first step, let's assume that the pore pressure is identical in the two configurations. We define δu_i as the differences between the configurations $\tau 1$ and $\tau 2$.

$$x_i^{\tau 2} = x_i^{\tau 1} + \delta u_i$$

Evaluation of the left-hand term of the equation yields:

$$\sigma_{ij}^{\tau 2} (\delta_{jk} - \frac{\partial \delta u_k}{\partial x_j^{\tau 2}}) \det F - \sigma_{ik}^{\tau 1}$$

$$= \sigma_{ik}^{\tau 2} \det F - \sigma_{ij}^{\tau 2} \frac{\partial \delta u_k}{\partial x_j^{\tau 2}} \det F - \sigma_{ik}^{\tau 1}$$

$$= (\sigma_{ik}^{\tau 2} - \sigma_{ik}^{\tau 1}) - \sigma_{ij}^{\tau 2} \frac{\partial \delta u_k}{\partial x_i^{\tau 2}} \det F + \sigma_{ik}^{\tau 2} (\det F - 1)$$

Assuming that the two configurations are close, we may assume that δu_i tends to du_i , and the det F can be rewritten as:

$$\det F = 1 + \frac{\partial du_l}{\partial x_l^t}$$

Using a Taylor expansion of the equation and discarding terms of degree greater than one yields after some algebra :

$$d\sigma_{ik}^t - \sigma_{ij}^t \frac{\partial du_k}{\partial x_j^t} + \sigma_{ik}^t \frac{\partial du_l}{\partial x_l^t}$$

The increment of total stress can be expressed as follow:

$$d\sigma_{ik}^t = C_{iklj} \frac{\partial du_l}{\partial x_j^t} - dp\ \delta_{ik}$$

The following expression of the stiffness matrix holds:

Small strain term

HM coupling term

$$\int_{\Omega^t} \frac{\partial u_i^*}{\partial x_k^t} \left(C_{ijkl} \frac{\partial du_l}{\partial x_j^t} - \sigma_{ij}^t \frac{\partial du_k}{\partial x_j^t} + \sigma_{ik}^t \frac{\partial du_l}{\partial x_l^t} \right) d\Omega^t + \int_{\Omega^t} \frac{\partial u_i^*}{\partial x_k^t} \left(-dp^t \delta_{ik} \right) d\Omega^t = \int_{\Omega^t} F_i^{HE} u_i^*\, d\Omega^t$$

Large strain term: stress matrix

Let's consider now the fluid mass balance equation and follow the same procedure.

Assuming the same configuration in $\tau 1$ and $\tau 2$ but different pore pressure $p^{\tau 2} = p^{\tau 1} + \delta p$ we obtain the classical flow stiffness matrix:

$$\int_{\Omega^t} p^* \left(\rho^{w,t} \frac{dp}{k^w} \frac{\phi^t}{k^w} \dot{p}^t + \rho^{w,t} \frac{\phi^t}{k^w} \frac{dp}{dt} + \rho^{w,t} \frac{dp}{k^w} \frac{\dot{\Omega}^t}{\Omega^t} \right) d\Omega^t -$$

$$\int_{\Omega^t} \frac{\partial p^*}{\partial x_k^t} \left(-\rho^{w,t} \frac{dp}{k^w} \frac{\kappa}{\mu} \left(\frac{\partial p^t}{\partial x_k^t} + \rho^{w,t} . g_k \right) - \rho^{w,t} \frac{\kappa}{\mu} \left(\frac{\partial dp}{\partial x_k^t} + \rho^{w,t} \frac{dp}{k^w} . g_k \right) \right) d\Omega^t = \int_{\Omega^t} F_p^{HE} p^* \, d\Omega^t$$

Considering now the influence of the configuration provides us the HM coupling terms:

HM coupling term

$$\int_{\Omega^t} p^* \left(\rho^{w,t} \frac{1-\phi^t}{k^w} \dot{p}^t \frac{1}{\Omega^t} \frac{\partial du_i}{\partial x_i^t} + \rho^{w,t} \left(\frac{1}{\Omega^t . dt} - \frac{\dot{\Omega}^t}{\Omega^t} \frac{1}{\Omega^t} \right) \frac{\partial du_i}{\partial x_i^t} + \dot{M} \frac{\partial du_i}{\partial x_i^t} \right) d\Omega^t -$$

$$\int_{\Omega^t} \frac{\partial p^*}{\partial x_k^t} \left(\rho^{w,t} \frac{\kappa}{\mu} \frac{\partial p^t}{\partial x_k^t} \frac{\partial du_i}{\partial x_k^t} + m_i \frac{\partial du_k}{\partial x_i^t} + m_k \frac{\partial du_i}{\partial x_k^t} \right) d\Omega^t = \int_{\Omega^t} F_p^{HE} p^* \, d\Omega^t$$

Large strain term: « stress matrix »

We have now the expression of the iteration matrix, necessary to find the corrections of the displacement fields *du_i* and the corrections of the pressure *dp* to be added to their respective current values to obtain a new current configuration, and a new pore pressure field closer to a well-balanced configuration:

$$\begin{bmatrix} F_x^{HE} \\ F_y^{HE} \\ F_p^{HE} \end{bmatrix} = \underline{\underline{K}} \begin{bmatrix} du_x \\ du_y \\ dp \end{bmatrix} \qquad \underline{\underline{K}} = \begin{bmatrix} K_{MM}(2\times 2) & K_{WM}(2\times 1) \\ K_{MW}(1\times 2) & K_{WW}(1\times 1) \end{bmatrix}$$

The classical matrices are located on the diagonal. The K_{MM} submatrix takes into account for the material and geometrical non linearities. The two other submatrices contain the effect of the Hydro-mechanical couplings.

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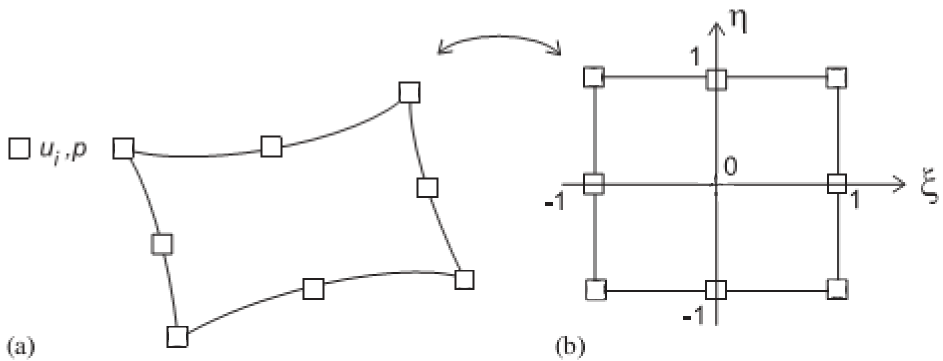
The field equations are spatially discretized using 2D plane strain isoparametric finite elements with eight nodes for u_i and dp. The usual quadratic serendipity shape function are used.

$$X_i = \phi_L \, X_{iL}$$

$$x_i = \phi_L \, x_{iL}$$

$$p = \phi_L \, p_L$$



(a) Quadrilateral element (b) parent element

In the element, the internal virtual work equations are computed:

$$\partial W_I^{Meca} = \int_\Omega \sigma_{ij} \dot{\varepsilon}_{ij}^* d\Omega = \int_\Omega \sigma_{ij} \frac{1}{2}\left(\frac{\partial \dot{u}_i^*}{\partial x_j} + \frac{\partial \dot{u}_j^*}{\partial x_i} \right) d\Omega$$

$$\partial W_I^{Fluid} = \int_\Omega \dot{M}.p^* - m_i \frac{\partial p^*}{\partial x_i} d\Omega$$

Where the virtual quantities (displacement rate and pore pressure vairation) are expressed as a function of nodel values:

$$\underline{\dot{u}}^* = \phi_L . \underline{\dot{u}}_L^* \qquad p^* = \phi_L . p_L^*$$

In 2D plane strain state, we obtain the expression of the nodal forces and flux:

$$F_{1L} = \sum_{PI} (\sigma_{11} \frac{\partial \phi_L}{\partial x_1} + \sigma_{12} \frac{\partial \phi_L}{\partial x_2}) t \,|\underline{J}|\, W_{PI}$$

$$F_{2L} = \sum_{PI} (\sigma_{12} \frac{\partial \phi_L}{\partial x_1} + \sigma_{22} \frac{\partial \phi_L}{\partial x_2}) t \,|\underline{J}|\, W_{PI}$$

$$F_{pL} = \sum_{PI} \left(\dot{M}.\phi_L - m_i \frac{\partial \phi_L}{\partial x_i} \right) .t. |\underline{J}| W_{PI}$$

Time discretization

A time step is defined by time t^A (beginning of the step) and time t^B (end of the step).

Pressure will be assumed to vary linearly on the time step.

Using a isoparametric formalism, it comes that :

$$t = N^A t^A + N^B t^B$$

$$p = N^A p^A + N^B p^B$$

$$N^A = 1 - \xi$$

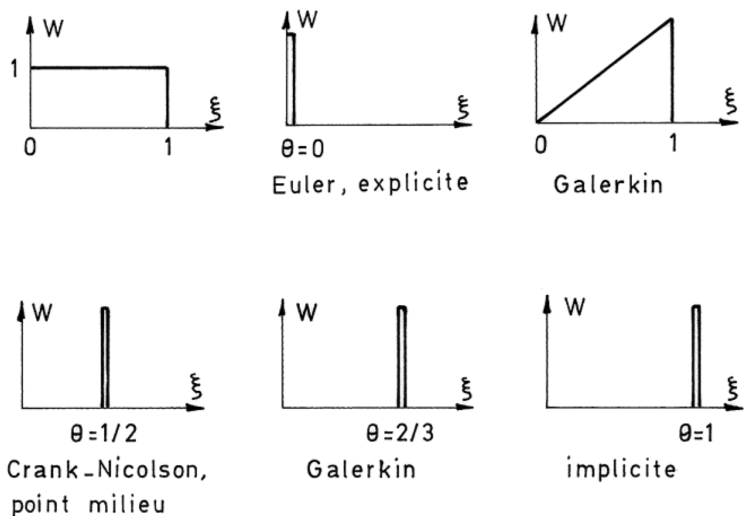
$$N^B = \xi$$

$$\xi \in [0,1]$$

Equilibrium equation

It is obvious that we can not ensure the equilibrium at any time. It must therefore be respected on average over the time step. To do this, we can use the method of weighted residuals, with a weighting function W varying over time. The temporally and spatially discretized balance equation is then written:

$$\int_{t_A}^{t_b} W(t)\, F_L^{\text{extérieur}}\, dt = \int_{t_A}^{t_B} W(t)\, F_L^{\text{intérieur}}\, dt$$



The value of θ is defined in the loading file (5th line, STRAT(2) coefficient).

The default value is 1 (implicit).

Values of θ higher than 0.5 guarantee stability.

1. General principal

When equilibrium is not met, a new configuration should be find for which the out of banlance forces vanish. Based on the mathematical formulation of the auxiliary linear problem and introducing the isoparametric function, we can define the stiffness matrix:

$$\int_{\Omega^t} \frac{\partial \phi_L}{\partial x_k^t} u_{i,L}^* \left(\boxed{C_{ijkl} \frac{\partial \phi_J}{\partial x_j^t}} du_{l,J} - \boxed{\sigma_{ij}^t \frac{\partial \phi_J}{\partial x_j^t} du_{k,J} + \sigma_{ik}^t \frac{\partial \phi_J}{\partial x_l^t} du_{l,J}} \right) d\Omega^t + \int_{\Omega^t} \frac{\partial \phi_L}{\partial x_k^t} u_i^* \boxed{\left(-\phi_J dp_J \delta_{ik} \right)} d\Omega^t = \int_{\Omega^t} F_i^{HE} \phi_L u_{i,L}^* \, d\Omega^t$$

$$\int_{\Omega^t} \phi_L p_L^* \left(\boxed{\rho^{w,t} \frac{\phi_J dp_J}{k^w} \frac{\phi^t}{k^w} \dot{p}^t + \rho^{w,t} \frac{\phi^t}{k^w} \frac{\phi_J dp_J}{dt} + \rho^{w,t} \frac{\phi_J dp_J}{k^w} \frac{\dot{\Omega}^t}{\Omega^t}} \right) d\Omega^t +$$

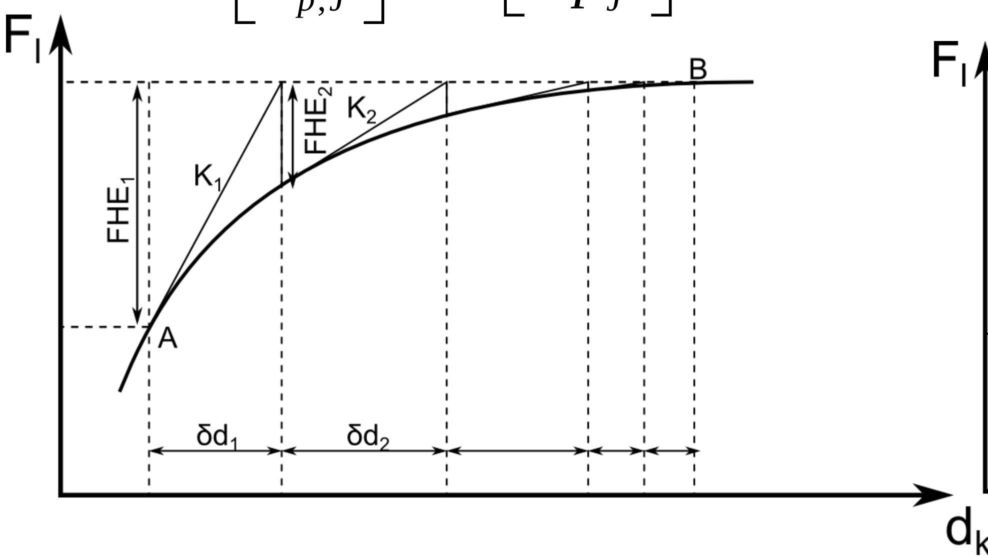
$$\int_{\Omega^t} \phi_L p_L^* \left(\boxed{\rho^{w,t} \frac{1-\phi^t}{k^w} \dot{p}^t \frac{1}{\Omega^t} \frac{\partial \phi_J}{\partial x_i^t} du_{i,J} + \rho^{w,t} \left(\frac{1}{\Omega^t . dt} - \frac{\dot{\Omega}^t}{\Omega^t} \frac{1}{\Omega^t} \right) \frac{\partial \phi_J}{\partial x_i^t} du_{i,J}} + \boxed{\dot{M} \frac{\partial \phi_J}{\partial x_i^t} du_{i,J}} \right) d\Omega$$

