MIKE
Powered by DHI

FEFLOW Hydromechanical Coupling Plugin

Reference and User Manual

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1   Introduction

This plugin describes the application of a modified Hooke's law to evaluate the hydro-dispersive parameters hydraulic conductivity, porosity, and storage coefficient, as a function of effective stress.

Model functions relating effective stress σ' to hydraulic conductivity $\mathbf{K}$, porosity θ and storage coefficient S_s (see Preisig *et al.* [2012, 2013]) have been developed from Hooke's law of elasticity and implemented in the FEFLOW software. They look at porous (granular) medias and fractured media in a specific manner using appropriate conceptualizations of model hydro-parameters.

Effective stress $\sigma'(\sigma, p)$ describes the stress state of a saturated rock and results from (e.g. Terzaghi [1923, 1936]):
- Load of principal stress (σ) on contacting grains
- Fluid pressure (p) in voids

An increase in σ' results from an increase in σ or a decrease in p. Changes in σ' induce reductions in the intrinsic hydrodynamic parameters ($\mathbf{K}$, S_s, θ) [e.g. overexploited basins / fracturing]:

$$\sigma' = \sigma - p$$
$$\sigma = c\gamma_r d$$
$$p = \alpha\gamma_w h$$
$$\gamma_r = \rho_r g$$
$$\gamma_w = \rho_w g$$
$$\alpha = 1 - \frac{E_p}{E_s}$$

With

σ = Total vertical/lithostatic stress [Pa], [kg/m/s^2]
c = Medium correction factor [−]
p = Pore pressure [Pa]
d = Depth [m]
h = Pressure head [m]
ρ_r = Rock/soil density [kg/m^3]
ρ_w = Water density [kg/m^3]
γ_r = Rock specific weight [kg/m^2/s^2]
γ_w = Water specific weight [kg/m^2/s^2]
g = Acceleration due to gravity [m/s^2]
α = Biot-Willis constant (close to 1)
E_s = Solid rock elastic modulus (bulk modulus of the rock) [Pa]
E_p = Drained bulk modulus of the porous medium [Pa]

2 Implementation and usage

The plugin allows the association of pre-defined elemental selections to the effective-stress models for fractured and granular media of Preisig *et al.* [2012, 2013]. Given the choice of model and parameterization, elements contained by these selections will be assigned the stress-dependent hydro-dispersive parameters. Portions of the mesh with no such associations are operating as usual, so the user needs to make sure the proper parameterization in FEFLOW exists for such mesh elements. In a similar way, discrete-feature selections can be used and assigned a stress-dependent fracture model. The discrete elements must be assigned the Hagen-Poiseuille law for the stress-dependent model to operate.

All stress-dependent formulations rely on the regionalization of the total stress field $\sigma(x, y, z)$. This is to be realized in a user *nodal reference distribution* where total stress is assigned in Pa. When not informed, only in the case of 3D layered mesh configurations will the plugin proceed with an automatic evaluation of lithostatic stress $\sigma(x, y, z) = g \int_z^{Z_{surface}} \rho_r(u) du$. Techniques for obtaining this information are given in Note Tricks and tips:

An optional *elemental reference distribution* for porosity under no stress conditions can be used. When not used, only problem classes with porosity definitions will allow such a porosity to be accounted for (first looking at variable saturation porosity, then mass and heat). A porosity value is eventually to be defined as a fallback in the absence of its definition through either a user distribution or a FEFLOW material entry.
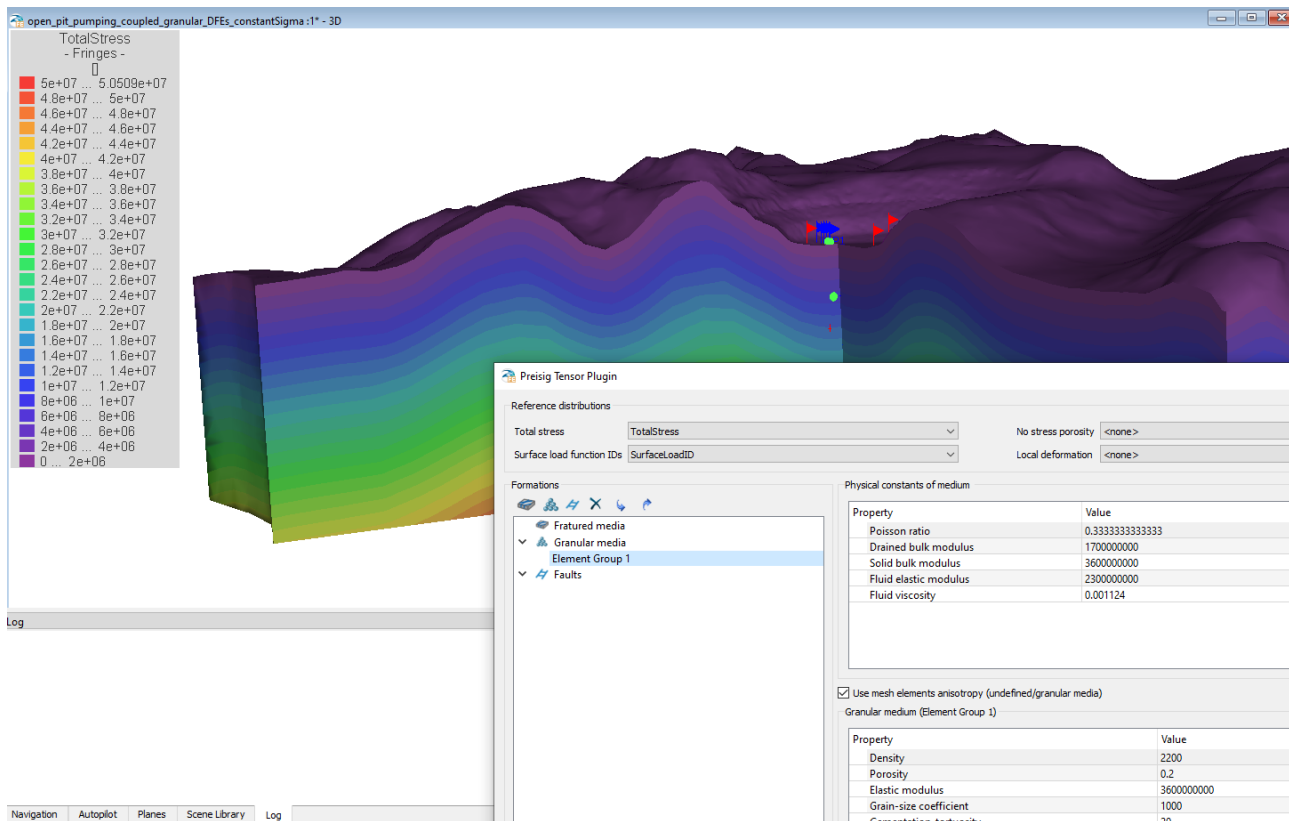

Figure 1 The user nodal reference distribution used to store the total stress field $\sigma(x, y, z)$.

