COMSOL CONFERENCE 2016 MUNICH

M4B: A Tool for the Multiphysics Analysis of the Deformational Behaviour of Soils and its Interaction with Building Foundations

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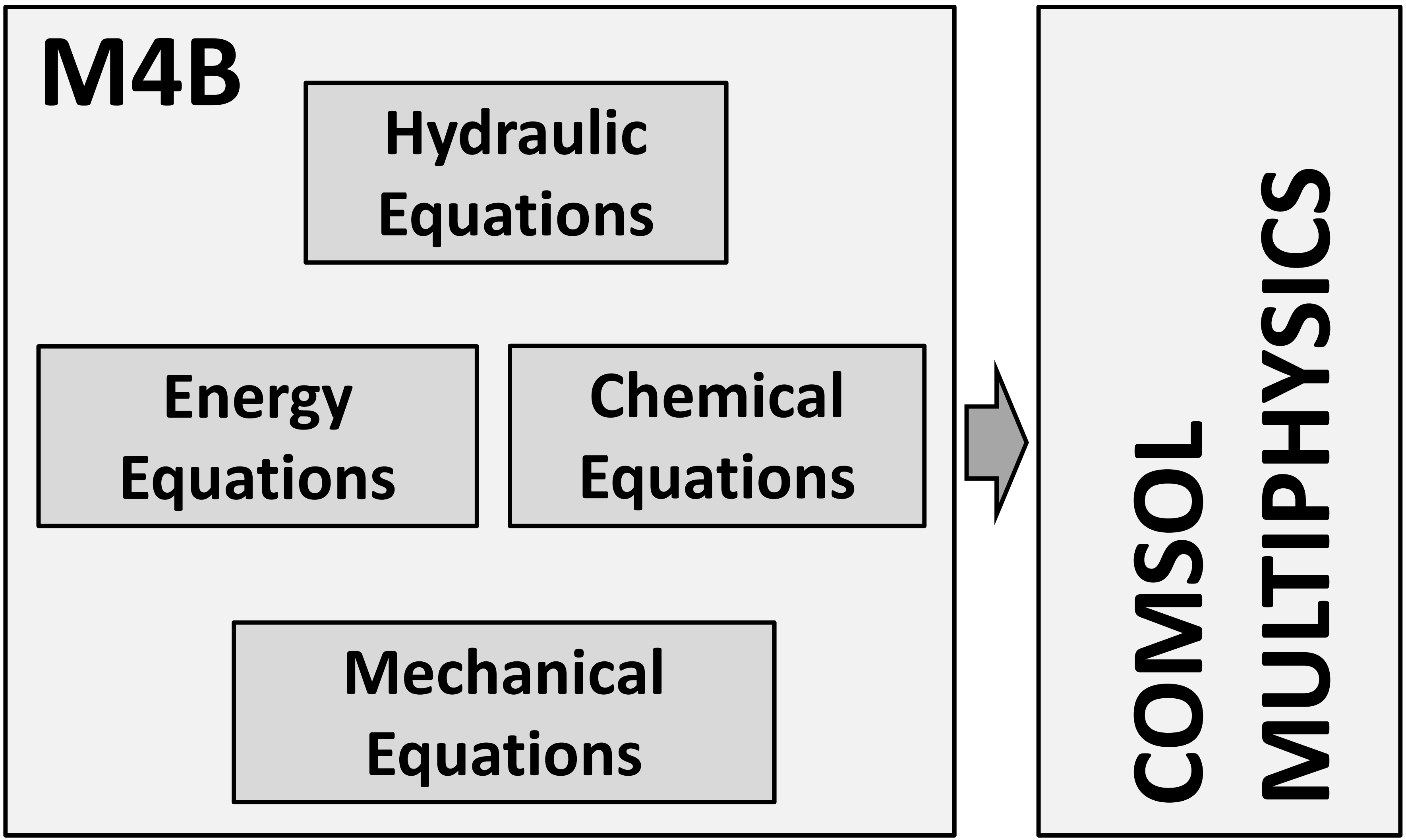
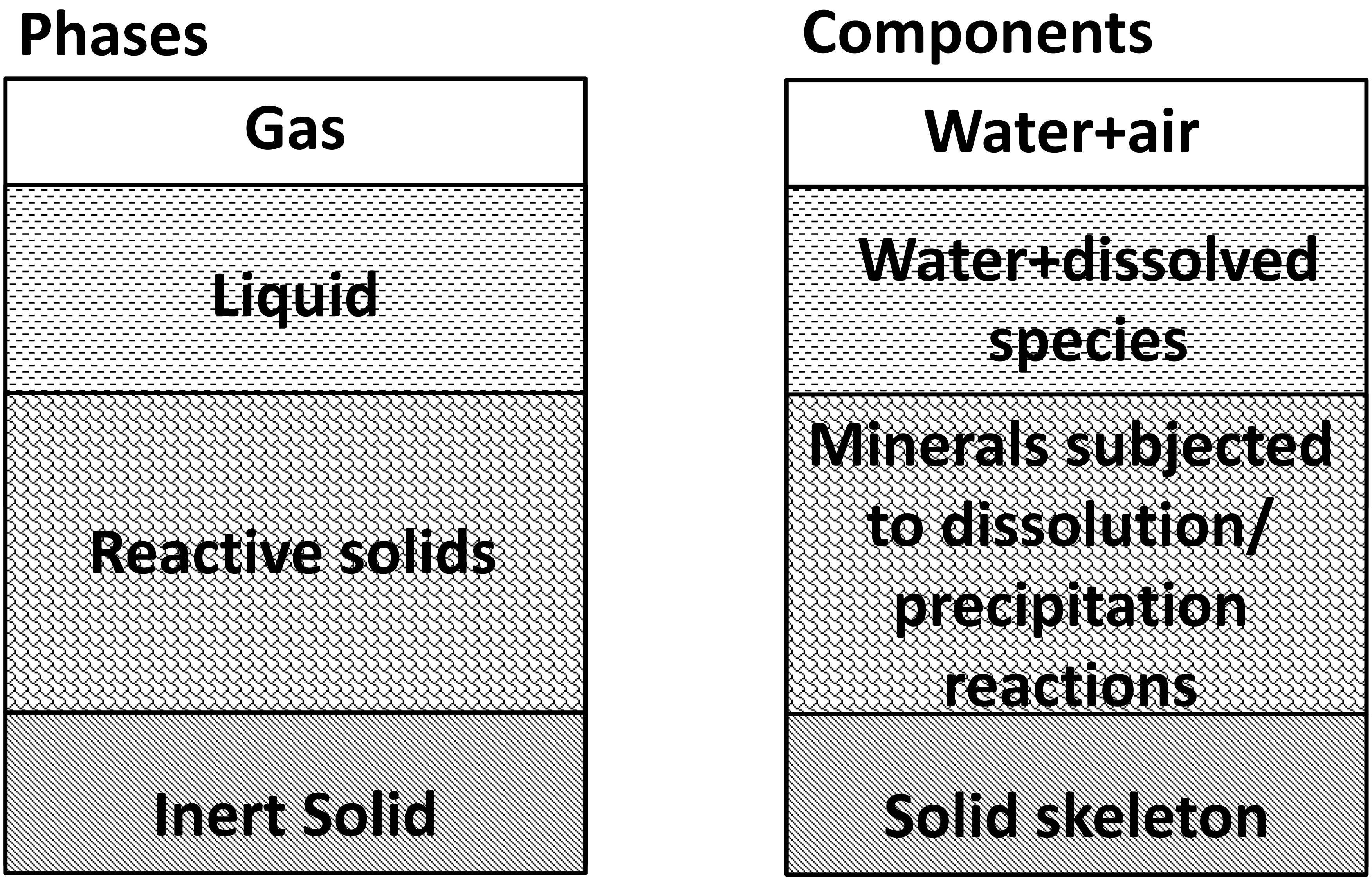
Introduction