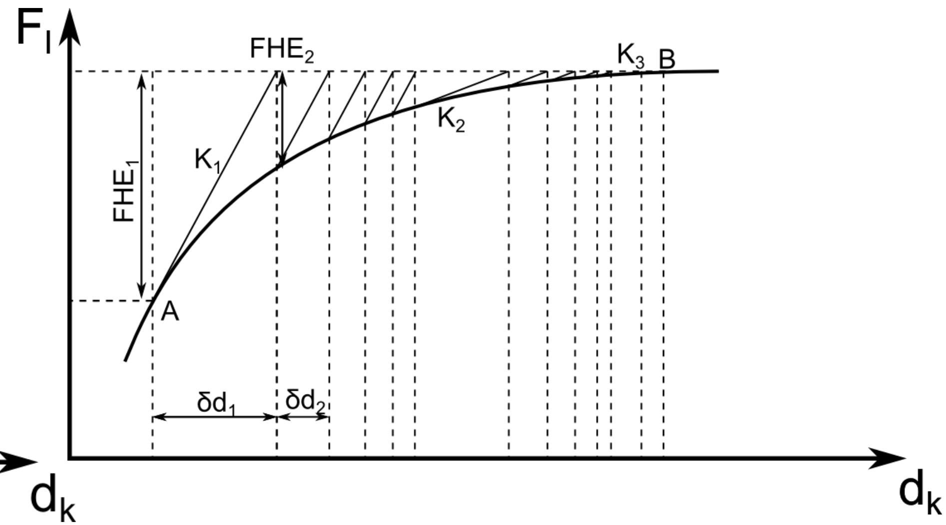
$$- \int_{\Omega^t} \frac{\partial \phi_L}{\partial x_k^t} p_L^* \left(\boxed{- \rho^{w,t} \frac{\phi_J dp_J}{k^w} \frac{\kappa}{\mu} \left(\frac{\partial p^t}{\partial x_k^t} + \rho^{w,t} . g_k \right) - \rho^{w,t} \frac{\kappa}{\mu} \left(\frac{\partial \phi_J}{\partial x_k^t} dp_J + \rho^{w,t} \frac{\phi_J dp_J}{k^w} . g_k \right)} \right) d\Omega^t$$

$$- \int_{\Omega^t} \frac{\partial \phi_L}{\partial x_k^t} p_L^* \left(\boxed{\rho^{w,t} \frac{\kappa}{\mu} \frac{\partial p^t}{\partial x_k^t} \frac{\partial \phi_J}{\partial x_k^t} du_{i,J} + m_i \frac{\partial \phi_J}{\partial x_i^t} du_{k,J} + m_k \frac{\partial \phi_J}{\partial x_k^t} du_{i,J}} \right) d\Omega^t = \int_{\Omega^t} F_p^{HE} \phi_L . p_L^* \, d\Omega^t$$

$$\begin{bmatrix} F^{HE}_{x,J} \\ F^{HE}_{y,J} \\ F^{HE}_{p,J} \end{bmatrix} = \underline{\underline{K}} \begin{bmatrix} du_{x,J} \\ du_{y,J} \\ dp_J \end{bmatrix}$$

$$\underline{\underline{K}} = \begin{bmatrix} K_{MM}(2\times 2) & K_{WM}(2\times 1) \\ K_{MW}(1\times 2) & K_{WW}(1\times 1) \end{bmatrix}$$



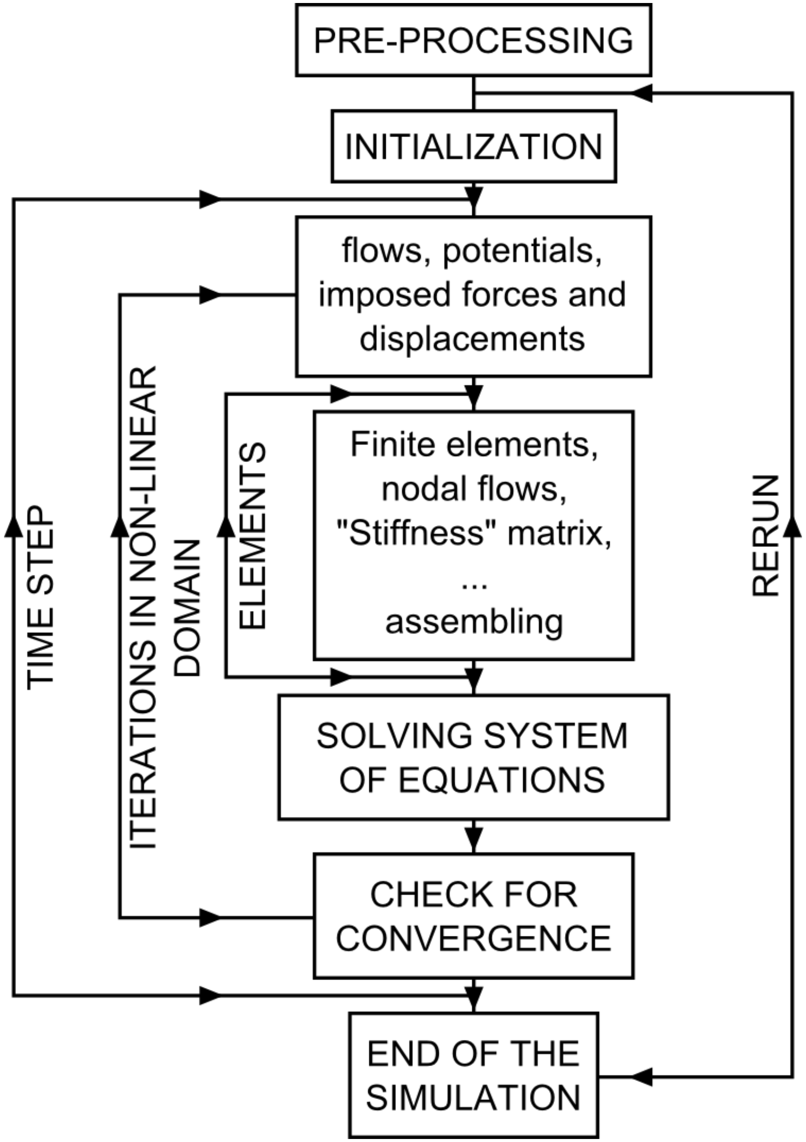


ISTR(1)=1; ISTR(2)=2; ISTR(3)=1

ISTR(1)=1; ISTR(2)=5; ISTR(3)=5

Computing all the terms and assembling the matrix is time consuming, it is possible to evaluate the matrix after each iteration or not (3rd line, ISTR(1), ISTR(2) and ISTR(3) in the loading file).
For hydro-mechanical problem, the global stiffness matrix is non-symmetric.

2. General Algorithm



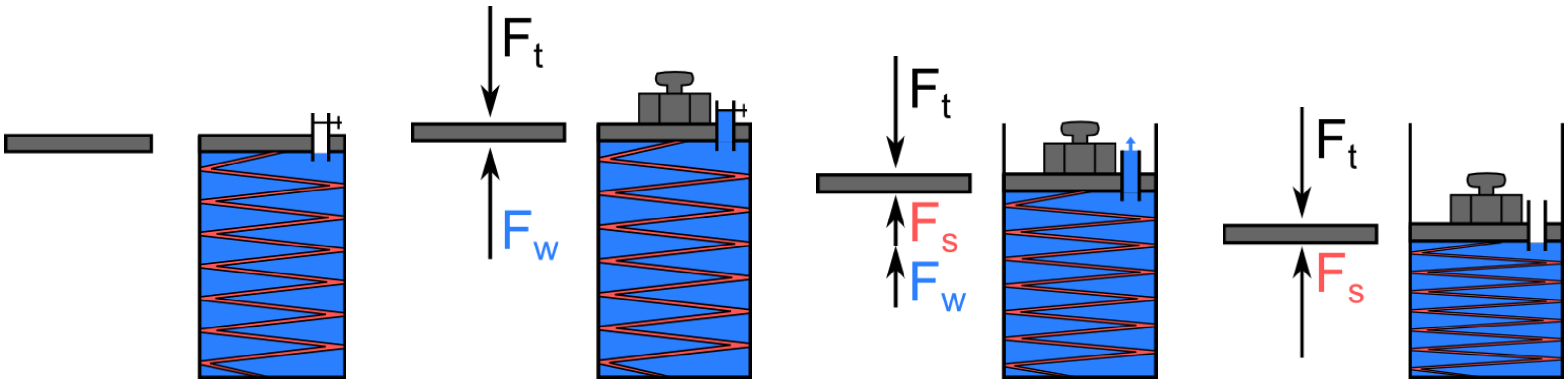
3. Convergence norm

By default the norm of the out of balance forces is evaluated through the following relationship:

$$\left\| F^{HE} \right\| = \frac{\sqrt{\dfrac{\sum \left(F^{HE}\right)^2}{N_{equation}}}}{\sqrt{\dfrac{\sum \left(F^{imp}\right)^2}{N_{Force}} + \dfrac{\sum \left(F^{react}\right)^2}{N_{React}}}}$$

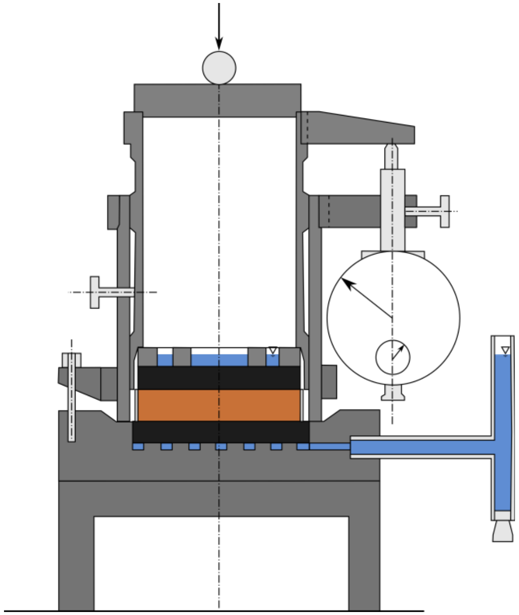
Knowing that the order of magnitude of the out of balance forces for the mechanical problem and the flow problem respectively are really different. It is therefore necessary to sum the norm of each problem computed separately:

$$\left\| F^{HE} \right\| = \left\| F^{HE} \right\|^{Meca} + \left\| F^{HE} \right\|^{hydro}$$

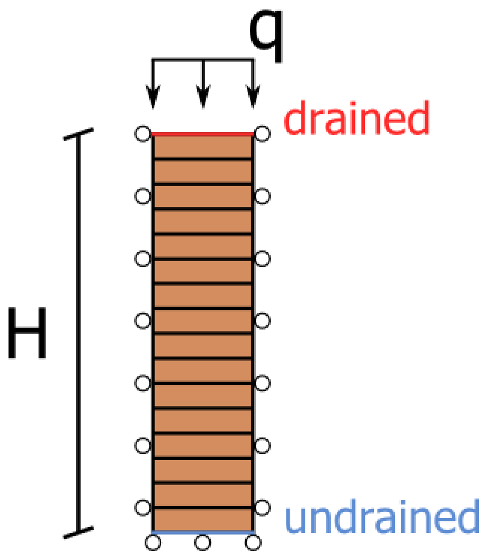


STEP	Load	Drainage	Stress (soil)	Overpressure (water)
1	No	No	No	No
2	Yes	No	No	Maximum
3	Yes	Yes	Increasing	Decreasing
4	Yes	Yes	Maximum	No

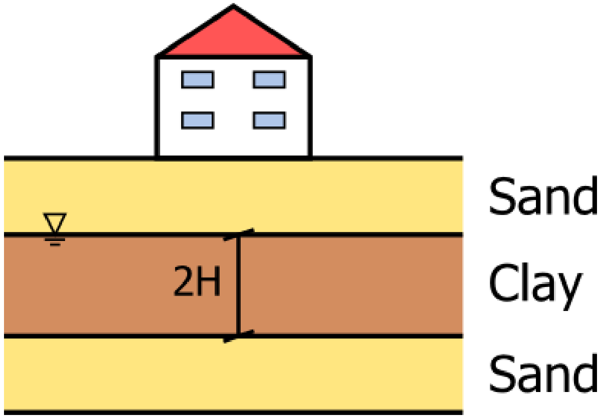
Oedometer test



Numerical model



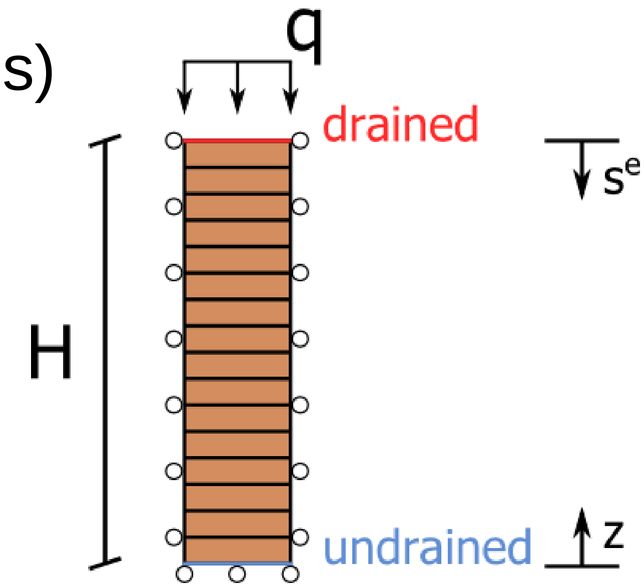
Reality



Characteristics :

