

CODE_BRIGHT

2023

USER'S GUIDE



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CODE_BRIGHT 2023 User's Guide

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https://deca.upc.edu/en/projects/code_bright



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I. CODE_BRIGHT. FOREWORD

I.1. INTRODUCTION

The program described here is a tool designed to handle coupled problems in geological media. The computer code, originally, was developed on the basis of a new general theory for saline media. Then the program has been generalised for modelling thermo-hydro-mechanical (THM) processes in a coupled way in geological media. Basically, the code couples mechanical, hydraulic and thermal problems in geological media.

The theoretical approach consists in a set of governing equations, a set of constitutive laws and a special computational approach. The code is written in FORTRAN and it is composed by several subroutines. The program does not use external libraries.

CODE_BRIGHT uses GiD system for preprocessing and post-processing. GiD is developed by the International Center for Numerical Methods in Engineering (CIMNE). GiD is an interactive graphical user interface that is used for the definition, preparation and visualisation of all the data related to numerical simulations. This data includes the definition of the geometry, materials, conditions, solution information and other parameters. The program can also generate the finite element mesh and write the information for a numerical simulation program in its adequate format for CODE_BRIGHT. It is also possible to run the numerical simulation directly from the system and to visualize the resulting information without transfer of files.

For geometry definition, the program works quite like a CAD (Computer Aided Design) system. The most important difference is that the geometry is developed in a hierarchical mode. This means that an entity of higher level (e.g. a volume) is constructed over entities of lower level (e.g. a surface); two adjacent entities (e.g. two volumes) will then share the same lower level entity (e.g. a surface).

All materials, conditions and solution parameters can also be defined on the geometry without the user having any knowledge of the mesh. The meshing is performed once the problem has been fully defined. The advantages of doing this are that, using associative data structures, modifications can be made on the geometry and all other information will be updated automatically.

Full graphic visualisation of the geometry, mesh and conditions is available for comprehensive checking of the model before the analysis run is started. More comprehensive graphic visualisation features are provided to evaluate the solution results after the analysis has been performed. This post-processing user interface is also customisable depending on the analysis type and the results provided.

A query window appears for some confirmations or selections. This feature is also extended to the end of a session, when the system prompts the user to save the changes, even when the normal ending has been superseded by closing the main window from the Window Manager, or in most cases with incorrect exits.

I.2. SYSTEM BASICS

GiD is a geometrical system in the sense that, having defined the geometry, all the attributes and conditions (i.e., material assignments, loading, conditions, etc.) are applied to the geometry without any reference or knowledge of a mesh. Only once everything is defined, should the meshing of the geometrical domain be carried out. This methodology facilitates alterations to

the geometry while maintaining the attributes and conditions definitions. Alterations to the attributes or conditions can simultaneously be made without the need of reassigning to the geometry. New meshes or small modifications on the obtained mesh can also be generated if necessary and all the information will be automatically assigned correctly.

The system does provide the option for defining attributes and conditions directly on the mesh once this has been generated. However, if the mesh is regenerated, it is not possible to maintain these definitions and therefore all attributes and conditions must be redefined. In general, the complete solution process can be described as:

1. Define geometry - points, lines, surfaces, volumes.
 - Use other facilities.
 - Import from CAD.
2. Define attributes and conditions.
3. Generate mesh.
4. Carry out simulation.
5. View results.

Depending upon the results in step (5) it may be necessary to return to one of the steps (1), (2) or (3) to make alterations and rerun the simulations.

Building a geometrical domain in GiD is based on the 4 geometrical levels of entities: points, lines, surfaces and volumes. Entities of higher level are constructed over entities of lower level; two adjacent entities can therefore share the same level entity.

All domains are considered in 3-dimensional space but if there is no variation in the third coordinate (into the screen) the geometry is assumed to be 2-dimensional for analysis and results visualisation purposes. Thus, to build a geometry, the user must first define points, join these to form lines, create closed surfaces from the lines and define closed volumes from the surfaces. Many other facilities are available for creating the geometrical domain; these include: copying, moving, automatic surface creation, etc.

The geometrical domain can be created in a series of layers where each one is a separate part of the geometry. Any geometrical entity (points, lines, surfaces or volumes) can belong to a particular layer. It is then possible to view and manipulate some layers and not others. The main purpose of the use of layers is to offer a visualisation and selection tool, but they are not used in the analysis.

The system has the option of importing a geometry or mesh that has been created by a CAD program outside GiD; at present, this can be done via a DXF, IGES or NASTRAN interface.

Once the geometry and attributes have been defined, the mesh can be generated using the **mesh generation tools** supplied within the system. Structured and unstructured meshes containing triangular and quadrilateral surface meshes or tetrahedral and hexahedral volume meshes may be generated. The automatic mesh generation facility utilizes a background mesh concept for which the users are required to supply a minimum number of parameters.

Simulations are carried out by using the calculate menu. The final stage of **graphic visualisation** is flexible in order to allow the users to critically evaluate the results quickly and easily. The menu items are generally determined by the results supplied by the solver module: this not only reduces the amount of information stored but also allows a certain degree of user customisation. The post solver interface may be included fully into the system so that it runs automatically once the simulation run has terminated.

I.3. USING THIS MANUAL

This User Manual has been split into several differentiated parts. The part, **THEORETICAL ASPECTS**, contains the theoretical basis of **CODE_BRIGHT**, and the numerical solution. In **CODE_BRIGHT. PREPROCESS. PROBLEM DATA**, it is described how to enter the data of the problem, i. e. general data, constitutive laws, boundary conditions, initial conditions and interval data. The referred as **CODE_BRIGHT. PROCESS** is related to the calculation process. This part also contains the description of input files. The part, **CODE_BRIGHT. CONSTITUTIVE LAWS** contains a description of hydraulic, thermal and mechanical constitutive laws and phase properties. Finally, **CODE_BRIGHT. TUTORIAL**, introduces guided examples for a fast and easy familiarization with the system.

II. CODE_BRIGHT. PRE-PROCESS. PROBLEM DATA.

Problem data include all the parameters, conditions (see section Conditions), materials properties (see section Materials), problem data (see section Problem Data) and intervals data (see section Interval Data) that define the project. Conditions and materials should be assigned to geometrical entities.

II.1. PROBLEM TYPE

This option permits to select among all available problem types. When selecting a new problem type, all information about materials, conditions and other that has already been selected or defined will be lost. *Select CODE_BRIGHT*. If an existing project has been created with an old version of CODE_BRIGHT, use the option '**Transform to new problem type**' and data will be converted to update the problem type. Be aware in some cases some information may be lost, which would be indicated in a window that appears in the screen.

II.2. CODE_BRIGHT INTERFACE

CODE_BRIGHT program reads data from two files: *ROOT_GEN.DAT* and *ROOT_GRI.DAT*. These files are identified by the *ROOT* argument (previously read in a file called *ROOT.DAT*). The information data files are structured in 'Cards' which are described in CODE_BRIGHT. PROCESS: 'Data files'. Working into CODE_BRIGHT interface, the information needs to be introduced in a four concept scheme:

<u>Interface (inputs)</u>	<u>Information Data Files (numerical program)</u> (File structure - obtained with CALCULATE)
CONDITIONS	ROOT.DAT
MATERIALS	ROOT_GEN.DAT
PROBLEM DATA	ROOT_GRI.DAT
INTERVAL DATA	

In order to build the data files *ROOT_GEN.DAT* and *ROOT_GRI.DAT*, data is introduced into several window statements associated with these concepts (interface inputs).

Once the geometry has been prepared, it is necessary to go through the different Interface steps, i.e. PROBLEM DATA, MATERIALS, CONDITIONS, and INTERVAL DATA. See the tutorials for a guided introduction to the interface between GiD and CODE_BRIGHT.

II.2.1. PROBLEM DATA

Problem data include all data that is general to the problem. This means that it is not related to a geometrical entity and it does not change in every time interval. It can be entered with the command `ProblemData` or in the problem data window. If entered in a window, the data is not accepted until the button `Accept` is pressed. This data can be entered before or after meshing. A description of the problem data features can be found in the following tables:

GENERAL DATA	
Title of the problem	Interface Default: Coupled problem in geological media
Execution	Only data file generation: ROOT_gen.dat and ROOT_gri.dat are built Full execution: Calculation with the finite element program CODE BRIGHT is performed (default option)
Backup (IMBACKUP in root_gen.dat)	No Backup Save Last: Allows restart the calculation from the last time step computed. Information is saved in file root_save.dat Save All: Allows restart the calculation from any time step computed. Information is saved in different files root_tnum_save.dat for each interval data computed (<i>tnum</i>). To restart the calculation, rename the file root_tnum_save.dat to root_save.dat
Axisymmetry (IAXISYM in root_gen.dat)	No, Around y-axis In 2-D axisymmetry the principal stresses are: σ_r (radial), σ_y (axial), σ_θ (circumferential)
Gravity X (2-D and 3-D) component	Interface Default: 0.0
Gravity Y (3-D) component	Interface Default: 0.0
Gravity Y (2-D) or Z (3-D) component	Interface Default: -9.81
EQUATIONS SOLVED	
Stress equilibrium (unknown displacement u) (IOPTDISPL in root_gen.dat)	Yes, No
Updated lagrangian method (IUPDC in root_gen.dat)	Yes, No. Updated lagrangian method, i.e. coordinates are modified after each time increment is solved. If deformations are very large, some elements may distort. If distortion is very large the volume of an element may become negative and the execution will terminate immediately.
Mass balance of water (unknown liquid pressure Pl) (IOPTPL in root_gen.dat)	Yes, No
Constant Pl	Constant liquid phase pressure for problems not including the mass balance of water equation
Mass balance of air (unknown liquid pressure Pg) (IOPTPG in root_gen.dat)	Yes, No
Constant Pg	Constant gas phase pressure for problems that do not include the equation of mass balance of air. Usually equal to 0.1 MPa.
Dissolved air into liquid phase (IOPTXAL in root_gen.dat)	Allowed, Not allowed
Energy balance (unknown temperature) (IOPTTEMP in root_gen.dat)	Yes, No
Vapour into gas phase (IOPTXWG in root_gen.dat)	Allowed, Not Allowed
Constant Temp	Constant temperature for problems that do not include the equation of energy balance.
Mass balance of conservative species (unknown concentration) (IOPTXWS in root_gen.dat)	Yes, No

Combinations of solving options are described below:

P_l	P_g	T	Variable
1	0	0	Compressible water flow, one phase, one species, air is not considered.
0	1	0	Compressible air flow, one phase, one species.
0	0	1	Heat flow (only conduction).
1	1	0	Two phase flow (liquid + gas), air dissolved permitted, vapour not permitted.
1	0	1	Water two phase non-isothermal flow, vapour allowed, gas phase at constant pressure.
0	1	1	Compressible non-isothermal gas flow, one phase, one species.
1	1	1	Non-isothermal two phase (liquid + gas) flow, vapour and air dissolved are allowed.