Introduction



HYDRAULIC EQUATIONS

- Water mass balance

$$\frac{D_S m^{\mathrm{W}}}{Dt} + m^{\mathrm{W}} \nabla \cdot \boldsymbol{v}_s + \nabla \cdot (\rho^{\mathrm{W}} \boldsymbol{q}^{\mathrm{W}}) = 0$$

- Water content

$$m^{\mathrm{W}} = n S_{\mathrm{L}} \rho_{\mathrm{L}}^{\mathrm{W}} + n S_{\mathrm{G}} \rho_{\mathrm{G}}^{\mathrm{W}}$$

- Mass water flux

$$\rho^{W} \boldsymbol{q}^{W} =$$

$$-\rho_L^{\mathrm{W}} \frac{\boldsymbol{K}_L k_{\mathrm{r}L}^{\mathrm{W}}}{\mu_L} (\nabla P_L + \rho g \nabla z) - S_{\mathrm{G}} n \, \tau \, D_v \nabla \cdot \rho_G^{\mathrm{W}}$$

- Vapour density

$$\rho_G^{\mathrm{W}} = \frac{W_W P_V}{RT}$$

- Vapour pressure

$$P_V = H P_V^0$$

$$H = \exp\left[\frac{W_W s}{\rho_L RT}\right]$$

HEAT EQUATIONS

- Energy Conservation Equation

$$\frac{\partial E}{\partial t} + \nabla\left(\boldsymbol{l}_E\right) = f^Q$$

$$E = E_S + E_L + E_G$$

- Internal Energy

$$E_G = c_G^W \rho_G^W S_G n T + l \rho_G^W S_G n$$

$$E_S = c_S \rho_S \left(1 - n\right) T$$

$$E_L = c_L^W \rho_L^W S_L n\ T$$

- Heat Flux

$$\boldsymbol{l}_E = \boldsymbol{i}_{\boldsymbol{C}} + \boldsymbol{l}_S + \boldsymbol{l}_L + \boldsymbol{l}_G$$

- Advection

$$\boldsymbol{l}_{\boldsymbol{G}} = \boldsymbol{q}_{\boldsymbol{G}}^W E_G + E_G \boldsymbol{v}_s$$

$$\boldsymbol{l}_{\boldsymbol{L}} = \boldsymbol{q}_{\boldsymbol{L}}^W E_L + E_L \boldsymbol{v}_s$$

$$\boldsymbol{l}_{\boldsymbol{S}} = E_S \rho_S \left(1 - n\right) \boldsymbol{v}_s$$

- Conduction

$$\boldsymbol{i}_{\boldsymbol{C}} = -\lambda\left(\boldsymbol{T}\right) \nabla T$$

$$\lambda = \lambda_S^{1-n} \lambda_L^{S_L n} \lambda_G^{\left(1 - S_L\right) n}$$

EQUATIONS

- Conservation of individual species

$$\frac{\partial n S_L C_i}{\partial t} + \nabla \boldsymbol{j}_i = n S_L (R_i + R_i^{MIN})$$

$$\frac{\partial m_{MIN,i}}{\partial t} = -m_{MIN,i} \nabla \cdot \boldsymbol{v}_s + R_i^{MIN}$$

- Massic flux of individual species

$$\boldsymbol{j}_i = \boldsymbol{q}^W C_i - n S_L D_i \nabla C_i$$

- Conservation of conserved substances

$$\sum_{i=1}^{N} \alpha_{ik} \left(\frac{\partial n S_L \left(C_i + C_i^a \right)}{\partial t} + \nabla \boldsymbol{j}_i = n S_L R_i \right) = 0$$

$$k = 1, \ldots, M$$

$$\sum_{i=1}^{N} \alpha_{ik} R_i = 0$$

- Conservation of conserved substances

$$T_k = \sum_{i=1}^{N} \alpha_{ik} \left(C_i + C_i^a \right) \qquad \forall k = 1, \ldots, M$$

$$\frac{\partial n S_L T_k}{\partial t} + \sum_{i=1}^{N} \alpha_{ik} \nabla \boldsymbol{j}_i = 0 \qquad k = 1, \ldots, M$$

- Electroneutrality condition $\sum_{i=1}^{N} z_i C_i = 0$

CONSERVED SUBSTANCES	H^+, CO_3^{2-}, SO_4^{2-}, Ca^{2+}, Mg^{2+}, Na^+, K^+, Cl^-
SPECIES	HCO_3^-, OH^-, H_2CO_3, HSO_4^-, H_2SO_4, $CaHCO_3^+$, $CaCO_3$, $CaHSO_4^+$, $CaSO_4$, $CaOH^+$, $MgHCO_3^+$, $MgCO_3$, $MgSO_4$, $MgOH^+$, $NaHCO_3$, $NaCO_3^-$, $NaSO_4^-$, NaOH, KOH, H^+, CO_3^{2-}, SO_4^{2-}, Ca^{2+}, Mg^{2+}, Na^+, K^+, Cl^-