- Soil height : 2H
- Vertical displacement only
- Drained bases
- Constant load

Analytical Solution (two drained bases)



Maximum settlement :

$$s^e_{\max} = \frac{H}{m_v \cdot q}$$

Adimensional time :

$$T_v = \frac{c_v \cdot t}{H^2}$$

Adimensional settlement :

$$\frac{s(T_v)}{s^e_{\max}} = 1 - \sum_{n=1,2}^{N} \frac{8}{n^2 \cdot \pi^2} \cdot \exp\left(- \frac{n^2 \cdot \pi^2}{4} \cdot T_v \right)$$

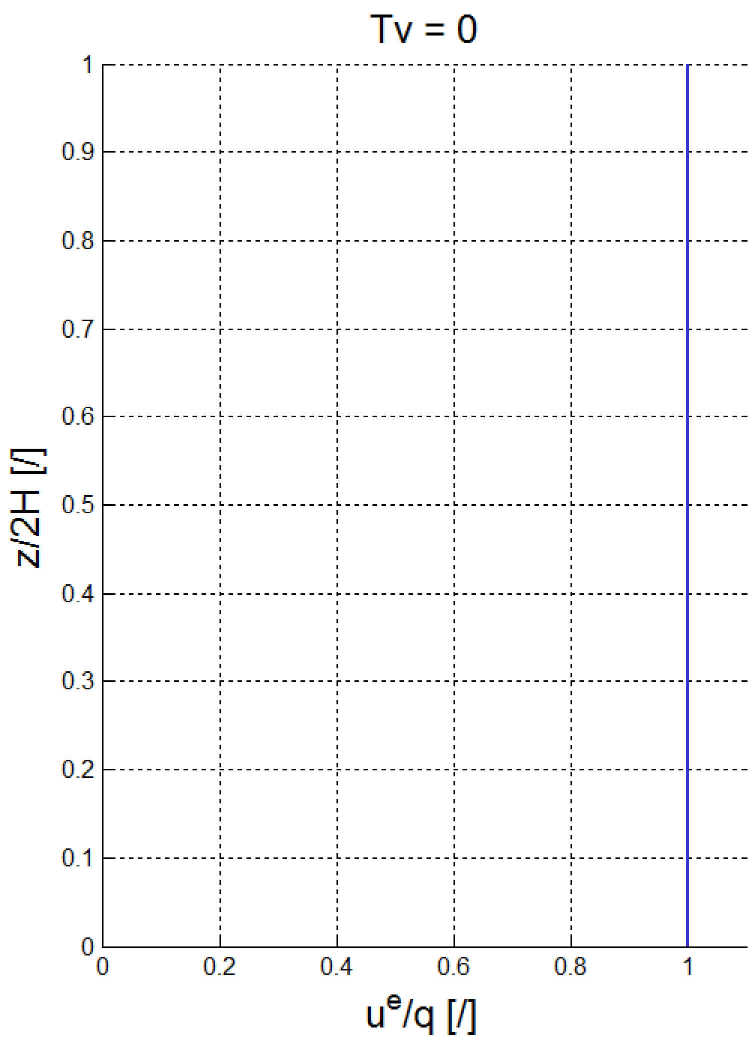
Adimensional pore pressure distribution :

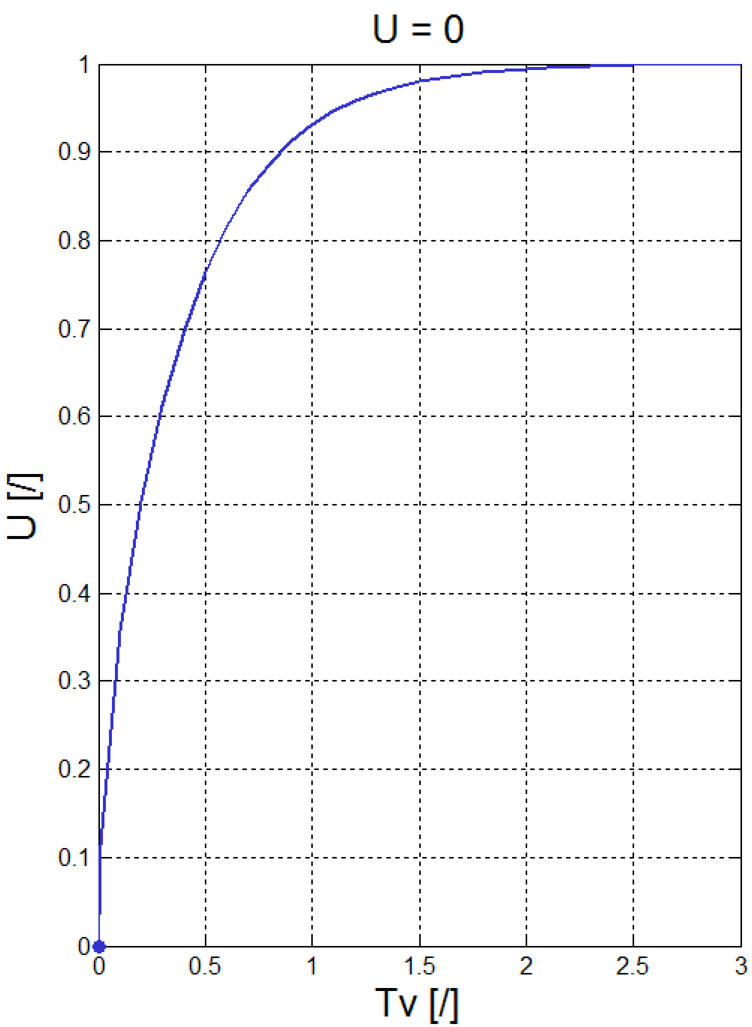
$$\frac{u^e(z, T_v)}{q} = \sum_{n=1}^{N} \frac{-2}{n \cdot \pi} \cdot (-1)^n \cdot \exp\left(- \frac{n^2 \cdot \pi^2}{4} \cdot T_v \right) \cdot \sin\left(\frac{\pi \cdot n}{2 \cdot H} \cdot z \right)$$

Soil parameters

$$m_v = \frac{1}{E} \cdot \left(1 - \frac{2 \cdot \nu^2}{1 - \nu} \right)$$

$$c_v = \frac{K_0}{\gamma_w \cdot m_v}$$


Tv = 0
z/2H [/]
u^e/q [/]
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0.2
0.4
0.6
0.8


U = 0
U [/]
Tv [/]
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0.5
1.5
2
2.5
3

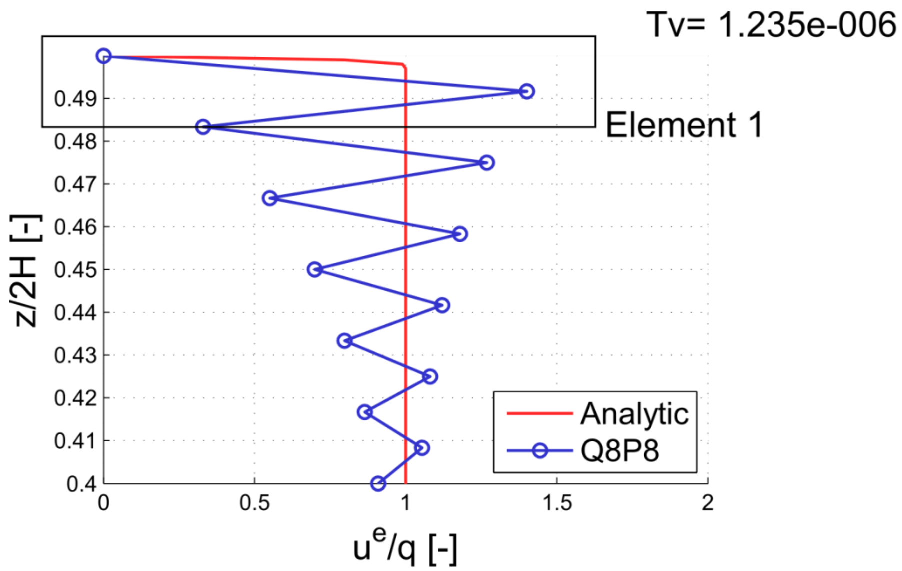
Comparison : Analytic solution & LAGAMINE

E [Pa]	**υ [-]**	**k [m²]**	**H [m]**
10^{7}	0.2	10^{-18}	0.03

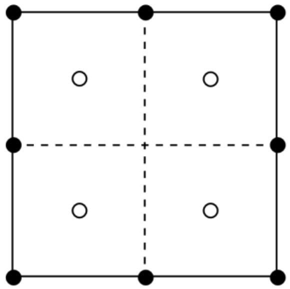
Geometry : 30 elements CSOL2

	Q8P8	**Q8P4**	**Q25P25**
DoF's	300	241	1563

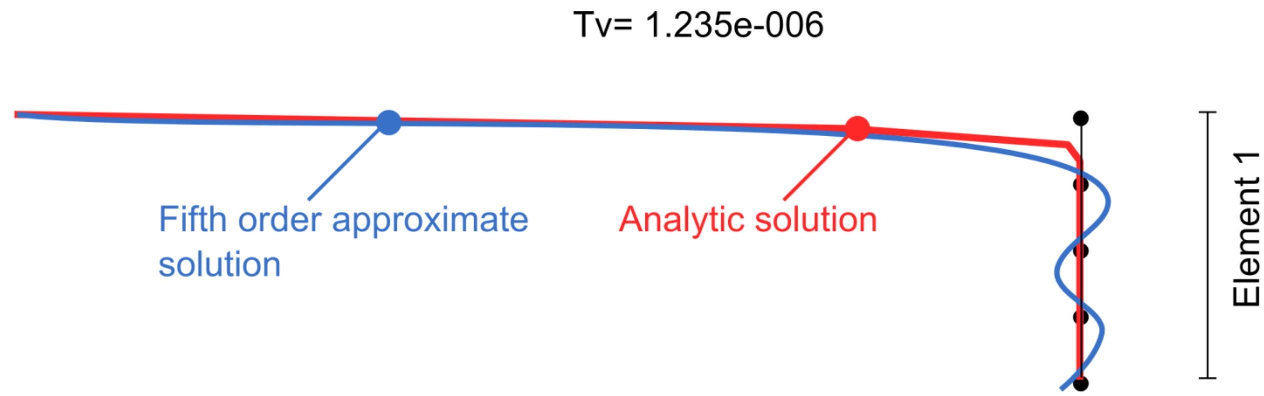
Application of HM problem: consolidation

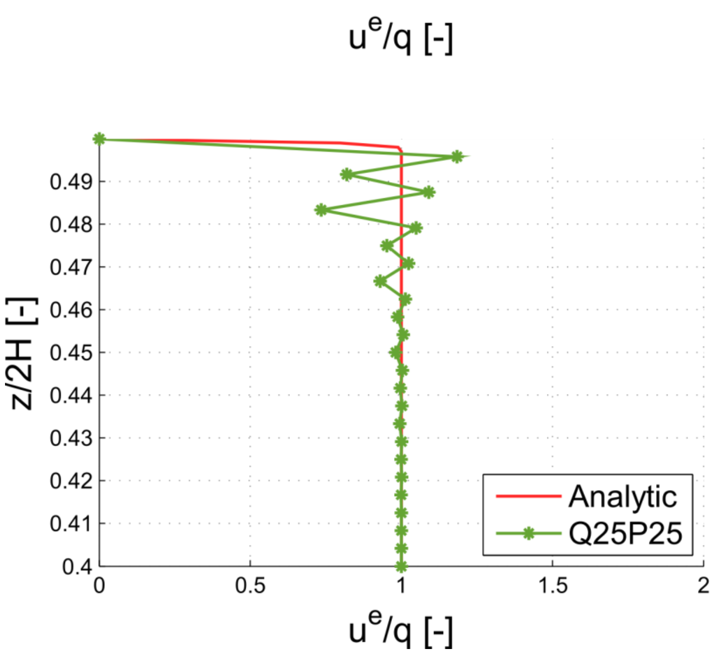


Q8P8 :
- meca : 8 nodes
  => parabolic shape function
- hydro : 8 nodes
  => parabolic shape function

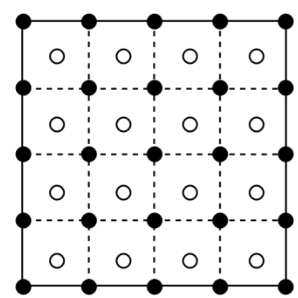


Application of HM problem: consolidation

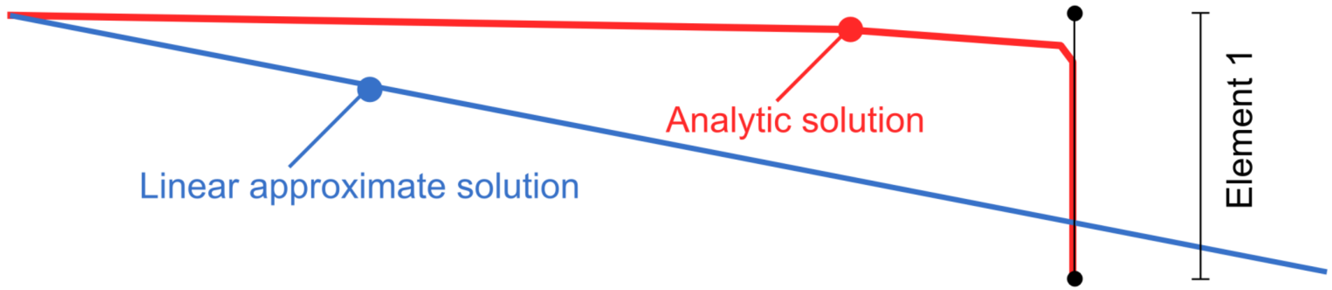




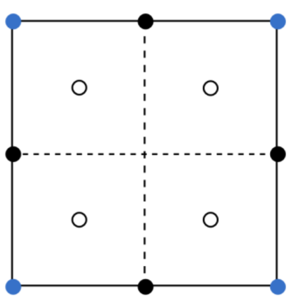
Q25P25 :
- meca : 25 nodes
  => 5th order shape function
- hydro : 25 nodes
  => 5th order shape function