SOLUTION STRATEGY		
Epsilon (intermediate time for nonlinear functions)	Position of intermediate time $t^{k+\epsilon}$ for matrix evaluation, i.e. the point where the non-linear functions are computed. (usual values: 0.5, 1). See details on Numerical Method. Default: 1.0	
Theta (intermediate time for implicit solution)	Position of intermediate time $t^{k+\theta}$ for vector evaluation, i.e. the point where the equation is accomplished. Default: 1.0	
Time step control (ITIME in root_gen.dat) Default: 1	<p><u>0-4: Time step control based on N-R iterations:</u></p> <p>0: no time step prediction is performed. 1: predicts time stepping according to a limit of 4 iterations. 2: predicts time stepping according to a limit of 3 iterations. 3: predicts time stepping according to a limit of 2 iterations. 4: predicts time stepping according to a limit of 1 iteration.</p> <p><u>6-9: Time step control based on error estimation:</u></p> <p>6: controls time stepping by means of a prediction based on the relative error deviation in the variables (relative error lower than 0.01). 7: same as 6 but with a tolerance equal to 0.001. 8: same as 6 but with a tolerance equal to 0.0001. 9: same as 6 but with a tolerance equal to 0.00001.</p> <p><i>Note: a time step control = 1 will always be considered for negative time.</i></p>	
Max. number of iterations per time step (ITERMAX in root_gen.dat)	Maximum number of Newton Raphson iterations per time step. If the prescribed value is reached, time step is reduced. Default: 10	
Solver type (ISOLVE in root_gen.dat)	Direct: LU + BACK Iterative: Sparse + CGS	
Solver type = Iterative: Sparse + CGS	Max number of solver iterations	Default: 5000
	Max abs solver error variable	Default: 1.e-9
	Max abs solver error residual	Default: 0
	Max rel solver error residual	Default: 0
	Max threads parallel	Default: 1

Elemental relative permeability computed from: (IOPTPC in root_gen.dat)	Elemental suction (consistent approach) Average nodal degrees of saturation (default) Average nodal relative permeabilities Average nodal relative permeabilities (applies also for derivatives) Maximal nodal relative permeability	
Stress equilibrium (unknown displacement u) = yes	Max Abs Displacement (m) (DELMXU in root_gen.dat)	Maximum (absolute) displacement error tolerance (m). When correction of displacements (displacement difference between two iterations) is lower than this value, convergence has been achieved. Default: 1e-6
	Max Nod Bal Forces (MN) (DELFMX in root_gen.dat)	Maximum nodal force balance error tolerance (MN). If the residual of forces in all nodes are lower than this value, convergence has been achieved. Default: 1e-10
	Displacement Iter Corr (m) (DUMX in root_gen.dat)	Maximum displacement correction per iteration (m) (time increment is reduced if necessary). Default: 1e-1
Mass balance of water (unknown liquid pressure Pl) = yes	Max Abs Pl (MPa) (DELMXPL in root_gen.dat)	Maximum (absolute) liquid pressure error tolerance (MPa). Default: 1e-3
	Max Nod Bal Forces (MN) (DELQWMX in root_gen.dat)	Maximum nodal water mass balance error tolerance (kg/s). Default: 1e-10
	Pl Iter Corr (MPa) (DPLMX in root_gen.dat)	Maximum liquid pressure correction per iteration (MPa) (time increment is reduced if necessary). Default: 1e-1
Mass balance of air (unknown liquid pressure Pg) = yes	Max Abs Pg (MPa) (DELMXPG in root_gen.dat)	Maximum (absolute) gas pressure error tolerance (MPa). Default: 1e-3
	Max Nod Air Mass (kg/s) (DELQAMX in root_gen.dat)	Maximum nodal air mass balance error tolerance (kg/s). Default: 1e-10
	Pg Iter Corr (MPa) (DPGMX in root_gen.dat)	Maximum gas pressure correction per iteration (MPa) (time increment is reduced if necessary). Default: 1e-1
Energy balance (unknown temperature) = yes	Max Abs Temp (C) (DELMXT in root_gen.dat)	Maximum (absolute) temperature error tolerance (C). Default: 1e-3
	Max Nod Energy (J/s) (DELQMX in root_gen.dat)	Maximum nodal energy balance error tolerance (J/s). Default: 1e-10
	Temp Iter Corr (C) (DTMX in root_gen.dat)	Maximum temperature correction per iteration (C) (time increment is reduced if necessary). Default: 1e-1
Mass balance of conservative species (unknown concentration) = yes	Max Abs Solute (DELMXI in root_gen.dat)	Maximum (absolute) concentration error tolerance. Default: 1e-3
	Max Nod Solute mass balance (DELIMX in root_gen.dat)	Maximum nodal solute mass balance error tolerance. Default: 1e-10
	Solute Iter Corr (DIMX in root_gen.dat)	Maximum solute concentration correction per iteration (time increment is reduced if necessary). Default: 1e-1

Comments regarding the use of tolerances

In order to illustrate the use of tolerances the thermal problem is considered with the following tolerances:

Max Abs Temp (C)	$T1$
Max Nod Energy (J/s)	$T2$
Temp Iter Corr (C)	$T3$

Convergence can be achieved in two ways: the one when $\delta T < T1$ for all nodes (condition *A*) and the second when ($q_h < T2$) also for all nodes (q_h represents here the energy balance or residual at a node) (condition *B*).

It is to be mentioned that convergence in terms of δT and convergence in terms of q_h should be reached simultaneously because the Newton - Raphson method is used. For this reason, the program stops the iteration process when one of the two conditions (*A* or *B*) is achieved.

When more than one degrees of freedom are solved per node and one of the recommended options is used (convergence by variable OR residual), convergence in terms of variable or residual should be achieved by all the variables simultaneously. In other words, it is not possible that the mechanical problem converges by residual and the thermal problem converges by the variable.

Finally, if ($\delta T > T3$), time increment will be reduced. This parameter controls the accuracy of the solution in terms of how large time increments can be. A low value of $T3$ will force to use small time increments when large variations of temperature take place.

OUTPUT	
Write numerical process information (IOWIT in root_gen.dat)	<p>Iteration information is written in file <i>ROOT_GEN.OUT</i> according to:</p> <p>NONE: no information about convergence is written. This option should be used if the user is very confident with the time discretization and not interested in details at every time step or problems with time increment reductions. Usually this happens when previous runs have shown that convergence and time discretization work very well.</p> <p>PARTIAL: partial information is written. Time intervals and time-values, number of iterations, CPU-time values, etc. are written. Convergence information (e.g. residuals) is only written if time increment reductions take place.</p> <p>ALL: all iteration information is written. Convergence information is written for all iterations and all time increments. This option may result in a very large file <i>ROOT GEN.OUT</i></p>

<p>Writing frequency (INTER in root_gen.dat)</p>	<p>Writing results frequency in output files according to the number of time steps (positive integer value) or according to a given time increment (negative integer value).</p> <p>If it is positive, e.g. is set to 20, results for the complete mesh will be written only every 20 calculated time increments.</p> <p>If it is negative, then we can obtain the output values in a specified time: e.g. setting a value of -10 will produce output for 0, 10, 20, 30, ... units of time. Note that you may need to set a suitable maximum time step in the interval data in order for this implementation to work well (the maximum time step should be around one order of magnitude lower than the writing time frequency). See Figures II.2.1a, b and c.</p>
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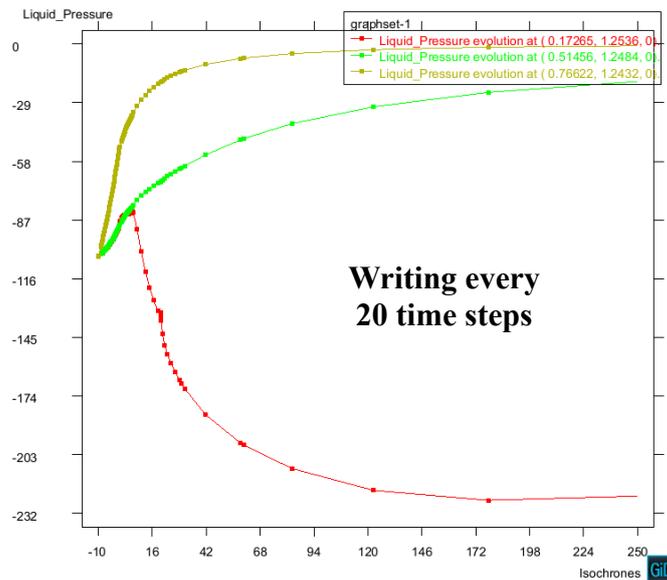


Figure II.2.1a. Writing every 20 time steps (Writing frequency = 20).

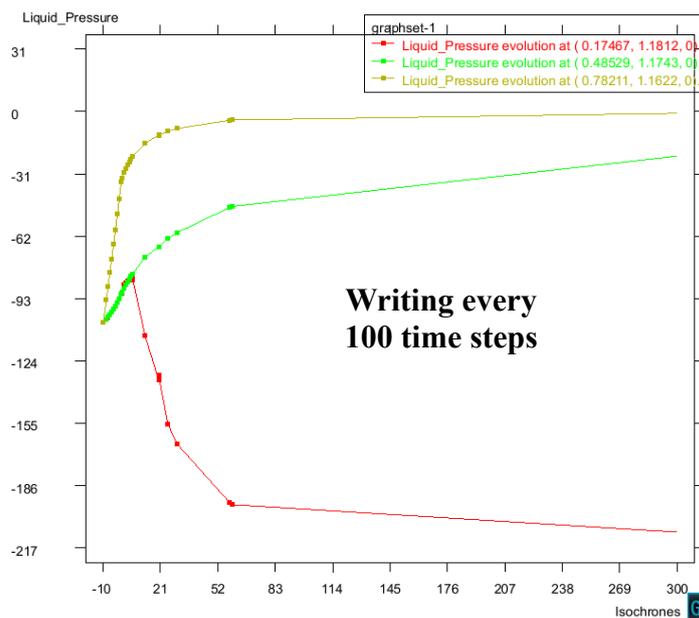


Figure II.2.1b. Writing every 100 time steps (Writing frequency = 100).