EQUATIONS

Nombre	*Fórmula*	*log k*	*Base de datos*	*Reacción*
Anhidrita*	$Ca(SO_4)$	-4.440	ANDRA	$Ca(SO_4) \leftrightarrow Ca^{+2} + SO_4^{-2}$
Antarcticita	$CaCl_2{:}6H_2O$	3.940	ANDRA	$CaCl_2{:}6H_2O \leftrightarrow Ca^{+2} + 2Cl^- + 6H_2O$
Aragonito	$CaCO_3$	-8.310	ANDRA	$CaCO_3 \leftrightarrow Ca^{+2} + CO_3^{-2}$
Arcanita	K_2SO_4	-1.850	ANDRA	$K_2SO_4 \leftrightarrow 2K^+ + SO_4^{-2}$
Artinita	$Mg_2(CO_3)(OH)_2{:}3H_2O$	9.810	ANDRA	$Mg_2(CO_3)(OH)_2{:}3H_2O \leftrightarrow 2Mg^{+2} - 2H^+ + CO_3^{-2} + 5H_2O$
Basanita	$CaSO_4{:}0.5H_2O$	-3.920	ANDRA	$CaSO_4{:}0.5H_2O \leftrightarrow Ca^{+2} + SO_4^{-2} + 0.5H_2O$
Bischofita	$MgCl_2{:}6H_2O$	4.460	ANDRA	$MgCl_2{:}6H_2O \leftrightarrow Mg^{+2} + 2Cl^- + 6H_2O$
Bloedita*	$Na_2Mg(SO_4)_2{:}4H_2O$	-2.350	ANDRA	$Na_2Mg(SO_4)^2{:}4H_2O \leftrightarrow Mg^{+2} + 2Na^+ + 2SO_4^{-2} + 4H_2O$
Brucita	$Mg(OH)_2$	17.100	ANDRA	$Mg(OH)_2 \leftrightarrow Mg^{+2} - 2H^+ + 2H_2O$
Burkeita	$Na_6(CO_3)(SO_4)_2$	-0.770	ANDRA	$Na_6(CO_3)(SO_4)^2 \leftrightarrow 6Na^+ + CO_3^{-2} + 2SO_4^{-2}$
$Ca_2Cl_2(OH)_2{:}H_2O(s)$	$Ca_2Cl_2(OH)_2{:}H_2O$	26.530	ANDRA	$Ca_2Cl_2(OH)_2{:}H_2O \leftrightarrow 2Ca^{+2} - 2H^+ + 2Cl^- + 3H_2O$
$Ca_4Cl_2(OH)_6{:}13H_2O(s)$	$Ca_4Cl_2(OH)_6{:}13H_2O$	68.730	ANDRA	$Ca_4Cl_2(OH)_6{:}13H_2O \leftrightarrow 4Ca^{+2} - 6H^+ + 2Cl^- + 19H_2O$
$CaCl_2{:}2H_2O(cr)$	$CaCl_2{:}2H_2O$	7.950	ANDRA	$CaCl_2{:}2H_2O \leftrightarrow Ca^{+2} + 2Cl^- + 2H_2O$
$CaCl_2{:}4H_2O(cr)$	$CaCl_2{:}4H_2O$	5.350	ANDRA	$CaCl_2{:}4H_2O \leftrightarrow Ca^{+2} + 2Cl^- + 4H_2O$
$CaCl_2{:}H_2O(s)$	$CaCl_2{:}H_2O$	7.850	ANDRA	$CaCl_2{:}H_2O \leftrightarrow Ca^{+2} + 2Cl^- + H_2O$
$CaCO_3{:}H_2O(s)$	$CaCO_3{:}H_2O$	-7.600	ANDRA	$CaCO_3{:}H_2O \leftrightarrow Ca^{+2} + CO_3^{-2} + H_2O$
Calcita*	$CaCO_3$	-8.480	ANDRA	$CaCO_3 \leftrightarrow Ca^{+2} + CO_3^{-2}$
$CaMg_3(CO_3)_4(s)$/Huntita	$CaMg_3(CO_3)_4$	-30.810	ANDRA	$CaMg_3(CO_3)_4 \leftrightarrow Ca^{+2} + 3Mg^{+2} + 4CO_3^{-2}$
Carnalita	$KMgCl_3{:}6H_2O$	4.330	ANDRA	$KMgCl_3{:}6H_2O \leftrightarrow Mg^{+2} + K^+ + 3Cl^- + 6H_2O$
Dolomita*	$CaMg(CO_3)_2$	-17.120	ANDRA	$CaMg(CO_3)_2 \leftrightarrow Ca^{+2} + Mg^{+2} + 2CO_3^{-2}$
Epsomita*	$Mg(SO_4){:}7H_2O$	-1.880	ANDRA	$Mg(SO_4){:}7H_2O \leftrightarrow Mg^{+2} + SO_4^{-2} + 7H_2O$
Gaylussita	$CaNa_2(CO_3)_2{:}5H_2O$	-9.430	ANDRA	$CaNa_2(CO_3)_2{:}5H_2O \leftrightarrow Ca^{+2} + 2Na^+ + 2CO_3^{-2} + 5H_2O$
….				