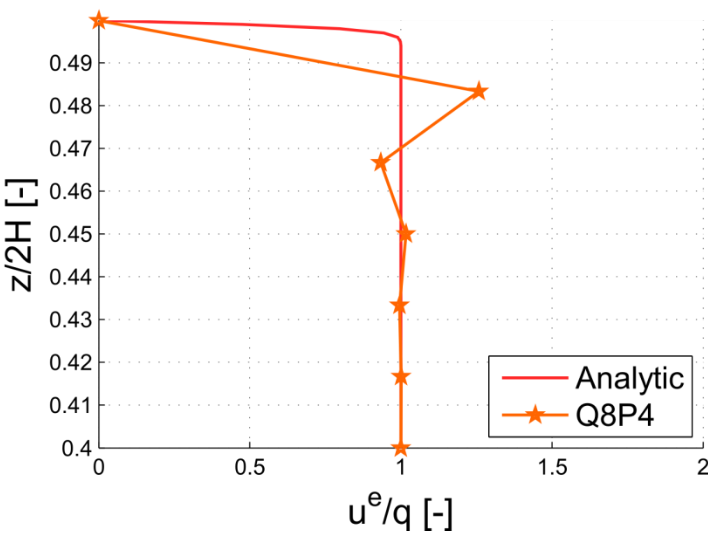


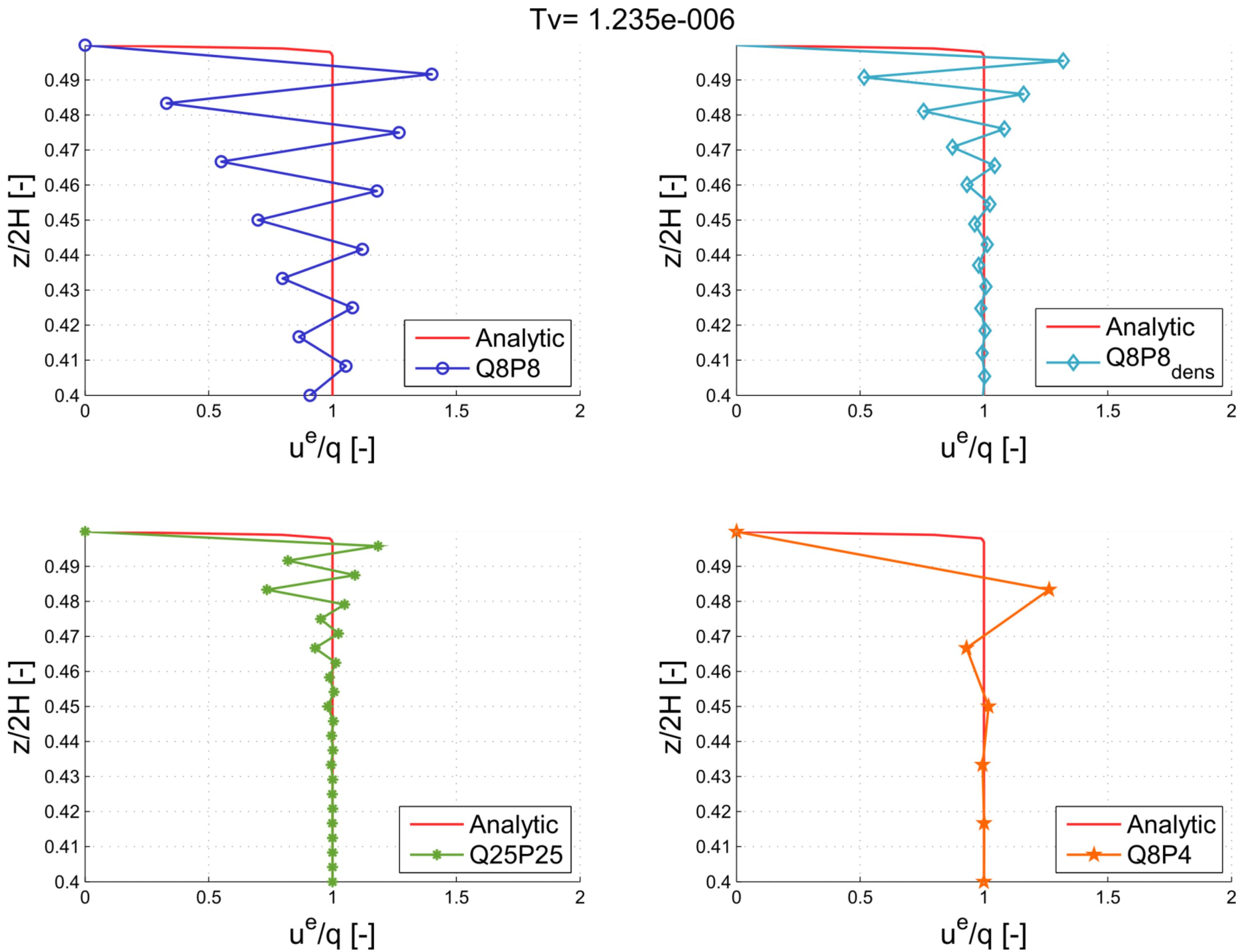
Tv= 1.235e-006



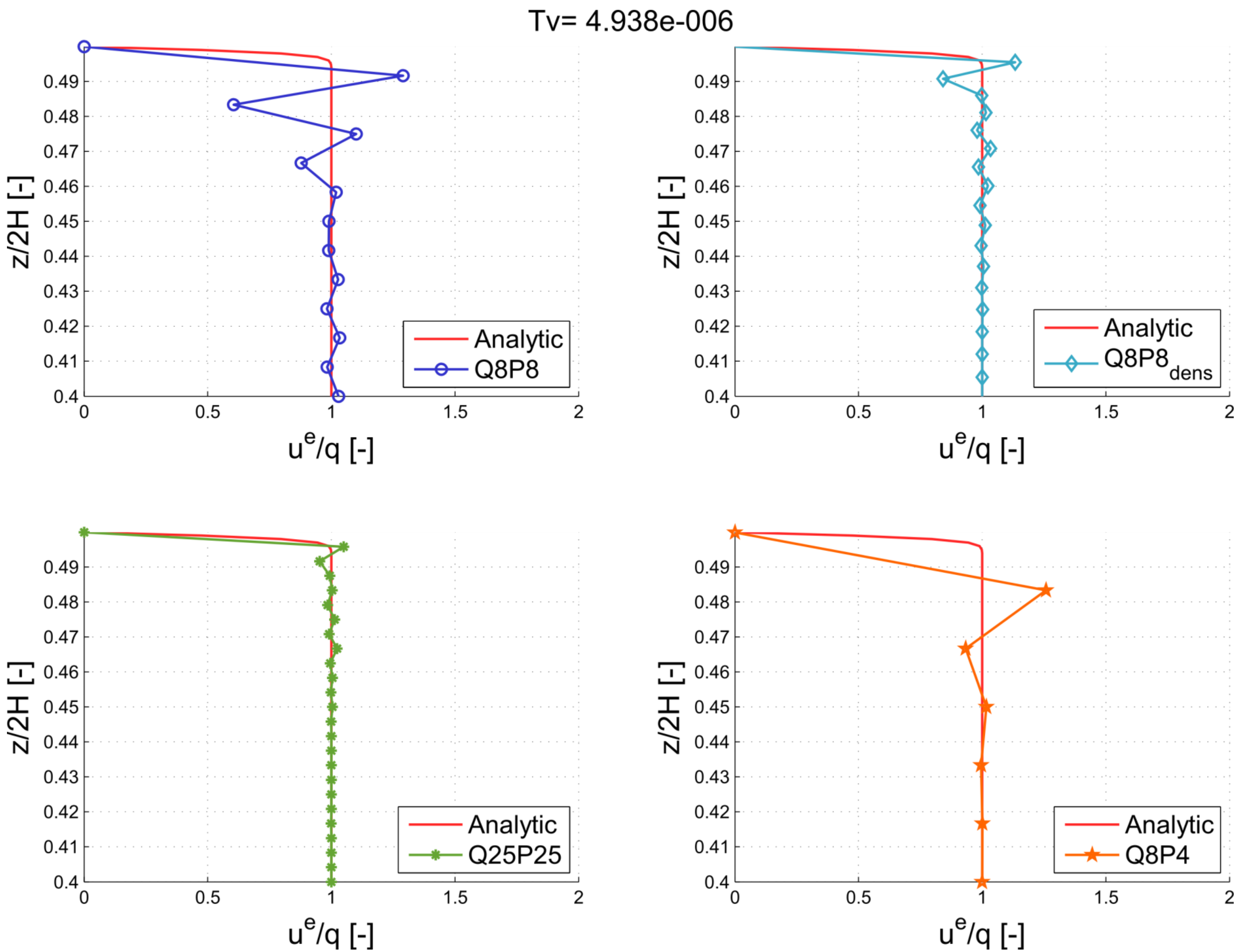
Q8P4 :
- meca : 8 nodes
  => parabolic shape function
- hydro : 4 nodes
  => **linear** shape function



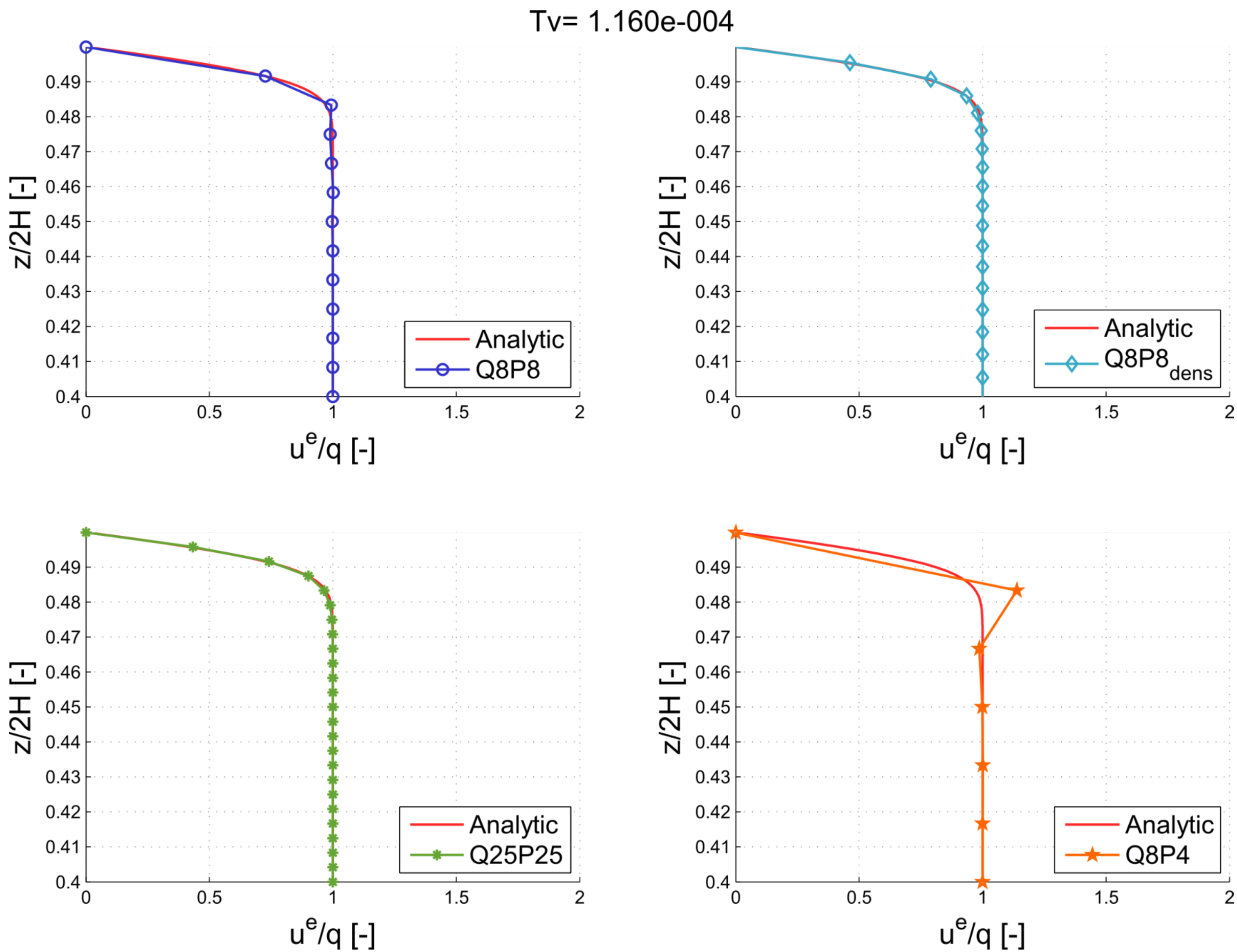



Tv= 1.235e-006
z/2H [-]
u^e/q [-]
0.4
0.41
0.42
0.43
0.44
0.45
0.46
0.47
0.48
0.49
0
0.5
1
1.5
2
Analytic
Q8P8
Analytic
$Q8P8_{dens}$
Analytic
Q25P25
Analytic
Q8P4