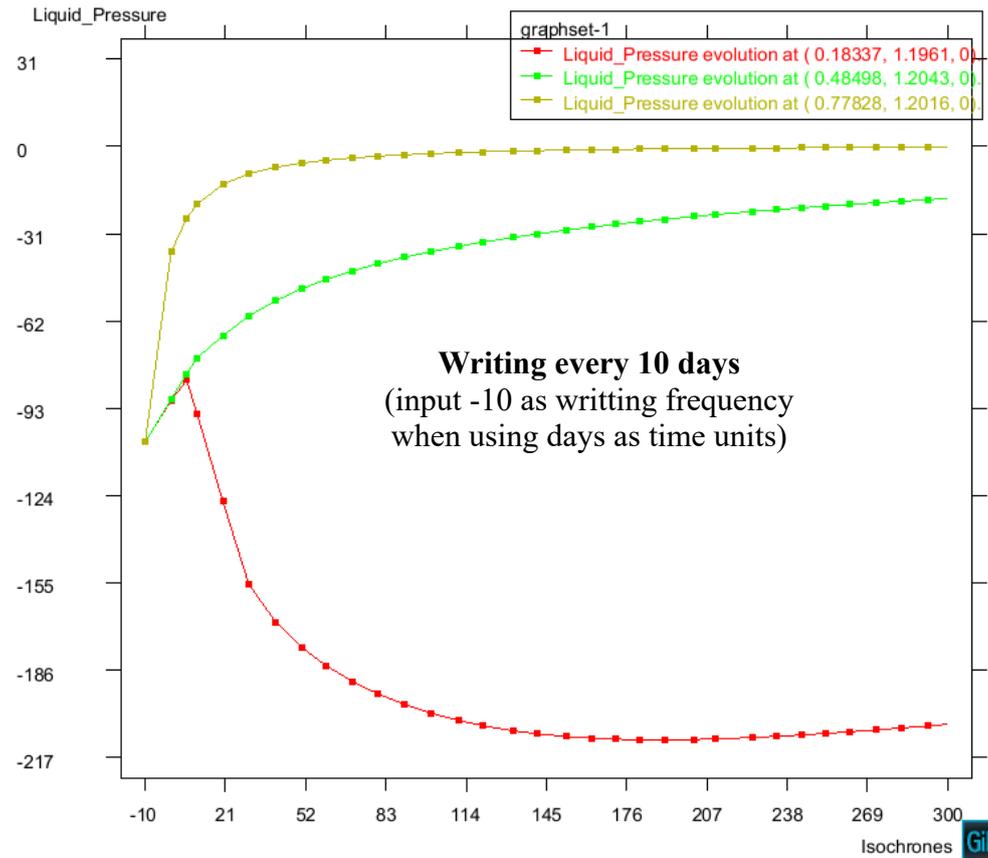


Figure II.2.1c. Writing every 10 days (Writing frequency = -10 and days selected in the interval data).

OUTPUT (continuation)	
Write piezometric head	Yes, No
Write boundary flow rates in additional file	No (Default option) Use writing frequency Write all
Write boundary reactions in additional file	No (Default option) Use writing frequency Write all
Output points (IOWCONTOURS in root_gen.dat)	Nodes Gauss points: (Default option)
Write all information (IWRALL in root_gen.dat)	Yes (default option), No If No is selected, the following option appears: Separated output files (IPOLYFILES in root_gen.dat) : Yes, No and user go to Select output window .

SELECT OUTPUT

(If Write all information=**No**)

Select outputs option is necessary when working with complex problems in which separated output files are used to facilitate the post-processing. The following options are available:

Write Displacements	Yes, No
Write Liquid Pressure	Yes, No
Write Gas Pressure	Yes, No
Write Temperature	Yes, No
Write solute concentration	Yes, No
Write Halite Concentration	Yes, No
Write Vapour Concentration	Yes, No
Write Gas Density	Yes, No
Write Dissolved air concentration	Yes, No
Write Liq Density	Yes, No
Write porosity	Yes, No
Write Liquid Saturation Degree	Yes, No
Write heat fluxes: qT	Yes, No
Write liquid fluxes: qL	Yes, No
Write gas fluxes: qG	Yes, No
Write diffusive heat fluxes: iT	Yes, No
Write diffusive water fluxes: iL	Yes, No
Write diffusive air fluxes: iG	Yes, No
Write diffusive solute fluxes: isolute	Yes, No
Write Stresses	Yes, No
Write Effective sStresses	Yes, No
Write stress invariants	Yes, No
Write strains	Yes, No
Write strains invariants	Yes, No
Write P0s TEP model	Yes, No
History variables of Viscoplastic model	Yes, No
History variables of Joint model	Yes, No
History variables of Argillite model	Yes, No
History variables of BExM model	Yes, No
History variables of CASM model	Yes, No

II.2.2. MATERIALS

All materials must be defined from a generic material. The following steps show how to assign materials and do modifications:

- Creating new materials: In order to create new materials, one should write a material name and complete the necessary constitutive laws and do an *Accept Data* to validate the data entered. It is necessary to create a material before assigning it on the geometry.
- Assignment must respect hierarchical structure of entities (i.e. cannot assign a material on a line belonging to a surface that have just been identified with another material). This type of error may create conflicts.
- Posterior modifications on the parameters of assigned materials do not require a re-meshing process.
- Material names: When introducing a name for a material, it is strongly recommended to avoid spaces or underscores (e.g. use *mat1* instead *mat_1* or *mat 1*). The use of spaces or underscores (`_`) might create conflicts when the material is read.

Constitutive Laws in CODE_BRIGHT

Properties for materials can vary at each interval or maintain constant. Every constitutive law is defined with 3 data types:

- Number of intervals. A box near the constitutive law name should be used for this purpose. Usually parameters will be entered only for the first interval.
- Each constitutive law is differentiated by the index ICL. For instance, ICL=6 is the retention curve. Groups of ICL are considered, for instance ICL=21 to 27 is used for the thermoelastoplastic model for unsaturated soils.
- Parameters for constitutive law. A series of parameters should be entered for each constitutive law, these are: ITYCL, P1, P2, P3, P4, P5, P6, P7, P8, P9, P10. The first one (ITYCL) is an integer that indicates which option among the available ones is used. For instance, thermal conductivity, permits different options depending the type of dependence of porosity and degree of saturation that is desired. P1 to P10 are numbers that correspond to parameters in a given equation.

ITYCL	P1	P2	P3	P4	P5	P6	P7	P8	P9	P10

A number indicates the intervals where the law will be defined. This number fixes the number of lines for VALUES to be entered. Every *Interval line* assumes parameters of INTERVAL DATA according to the same order.

The following constitutive laws are available:

<p>HYDRAULIC AND THERMAL CONSTITUTIVE MODELS (a) RETENTION CURVE INTRINSIC PERMEABILITY LIQUID PHASE RELATIVE PERMEABILITY GAS PHASE RELATIVE PERMEABILITY DIFFUSIVE FLUXES OF MASS DISPERSIVE FLUXES OF MASS AND ENERGY CONDUCTIVE FLUX OF HEAT</p>	<p>MECHANICAL CONSTITUTIVE MODELS ELASTICITY (b) NONLINEAR ELASTICITY (b) VISCOPLASTICITY FOR SALINE MATERIALS (b) VISCOPLASTICITY FOR SATURATED SOILS AND ROCKS (b) VISCOPLASTICITY - GENERAL (b) DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS (c) THERMOELASTOPLASTIC MODEL FOR SOILS (d) BARCELONA EXPANSIVE MODEL FOR SOILS (e) CASM's FAMILY MODELS (f)</p>
<p>PHASE PROPERTIES (a) SOLID PHASE PROPERTIES LIQUID PHASE PROPERTIES GAS PHASE PROPERTIES</p>	<p>EXCAVATION PROCESS (g)</p>

Description of each law is included in Chapter VI.

Assign material

With this instruction, the material is assigned to the selected entities. If assigning from a window, every time the assigned material changes, the button `Assign` must be pressed again. The user must select the entity on which to assign the materials, i.e.: `line`, `surface` or `volume` when working in `geometry` mode or directly over the `elements` when working in `mesh` mode. It is recommended to assign the materials on the geometry entities rather than on the elements.

If assigning from the command line, option `UnAssignMat` erases all the assignments of this particular material.

When a mesh has been already generated, and changes in the assigned materials are required, then it is necessary to re-mesh again or assign the materials directly on the mesh.

Draw material

Draws a color indicating the selected material for all the entities that have the required material assigned. It is possible to draw just one or draw all materials. To select some of them the users should use `a:b` and all material numbers that lie between `a` and `b` will be drawn.

When drawing materials in 3 dimensions, it may be necessary to change the viewing mode to `polygons` or `render` (see section `Render`) to differentiate the front and back of the objects.

Unassign material

Command `Unassign` unassigns all the materials from all the entities. For only one material, use `UnAssignMat` (see section `Assign material`).

New material

When the command `NewMaterial` is used, a new material is created taking an existing one as a base material. Base material means that the new one will have the same fields as the base one. Then, all the new values for the fields can be entered in the command line. It is possible to redefine an existing material.

To create a new material or redefine an existing one in the materials window, write a new name or the same one and change some of the properties. Then push the command `Accept`.

Element types in CODE_BRIGHT

When an element is selected to generate a finite element mesh it has to be available in `CODE_BRIGHT`. The types of elements available in `CODE_BRIGHT` are:

DIM=2	TYPE 1	Linear triangle: mainly used in flow problems, i.e. when the mechanical problem is not solved. Linear triangles are not adequate for incompressible media. Analytical integration.
	TYPE 12	Quadratic triangle. Corner nodes: 1, 2, 3; side nodes: 4, 5, 6. Numerical integration with 3 internal points.
	TYPE 5	Linear quadrilateral. Selective integration by means the modification of the matrix B (Hughes, 1980). This avoids locking when the medium is highly incompressible. Numerical integration with 4 points (recommended quadrilateral element).
	TYPE 16	Zero thickness or joint element.
	TYPE 8	Segment with a default thickness of 0.001 m and a default porosity of 0.9.
DIM=3	TYPE 1	Linear tetrahedron. Analytical integration. For $n1 \neq n2 \neq n3 = n4$ a triangular element is recovered. A default thickness of 0.001 m is considered.
	TYPE 26	Linear triangular prism. Numerical integration with 6 points.
	TYPE 3	Linear quadrilateral prism element. Numerical integration (selective) with 8 points.
	TYPE 33	Quadratic tetrahedron. Numerical integration with 4 integration points.

These types of elements are assigned by the interface between GiD and `CODE_BRIGHT`.

Note that linear triangular elements or linear tetrahedrons, which have been proven to be very adequate for flow problems, should be avoided for mechanical problems. This is because if the medium is nearly-incompressible (creep of rocks takes place with very small volumetric deformation), locking takes place (not all displacements are permitted due to element restrictions).

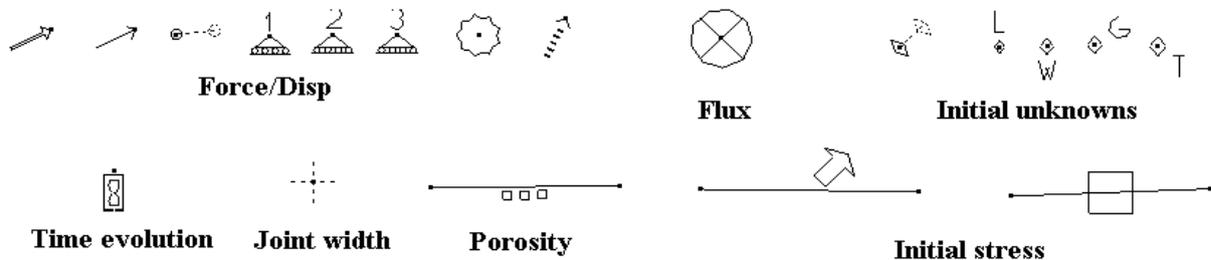
II.2.3. CONDITIONS

Conditions are all the properties of a problem –excluding materials– that can be assigned to an entity. In this concept several types of conditions have been included: Force/displacement conditions, flux conditions, initial unknowns, porosity (and other variables), initial stress, joint element width, time evolution location, etc. The condition window permits to choose entities to assign on (Point, Line, Surface or Volume in geometry display mode; and Node or Element in mesh display mode) and select different types of conditions. It must be taken into account that conditions assigned in mesh display mode will be unassigned in every new meshing process.