2.1 Parametric model for fractured media

The effective-stress model for fractured regions after Preisig *et al.* [2012] reads

$$\mathbf{K} = \sum_{i=1}^{N_f} \Phi[i] K_f[i] (\mathbf{I} - \mathbf{n}[i] \otimes \mathbf{n}[i]) + \mathbf{K}_m$$

$$\theta = \sum_{i=1}^{N_f} \Phi[i] \theta_f[i] + \theta_m$$

$$S_s = \sum_{i=1}^{N_f} S_f[i] + S_m$$

$$\Phi[i] = \left(1 - r[i]^{\frac{1}{m[i]}}\right)^3 \in [0:1], \qquad r[i] = \frac{\sigma'}{\sigma_c[i]} \in [0:1]$$

$$c[i] = \lambda[i]\left(n_x^2[i] + n_y^2[i]\right) + n_z^2[i] \in [0:1]$$

$$\lambda[i] = \frac{\nu[i]}{1 - \nu[i]} \in [0:1]$$

$$K_f[i] = \frac{\gamma_w}{\mu} \frac{f[i] a[i]^3}{12}$$

$$\theta_f[i] = f[i] a[i] \theta_{fm}[i]$$

$$S_f[i] = \frac{\gamma_w}{E_w} \theta_f[i]$$

with

$\mathbf{K}$ = Hydraulic conductivity tensor for the matrix-fracture equivalent [m/s]

$\mathbf{K}_m$ = Matrix hydraulic conductivity diagonal tensor [m/s]

θ_m = Matrix porosity [−]

S_m = Matrix storage coefficient [m^{-1}]

μ = Fluid dynamic viscosity [kg/m/s]

E_w = Water elastic modulus [Pa]

N_f = Number of fracture families

$\mathbf{I}$ = Identity matrix

$\mathbf{n}[i]$ = Fracture family plane unit normal vector

$\otimes$ = Tensor product operator

$a[i]$ = Fracture family aperture [m]

$f[i]$ = Fracture family frequency [m^{-1}]

$K_f[i]$ = Fracture family hydraulic conductivity [m/s]

$S_f[i]$ = Fracture family storage coefficient [m^{-1}]

$\theta_f[i]$ = Fracture family porosity [−]

$\theta_{fm}[i]$ = Fracture plane fill-in material porosity (default 1.0) [−]

$\sigma_c[i]$ = Critical lithostatic stress or fracture closure limit [Pa]

$\lambda[i]$ = Fracture family geometric factor [−]

$\nu[i]$ = Poisson ratio [−] (Horizontal to vertical stress ratio, $\nu \sim 0.25$ in crystalline rocks)

$m[i]$ = Geometric exponent [−] (related to the statistical distribution of fracture asperities)
      Large asperities: $m \in [1.0 - 3.1]$; Small asperities: $m \in [3.1 - 11.0]$

The plugin allows for an association of an arbitrary number of elemental selections to fractured medium representations.

Such regions can be created and parameterized by adding new fractured medium formations . This results in selecting an available elemental selection to which the fracture families are to be defined in the corresponding table. Fracture family's orientation is given by the definition of their normal unit vectors by means of a two-angles, yaw and pitch formalism.
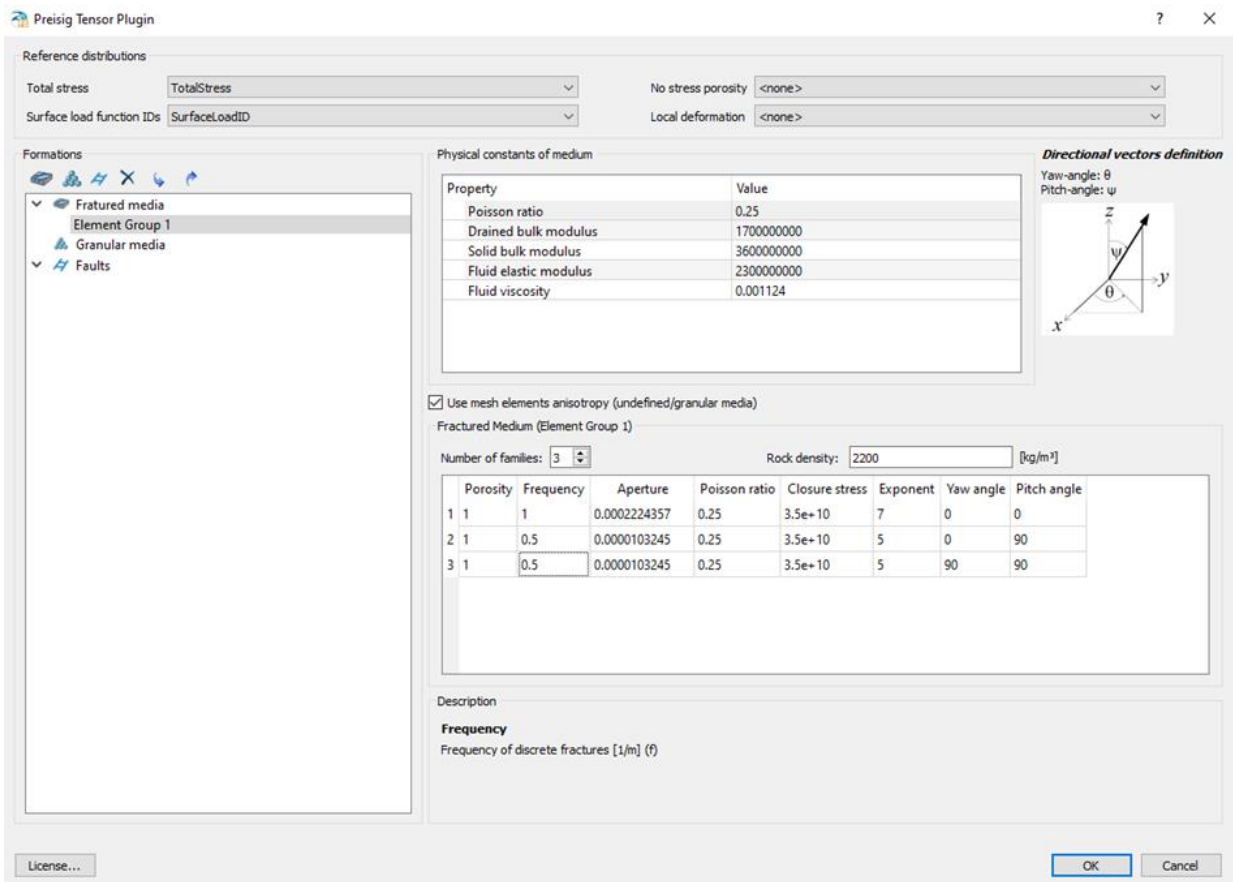
Figure 2 Fractured medium input parameter table with elemental selection relationship. Here the elemental selection named "Element Group 1" has been chosen and 3 families of fractures have been parameterized

Table 1 Indicative ranges for fracture closure limit effective stress and vertical elasticity.

Rock type	E_v [Pa] Vertical elasticity	η [1/m^2] Number of asperities per area	s [m^2] Asperity section	$\sigma_0' = \eta E_v s$ [MPa] Limit effective stress for fracture closure
Fractured granite / gneiss	$10^{10} - 10^{11}$	$1000 - 2000$	$0.001^2\pi$	$100 - 1000$
Fractured limestone	10^{10}	$1000 - 2000$	$0.001^2\pi$	$50 - 500$
Fractured schist / marl	$10^{09} - 10^{10}$	$1000 - 2000$	$0.001^2\pi$	$50 - 500$

2.2 Parametric model for single fractures

The effective-stress model for fractured regions after Preisig *et al.* [2012] applied to sets of discrete feature elements reads

$$K_f = \Phi \frac{\gamma_w}{\mu} \frac{a^3}{12}$$

$$\theta_f = \Phi a \theta_{fm}$$

$$S_f = \frac{\gamma_w}{E_w} \theta_f$$

$$\Phi = \left(1 - \frac{\sigma'^{\frac{1}{m}}}{\sigma_c}\right)^3 \in [0:1]$$

$$c = \frac{\nu}{1-\nu}(n_x^2 + n_y^2) + n_z^2$$

with

K_f = Fracture hydraulic conductivity [m/s]

θ_f = Fracture porosity [−]

θ_{fm} = Fracture plane fill-in material porosity (default 1.0) [−]

S_f = Fracture storage coefficient [m⁻¹]