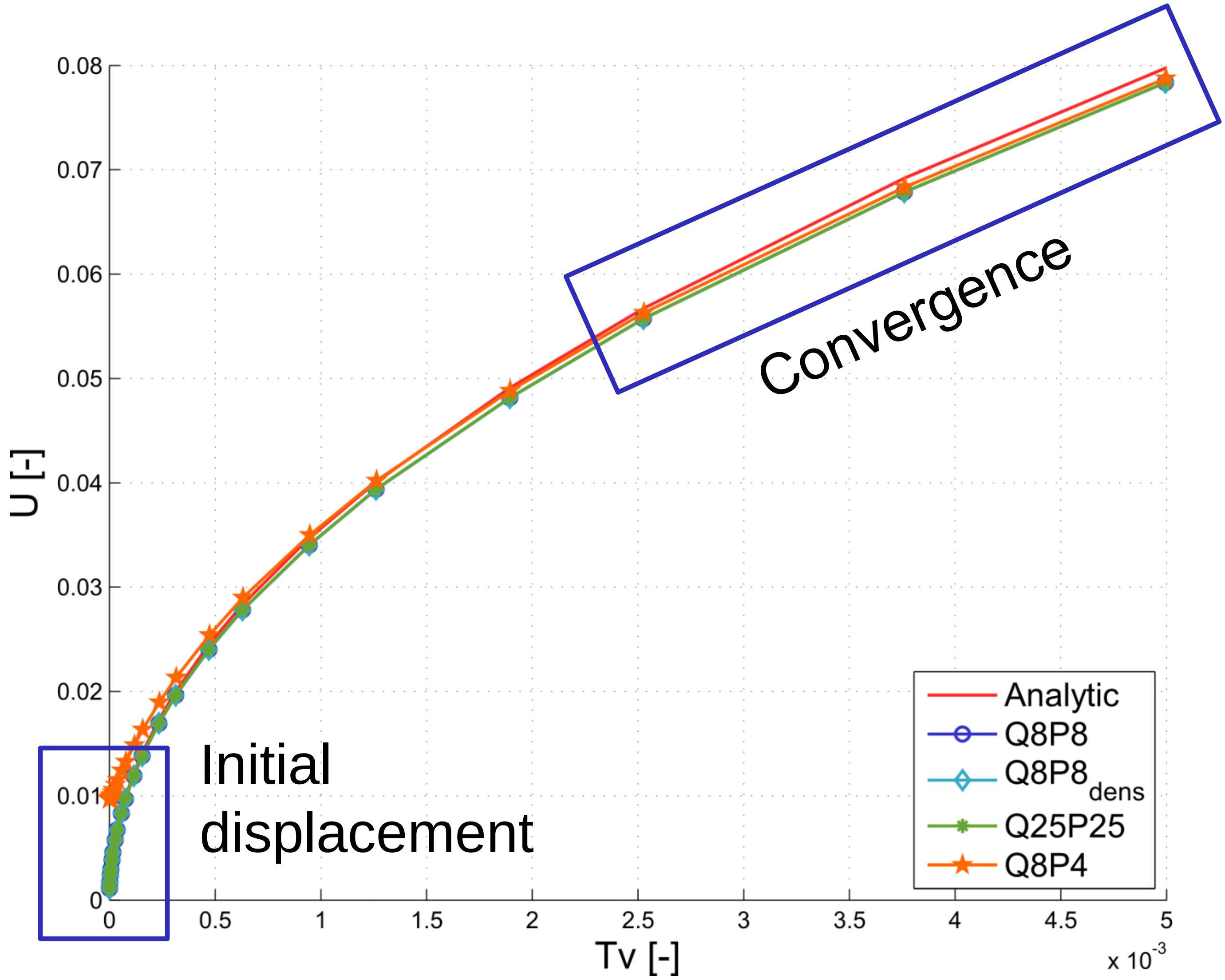
Application of HM problem: consolidation



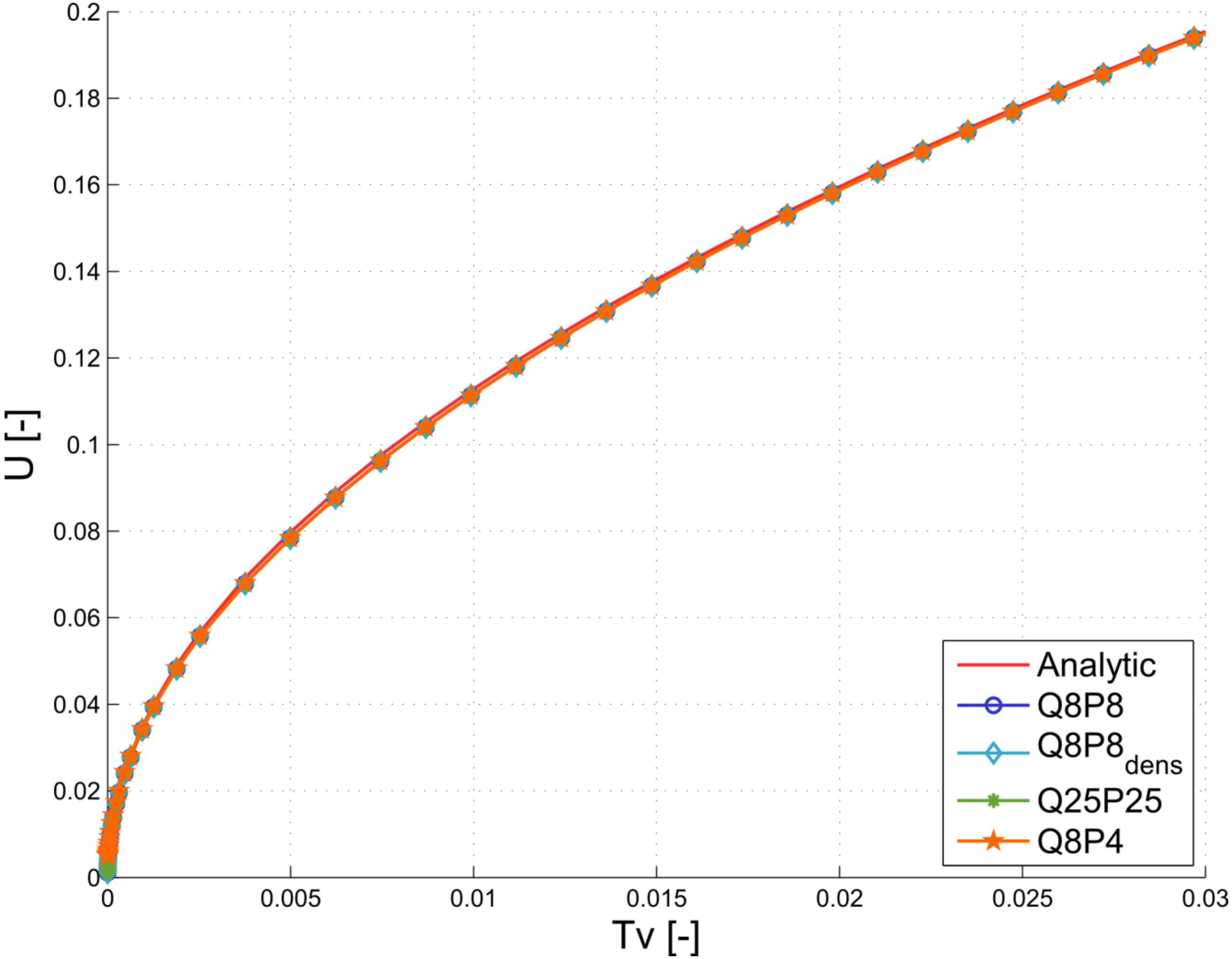
Application of HM problem: consolidation



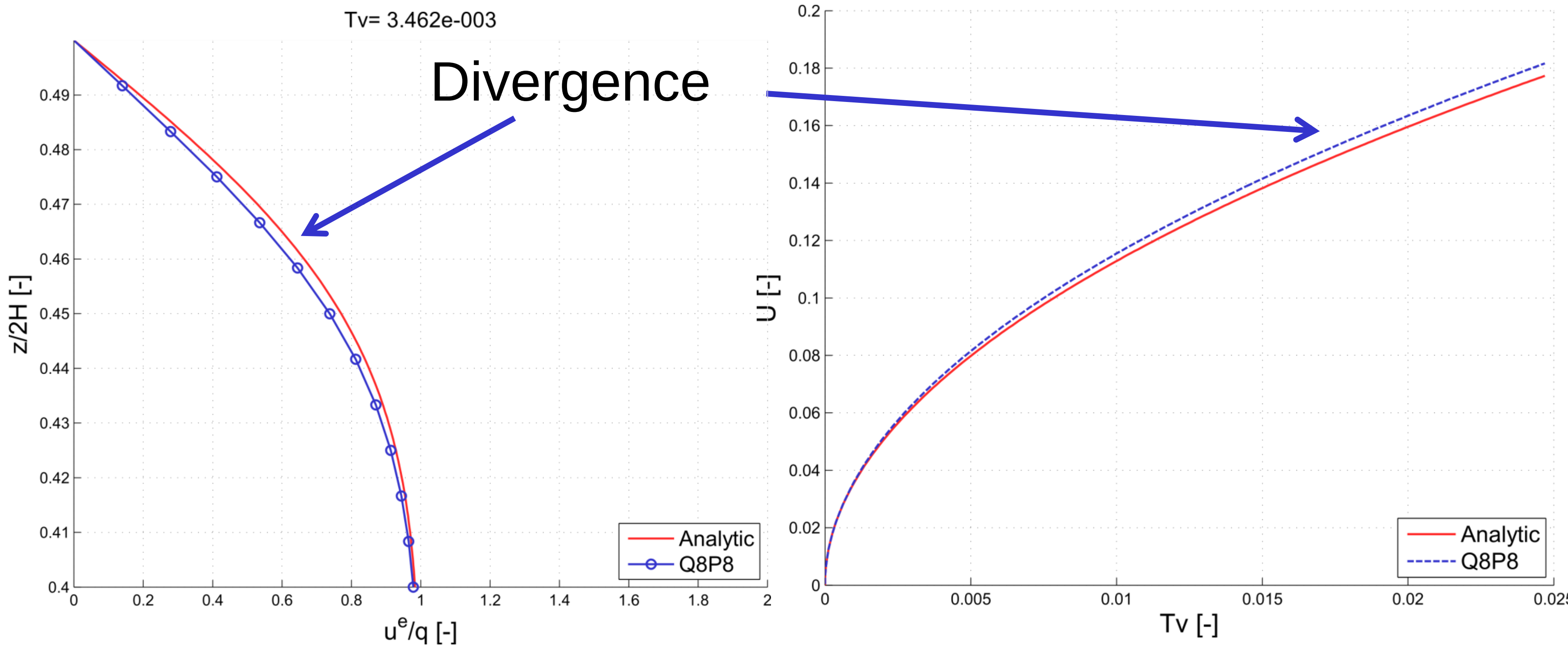
Application of HM problem: consolidation



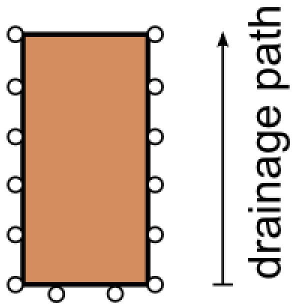
Application of HM problem: consolidation