In addition, the following points should be taken into account:

- Force/displacement conditions add up all conditions assigned at every node, except for variables *Index* (takes last value encountered) and *Multiplier* (takes the biggest).
- Flux conditions, initial unknowns, porosity (and other variables), initial stress and joint element width are assigned with entities priority from lower to higher level i.e. in the following order: Points, Lines, Surfaces and Volumes (i.e. the node takes a Flux_Point_B.C. refusing a Line_Flux_B.C. assigned previously).
- When dealing with nodes shared by entities of the same level (e.g. surfaces) with different initial values, it is recommended –especially in the case of thin interfaces– to assign initial conditions on the entities containing those shared nodes (e.g. lines), so we are able to effectively control the initial values on those nodes.

If a mesh has already been generated, for any change in the condition assignments, it is necessary to re-mesh again to transfer these new conditions to the mesh.



Conditions description

II.2.3.1 Force/displacement conditions

The mechanical boundary conditions only exist if the mechanical problem is solved (Solve displacement). For each time interval only the types that undergo changes should be read.

X direction force/stress	Value in MN or $\text{MN/m}^2 = \text{MPa}$
Y direction force/stress	Value in MN or $\text{MN/m}^2 = \text{MPa}$
Z direction force/stress	Value in MN or $\text{MN/m}^2 = \text{MPa}$

X displacement rate prescribed	Value in m/s
Y displacement rate prescribed	Value in m/s
Z displacement rate prescribed	Value in m/s
X direction prescribed	When selected, displacement rate will be prescribed in the X direction. Its value is given in the cells above.
Y direction prescribed	When selected, displacement rate will be prescribed in the Y direction. Its value is given in the cells above.
Z direction prescribed	When selected, displacement rate will be prescribed in the Z direction. Its value is given in the cells above.
γ (<i>multiplier</i>)	The units of this parameter depend on whether force or stress is applied: When applying a force: $\frac{\text{MN}}{\text{m}}$ When applying a stress: $\frac{\text{MPa}}{\text{m}}$
Δf_x^o obtained as ramp loading during the current interval.	
Δf_y^o obtained as ramp loading during the current interval.	
Δf_z^o obtained as ramp loading during the current interval.	

The general boundary condition is applied by means a forces/stresses computed as:

$$f_x = f_x^o + \gamma \left(i_{x,x} \quad \cdot \quad \cdot \right)$$

$$f_y = f_y^o + \gamma \left(i_{y,y} \quad \cdot \quad \cdot \right)$$

$$f_z = f_z^o + \gamma \left(i_{z,z} \quad \cdot \quad \cdot \right)$$

This condition incorporates a von Newman type boundary condition plus a Cauchy type boundary condition. A very large value of γ can be used to impose a fixed displacement rate. If displacement rate is zero ($i_{x,x} = 0$) and γ is very large, displacement is not permitted in that direction.

If γ is insufficiently large, however, the prescription of the displacement rate will be inaccurate. On the contrary, extremely large values can cause matrix ill conditioning. Each specific problem requires an adjusted value if displacement rate should be prescribed.

Depending on the geometric entity on which the condition should be applied, the following options are encountered:

Points (2-D or 3-D)	Lines (usually 2-D)	Surfaces (usually 3-D)	Volumes (3-D)
Forces	Forces Boundary stresses	Forces Boundary stresses	Forces

II.2.3.2 Flux Boundary Condition

Mass or heat transport problems. These conditions only exist if any balance (water, air, energy flow) problem is solved. For each time interval, only the types that undergo changes need to be read.

The boundary condition is incorporated by adding a flux or flow rate. The mass flux or flow rate of species $i = w$ as a component of phase $\alpha = g$ (i.e. the inflow or outflow of vapour) is calculated as:

$$j_g^w = (\omega_g^w)^0 j_g^0 + (\omega_g^w)^0 \gamma_g (P_g^0 - P_g) + \beta_g \left((\rho_g \omega_g^w)^0 - (\rho_g \omega_g^w) \right)$$

where the superscript ⁰ stands for the prescribed values, ω is mass fraction, ρ is density, P_g is gas pressure, j_g^0 is a prescribed gas flow and γ_g and β_g are two parameters of the boundary condition. Particular cases of this boundary condition are obtained for instance in the following way:

Description	$(\omega_g^w)^0$	j_g^0	γ_g	P_g^0	(ρ_g)	β_g
A prescribed mass flow rate of gas with 0.02 kg/kg of vapor and 0.98 kg/kg of air is injected	0.02	1e-5 kg/s				
If $P_g < P_g^0 = 0.1 \Rightarrow$ a variable mass flow rate of gas with 0.02 kg/kg of vapor and 0.98 kg/kg of air is injected. If $P_g < P_g^0 = 0.1 \Rightarrow$ a variable mass flow rate of gas with variable composition outflows.	0.02		10	0.1		
Humidity in the boundary is prescribed to 0.0112 kg/m ³ . This is equivalent to a relative humidity of 0.0112/0.0255 = 0.44 = 44%	0.01				1.12	10

Vapour pressure at $T = 27$ °C is calculated as:

$$p_v = 136075 \exp(-5239.7/(273 + T)) = 0.003536 \text{ MPa} = 3536 \text{ Pa}$$

and the corresponding density is:

$$\rho_v = \frac{p_v M}{R(273 + T)} = \frac{3536 \text{ Pa} \times 0.018 \text{ kg/mol}}{8.3143 \text{ J/mol/K} \times (273 + 27) \text{ K}} = 0.02551 \text{ kg/m}^3$$

Associated to the same parameters but for component air, the following equation can be written:

$$j_g^a = (\omega_g^a)^0 j_g^0 + (\omega_g^a)^0 \gamma_g (P_g^0 - P_g) + \beta_g \left((\rho_g \omega_g^a)^0 - (\rho_g \omega_g^a) \right)$$

where:

$$(\omega_g^a)^0 = 1 - (\omega_g^w)^0$$

which comes from the mass fraction definition.

On the other hand, for liquid phase a similar set of equations can be considered. These are:

$$j_l^a = (\omega_l^a)^0 j_l^0 + (\omega_l^a)^0 \gamma_l (P_l^0 - P_l) + \beta_l \left((\rho_l \omega_l^a)^0 - (\rho_l \omega_l^a) \right)$$

$$j_l^w = (\omega_l^w)^0 j_l^0 + (\omega_l^w)^0 \gamma_l (P_l^0 - P_l) + \beta_l \left((\rho_l \omega_l^w)^0 - (\rho_l \omega_l^w) \right)$$

$$(\omega_l^w)^0 = 1 - (\omega_l^a)^0$$

Positive values of mass flow rate indicate injection into the medium.

For energy, the boundary condition has the general form:

$$j_e = j_e^0 + \gamma_e (T^0 - T) + E_g^w (j_g^w) + \dots$$

In other words, a von Newman type term plus a Cauchy type term and a series of terms that represent the energy transfer caused by mass inflow and outflow through the boundary.

The set of parameters that are required for these equations are (note that the symbols used by Gerard et al., 2009, are not the same):

ω_g^w	Prescribed mass fraction (kg/kg)
j_g	Prescribed gas flow rate *
Δj_g	Prescribed increment of j_g during the time step *
P_g	Prescribed gas pressure (MPa)
ΔP_g	Prescribed increment of P_g during the time step (MPa)
γ_g	Parameter for gas pressure term *
β_g	Parameter for humidity term *
ρ_g	Prescribed gas density (kg/m ³)

ω_l^h	Prescribed solute concentration (kg/kg)
ω_l^a	Prescribed mass fraction of air (kg/kg)
j_l	Prescribed liquid flow rate *
Δj_l	Prescribed increment of j_l during the time step *
P_l	Prescribed liquid pressure (MPa)
ΔP_l	Prescribed increment of P_l during the time step (MPa)
γ_l	Parameter needed to be $\neq 0$ when P_l is prescribed *
β_l	Parameter needed only when mass transport problem is considered *
ρ_l	Prescribed liquid density (kg/m ³)

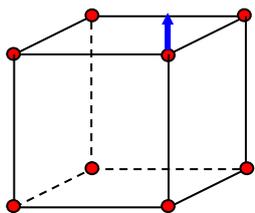
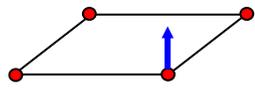
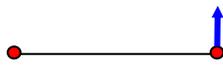
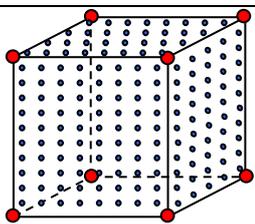
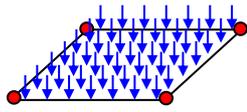
j_e	Prescribed heat flow rate *
Δj_e	Prescribed increment of j_e *
T	Prescribed temperature (C)
ΔT	Prescribed increment of T during the time step (C)
γ_e	Parameter needed to be $\neq 0$ when T is prescribed *
λ_e	Positive values: [$j_e = j_e \times \exp(-\text{abs}(\lambda_e) t)$] is used (1/s). Negative values: [$j_e = j_e t^{-\text{abs}(\lambda_e)}$] is used (1/s).
δ	Parameter for smoothing the seepage condition (outflow of water only) boundary condition.

* Units depend on problem dimension and parameter *index*. See Table II.2.1 (below) with a summary of the units for each case.

For a positive value of δ a parabolic curve is used; for a negative value an exponentially decaying curve is used. δ is the distance from the reference pressure to the point of change.

<i>Index</i> (auxiliary index)	→ +1.0 means that all flow rates are nodal values. For instance, a pumping well boundary condition.
	→ -1.0 means that all flow rates are per unit volume (3-D), area (2-D) or length (1-D) of medium (internal source or sink). For instance, a recharge due to rain in a 2-D case.
	→ +2.0 means that all flow rates are per unit area (3-D) or length (2-D) (lateral fluxes). For instance, lateral fluxes from neighbour aquifers.