EQUATIONS

- Equilibrium equation

$$\nabla \boldsymbol{\sigma}_{\mathrm{TOT}} + \rho g \nabla z = 0$$

- Constitutive stresses

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_{\mathrm{TOT}} - P_{\phi} \boldsymbol{m}$$

$$P_{\phi} = \max(P_{\mathrm{G}}, P_{\mathrm{L}})$$

- Incremental stresses

$$d\boldsymbol{\sigma} = \boldsymbol{D}^{el} \left(d\boldsymbol{\varepsilon} - d\boldsymbol{\varepsilon}^{S} - d\boldsymbol{\varepsilon}^{CH} - d\boldsymbol{\varepsilon}^{m} - d\boldsymbol{\varepsilon}^{P} \right)$$

- Porosity variations

$$\frac{D_S n}{Dt} = (1 - n) \nabla \cdot \boldsymbol{v}_s - \sum_i \frac{1}{\rho_i} W_{\mathrm{i}} R_i^{MIN}$$

- Strain component due to suction changes

$$d\boldsymbol{\varepsilon}^{S} = \frac{\kappa_S}{\left(s + P_{atm}\right)} ds$$

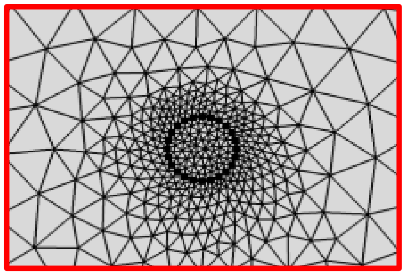
- Strain component due to dissolution/precipitation

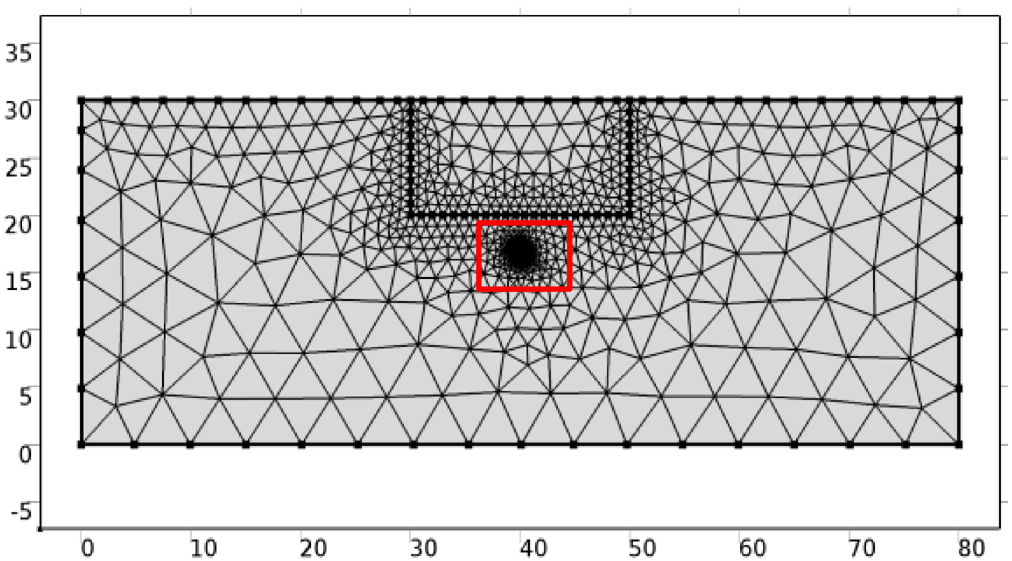
$$d\boldsymbol{\varepsilon}_V^{CH} = \sum_i \frac{\gamma_i}{\rho_i} W_{\mathrm{i}} R_i^{MIN}$$