The plugin allows for an association of an arbitrary number of fracture selections to fractured medium representations, using the button ⟨icon⟩. The Hagen-Poiseuille law must have been selected for these discrete feature elements for the plugin to apply the effective stress model. The components of the fracture normal unit vector are evaluated at the fracture element plane level given its orientation.
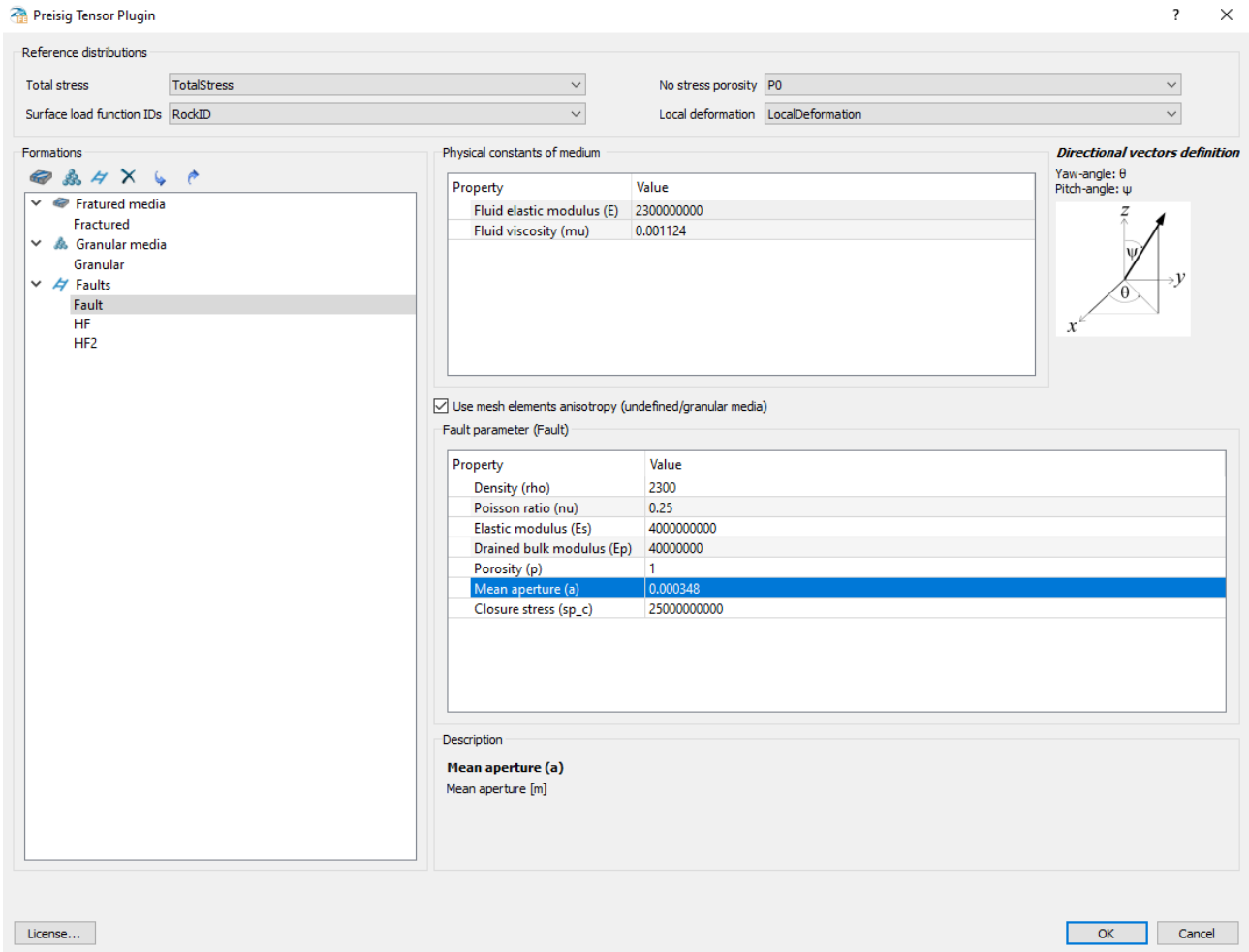
Figure 3 Assigning the effective stress fracture model to discrete feature elements selections.

2.3   Parametric model for granular media

The granular medium model with $c = 1$ after Preisig *et al.* [2013] reads

$$\mathbf{K} = \frac{\gamma_w}{\mu} \mathbf{R} \begin{pmatrix} k & 0 & 0 \\ 0 & r_{xy}k & 0 \\ 0 & 0 & r_{xz}k \end{pmatrix} \mathbf{R}^{-1}$$

$$k = \frac{bC^2\theta^3}{9S_0{}^2}$$

$$\theta = 1 - S_0$$

$$S_s = \gamma_w \left(\frac{1}{E_s} + \frac{\theta}{E_w} \right)$$

$$S_0 = (1 - \theta_0)^{1-r}$$

$$r = \frac{\sigma'}{\sigma_c} \in [0:1]$$

$$\sigma_c = -E \log(1 - \theta_0)$$

with

k = Geometric permeability [m²]

K = Hydraulic conductivity [m/s], $K = \frac{\gamma_w}{\mu} k = \mathbf{K}_{11}$

θ_0 = Porosity under no stress conditions [−]

σ_c = Critical lithostatic stress / void space closure pressure [Pa]

E = Vertical elasticity coefficient at full saturation [Pa]

E_s = Elastic modulus of the aquifer [Pa]

E_w = Water elastic modulus [Pa]

C = Coefficient depending on the distribution of grains size [1/m]

b = Cementation-tortuosity factor (10 < b < 30) [−]

r_{xy} = Anisotropy ratio in the XY-plane [−], $r_{xy} = \mathbf{K}_{22}/\mathbf{K}_{11}$

r_{xz} = Anisotropy ratio in the XZ-plane [−], $r_{xz} = \mathbf{K}_{33}/\mathbf{K}_{11}$

$\mathbf{R}$ = Rotation matrix $\mathbf{R} = \mathbf{R}_{313} = \mathbf{R}(\phi, \theta, \psi)$ (see Note 8 in section Notes)