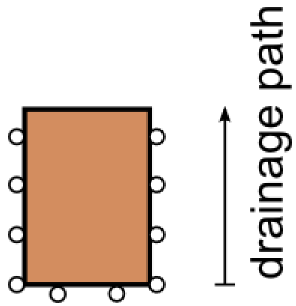
Comparison for E=10^6 Pa



Initial Sample & Analytic Solution

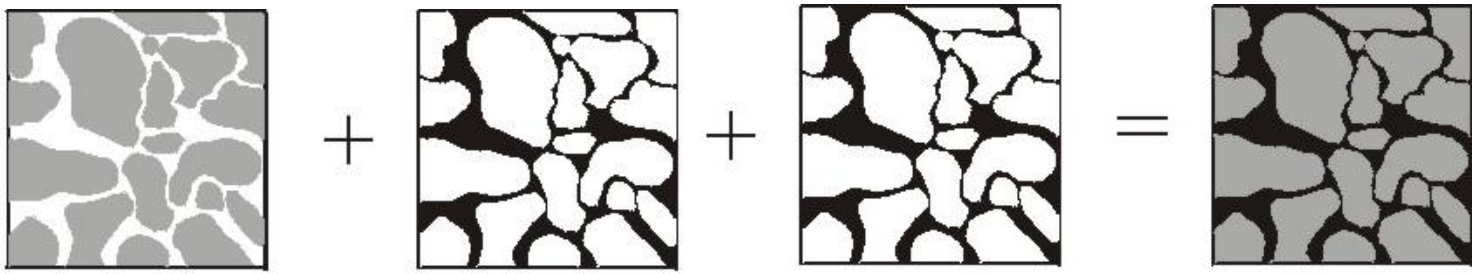


Deformed Sample

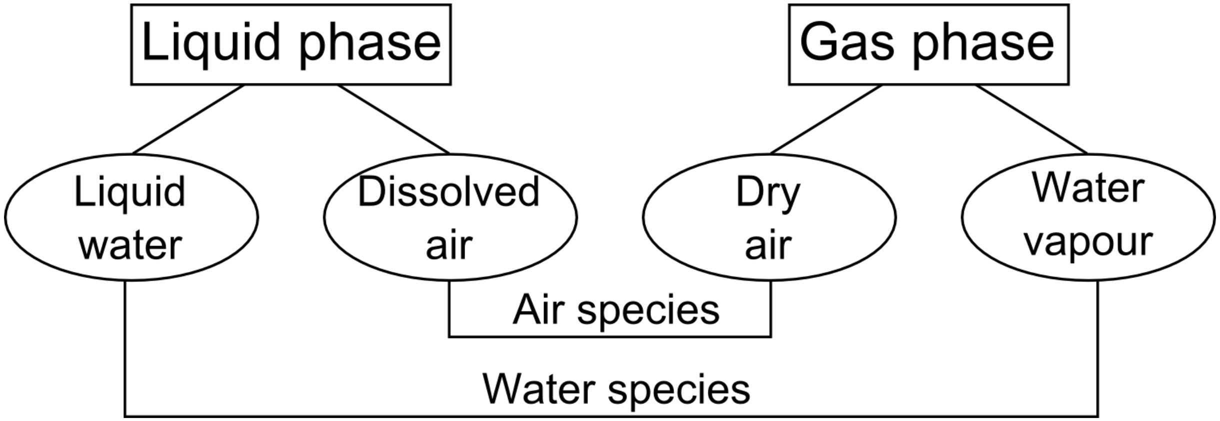


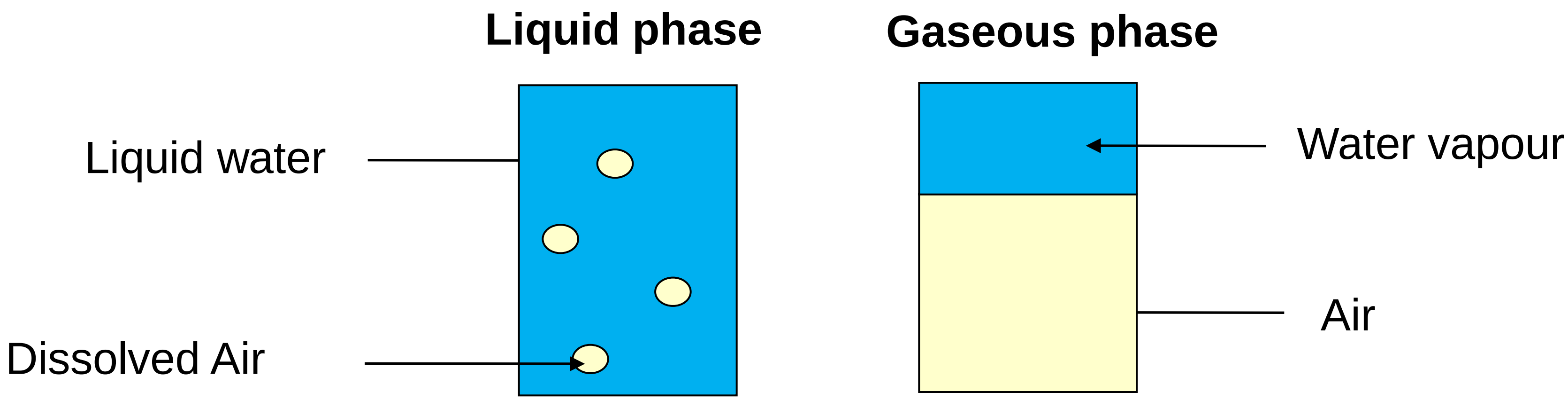
- Introduction
- Mathematical formulation of HM problem
- Finite element formulation (CSOL2)
- **Mathematical formulation of THM problem (MWAT2)**
- Mathematical formulation of C/B-THM problem
- Conclusion

Unsaturated porous medium



Solid skeletton Pore Fluid 1 Pore fluid 2 Porous medium





Water mass balance

$$div\left(\underline{f}_w\right)+div\left(\underline{f}_v\right)+\dot{S}_w+\dot{S}_v-Q_{H_2O}=0$$

Air mass balance

$$div\left(\underline{f}_a\right)+div\left(\underline{f}_{a-d}\right)+\dot{S}_a+\dot{S}_{a-d}-Q_a=0$$

Momentum balance

$$div(\sigma_{ij})+\rho g_i=0$$

Liquid phase: *Liquid water + Dissolved air*

- Liquid phase advection (unsaturated Darcy's flow) $\underline{q}_l = -\frac{k k_r^w (S_{r,w})}{\mu_w} (\underline{\nabla} p_w + \rho_w g \underline{\nabla} z)$
- Dissolved air diffusion (Fick's law) $\underline{i}_{(Ar)_d} = -\rho_w S_{r,w} D_{Ar}^{H_2O} \underline{\nabla} \left(\frac{\rho_{Ar}^w}{\rho_w} \right)$

Henry's law $\rho_{Ar}^w = H_{Ar}(T).\rho_{Ar}^g$

Gaseous phase: *Water vapour + dry air*

- Gaseous phase advection $\underline{q}_g = -\frac{k k_r^g (S_{r,g})}{\mu_g} (\underline{\nabla} p_g + \rho_g g \underline{\nabla} z)$
- Dry air – water vapour diffusion $\underline{i}_{(Ar)_g} = -\rho_g S_{r,g} D_{Ar}^{vapeur} \underline{\nabla} \left(\frac{\rho_{Ar}^g}{\rho_g} \right) = -\underline{i}_{(H_2O)_g}$

Liquid water: $\dot{S}_{(H_2O)_l} + div(\underline{f}_{(H_2O)_l}) + \dot{E}^{l\to g}_{H_2O} = Q_{(H_2O)_l}$

Water vapour: $\dot{S}_{(H_2O)_g} + div(\underline{f}_{(H_2O)_g}) - \dot{E}^{l\to g}_{H_2O} = Q_{(H_2O)_g}$

$\dot{S}_{(H_2O)_l} / \dot{S}_{(H_2O)_g}$: Storage term liquid water / water vapour

$\underline{f}_{(H_2O)_l} / \underline{f}_{(H_2O)g}$: mass flow of liquid water / water vapour

$\dot{E}^{l\to g}_{H_2O}$: Evaporation mass rate

$Q_{(H_2O)_l} / Q_{(H_2O)g}$: Production – consumation of liquid water / water vapour

$$\underline{f}_{(H_2O)_l} = \rho_w . \underline{q}_l$$

$$\underline{f}_{(H_2O)_g} = \rho^g_{H_2O} . \underline{q}_g + \underline{i}_{(H_2O)_g}$$

$\underline{q}_l$ et $\underline{q}_g$: liquid and gas phase flow

$\underline{i}_{(H_2O)_g}$: diffusive water vapour flow

$$\Rightarrow \frac{\partial}{\partial t}(\rho_w . \varphi . S_{r,w} + \rho^g_{H_2O} . \varphi . S_{r,g}) + div\left(\rho_w . \underline{q}_l\right) + div\left(\underline{i}_{(H_2O)_g} + \rho^g_{H_2O} . \underline{q}_g\right) - Q_{H_2O} = 0$$

Q_{H_2O} Production – consumation of water

Gaseous air: $$\dot{S}_{(Air)_g} + div(\underline{f}_{(Air)_g}) + \dot{E}^{g\rightarrow d}_{Air} = Q_{(Air)_g}$$

Dissolved air: $$\dot{S}_{(Air)_d} + div(\underline{f}_{(Air)_d}) - \dot{E}^{g\rightarrow d}_{Air} = Q_{(Air)_d}$$

$\dot{S}_{(Air)_g} / \dot{S}_{(Air)_d}$: Storage term dry air / dissolved air

$\underline{f}_{(Air)_g} / \underline{f}_{(Air)_d}$: mass flow of dry air / dissolved air

$\dot{E}^{g\rightarrow d}_{Air}$: Dissolution mass rate

$Q_{(Air)_g} / Q_{(Air)_d}$: Production – consumation of dry air / dissolved air

$$\underline{f}_{(Air)_g} = \rho^g_{Air}.\underline{q}_g + \underline{i}_{(Air)_g}$$

$$\underline{f}_{(Air)_d} = \rho^g_{Air}.H_{Air}.\underline{q}_l + \underline{i}_{(Air)_d}$$

$\underline{q}_l$ et $\underline{q}_g$: liquid and gas phase flow

$\underline{i}_{(Air)_g} / \underline{i}_{(Air)_d}$: diffusive dry air and dissolved air flow

→

$$\frac{\partial}{\partial t}(\rho^g_{Air}.\varphi.S_{r,g} + \rho^g_{Air}.H_{Air}.\varphi.S_{r,w}) + div(\rho^g_{Air}.\underline{q}_g + \underline{i}_{(Air)_g}) + div(\rho^g_{Air}.H_{Air}.\underline{q}_l + \underline{i}_{(Air)_d}) - Q_{(Air)} = 0$$

$Q_{(Air)}$: Production – consumation of air

Thermo-hydro-mechanical problem

$$\underline{\text{Heat transfer}}: \quad \dot{S}_T + \dot{E}^{w\rightarrow v}_{H_2O}.L + div(\underline{f}_T) - Q_T = 0$$

$\dot{S}_T$	: Storage term of heat
$\underline{f}_T$	: Heat flow
$\dot{E}^{g\rightarrow d}_{Air}$	: Evaporation mass rate
Q_T	: Production – consumation of heat
L	: Evaporation Latent Heat

$$\underline{f}_T = \underline{i}_{cond} + \sum_i H_i.\underline{f}_i^{eff}$$

$$\underline{i}_{cond} = -\Gamma_m.\underline{grad}(T)$$

H_i	: Enthalpy of species i
$\underline{i}_{cond}$	: Conductive heat flow

$$\dot{S}_T + \dot{S}_v.L + div(\underline{V}_v).L + div(\underline{i}_{cond} + \sum_i H_i.\underline{V}_i^{eff}) - Q_T = 0$$

$Q_{(Air)}$: Production – consumation of heat

This formulation can be adapted for many applications with various materials, fluids.

Some parameters are related to the physical processes:

IKW, IKA, ISRW, ITHERM, IENTH: definition of the relative permeability curves, retention curve, thermal conductivity evolution and heat capacity expression (See appendix 8)

IVAP : water vapour taken into account

ICONV : heat convection taken into account

IGAS: 0 = air ; 1 = hydrogen ; 2 = nitrogen ; 3 = argon ; 4 = helium ; 5 = CO_2 ;
6 = CH_4

Other parameters are related to the numerical purposes:

ITEMOIN: stiffness matrix computed analyticaly or numerically

IFORM: secant or tangent formulation of the storage term.

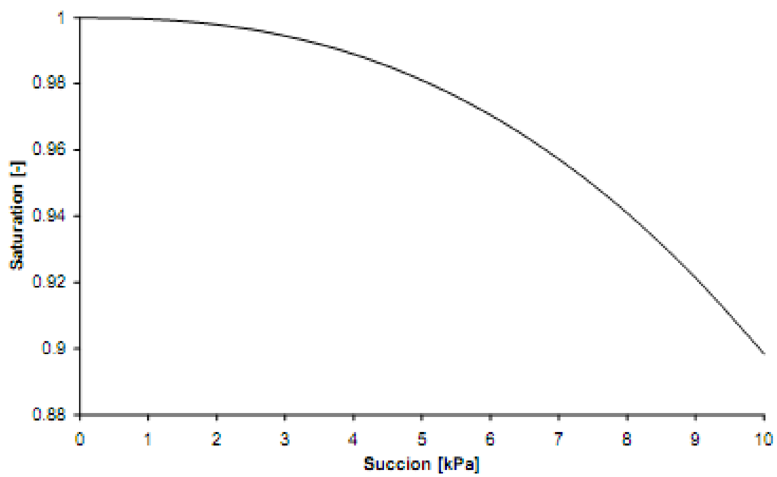
As an extension of the hydro-mechanical problem, the stiffness matrix of the MWAT2 element has the following expression:

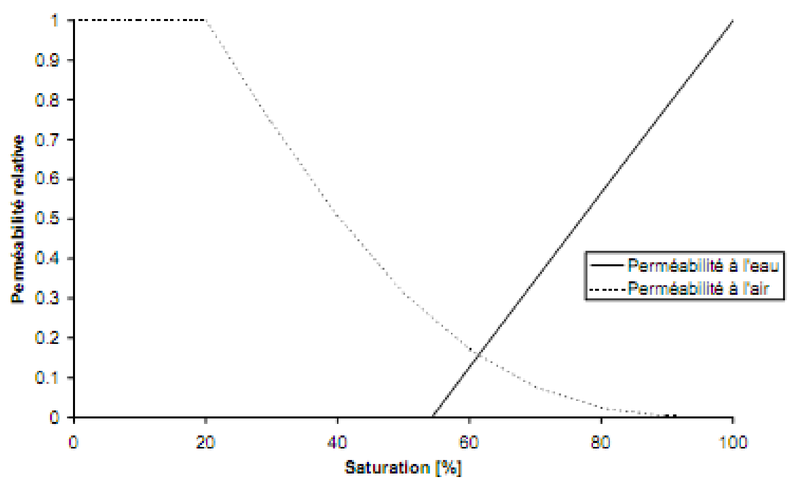
$$\begin{bmatrix} F_x^{HE} \\ F_y^{HE} \\ F_{p_w}^{HE} \\ F_{p_g}^{HE} \\ F_T^{HE} \end{bmatrix} = \underline{\underline{K}} \begin{bmatrix} du_x \\ du_y \\ dp_w \\ dp_g \\ dT \end{bmatrix} \qquad \underline{\underline{K}} = \begin{bmatrix} K_{MM}(2\times2) & K_{WM}(2\times1) & K_{GM}(2\times1) & K_{TM}(2\times1) \\ K_{MW}(1\times2) & K_{WW}(1\times1) & K_{GW}(1\times1) & K_{TW}(1\times1) \\ K_{MG}(1\times2) & K_{WG}(1\times1) & K_{GG}(1\times1) & K_{TG}(1\times1) \\ K_{MT}(1\times2) & K_{WT}(1\times1) & K_{GT}(1\times1) & K_{TT}(1\times1) \end{bmatrix}$$