- Dissolution/precipitation rates

$$R_i^{MIN} = \frac{1}{W_{\mathrm{i}}} \sigma_c k \xi_i \phi_i \left\{ \left| \frac{IAP_i}{K_i} \right|^{\theta} - 1 \right\}^{n}$$

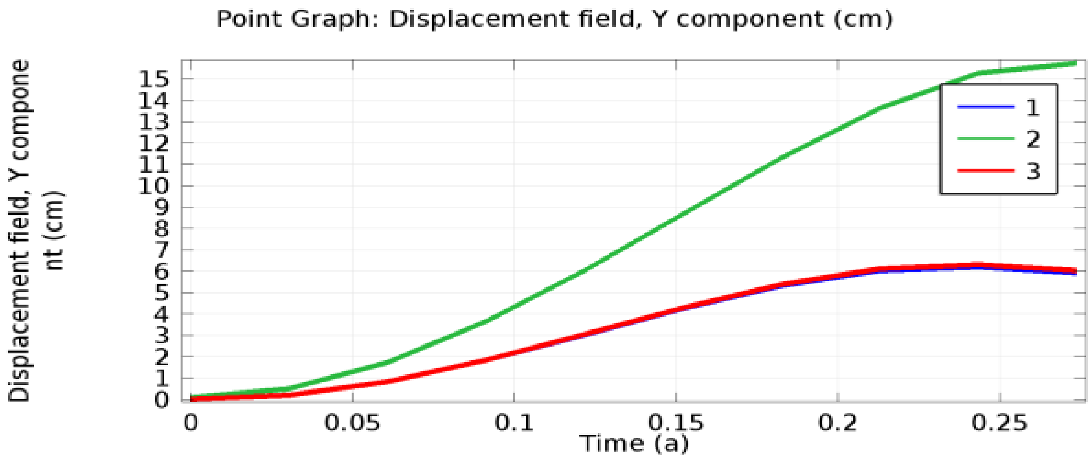
Example Model. Excavation and gypsum dissolution