ϕ = Euler 1st sequential rotation angle around the Z-axis

θ = Euler 2nd sequential rotation angle around the X-axis

ψ = Euler 3rd sequential rotation angle around the Z-axis

The plugin allows for an association of an arbitrary number of elemental selections to granular medium representations. Such regions can be created and parameterized by adding new granular medium formations . This results in selecting an available elemental selection to which the granular medium parameters are to be defined in the corresponding table.
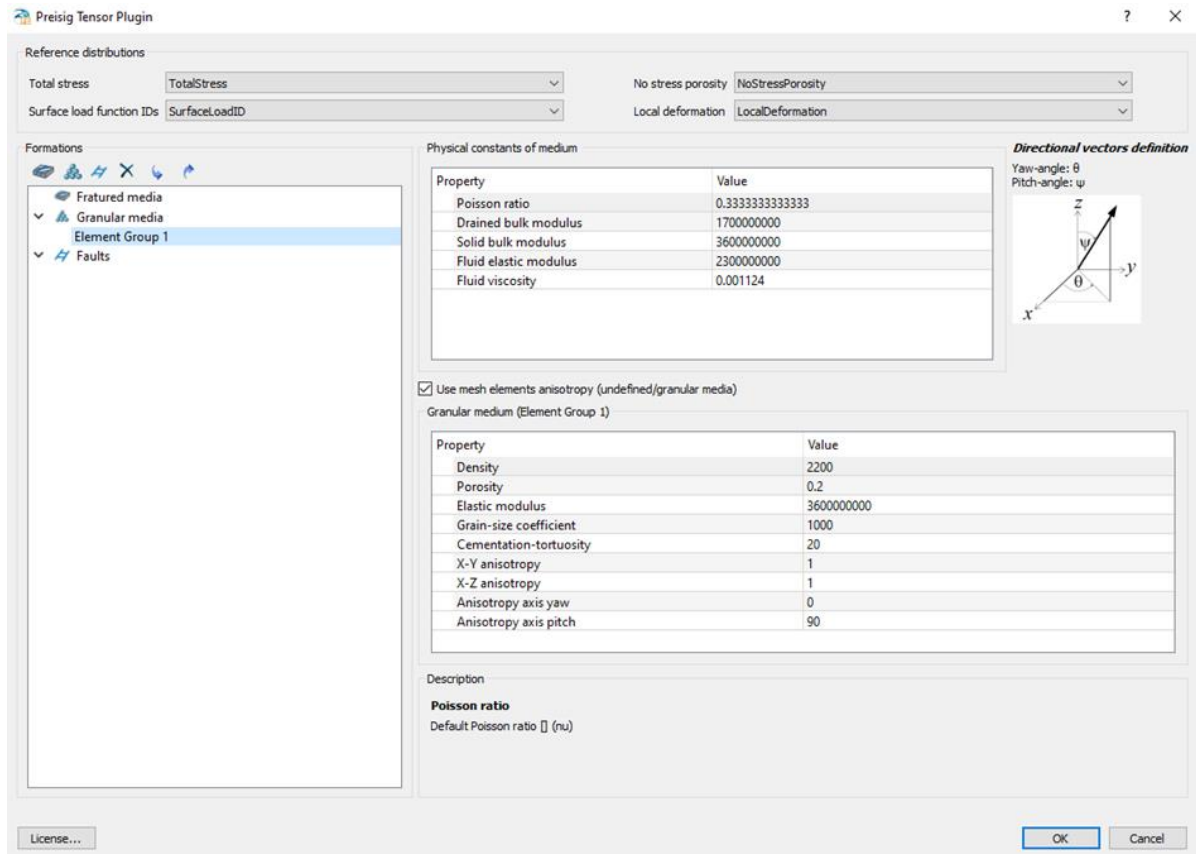
Figure 4 Granular medium input parameter table with elemental selection relationship. Here the elemental selection named "Element Group 1" has been chosen and the granular model has been parameterized.

Table 2 Indicative ranges for porosity closure limit effective stress and vertical elasticity.

Soil type	E_s [Pa] Vertical elasticity	ϕ_0 [-] Porosity	σ_0' [Pa] Limit effective stress for pore closure
Peat	$10^6 - 10^7$	$0.1 - 0.2$	$10^5 - 10^6$
Silty clay	$10^7 - 10^8$	$0.1 - 0.2$	$10^6 - 10^7$
Sand - gravel	$10^8 - 10^9$	$0.2 - 0.3$	$10^7 - 5 \times 10^8$

Table 3 Indicative ranges for the grain size distribution coefficient C.

Soil type	C [1/m]
Pebble gravel stream channel	~ 1000
Sandy gravel	~ 3500
Fine sand	~ 7000
Alluvial sandy gravel	$\sim 13'500$
Sandy-silty gravel moraine	$\sim 36'000$
Silty sand	$\sim 36'500$
Lacustrine clayey silt	$\sim 205'500$

2.4 Validation for granular media

The granular medium model implementation is validated against an analytical solution at steady-state. A vertical sand column of 100 meters and of section 1 m² is considered. It is subject to the constant heads $H(Z = 100) = 100$ and $H(Z = 0) = 0$, generating a uniform flow from top to bottom. The formation has the following characteristics:

$$\theta_0 = 0.25 \, [-]$$
$$\rho_r = 1800 \, [\text{kg/m}^3]$$
$$E_s = 20 \, [\text{MPa}]$$
$$\sigma_c = -E \log(1 - \theta_0) = 11.5 \, [\text{MPa}]$$
$$C = 1000 \, [1/\text{m}]$$
$$b = 20 \, [-]$$

Hydraulic conductivity and discharge rate at no stress conditions read:

$$K_0 = K(\sigma' = 0) = 0.00134613 \, [\text{m/s}]$$
$$q_0 = q(\sigma' = 0) = -K \frac{dH}{dz} = 0.000788627966 \, [\text{m}^3/\text{s}]$$
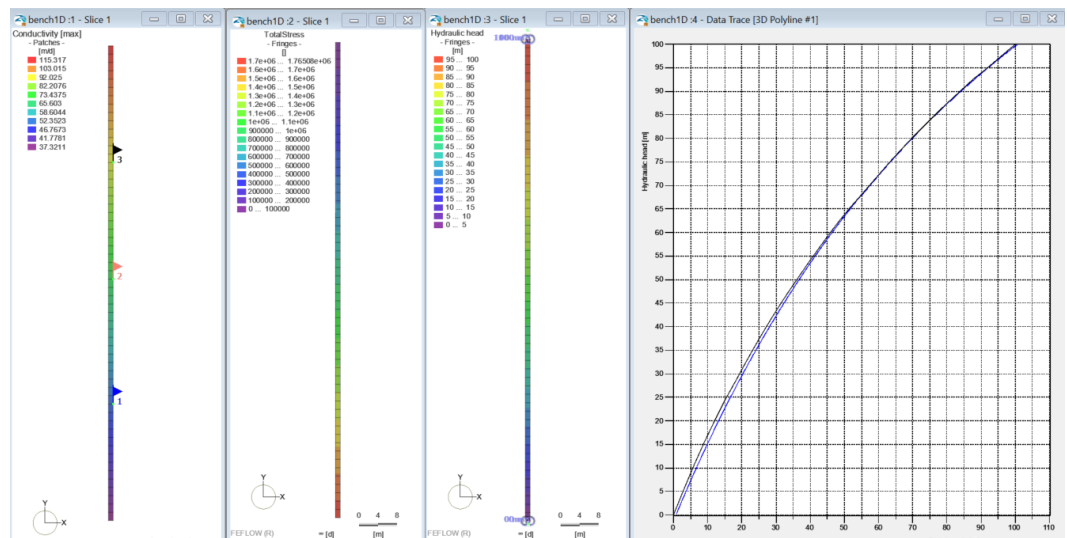

Figure 5 Solution vertical profiles with head compared to an analytical solution.

2.5 Validation for fractured media

This 3D validation considers a block of fractured rock mass of 2000 m x 1000 m x 1000 m. Permeability is generated by a single family of horizontally fractures with aperture 0.1 mm and frequency 100 (1/m).

The rock density is $\rho_r = 2500$ kg/m³, closure stress is $\sigma'_0 = 350$ MPa, and Poisson ratio is taken as $\nu = 0.5$. Fractures being horizontal, only vertical closure is occurring. Without stress, the equivalent hydraulic conductivity tensor is

$$\mathbf{K} = \begin{bmatrix} K_0 & 0 & 0 \\ 0 & K_0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad K_0 = 7.27 \times 10^{-5} \text{m/s}$$

One border of the rock is at a constant hydraulic head $H_0 = 1000$ m while the opposite border is at constant atmospheric pressure. Initial head conditions hydrostatic conditions. The simulation is running until equilibrium is met. Rock consolidation becomes consequence of the change from hydrostatic to hydrodynamic conditions.

Analytical solutions for the steady flow rate and for the pressure head field can be derived only for the case of a model exponent $m = 1$ (Preisig, 2014). The steady-state groundwater flow rate through the fractured rock mass and pressure head distributions read:

$$Q = W \int_{z=0}^{z=H_0} q(x,z)dz$$

$$q(x,z) = K_0 \int_0^L \left(1 - \left(\frac{\alpha D - h(x,z)}{s_0} \right) \right)^3 dH$$

$$h(x,y,z) = \left[(\alpha D - h_0 - s_0)^4 - \frac{xh_0^2}{l}(2\alpha D - h_0 - 2s_0)^2 \right.$$
$$\left. + \frac{h_0 x^2}{l}(2\alpha D - h_0 - 2s_0)(\alpha D - s_0)^2 \right]^{1/4} - s_0 + \alpha D$$

where W is width (1000 m), D is depth, L is the length of fractures in the *X*-direction, l is length along the *X*-axis, $h_0 = 1000 - z$, and with $\alpha = \frac{\rho_r}{\rho_w}$ and $s_0 = \frac{\sigma'_0}{\rho_w g}$.