Prescribed gas, liquid and heat flows must be given in terms of flow units depending on the way these flows are considered, i.e., depending on the kind of element they pass through and on the problem dimension. The required units for each case are graphically specified below:

<i>INDEX</i> PARAMETER	PROBLEM DIMENSION	ILLUSTRATION	FLOW UNITS
<i>Index = 1.0</i>	3-D		<i>Mass:</i> $\frac{\text{kg}}{\text{s}}$
			<i>Heat:</i> $\frac{\text{J}}{\text{s}}$
	2-D		<i>Mass:</i> $\frac{\text{kg}}{\text{s}}$
			<i>Heat:</i> $\frac{\text{J}}{\text{s}}$
	1-D		<i>Mass:</i> $\frac{\text{kg}}{\text{s}}$
			<i>Heat:</i> $\frac{\text{J}}{\text{s}}$
<i>Index = -1.0</i>	3-D		<i>Mass:</i> $\frac{\text{kg}}{\text{m}^3 \text{ s}}$
			<i>Heat:</i> $\frac{\text{J}}{\text{m}^3 \text{ s}}$
	2-D		<i>Mass:</i> $\frac{\text{kg}}{\text{m}^2 \text{ s}}$
			<i>Heat:</i> $\frac{\text{J}}{\text{m}^2 \text{ s}}$
	1-D		<i>Mass:</i> $\frac{\text{kg}}{\text{m s}}$
			<i>Heat:</i> $\frac{\text{J}}{\text{m s}}$

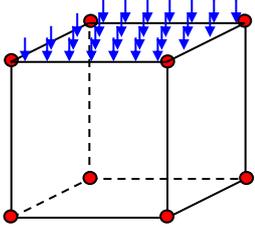
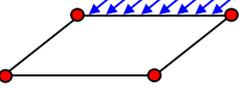
Index = 2.0	3-D		Mass: $\frac{\text{kg}}{\text{m}^2 \text{ s}}$
			Heat: $\frac{\text{J}}{\text{m}^2 \text{ s}}$
	2-D		Mass: $\frac{\text{kg}}{\text{m s}}$
			Heat: $\frac{\text{J}}{\text{m s}}$

Table II.2.1. Summary of units used for different variables, depending on problem dimension and parameter *index*

<i>index</i>	Problem dimension	Required units					
		Gas flow rate j_g	Liquid flow rate j_l	Parameters γ_g and γ_l	Parameters β_g and β_l	Heat flow rate j_e	Parameter γ_e
1.0	---	$\frac{\text{kg}}{\text{s}}$	$\frac{\text{kg}}{\text{s}}$	$\frac{\text{kg}}{\text{s MPa}}$	$\frac{\text{m}^3}{\text{s}}$	$\frac{\text{J}}{\text{s}}$	$\frac{\text{J}}{\text{s C}}$
-1.0	1D	$\frac{\text{kg}}{\text{m s}}$	$\frac{\text{kg}}{\text{m s}}$	$\frac{\text{kg}}{\text{m s MPa}}$	$\frac{\text{m}^3}{\text{m s}} = \frac{\text{m}^2}{\text{s}}$	$\frac{\text{J}}{\text{m s}}$	$\frac{\text{J}}{\text{m s C}}$
	2D	$\frac{\text{kg}}{\text{m}^2 \text{ s}}$	$\frac{\text{kg}}{\text{m}^2 \text{ s}}$	$\frac{\text{kg}}{\text{m}^2 \text{ s MPa}}$	$\frac{\text{m}^3}{\text{m}^2 \text{ s}} = \frac{\text{m}}{\text{s}}$	$\frac{\text{J}}{\text{m}^2 \text{ s}}$	$\frac{\text{J}}{\text{m}^2 \text{ s C}}$
	3D	$\frac{\text{kg}}{\text{m}^3 \text{ s}}$	$\frac{\text{kg}}{\text{m}^3 \text{ s}}$	$\frac{\text{kg}}{\text{m}^3 \text{ s MPa}}$	$\frac{\text{m}^3}{\text{m}^3 \text{ s}} = \frac{1}{\text{s}}$	$\frac{\text{J}}{\text{m}^3 \text{ s}}$	$\frac{\text{J}}{\text{m}^3 \text{ s C}}$
2.0	2D	$\frac{\text{kg}}{\text{m s}}$	$\frac{\text{kg}}{\text{m s}}$	$\frac{\text{kg}}{\text{m s MPa}}$	$\frac{\text{m}^3}{\text{m s}} = \frac{\text{m}^2}{\text{s}}$	$\frac{\text{J}}{\text{m s}}$	$\frac{\text{J}}{\text{m s C}}$
	3D	$\frac{\text{kg}}{\text{m}^2 \text{ s}}$	$\frac{\text{kg}}{\text{m}^2 \text{ s}}$	$\frac{\text{kg}}{\text{m}^2 \text{ s MPa}}$	$\frac{\text{m}^3}{\text{m}^2 \text{ s}} = \frac{\text{m}}{\text{s}}$	$\frac{\text{J}}{\text{m}^2 \text{ s}}$	$\frac{\text{J}}{\text{m}^2 \text{ s C}}$

The fact that units are different for 3D, 2D and 1D is due to the reduction of one dimension in 2D and two dimensions in 1D. However, if a 2D model is considered to have 1 m associated thickness, then units would be identical as in 3D. Similarly, if a 1D model is considered to have 1 m² associated surface then units would be identical as in 3D.

The above boundary conditions are rather general. They incorporate terms of von Newman type and Cauchy type. The equation includes three terms. The first one is the mass inflow or outflow that takes place when a flow rate is prescribed at a node. The second term is the mass inflow or outflow that takes place when a phase pressure is prescribed at a node. The coefficient γ is a leakage coefficient. This variable allows prescribing a pressure with more or less strength. If γ is very large, pressure will tend to reach the prescribed value (see Figures II.2.2 and II.2.3). However, an extremely large value can produce matrix ill conditioning and a lower one can produce inaccuracy in prescribing the pressure. However, it is not difficult to guess adequate

values for a given problem simply by trial. The third term is the mass inflow or outflow that takes place when species mass fraction is prescribed at a node.

A surface where seepage (only outflow for liquid phase is permitted) is a case that may be of interest. To indicate that only outflow is permitted γ_i is entered with negative sign. This negative sign only indicates that nodes with this kind of boundary condition allow seepage (i.e. only outflow).

If there is inflow of gas or liquid phase, it is very important to give values of the following variables: $(\omega_g^w)^o$, $(\omega_l^a)^o$, $(\rho_l)^o$, $(\rho_g)^o$ and T^o . Otherwise, they are assumed to be zero, which is not correct because they will be too far from equilibrium. If outflow takes place, this is not relevant because the values of the medium are used instead of the prescribed ones.

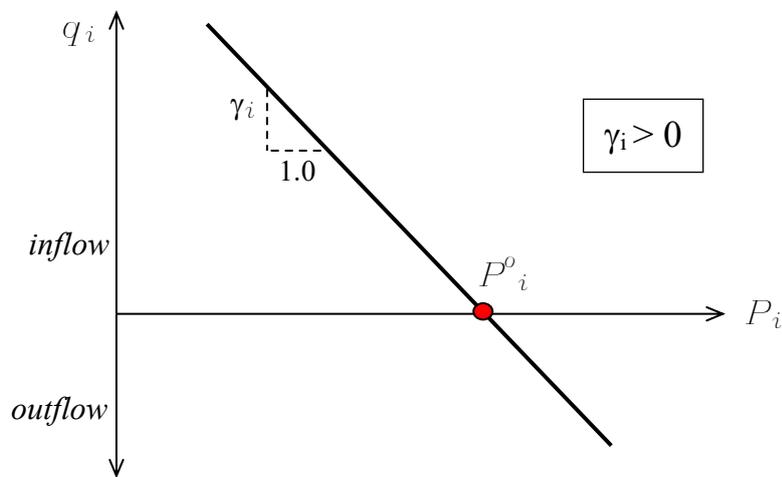


Figure II.2.2

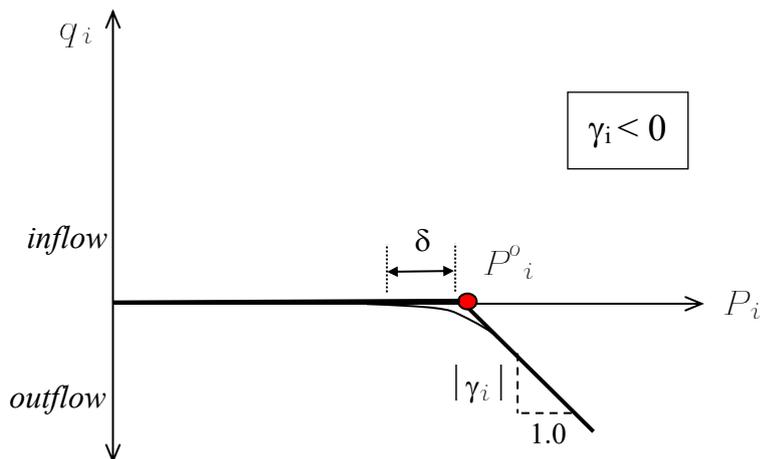


Figure II.2.3

Boundary conditions variable with time.

a) One boundary condition variable with time.

It is possible to assign a flux condition varying with time using an auxiliary file. In this case, the user must assign a value of **-999** to the particular variable for which a given variation wants to be assigned and include an ASCII file called “*root_bcf.dat*” in the GiD project folder with the variation with time of the given flux variable. The structure of the “*root_bcf.dat*” file is illustrated in Table II.2.2. Note that with *root* we mean the root name of the project: for example, if our project is *DAM.gid* then the file should be named *DAM_bcf.dat*.

Table II.2.2. Illustration of the format of the **root_bcf.dat** file

Number of data (N)				
Number of Flux variables (NF)	Id. variable (1)	Id. variable (2)	...	Id. variable (NF)
Time (1)	Value	Value	...	Value
Time (2)	Value	Value	...	Value
...
Time (N)	Value	Value	...	Value

It should be noted that the first line of the *root_bcf.dat* file must contain the number of data (N) that has to be read. The first column of the second line refers to the number of flux variables (NF) for which a given variation with time want to be assigned. The other columns of the second line contain a special flag (or indicator) of the flux variables to be changed. This indicator is shown in Table II.2.3. The following lines (from third to N) contain the time in the same unit considered at the interval data (in the first column) and the values of the flux variables assigned to the specific time (in the other columns).

Table II.2.3. Identification number (Id.) of the flux variables

Id.	Flux variable
1	ω_g^w prescribed mass fraction (kg/kg)
2	j_g prescribed gas flow rate (units in Table II.2.1)
3	P_g prescribed gas pressure (MPa)
4	γ_g parameter for gas pressure term (units in Table II.2.1)
5	β_g parameter for humidity term (units in Table II.2.1)
6	ρ_g prescribed gas density (kg/m ³)
7	ω_l^w prescribed mass fraction of solute (kg/kg)
8	ω_l^a prescribed mass fraction of air (kg/kg)
9	j_l prescribed liquid flow rate (units in Table II.2.1)
10	P_l prescribed liquid pressure (MPa)
11	γ_l parameter needed to be $\neq 0$ when P_l is prescribed (units in Table II.2.1)
12	β_l parameter needed only when mass transport problem is considered (Table II.2.1)
13	ρ_l prescribed liquid density (kg/m ³)
14	j_e prescribed heat flow rate (units in Table II.2.1)
15	T prescribed temperature (C)
16	γ_e parameter needed to be $\neq 0$ when T is prescribed (units in Table II.2.1)

b) Multiple boundary conditions variable with time.

For a value in a flux boundary condition that varies with time according to a function of time (list of values) the following actions have to be taken:

- Set the value of the variable equal to -99901.
- If you have more values for the same boundary condition or in another boundary condition, use the values -99902, -99903 up to -99999 if necessary.
- Prepare a file (`root_bcf.dat`) with the following structure:
 - First row: m , number of data values to be read (lines).
 - Second row: $-n$ 1 2 3 ... n where $n \leq 99$ number of variables that change with time.
 - m rows with `time_1 value_1 time_2 value_2 ... time_n value_n`.

II.2.3.3 Atmospheric boundary conditions module in CODE_BRIGHT

Introduction

Within Flux Boundary conditions in CODE_BRIGHT, the particular case of atmospheric boundary conditions¹ is eligible. These conditions encompass mass and heat conditions (in terms of atmospheric data) and suppose that mass and heat transport problems are to be solved. Atmospheric conditions are accessible from the “Flow rate” combo box in GiD or setting `index=5` (and giving the parameters as described in Table II.2.4) in CardGroup 20.