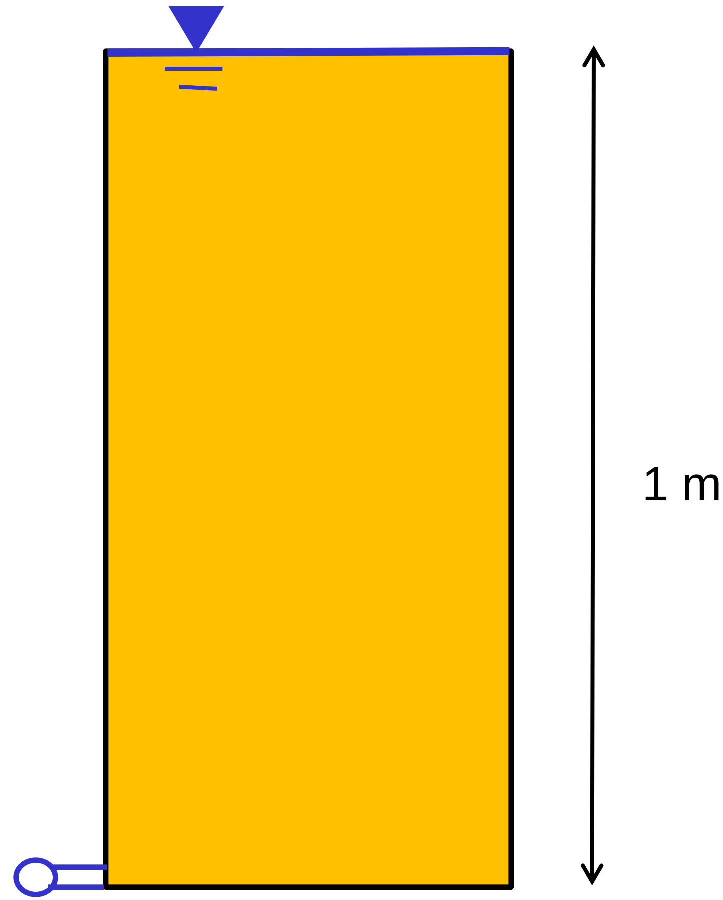
Knowing that the order of magnitude of the out of balance forces for the mechanical problem, the flow and the heat problem are really different, it is therefore necessary to sum the norm of each problem computed separately:

$$\left\| F^{HE} \right\| = \left\| F^{HE} \right\|^{Meca} + \left\| F^{HE} \right\|^{hydro+air} + \left\| F^{HE} \right\|^{Thermal}$$

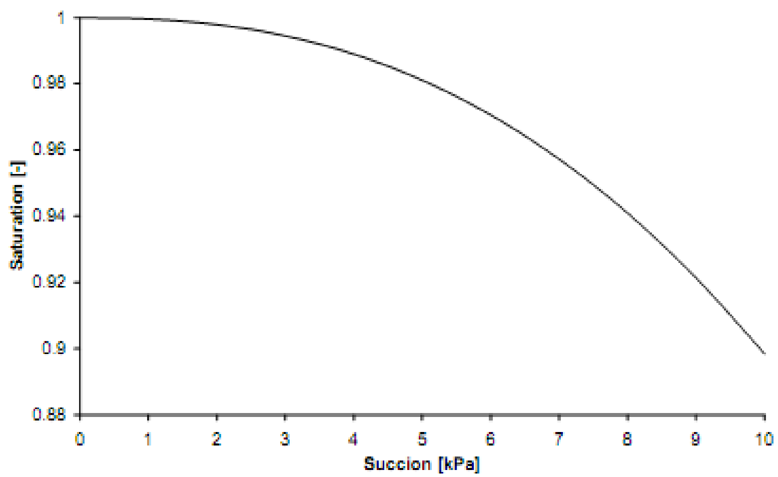
Application of a THM problem: sand column

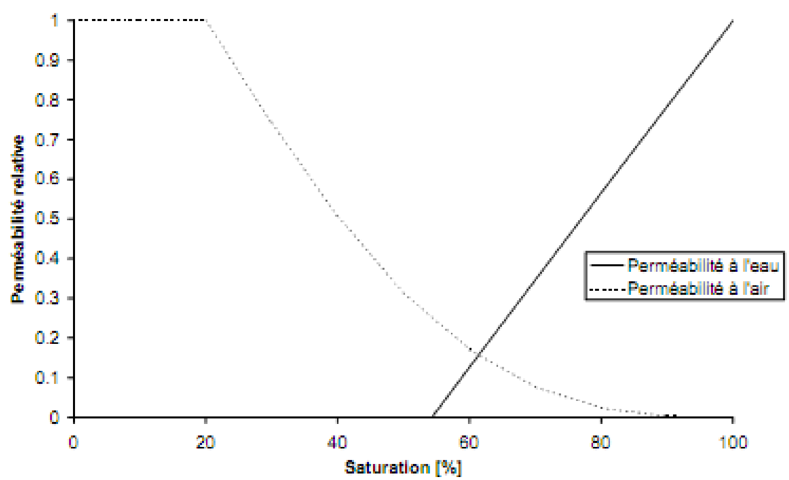


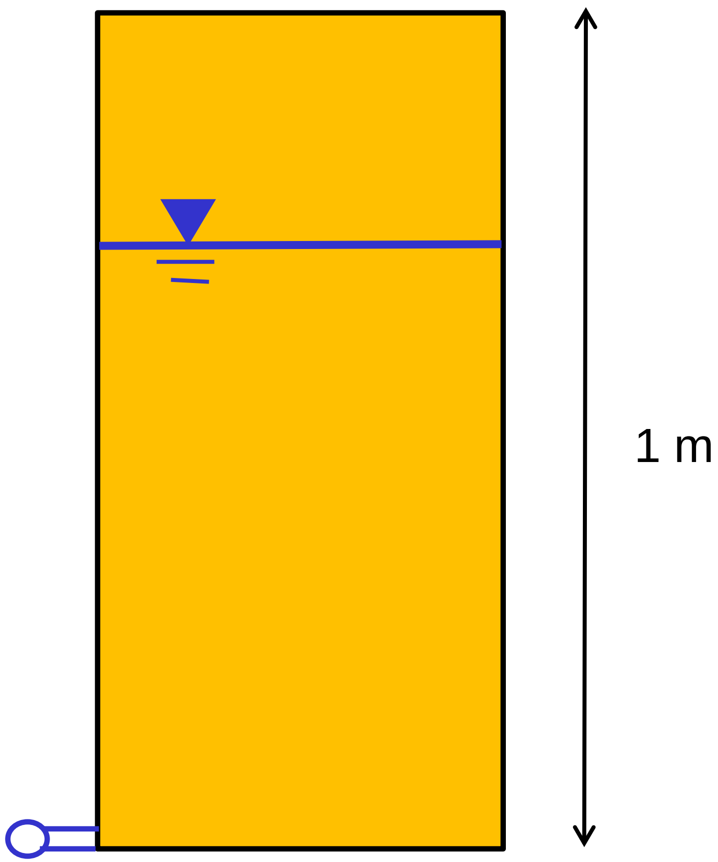


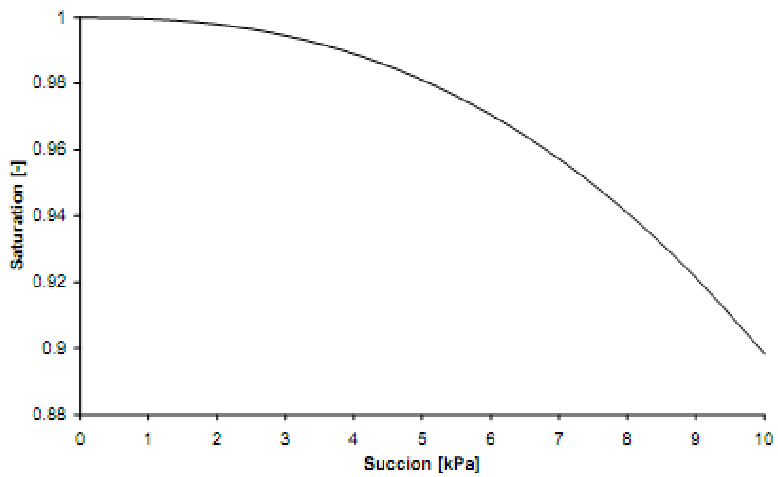


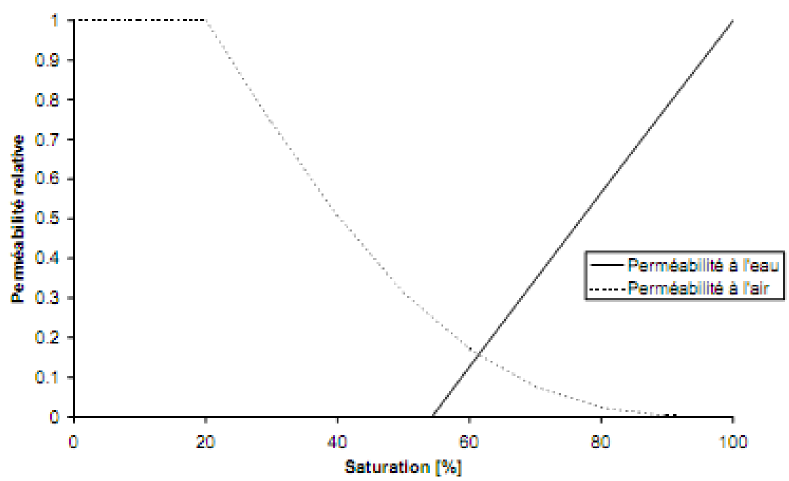
Application of a THM problem: sand column

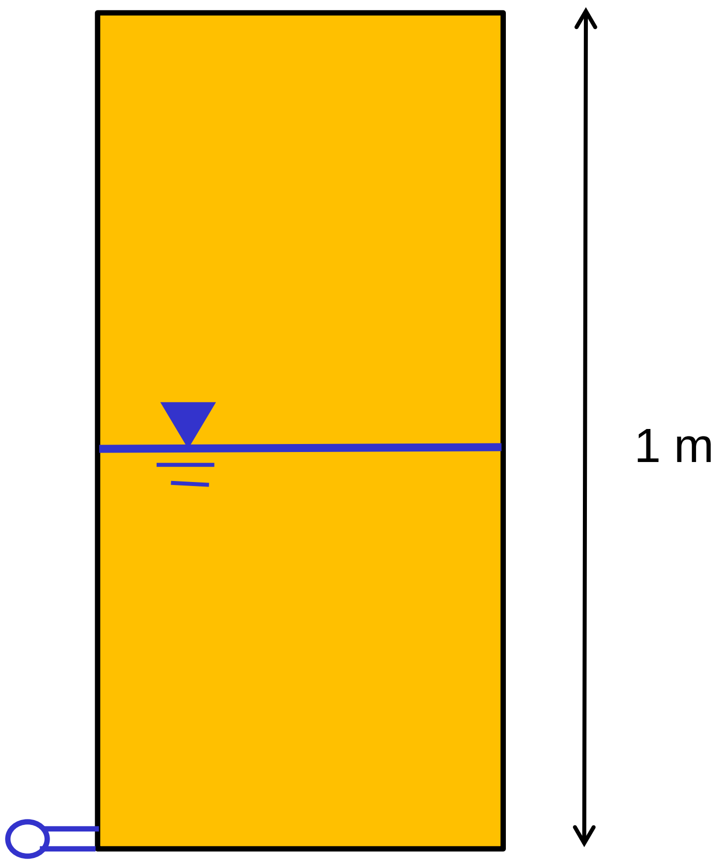




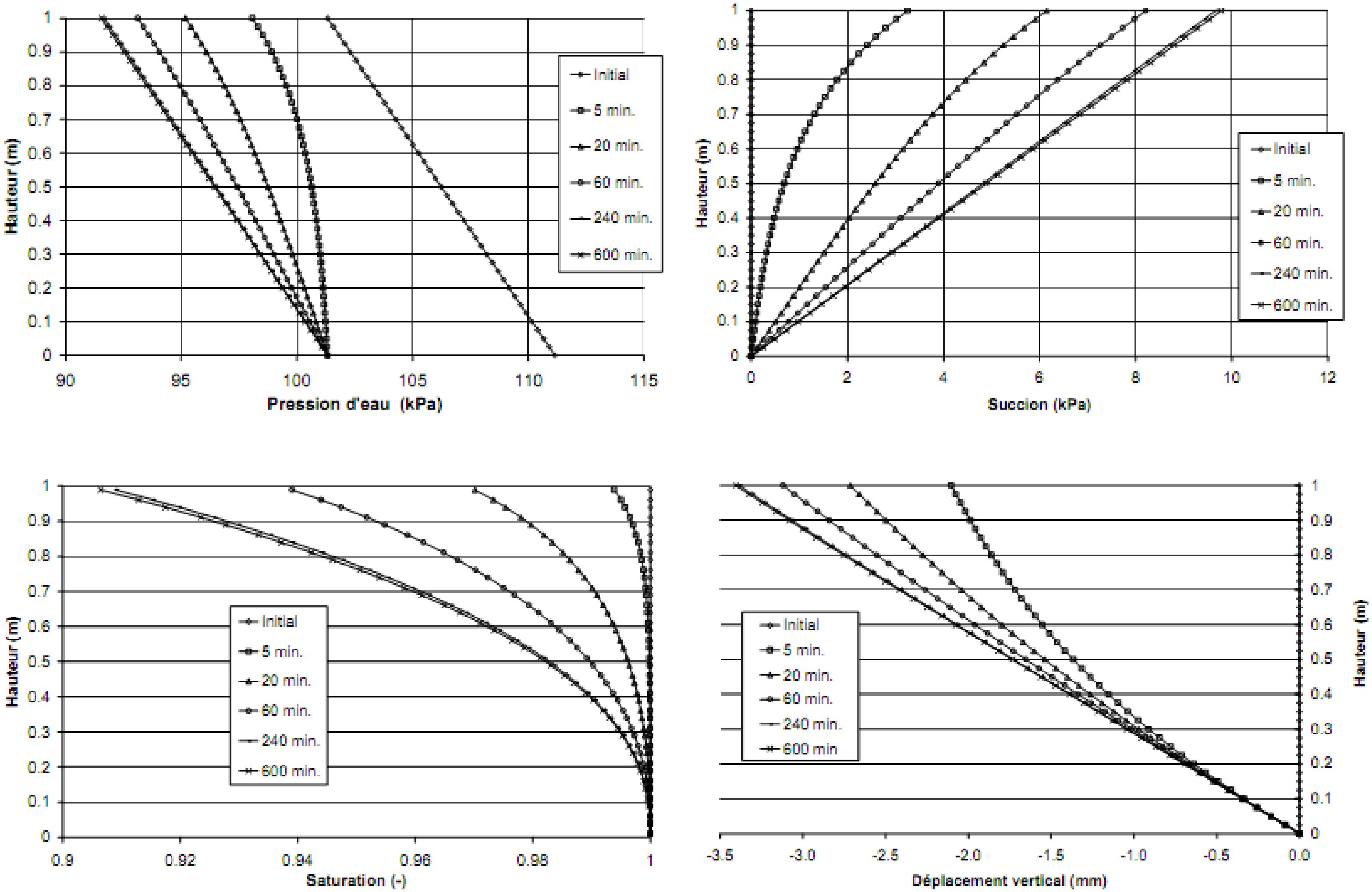



Saturation [-]
Succion [kPa]
1
0.98
0.96
0.94
0.92
0.9
0.88
0
1
2
3
4
5
6
7
8
9
10