Figure 6 shows the numerical results at equilibrium. The computed steady-state discharge (16.223 m³/s) matches the analytical value (16.222 m³/s).
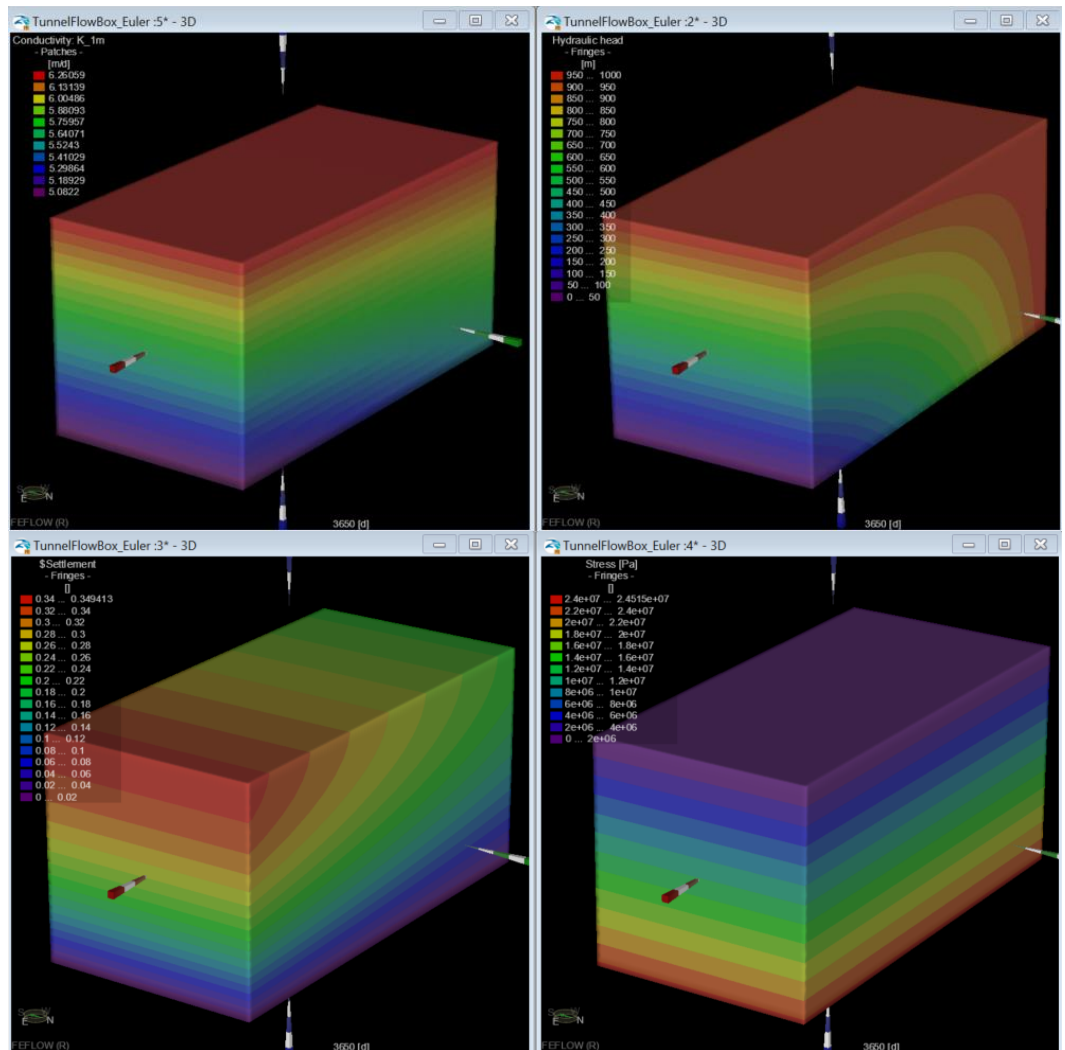
Figure 6 3D benchmark for the fractured medium case, with displayed heads, stresses, consolidation, and hydraulic conductivity at equilibrium.

2.6 Including surface overburden effects

Neuzil's 1D approach for surface load effects

Surface overburden effects are included following Neuzil's 1D vertical *loading efficiency* (2003) by formulating the following fluid source/sink function:

$$S_f(t) = \zeta \frac{S_s}{\rho_w g} \frac{d\sigma_v(t)}{dt}, \qquad \zeta = \frac{B(1+\nu)}{3(1-\nu) - 2B\alpha(1-2\nu)}, \qquad B = \frac{\frac{1}{E_p} - \frac{1}{E_s}}{\frac{1}{E_p} - \frac{1}{E_s} + \theta\left(\frac{1}{E_w} - \frac{1}{E_s}\right)}$$

with

S_f = Volumetric fluid source term [T^{-1}]

ζ = 1D vertical loading efficiency [−]

σ_v = Overburden vertical stress from material generating surface overload [Pa]

B = Skempton's coefficient [−]

The user needs to create an elemental reference distribution whose values point to the IDs of existing power functions. These power functions are used to represent in a discrete manner the arbitrary, time-varying surface load function(s) $\sigma_v(t)$ expressed in Pa. Elements having such a description defined in the elemental reference distribution are then receiving the Neuzil source/term S_f.

Validation

The 1-D vertical saturated sand column analytical benchmark case of Lemieux *et al.* [2008] is used to illustrate the effect of ice loading on hydraulic head distribution. A surface load function $\sigma_v(t)$ representing an ice sheet forming above an aquifer, is added at the inlet at constant intervals such that $\frac{d\sigma_v(t)}{dt}$ is a constant, i.e. the surface σ_v load function is linear. Surface load σ_v can further be converted to an equivalent water height using the freshwater density ρ_w, yielding to the surface function $\omega(t) = \frac{1}{\rho_w g} \frac{d\sigma_v}{dt}$.

The governing equation describing flow along the column with mechanical loading is $\frac{dH}{dt} = D\frac{d^2H}{dz^2} + \zeta\omega(t)$, where $D = K/S_s$ is hydraulic diffusivity and H is hydraulic head. For a column of semi-infinite length, initial and boundary conditions can be specified as follows: $H(z,0) = 0$, $H(0,t) = 0$, $dH(z=\infty,t)/dz = 0$.
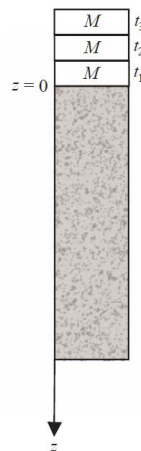

Figure 7 Schematic representation of the 1D vertical ice-loading model.