Atmospheric boundary condition option allows to impose boundary conditions in terms of evaporation, rainfall, radiation and heat exchanges thus simulating the complex soil-atmosphere interactions. These phenomena are expressed as flux boundary conditions for the three components (water, air and energy) as functions of the state variables (liquid pressure, gas pressure and temperature of the soil) or dependent variables (liquid saturation degree, fraction of water in the gas phase) and meteorological data that vary in time (atmospheric temperature and pressure, relative humidity, solar radiation, cloud index, rainfall and wind velocity).

Conventions used in this paper are:

- a filename is typed in an *italic shaped font*,
- a subroutine name or a variable is typed using `Courier font`,
- a filename in parentheses after a subroutine name refers to the file in which the subroutine is implemented.

Overview of the module

The file `bcond_atmos.f` contains 3 subroutines:

- `atmospheric_boundary_condition`
- `get_atm_data`
- `sun`

Figure 4 presents a general algorithm of `atmospheric_boundary_condition` subroutine.

¹The first implementation of this module is due to Maarten Saaltink.

The calls to `atmosferic_boundary_condition` subroutine appear in the following subroutines:

- `atm_boundary_conditions` (*bcond_flow.f*) itself called by `newton_raphson` (*nr.f*)
- `write_boundary_flows` (*write.f*) itself called by `main_calculate` (*code_bright_main.f*)

Running `atmosferic_boundary_condition` needs `index=52` as boundary condition type, this latter being passed in `FLUX(20)`. `FLUX` vector is read from file *root_gen.dat* by `read_boundary_conditions` (*read_general.f*). The index of this file is `iin1` (the concerned card is numbered 20).

It should be noted that flow rates computed by the `atmosferic_boundary_condition` subroutine are then treated as if `index = 2.0` (used in classic flux boundary conditions) were set *i.e.* as if flow rates are per unit area.

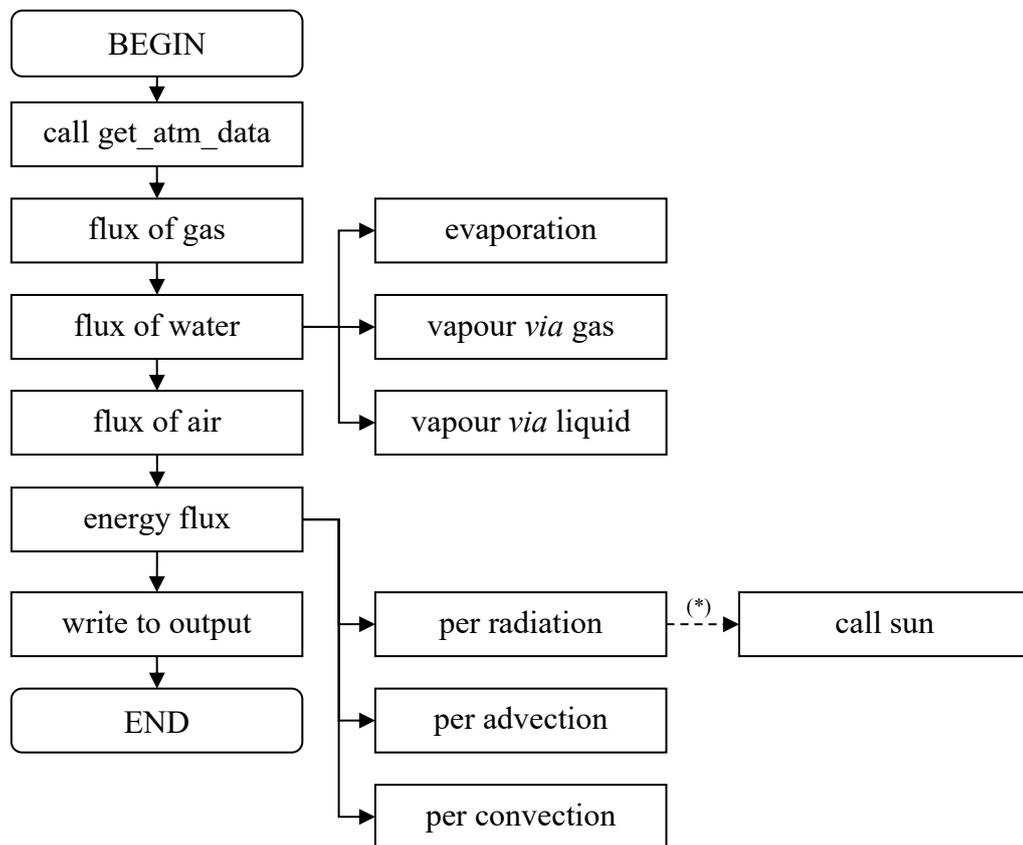


Figure II.2.4: General algorithm of `atmosferic_boundary_condition`.

(*) Subroutine `sun` is called if and only if `ISUN ≤ 1`.

²This variable is locally called `ICON`.

Input data

Problem data definition file (root_gen.dat)

When atmospheric boundary conditions are considered, the parameters presented in Table II.2.4 have to be entered in CardGroup 20 in file *root_gen.dat*. These conditions are activated via FL20, which should be set to 5. In Table II.2.4, latitude, time when autumn begins, time at noon, dry and wet albedos are used for calculating radiation when radiation type is lower than 3.

Roughness length, screen height and stability factor are used for evaporation estimation and for estimation of the advective energy flux.

Table II.2.4: Parameters to be entered in CardGroup 20.

FL1	Latitude (rad), λ
FL2	Time when autumn starts (s), t_s
FL3	Time at noon (s), t_m
FL4	Roughness length (m), z_0
FL5	Screen height (m), z_a
FL6	Stability factor (-), ϕ
FL7	Atmospheric gas density ($\text{kg}\cdot\text{m}^{-3}$), ρ_{ga}
FL8	Dry albedo (-), A_d
FL9	Wet albedo (-), A_w
FL10	Gas leakage coefficient ($\text{kg}\cdot\text{m}^{-2}\cdot\text{s}^{-1}\cdot\text{MPa}^{-1}$), γ_g
FL11	Liquid leakage coefficient ($\text{kg}\cdot\text{m}^{-2}\cdot\text{s}^{-1}\cdot\text{MPa}^{-1}$), γ_l
FL12	Factor with which rain is multiplied (-), k_{rain}
FL13	Factor with which radiation is multiplied (-), k_{rad}
FL14	Factor with which evaporation is multiplied (-), k_{evap}
FL15	Dip (rad)
FL16	Strike (rad)
FL17	Unused
FL18	Unused
FL19	= 0.0: radiation is calculated (see section 0) = 3.0: radiation data are read from input file <i>root_atm.dat</i>
FL20	index=5 means atmospheric boundary conditions

Table II.2.5 presents ranges of roughness lengths for different types of surfaces from which evaporation has to be calculated.

Table II.2.5: Roughness lengths for different types of surfaces after Chow et al. (1988).

<i>Type of surface</i>	<i>Height main roughness (m)</i>
Ice, mud flats	$1\cdot 10^{-5}$
Water	$1\cdot 10^{-4} - 6\cdot 10^{-4}$
Grass (up to 10 cm high)	$1\cdot 10^{-3} - 2\cdot 10^{-2}$
Grass (10 to 50 cm high)	$2\cdot 10^{-2} - 5\cdot 10^{-2}$
Vegetation (1–2 m)	0.2
Trees (10 – 15 m)	0.4 – 0.7

Atmospheric data input file (*root_atm.dat*)

General parameters are to be entered in the problem data file (see CardGroup 20 description here above) but time varying atmospheric data which are required to compute mass and heat fluxes should be entered within an ASCII file called *root_atm.dat*³. Data that can be read is summarized in Table II.2.6.

For each variable, the pair of columns containing available data is organised in the way schematically presented in Table II.2.4. More details about this file and time varying atmospheric data are given in section 0, dedicated to `get_atm_data` subroutine.

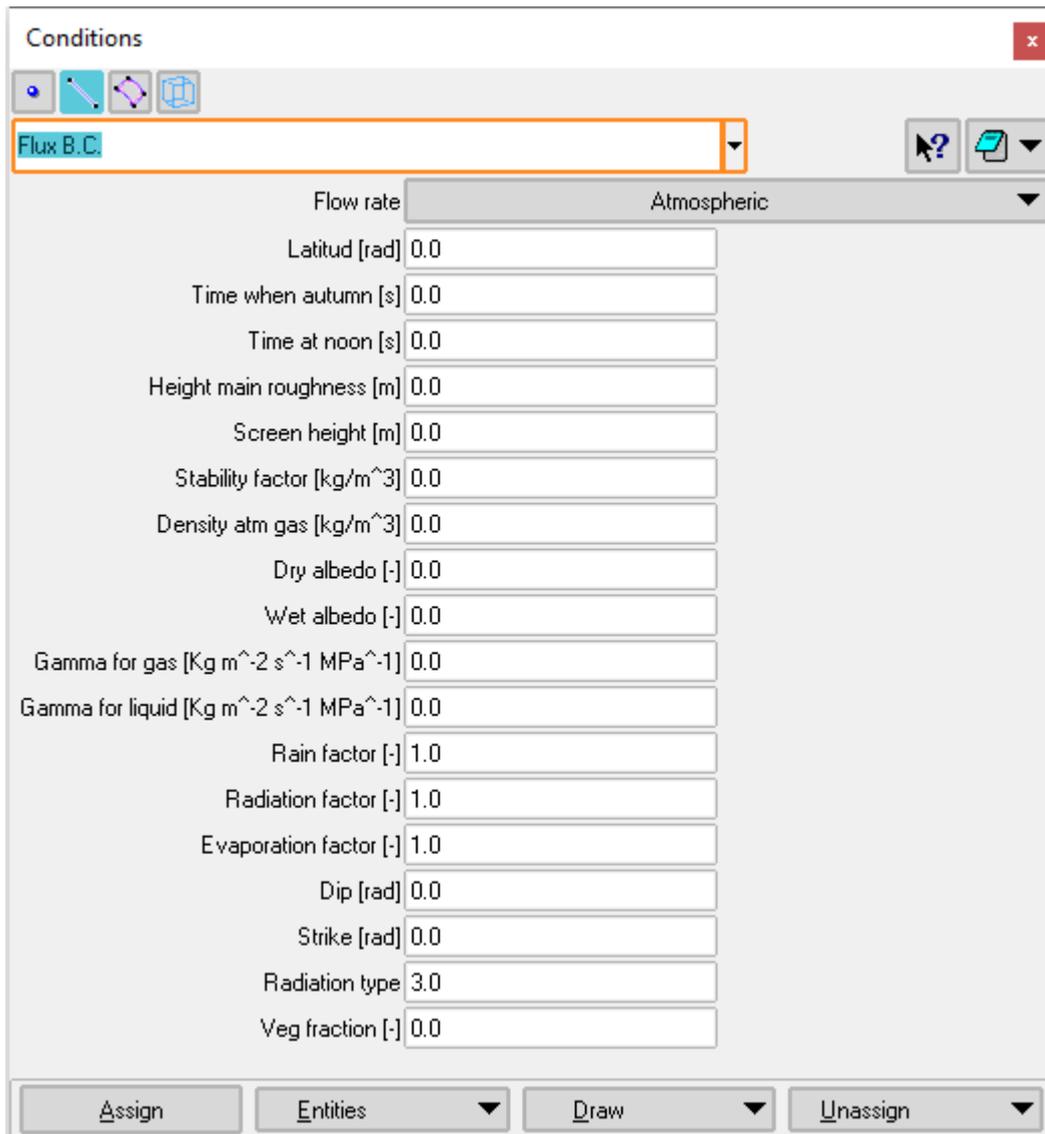


Figure II.2.5: Screenshot of GID atmospheric boundary conditions window.