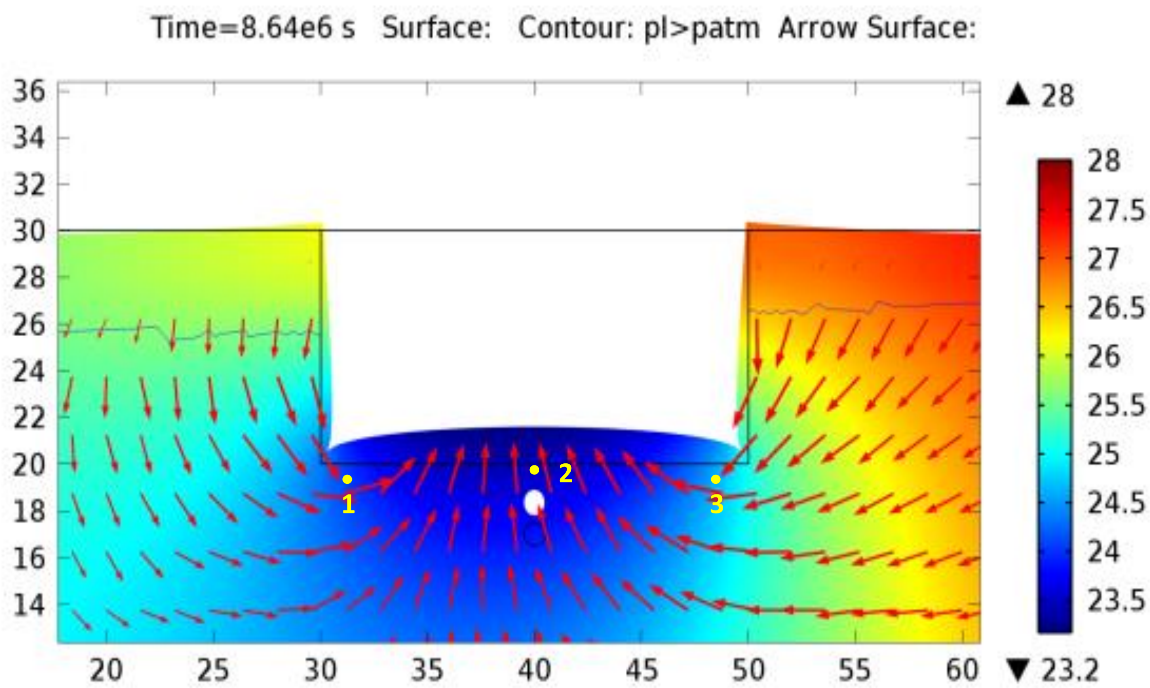




Parameter	Value
ρ_s , soil density	2650 kgm^{-3}
$k_{s,}$ bulk modulus related to suction changes	-0.02 MPa^{-1}
γ, coefficient related to crystal growth pressure	1
Elastic modulus	17 MPa
Poisson coefficient	0.3
Initial porosity, *n*	0.4
Intrinsic permeability, $\boldsymbol{K}_L$	1.00 x 10^{-17} m^2
Initial gypsum content	20 %
Initial sulphate concentration	0.002 mol l^{-1}
Initial calcium concentration	0.014 mol l^{-1}
$k\sigma_c$	3.4 x 10^{-04} $kgm^{-2}s^{-1}$

Excavation


Point Graph: Displacement field, Y component (cm)
Displacement field, Y component (cm)
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
0
0.05
0.1
0.15
0.2
0.25
Time (a)
1
2
3


Time=8.64e6 s Surface: Contour: pl>patm Arrow Surface:
36
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▲ 28
28
27.5
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26.5
26
25.5
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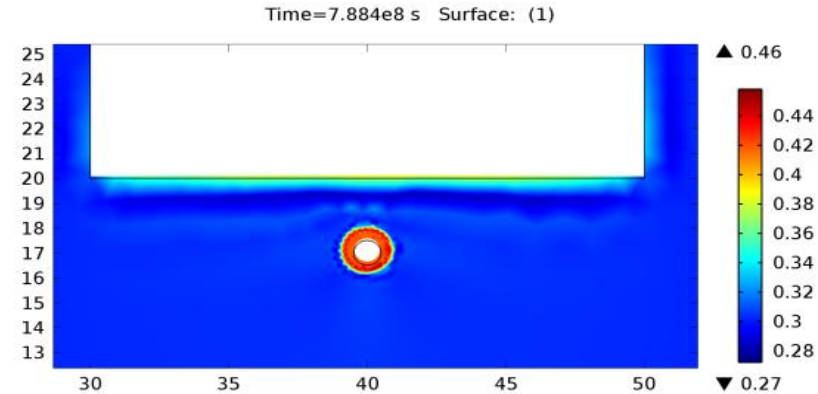
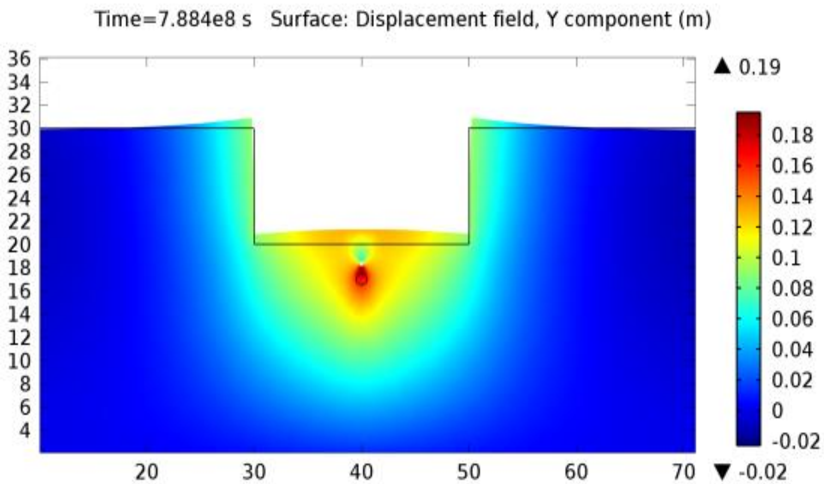
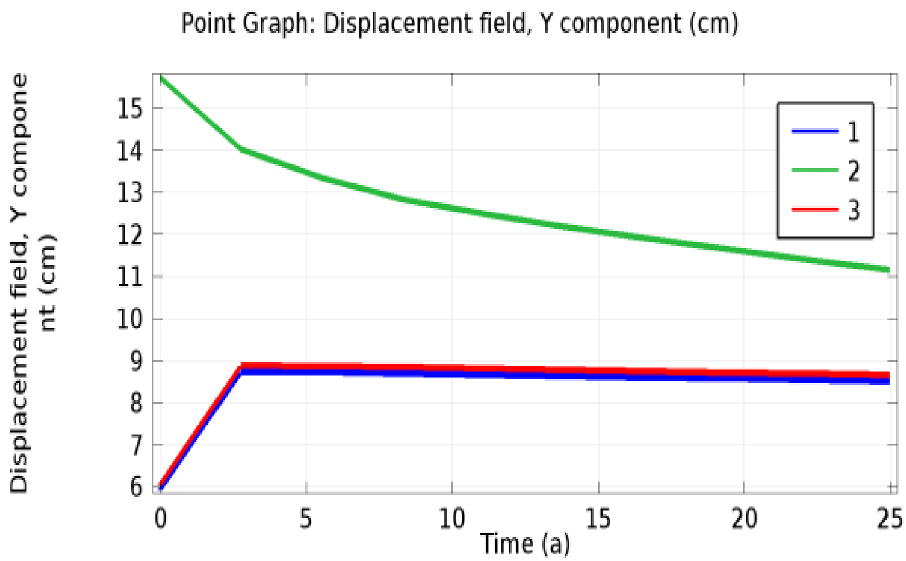
24
23.5
▼ 23.2