Using Laplace transforms, and using the fact that $\omega(t)$ is constant, one can derive an analytical solution to this boundary-value problem:

$$H(z,t) = \zeta\omega\left(t - \left(t + \frac{z^2}{2D}\right)\text{erfc}\left(\frac{z}{2\sqrt{Dt}}\right) + z\sqrt{\frac{t}{\pi D}}\exp\left(-\frac{z^2}{4Dt}\right)\right)$$

$$q(z,t) = -K\frac{dH(z,t)}{dz} = 2K\zeta\omega\left(\frac{z}{D}\text{erfc}\left(\frac{z}{2\sqrt{Dt}}\right) - \sqrt{\frac{t}{\pi D}}\exp\left(-\frac{z^2}{4Dt}\right)\right)$$

From the flux $q(z,t)$, the inlet flowrate is obtained at $z = 0$:

$$Q(t) = 2K\zeta\omega\sqrt{t/\pi D}$$
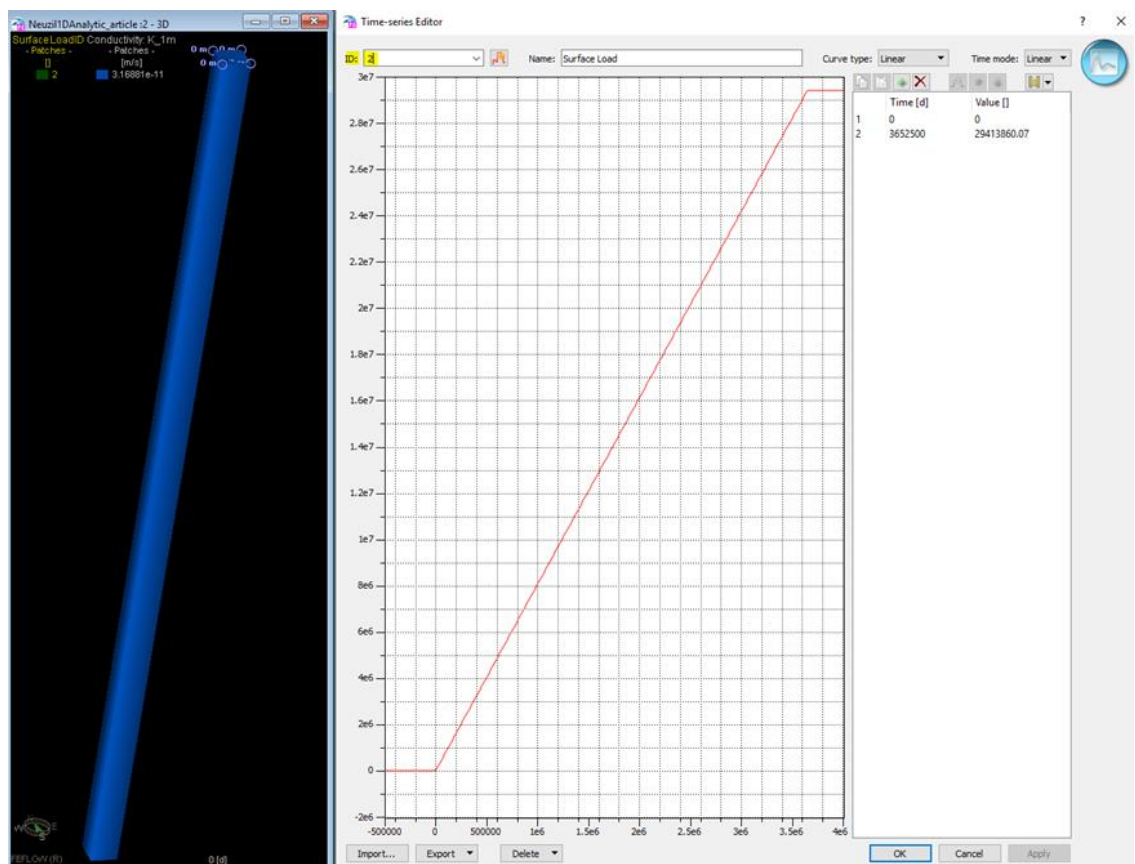
Figure 8 FEFLOW time-series editor displaying the surface ice load temporal function $\sigma_v(t)$ in Pa, and the elemental reference distribution used to point at the function ID (here 2).

In order to compare the numerical solutions with the analytical solutions, we make use of a 10'000 m length domain to which an ice sheet is taken to grow in thickness at a rate of 0.326 meters of ice per year, which is equivalent to 0.3 meters of water equivalent loading per year for 10'000 years (i.e. $\omega = 0.3$m/y) with an ice density of $\rho_{ice} = 920$kg/m³.

The surface overburden load function is the linear $\sigma_v(t) = \rho_{ice}gd_{ice}(t) \approx 8.052\ t$ [Pa], where time t is in days (Figure 8). The top of the column is drained and as such a specified head of 0.0m is assigned. The column bottom is a no-flow boundary.

The hydraulic and mechanical properties of the rock are $K = 10^{-3}$m/y, $S_s = 10^{-6}$1/m, $E_p = 1.7 \times 10^9$kg/s²/m, $E_s = 3.6 \times 10^9$kg/s²/m, $E_w = 2.3 \times 10^9$kg/s²/m, $\nu = 1/3$. Skempton's coefficient is $B = 0.868$ and the resulting loading efficiency is $\zeta = 0.683$.
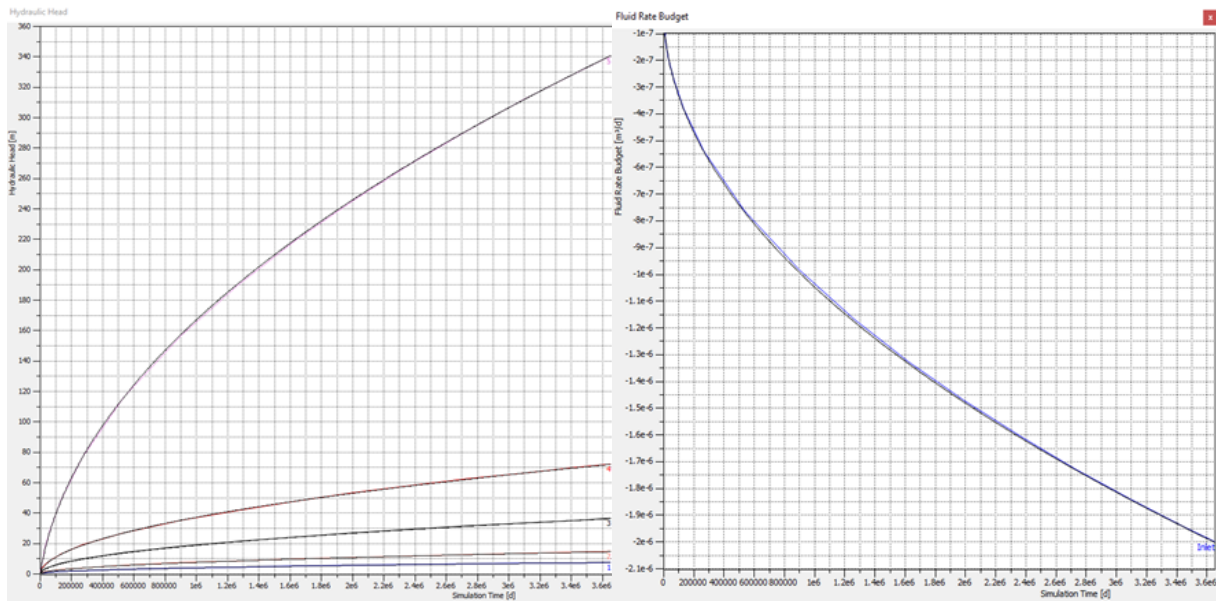
Figure 9 **Left:** FEFLOW (colored lines) vs analytical (black lines) hydraulic head results $H(z, t)$ at depths 10m (P1), 20m (P2), 50m (P3), 100m (P4), and 500m (P5). **Right:** FEFLOW (blue line) vs analytical (black line) inlet parabolic discharge $Q(t) = q(0, t) = 2K\zeta\omega\sqrt{t/\pi D}$