³The file *root_atm.dat* is read with a free format. A dedicated tool developed by J.M. Pereira (`atmdata.exe`) can be used to check its general format.

⁴In this table, light grey and bold grey cells respectively identify measured data and unused data (the former being constituted of time (*t_i*) and corresponding values (*x_i*) pairs for each quantity).

Table II.2.6: Time varying atmospheric data to be provided in file *root_atm.dat*.

<i>Data</i>	<i>Unit</i>
Atmospheric temperature, T_a	$^{\circ}\text{C}$
Atmospheric gas pressure, P_{ga}	MPa
Relative humidity, H_r	-
Radiation ⁵ , R_m	$\text{J m}^{-2} \text{s}^{-1}$
Cloud index ⁶ , I_n	-
Rainfall, P	$\text{kg m}^{-2} \text{s}^{-1}$
Wind velocity, v_a	m s^{-1}
Long wave Radiation ⁷ , R_l	$\text{J m}^{-2} \text{s}^{-1}$
Atmospheric transmissivity ⁸ , τ_a	-

Table II.2.7: Illustration of the format of *root_atm.dat* file (excluding first line).

	T_a	P_{ga}	H_r	R_m	I_n	P	v_a	R_l	τ_a	
Flag	0	0	0	0	0	0	0	0	0	
Annual mean	0	x_am	0	x_am	0	x_am	0	x_am	0	x_am
Annual ampl	0	x_aa	0	x_aa	0	x_aa	0	x_aa	0	x_aa
Annual gap (s)	0	x_ag	0	x_ag	0	x_ag	0	x_ag	0	x_ag
Daily ampl	0	x_da	0	x_da	0	x_da	0	x_da	0	x_da
Daily gap (s)	0	x_dg	0	x_dg	0	x_dg	0	x_dg	0	x_dg
Unused	0	0	0	0	0	0	0	0	0	0
Measures...	ti	xi	ti	xi	ti	xi	ti	xi	ti	xi
Measures...	ti	xi	ti	xi	ti	xi	ti	xi	ti	xi
Measures...	ti	xi	ti	xi	ti	xi	ti	xi	ti	xi
Measures...	ti	xi	ti	xi	ti	xi	ti	xi	ti	xi
Measures...

⁵Radiation data will be used only if “Radiation type” is different from ‘0’ or ‘1’ in the boundary conditions parameters. R_m will be the net radiation measurements if “Radiation type” is set “3”, otherwise, if “Radiation type” is set to 2, 4 or 5 R_m will be the short wave (solar) radiation measurements.

⁶Cloud index allows to account for a cloudy sky in the radiation computation ($I_n = 1$ for a clear sky and $I_n = 0$ for a completely cloudy sky).

⁷Long wave (atmospheric) radiation data will be used only if “Radiation type” is set to 4 in the boundary conditions parameters.

⁸Atmospheric transmissivity data will be used only if “Radiation type” is set to 0 or 1, or the atmospheric boundary condition is apply to a inclined surface ($\text{dip} > 0$, FLUX (15)).

Atmospheric transmissivity expresses the amount of external radiation that is absorbed by the atmosphere, it can be estimated from the relative sunshine hours as $\tau_a = 0.25 + 0.50 \frac{n}{N}$, where n is the hours of sunshine and N the hours of daylength. Or, τ_a can be estimated from the maximal (T_a^{max}) and minimal (T_a^{min}) daily temperature as $\tau_a = K_h \sqrt{T_a^{max} - T_a^{min}}$, where K_h is an empirical constant, $K_h = 0.16$ for interior and $K_h = 0.19$ for coastal regions.

It should be noted that the first line of the file *root_atm.dat* must contain the number of lines (excluding this one) and number of columns that has to be read. The second line refers to interpolation or simulation option: it corresponds to a special flag allowing the user to simulate the atmospheric data on the base of annual and daily characteristics that are furnished (see eq. (23)). This simulation will be processed if, for a given quantity, its flag is set to '0'. The values necessary to proceed to this simulation are provided in the 5 following lines and correspond to annual mean, amplitude and gap and daily amplitude and gap. On the contrary, if this flag is set to '1', CODE_BRIGHT will use the measured data provided in the rest of the lines of the data file and process to linear interpolations in order to obtain the value of a quantity for a given calculation time.

For atmospheric subroutines description, take a look at APPENDIX II.A. ATMOSPHERIC SUBROUTINES DESCRIPTION

II.2.3.4 Initial Unknowns

Initial values of the unknowns can be assigned on *surfaces/volumes* on the geometry. A constant or linear distribution is available.

Distribution:	Constant / Linear
Ux displacement	Value in m
Uy displacement	Value in m
Uz displacement	Value in m
Liquid pressure: Pl	Value in MPa
Gas pressure: Pg	Value in MPa
Temperature: T	Value in °C
Concentration	Value in kg/kg

If distribution is linear, information about unknowns' values at final point and the coordinates of the initial and final points are required.

In case of nodes with multiple initial conditions assigned, the ones assigned into entities of higher levels prevail. It is recommended to assign the materials on the geometry entities, but it is also possible to assign them directly into mesh elements in case is needed.

II.2.3.5 Initial porosity

A constant initial value of porosity can be assigned on *surfaces/volumes* on the geometry. Porosity value should be less than 1.

II.2.3.6 Initial stress

Initial values of the stresses and history variables (depends on the type of mechanical constitutive model) can be assigned on *surfaces/volumes* on the geometry. A constant or linear distribution is available.

Distribution:	Constant / Linear
X stress	Value in MPa
Y stress	Value in MPa
Z stress	Value in MPa

XY stress	Value in MPa
XZ stress	Value in MPa
YZ stress	Value in MPa
History variable 1	(depend on the constitutive model)
History variable 2	(depend on the constitutive model)

In chapter VI, the description of history variables required for elastoplastic and viscoplastic models is included.

If distribution is linear, information about stresses and history variables values at final point and the coordinates of the initial and final points are required.

II.2.3.7 Initial anisotropy.

Transverse isotropy can be assigned on *surfaces/volumes* in a hydraulic, thermal and/or mechanical problem. The direction of orthotropic axis is indicated by the two angles shown in Figure II.2.9. Transformation is done from physical plane (global axes) to anisotropy directions (local axes). First rotation is around z axis and the second rotation is around the new y' axis. For further help on how to model anisotropic properties please visit CODE_BRIGHT-Tutorial XVII in the Tutorial Manual.

First rotation: α (around z)	$\alpha > 0$ if directed from x to y α is the orientation of the dip with respect to y (usually the North)
Second rotation: β (around y')	$\beta > 0$ if directed from z' to x' β is the inclination of dip with respect to the horizontal plane

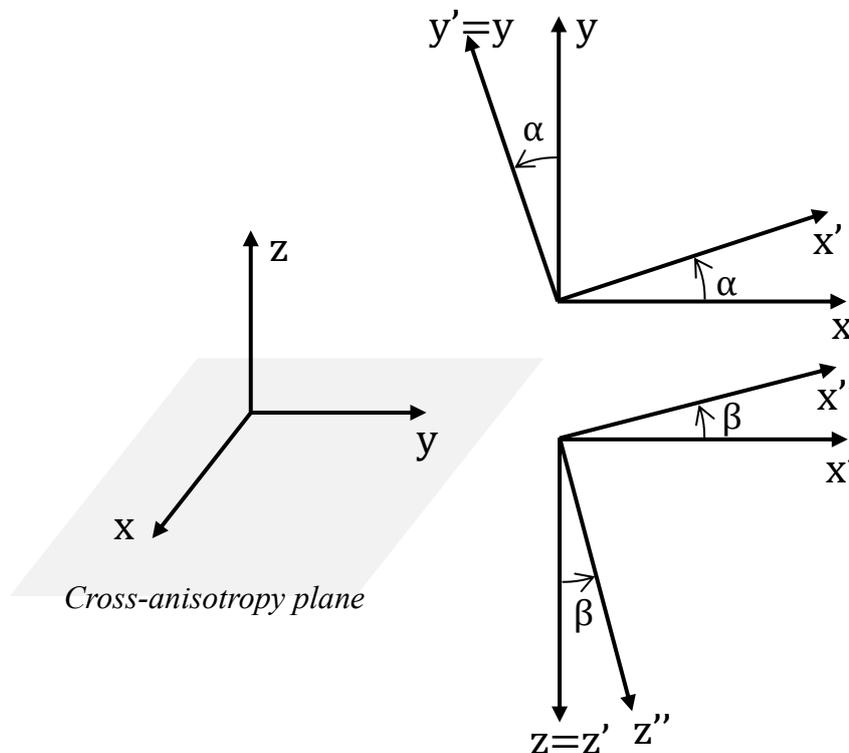


Figure II.2.9: Convention of reference axis for transverse isotropic material.

Parameters of elastic transverse isotropy can be assigned through the Damage-elastoplastic model for argillaceous rocks (ICL=71 to 79; see chapter VIc), while parameters of hydraulic transverse isotropy can be assigned through the intrinsic permeability law (ICL=7; see chapter VIa).

II.2.3.8 Time Evolution

CODE_BRIGHT offers the user the possibility of registering the evolution with time of specified problem variables either at specific points and surfaces/volumes on the geometry, or at specific nodes and elements on the mesh. In case that nodes and elements are specified by the user, special care must be taken when remeshing, yet information regarding time evolution will be lost.

The program does not admit more than 10 nodes and 10 elements (or, if the case, points and surfaces/volumes) for time evolution registration, whatever could be read from the introduced time evolution data. These data, on the other hand, have to be given to the program as referring to the first time interval of the problem.

However, Post-process interface in GiD has available the information of problem variables in all points/lines/surfaces/volumes of the geometry and nodes/elements of the mesh. Post-process offers the option to draw graphs of specified problem variables. Several graph types are available: point evolution against time, result 1 vs. result 2 over points, and result along a boundary line (see View results/graphs option of Post-process). It is possible to save or read a graph (see Files menu of Post-process). These advanced options of Post-process avoid the need to select specific points/surfaces/volumes in conditions for the time evolution, before to run the problem.

Assigning priorities

Conditions assigned on the *geometry* are distributed over the *mesh* with priorities. In general points have priority over lines, lines over surfaces and surfaces over volumes. At mesh level, nodes have priority over elements.

Mechanical boundary conditions on high entities are superimposed when they are applied to a lower entity. This means, for instance in a 2-D case, that a point that belongs to two lines will have the combination of boundary conditions coming from these two lines.

Assign condition

A condition is assigned to the entities with the given field values. If assigning from the command `AssignCond`, the option `Change` allows the definition of the field values. Do not forget to change these values before assigning. Option `DeleteAll` erases all the assigned entities of this particular condition. Conditions can be assigned both on the geometry and on the mesh but it is convenient to assign them on the geometry and the conditions will then be transferred to the mesh. If conditions are assigned on the mesh, any remeshing will cause the conditions to be lost.