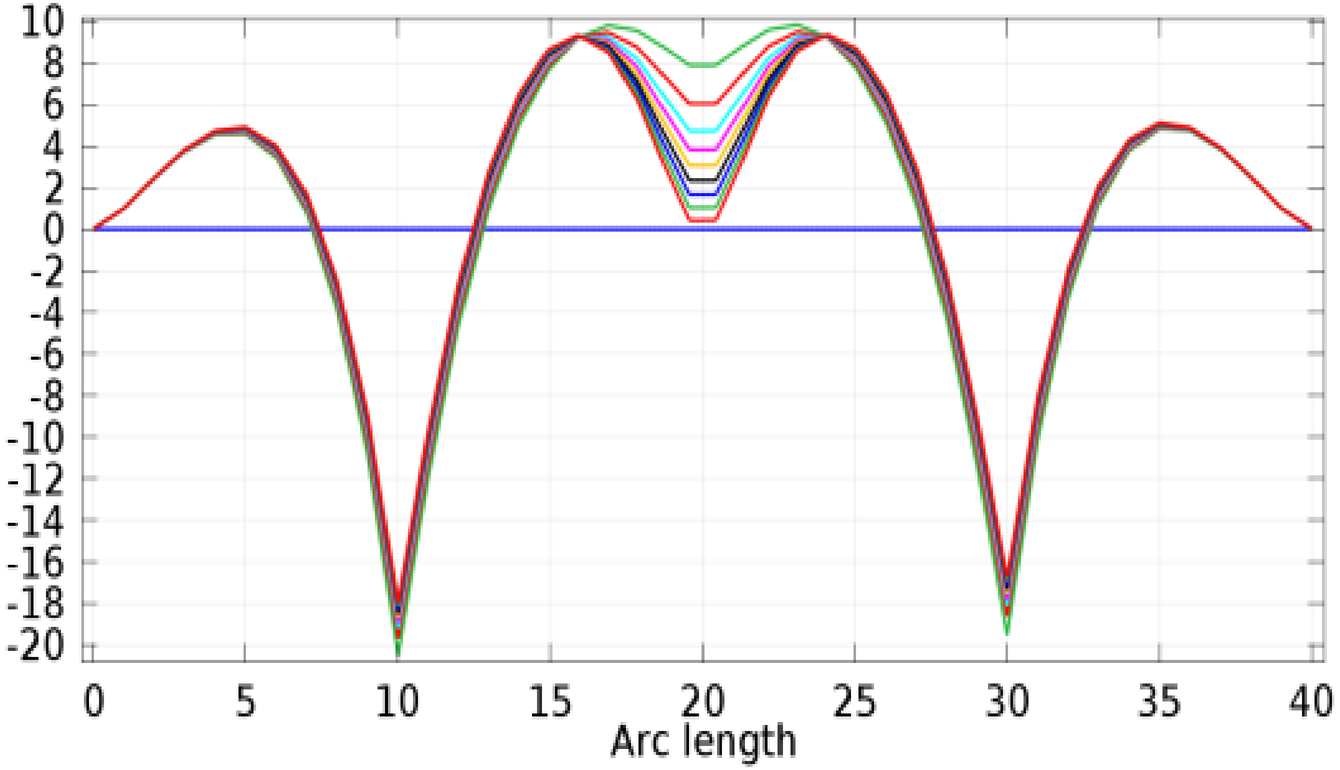
Dissolution







Section forces



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