2.7   Local deformation

Local deformation at post-timestep is optionally written in the indicated elemental reference distribution. It is the change in porosity on the element over the last period about the maximum porosity θ_0:

$$\Delta\theta = \theta(\sigma'_p) - \theta(\sigma') = \begin{cases} \theta_{f,0}\left(\left(\dfrac{\sigma'}{\sigma'_0}\right)^{\frac{1}{m}} - \left(\dfrac{\sigma'_p}{\sigma'_0}\right)^{\frac{1}{m}}\right)|n_z| & \text{Single fracture} \\[2em] \displaystyle\sum_{i=1}^{N_f}\theta_{f,0}[i]\left(\left(\dfrac{\sigma'[i]}{\sigma'_0[i]}\right)^{\frac{1}{m[i]}} - \left(\dfrac{\sigma'_p[i]}{\sigma'_0[i]}\right)^{\frac{1}{m[i]}}\right)|n_z[i]| & \text{Fractured medium} \\[2em] (1-\theta_0)^{1-\frac{\sigma'}{\sigma'_0}} - (1-\theta_0)^{1-\frac{\sigma'_p}{\sigma'_0}} & \text{Granular medium} \end{cases}$$

with σ'_p being the effective stress previous state. $\Delta\theta$ is positive in consolidation and negative in expansion.
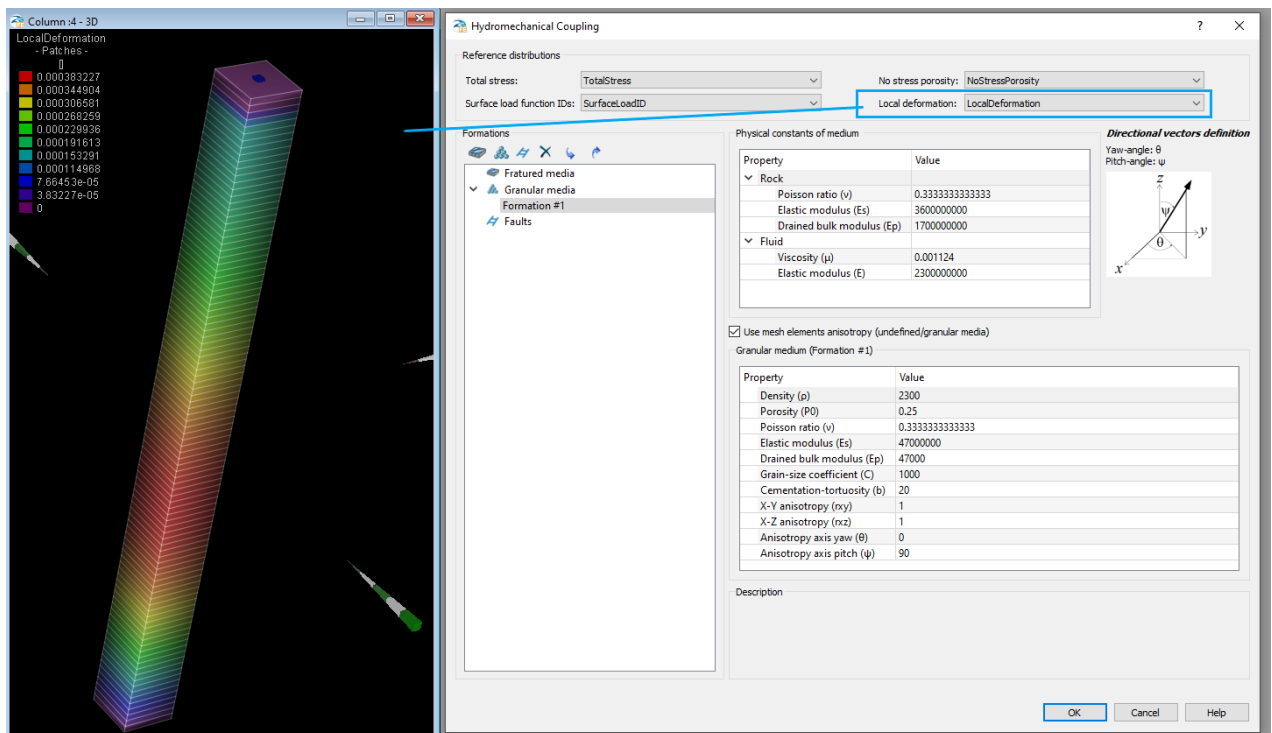
Figure 10 Providing an elemental reference distribution for dumping local deformation.

2.8   Settlement / consolidation

Settlement $S(x, y, z)$ evaluations can be obtained from local deformation by integration over the vertical from the bottom to the top of the mesh:

$$S(x, y, z) = \int_{Z_{bottom}}^{Z_{top}} \Delta\theta(x, y, z) dz$$

From version v1.1, and for the case of 3D layered meshes only, this explicit integration is performed if a **nodal reference distribution** is provided for writing the results. Results are mapped into this container in meters. For 2D and 3D meshes, this integration needs a special operation that will be released later (see in Tricks and tips: in Section Notes).
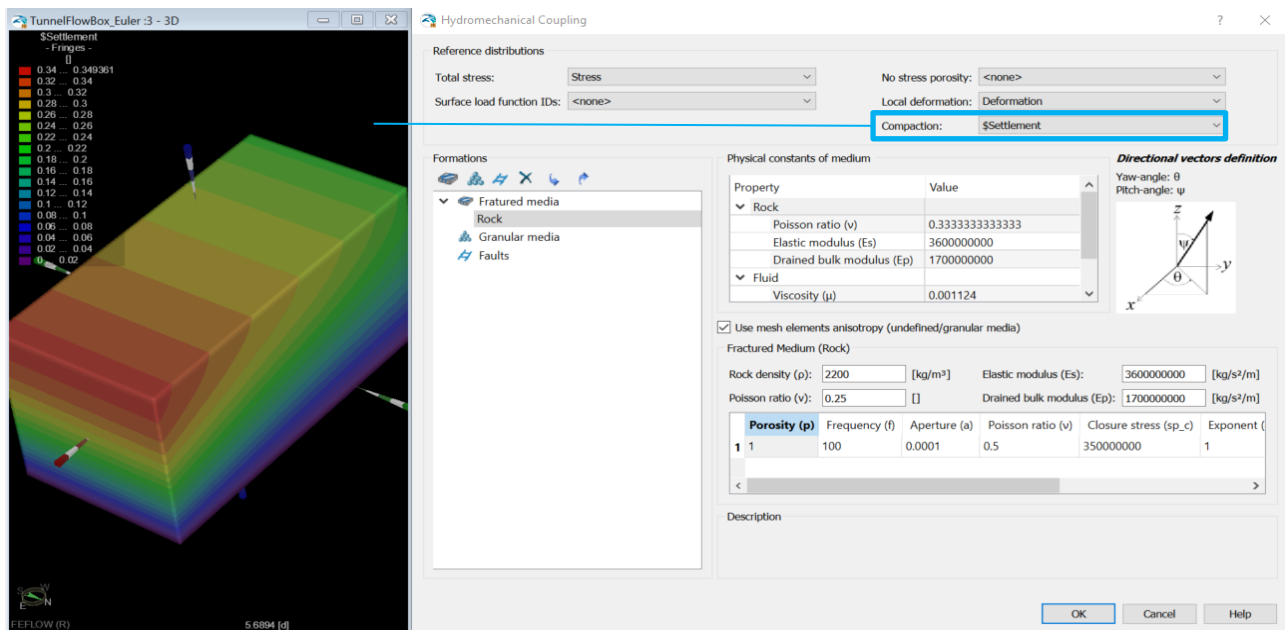

Figure 11 Providing a nodal reference distribution for dumping compaction / settlement.

3   Notes

1. In the absence of tectonic stresses, the principal stress is assumed to be the vertical component of the total stress tensor: $\sigma_v = \sigma_{ZZ}$, $\sigma_h = \sigma_{XX} = \sigma_{YY}$

2. Isotropic conditions are assumed for elastic compressible media not undergoing tectonic, erosional, or post-glacial stress

3. Vertical elasticity coefficient $E = E_s$ if water is assumed incompressible

4. In granular media, the law of elasticity is valid for small strains, and one assumes vertical deformation is exclusively driven by:

    -   Change in porosity due to the shifting of incompressible solid grains, and
    -   Closure of intergranular voids

5. In fractured media it is assumed:
    -   A fracture of aperture a is conceptualized as a pair of surfaces with a set of asperities whose length is given by a statistical distribution
    -   Each asperity satisfies Hooke's law

6. The range of applicability of the effective stress models implies that:
    -   The fracture / void space is closed: $r = \min(r, 1)$, and
    -   The case $\sigma' < 0$ pushes the model out of its applicability for it implies non-darcean quicksand effects: $r = \max(r, 0)$

7. The effective stress σ' may be enriched by extra terms:
    $$\sigma' = (\sigma - p) + \sigma_{SU} + \sigma_{CO}$$
    σ_{SU} = Soil suction stress [Pa] at the variably saturated state
    σ_{CO} = Apparent tensile stress [Pa] at the saturated state (or saturated cohesion) caused by cohesive or physio-chemical forces (from individual contributions from van der Waals attractions, electrical double layer repulsion, and chemical cementation effects).
    σ_{CO} is constant for different soil types, and $\sigma_{CO} \in [0: \sigma_{CO} \geq 100\text{kPa}]$.