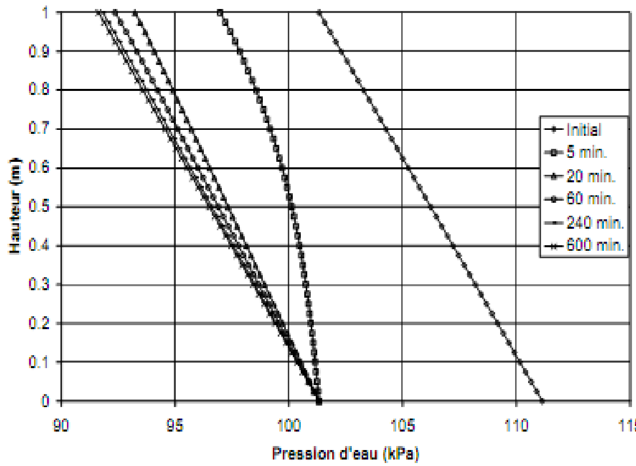

Perméabilité relative
Saturation [%]
Perméabilité à l'eau
Perméabilité à l'air
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
20
40
60
80
100

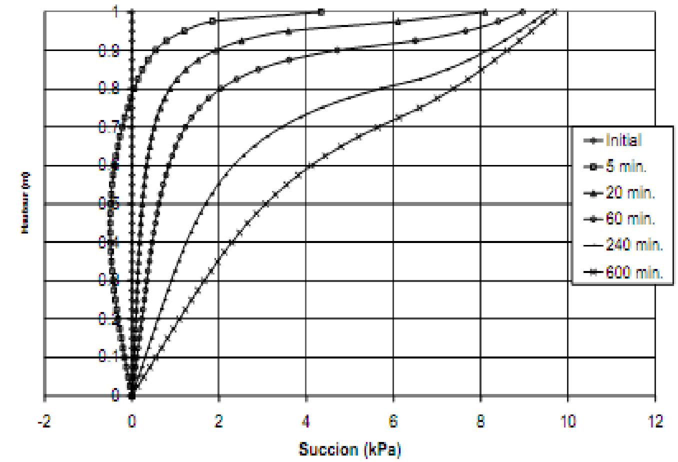

1 m

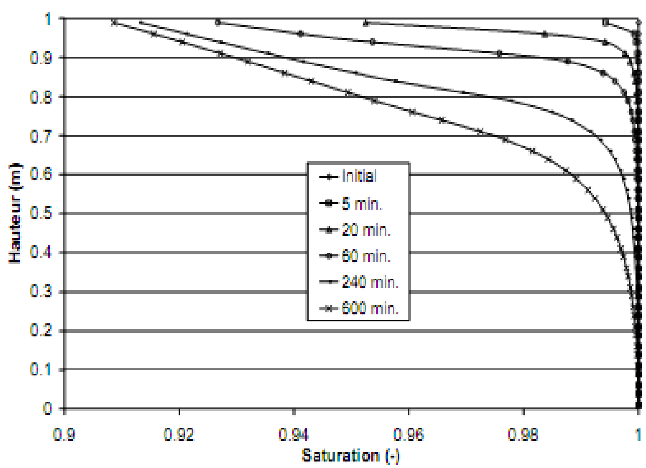
Modelling with fixed gas pressure

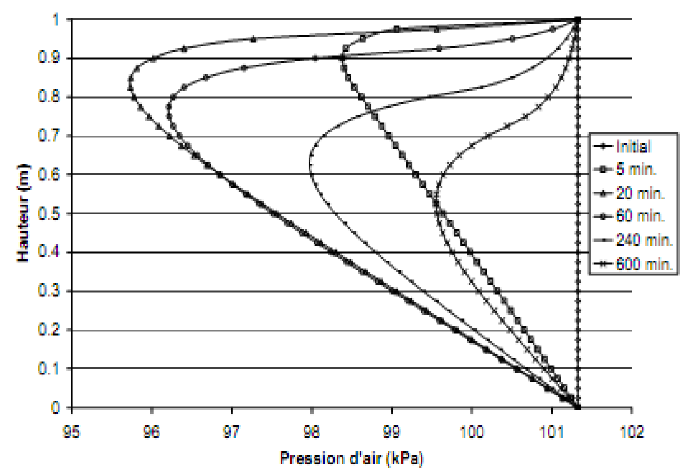


Modelling with variable gas pressure ($k_{r,min}$ <>0)

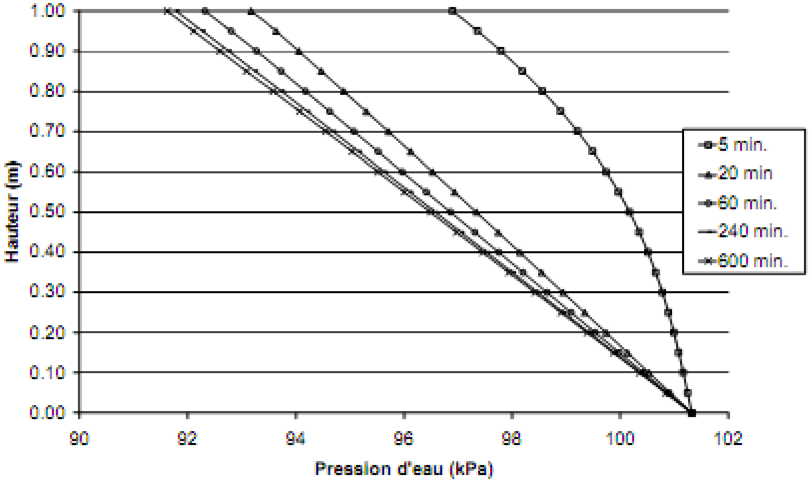


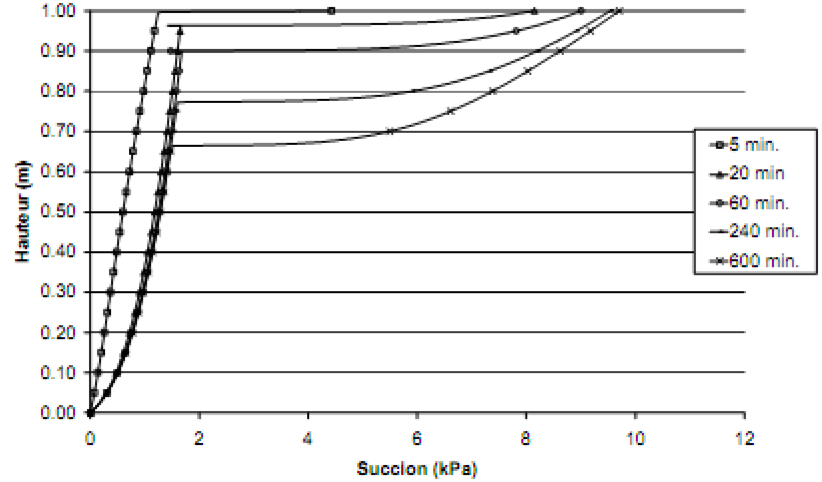


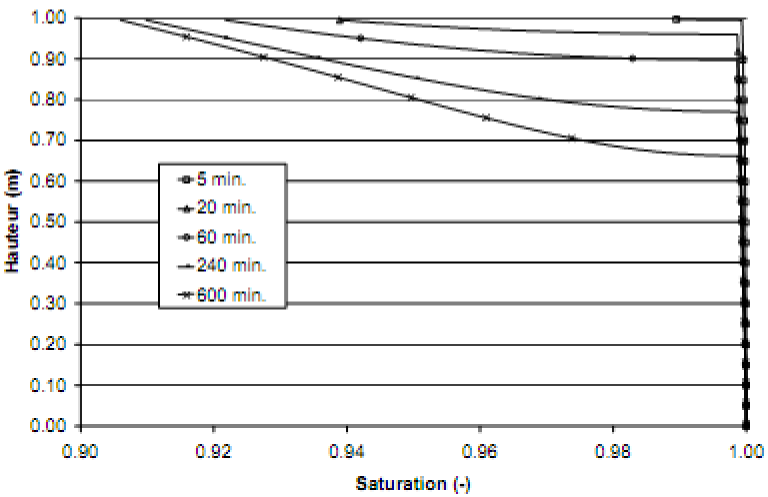


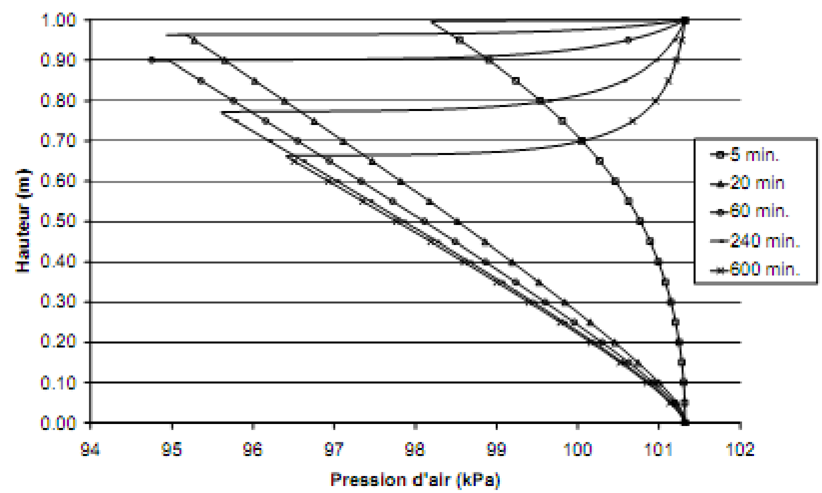


Modelling with variable gas pressure (+dissolved gas)









Modelling reactive medium in a THM context

$$\frac{\partial C_j}{\partial t} + S_j = 0 \text{ (j = coal (}f\text{) or solid product)}$$

$$S_f = -C_f C_{O_2} k_0 \exp\left(-\frac{E}{RT}\right)$$

Second-order Arrhenius-type reaction rate for coal

$$S_j = \left(\frac{v_j}{v_f}\right)\left(\frac{M_j}{M_f}\right) \cdot S_f$$

$$\frac{\partial \theta C_j}{\partial t} + \boldsymbol{q}\,\nabla C_j - \nabla \cdot \left(D_{ij} \nabla C_j\right) + S_j = 0 \text{ (j = O}_2\text{ or gaseous product)}$$

Transport part: $\boldsymbol{q}\,\nabla C_j - \nabla \cdot \left(D_{ij} \nabla C_j\right)$

Consumption part: S_j

Modelling reactive medium in a THM context

Darcy velocities of gas

MWAT2D → **ADVE2D**

NTECL

$$C_{O2} = C_{O2} + FIC(IN,IPI)*XY(6,KF)$$

Average O_2 concentration degradation rate in DELTAT

REACT → **ADVE2D**

New data transfer file: NTECF

Degradation term

As an extension of the THM problem, the stiffness matrix of the MWAT2+ADVEC elements has the following expression:

$$\begin{bmatrix} F_x^{HE} \\ F_y^{HE} \\ F_{p_w}^{HE} \\ F_{p_g}^{HE} \\ F_T^{HE} \\ F_C^{HE} \end{bmatrix} = \underline{\underline{K}} \begin{bmatrix} du_x \\ du_y \\ dp_w \\ dp_g \\ dT \\ dC \end{bmatrix} \qquad \underline{\underline{K}} = \begin{bmatrix} K_{MM}(2\times 2) & K_{WM}(2\times 1) & K_{GM}(2\times 1) & K_{TM}(2\times 1) & K_{CM}(2\times 1) \\ K_{MW}(1\times 2) & K_{WW}(1\times 1) & K_{GW}(1\times 1) & K_{TW}(1\times 1) & K_{CW}(1\times 1) \\ K_{MG}(1\times 2) & K_{WG}(1\times 1) & K_{GG}(1\times 1) & K_{TG}(1\times 1) & K_{CG}(1\times 1) \\ K_{MT}(1\times 2) & K_{WT}(1\times 1) & K_{GT}(1\times 1) & K_{TT}(1\times 1) & K_{CT}(1\times 1) \\ K_{MC}(1\times 2) & K_{WC}(1\times 1) & K_{GC}(1\times 1) & K_{TC}(1\times 1) & K_{CC}(1\times 1) \end{bmatrix}$$

Knowing that the order of magnitude of the out of balance forces for the mechanical problem, the flow, the heat problem and the reactive transport problem are really different, it is therefore necessary to sum the norm of each problem computed separately:

$$\left\|F^{HE}\right\| = \left\|F^{HE}\right\|^{Meca} + \left\|F^{HE}\right\|^{hydro+air} + \left\|F^{HE}\right\|^{Thermal} + + \left\|F^{HE}\right\|^{\mathrm{React}}$$

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