    Bishop [1959] provides a saturation-dependent formulation:
    $$\sigma' = \sigma - p_A + S_e(p_A - p)$$
    p_A = Air-entry pressure [Pa]
    S_e = Effective degree of saturation [−]

    Effective stress in variably-saturated formations is explained in Lu and Likos [2006] and Lu *et al.* [2010].

8. The rotation matrix $\mathbf{R}(\phi, \theta, \psi)$ according to FEFLOW's sequences of Euler angles (ϕ, θ, ψ) rotations is a 313 (or ZXZ) constructed matrix, $\mathbf{R} = \mathbf{R}_{313}$:
    $$\mathbf{R}_{313} = \begin{pmatrix} c\psi\, c\phi - c\theta\, s\phi\, s\psi & c\psi\, s\phi + c\theta\, c\phi \sin\psi & s\psi\, s\theta \\ -s\psi\, c\phi - c\theta\, s\phi\, c\psi & -s\psi\, s\phi + c\theta\, c\phi \cos\psi & c\psi\, s\theta \\ s\theta\, s\phi & -s\theta\, c\phi & c\theta \end{pmatrix}$$
    $$c\,\alpha = \cos(\alpha), s\alpha = \sin(\alpha)$$

    with

ϕ	=	Euler 1st sequential rotation angle around the Z-axis
θ	=	Euler 2nd sequential rotation angle around the Y-axis
ψ	=	Euler 3rd sequential rotation angle around the Z-axis

9. The fractured medium case builds an elemental full hydraulic conductivity tensor $\mathbf{K}$, which is then converted into the standard FEFLOW principal components / Euler angles formalism. This is accomplished by diagonalizing $\mathbf{K}$ and by extracting the 3 Euler angles of rotation from the eigenvectors column matrix:

$$\mathbf{K} = \mathbf{Q}\,\mathbf{D}\,\mathbf{Q}^{\mathrm{T}}$$

$$\mathbf{D} = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}$$

$$\mathbf{Q} = \mathrm{matrix}(\boldsymbol{\lambda}_1 \mid \boldsymbol{\lambda}_2 \mid \boldsymbol{\lambda}_3)$$

$$\mathbf{R} = \mathbf{Q}, \qquad \mathbf{R}^{\mathrm{T}} = \mathbf{R}^{-1}$$

$$\begin{pmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{pmatrix} = \begin{pmatrix} \mathrm{atan}(\mathbf{R}_{23}, \mathbf{R}_{33}) \\ -\mathrm{asin}(\mathbf{R}_{13}) \\ \mathrm{atan}(\mathbf{R}_{12}, \mathbf{R}_{11}) \end{pmatrix}$$

$$\begin{pmatrix} \phi \\ \theta \\ \psi \end{pmatrix} = \begin{pmatrix} \mathrm{atan}(-\,\mathrm{s}\,\theta_2, \mathrm{s}\,\theta_1\,\mathrm{c}\,\theta_2) \\ \mathrm{acos}(\mathrm{c}\,\theta_1\,\mathrm{c}\,\theta_2) \\ \mathrm{atan}(\mathrm{c}\,\theta_1\,\mathrm{s}\,\theta_2\,\mathrm{c}\,\theta_3 + \mathrm{s}\,\theta_1\,\mathrm{s}\,\theta_3, -\,\mathrm{c}\,\theta_1\,\mathrm{s}\,\theta_2\,\mathrm{s}\,\theta_3 + \mathrm{s}\,\theta_1\,\mathrm{c}\,\theta_3) \end{pmatrix}$$

with

$\mathbf{D}$ = Diagonalized tensor (principal components $\mathbf{D}_{ii} = \lambda_i$)
λ_i = Eigenvalues of $\mathbf{K}$
$\boldsymbol{\lambda}_i$ = Normalized eigenvectors of $\mathbf{K}$
$\mathbf{R}$ = Rotation matrix $\mathbf{R} = \mathbf{R}_{123} = \mathbf{R}(\theta_1, \theta_2, \theta_3)$
θ_1 = Euler 1st sequential rotation angle around the X-axis
θ_2 = Euler 2nd sequential rotation angle around the Y-axis
θ_3 = Euler 3rd sequential rotation angle around the Z-axis

10. Tricks and tips:

- The conversion from yaw angle θ and pitch angle ψ to obtain an explicit normal definition (n_x, n_y, n_z) for fracture family planes reads:

$$\begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix} = \begin{pmatrix} \cos(\theta)\cos\left(\psi - \dfrac{\pi}{2}\right) \\ \sin(\theta) \\ \cos(\theta)\sin\left(\dfrac{\pi}{2} - \psi\right) \end{pmatrix}$$

- For unstructured meshes (3D or 2D vertical), the evaluation of the nodal depth or lithostatic stress fields is not straightforward but can be achieved by solving an equation of type steady-state confined flow. One can e.g. either solve for nodal depth $d(x.y.z)$ or lithostatic stress $\sigma(x.y.z) = g \int_z^{Z_{top}} \rho_r(x, y, u)\,du$ by defining the following boundary-value problems:

$$\begin{cases} \nabla \cdot \boldsymbol{\Sigma}\nabla d(x, y, z) = 0 \text{ in } \Omega \\ d\left(x, y, z = Z_{top}\right) = 0 \\ -\boldsymbol{\Sigma}\nabla d(x, y, z = Z_{bottom}) \cdot \boldsymbol{n} = g \\ \boldsymbol{\Sigma} = \nabla z \otimes \nabla z = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \end{cases} \quad \text{Depth BVP}$$

and

$$\begin{cases} \nabla \cdot \boldsymbol{\Sigma}\nabla \sigma(x, y, z) = 0 \text{ in } \Omega \\ \sigma\left(x, y, z = Z_{top}\right) = 0 \\ -\boldsymbol{\Sigma}\nabla \sigma(x, y, z = Z_{bottom}) \cdot \boldsymbol{n} = g \\ \boldsymbol{\Sigma} = \dfrac{1}{\rho_r}\nabla z \otimes \nabla z = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1/\rho_r \end{bmatrix} \end{cases} \quad \text{Stress BVP}$$

A proper definition of top and bottom of the mesh is thus the key for obtaining meaningful solutions. By defining a steady-state confined flow problem class in FEFLOW, one simply needs to assign top and bottom nodal conditions. Zero prescribed heads on top of the mesh will represent zero depth or zero stress. Outflowing Neumann flux conditions on the bottom of the mesh will define the BVP. The manipulation of hydraulic conductivity tensor is the last operation to be done, letting $K_{zz} = 1/\rho_r$, $K_{xx} = K_{yy} = 0$ for the stress filed BVP, or $K_{zz} = 1$, $K_{xx} = K_{yy} = 0$ for the depth BVP. The stress field can therefore be obtained by solving its BVP, or deduced from the depth field, e.g. by making use of the equation editor in FEFLOW with the formula $\sigma(x.y.z) = \rho_r g d(x,y,z)$. Calculated heads will correspond to stresses in Pa (or depths in meters for the depth BVP) which can be copied to a nodal reference distribution for usage with the plugin.

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