Conditions that are to be attached to the boundary of the elements, are assigned to the elements and GiD searches the boundaries of the elements that are boundaries of the total mesh. Option `Unassign` inside `AssignCond`, permits to unassign this condition. It is also possible to unassign from only certain entities.

If a mesh has already been generated, for any change in the condition assignments, it is necessary to re-mesh again.

Draw condition

Option `Draw all` draws all the conditions assigned to all the entities in the graphical window. This means to draw a graphical symbol or condition number over every entity that has this condition. If one particular condition is selected, it is possible to choose between `Draw` and one of the fields. `Draw` is like `Draw all` but only for one particular condition. If one field is chosen, the value of this field is written over all the entities that have this condition assigned. When the condition has any field referred to the type of axes, the letters can be visualized by means of `Draw local axes`.

Unassign condition

In window mode, command `UnAssign` lets the user to choose between unassigning this condition from the entities that owe it or unassigning all the conditions or select some entities to unassign. In command mode `UnAssing`, do it for all the conditions. For only one condition, use command `Delete All` (see section `Assign condition`).

Entities

Create an information window with all entities assigned including values at every one.

II.2.4. INTERVALS DATA

Intervals are a way to change some conditions and, eventually, material properties.

Properties for materials can vary at each interval or remain constant. For a problem with several intervals, a window with more than one row can be used for each constitutive law (see figure below). Each row represents the properties for each interval. If the number of the current interval is higher than the number of rows, then the material will keep the properties of the last row. Usually, only the first line should be filled. The following lines may be left in blank if material properties are unchanged.

ITYCL	P1	P2	P3	P4	P5	P6	P7	P8	P9	P10

Boundary conditions may vary at each interval or remain constant. For conditions the correct way to proceed is to define all the invariable conditions first (i.e. those that remain unchanged during all intervals). Then, it is allowed to define as many intervals as desired with the command `NewInterval` or update the conditions in different intervals using the command `ChangeInterval`. It is possible to define as many conditions as necessary into particular intervals. The conditions which have not been duplicated when creating new intervals, are only considered for their interval.

Interval data parameters, describe temporal limits and time steps for each interval. They can be entered with the command `IntervalData` or in the intervals data window. If entered in a window, the data is not accepted until button `Accept` is pressed. This data can be entered before or after meshing.

Description

INTERVAL DATA	
Units of time discretization	Time units for defined interval. Options: Seconds, Minutes, Hours, Days, Weeks, Months, Years
Initial Time (interval starts) (TIMEI in root_gen.dat)	Initial time for the defined interval.
Initial Time Step (DTIME in root_gen.dat)	Initial time step for this time interval.
Final Time (interval ends) (TIMEF in root_gen.dat)	Final time for the defined interval.
Intermediate Time (TIME1 in root_gen.dat)	Time from which time increment is kept below the maximum allowed (advanced option).
Maximum Time Step (DTIMEC in root_gen.dat)	Maximum allowed time step constant value.
Reset displacements to zero	Yes / No This option puts displacement to zero at the first time step of the next time interval.

Using the advanced options, there is also possible to change the values of ‘epsilon’ or ‘time step control’ for a given interval (these two variables have been explained in chapter II.2.1). These changes will be mantained during the following intervals, unless the user explicitly change them.

In 'Writing results frequency', the intermittence for writing results is defined, i.e. only after a given number of time steps the results will be written. This may cause inconveniences if the user desires the results at precisely fixed times (for instance: 6 months, 1 year, 2 year, etc.). Moreover, if something changes between two runs (e.g. boundary conditions) and any time increment should be modified, the value of the times in which results are output will not be identical between these two runs. In this case, it would be difficult to make a comparison of the two analyses because the output results correspond to different times.

However, it is possible to decide the values of the times for output using a sequence of consecutive intervals. In this way, the results will be output for all 'Final time' defined, and if the user is only interested in these fixed times a very large value may be used for 'Writing results frequency' to avoid output at other times. Alternatively, this could be solved using a negative ‘writing frequency’ (see section II.2.1).



III.CODE_BRIGHT. PROCESS

III.1. CALCULATE

This part deals with the stage of the process that solves the numerical problem. The system would allow calling the Finite Element program without necessity of leaving from the work environment. Pressing Calculate the user can see a Process window, and clicking on Start the solver module runs.

The option Calculate from the beginning is useful in case that you need to calculate the project from the beginning (without using the saved files created in a previous calculate process). WARNING: Calculate from the beginning option will erase all the save type files from the working directory.

III.2. DATA FILES

If the solver program is required to be run outside GiD enviroment, i.e. in another computer or the user needs to check the data input for calculations; it is posible to see the data files. In the work directory there are the followings files:

- Root.dat
- *ROOT_GEN.DAT*
- *ROOT_GRI.DAT*

from which the program CODE_BRIGHT reads all the necessary data.

The name of these two files is composed by the extension **.DAT** which indicates that these files contain input data, a suffix (**_GEN** or **_GRI**) that follows the **ROOT** and which indicates a file with general information and a file with grid information, and a **ROOT** which is a name assigned by the user. The **ROOT** is previously read in a file called **ROOT.DAT**. For a run with another problem only this **ROOT.DAT** file must be changed and the files of the new problem will be used.

III.3. GENERAL INFORMATION FILE '*ROOT_GEN.DAT*'

See APPENDIX III.A.

III.4. GEOMETRICAL DESCRIPTION FILE: *ROOT_GRI.DAT*

See APPENDIX III.B.

III.5. SUMMARY-LIST OF CARDS

This section contains the list of **Cards** with the variables that are read in each one.

File *ROOT_GEN.DAT*

Card 1. Problem	HEAD
Card 2. Dimensions and options	NUMNP, NUMEL, NDIM, IAXISYM, NUMMAT, NHV
Card 3. Dimensions and options	MXDIFN, MBANDT, MFRONTH, NDF, MNVAL, ISOLVE
Card 4. Dimension boundary conditions	NFDTYPE, NFLUXTYPE
Card 5. Options. Unknowns to be calculated	IOPTDISPL, IOPTPL, IOPTPG, IOPTTEMP, IOPTXWS
Card 6. Other options	IOPTXHL, IUPDPOR, IOPTXWG, IOPTXAL, IOPTPC, IOPHYS, IUPDC
Card 7. Flags. Auxiliary options	IFLAG1, IFLAG2, IFLAG3, IFLAG4, IFLAG5
Card 8. Constants	EPSILON, THETA, PGCONS, TCONS, PLCONS
Card 9. Void	
Card 10. Options	IOWIT, INTER, ITERMAX, IOWCONTOURS, ITERMAXS, ITIME, IMBACKUP, IWRALL, IPOLYFILES
CardGroup 11. Convergence parameters	DELMXU, FACU, DELFMX, DUMX (Omit if IOPTDISPL=0) DELMXPL, FACPL, DELQWMX, DPLMX (Omit if IOPTPL=0) DELMXPG, FACPG, DELQAMX, DPGMX (Omit if IOPTPG=0) DELMXT, FACT, DELQMX, DTMX (Omit if IOPTTEMP=0) DELMXI, FACI, DELIMX, DIMX (Omit if IOPTXWS=0) DXS,DRS,DRSREL (Omit if ISOLVE not equal 5)
This group ends with -1	
Card 12. Gravity	GRAVITY(1), ..., GRAVITY(NDIM)
Card 13. Interval time variables	TIMEI, DTIME, TIME1, DTIMEC, TIMEF, FACTTIME
Card 14. Number of material	IMAT

Card 15. Number and name of constitutive law	ICL, TIT, ITYCL
CardGroup 16. Parameters constitutive law	TIT, PARCL(1,ICL,IMAT) TIT, PARCL(6,ICL,IMAT) TIT, PARCL(2,ICL,IMAT) TIT, PARCL(7,ICL,IMAT) TIT, PARCL(3,ICL,IMAT) TIT, PARCL(8,ICL,IMAT) TIT, PARCL(4,ICL,IMAT) TIT, PARCL(9,ICL,IMAT) TIT, PARCL(5,ICL,IMAT) TIT, PARCL(10,ICL,IMAT)
(group of Cards from IMAT=1 to NUMMAT and for every IMAT value from ICL=1 to NCL (not all ICL are required)) This group ends with -1 (ICL loop) This group ends with -1 (IMAT loop)	
Card 17. Type of boundary condition (Mechanical problem)	IF
CardGroup 18. Force/displacement prescribed	TIT, FORDISP(1,IF) TIT, FORDISP(2,IF) TIT, FORDISP(...,IF)
(group of Cards from IF=1 to NFDTYPE) (Omit if IOPTDISPL=0) This group ends with -1	
Card 19. Type of boundary condition. Mass or heat transport problems	IF
CardGroup 20. Flux problem boundary condition	TIT, FLUX(1,IF), TIT, FLUX(21,IF) TIT, FLUX(2,IF), TIT, FLUX(22,IF) TIT, FLUX(...,IF), TIT, FLUX(...,IF) TIT, FLUX(20,IF), TIT, FLUX(40,IF)
(group of Cards from IF=1 to NFLUXTYPE) (Omit if IOPTPL + IOPTPG +IOPTTEMP = 0) This group ends with -1	

The group of **Cards** from 13 to 20 can be repeated in order to make a simulation with several time intervals in which the boundary conditions and material properties are not the same. If any parameter is not read, the value in the previous interval is used. If a '-1' is read with IMAT, ICL and IF, then no change takes place in material properties and boundary conditions.

File *ROOT_GRI.DAT*

Card 1. Grid writing index	IOWGRI, IOFILE, IFMT
CardGroup 2. Node coordinates and boundary condition type	N, COORD(1, N), ..., COORD(NDIM, N), IFORDISP(1,N), IFORDISP(2,N), IFORDISP(3,N), IFLUXTYPE(1,N), IFLUXTYPE(2,N), IFLUXTYPE(3,N), WIDTH(N)
(group of Cards from N=1 to NUMNP)	
CardGroup 3. Node connectivities, material, element type,...	L, MTYPE, LTYPE, KXX(1,L),..., KXX(MNNEL,L)
(group of Cards with L=1 to NUMEL)	
CardGroup 4. Initial values of unknowns	N, XOLD(1,N), ..., XOLD(NDF,N)
(group of Cards with N=1 to NUMNP)	
CardGroup 5. Initial values of stresses	L, STRESSOLD(1, 1, L), ..., STRESSOLD(NSTREC, 1, L)
(group of Cards with L=1 to NUMEL) (Omit if IOPTDISPL=0)	
CardGroup 6. Other element wise properties	L, POROSITY(L), (FK(I, L), I=1,NDIM), ANISOTPER(1, L), ..., ANISOTPER(NISOT, L), THICKNESS (L), (FK(I,L), I=NDIM+1, NDIM+3)
(group of Cards with L=1 to NUMEL)	
Card 7. Time evolution of state or dependent variables at nodes	NOUTOT, IVOU(1), ..., IVOU(10), INTERNODE
Card 8. Nodes for time evolution	NODOUT(1), ..., NODOUT(NOUTOT)
Card 9. Piezometric head map	IWHEAD, NWHEAD
Card 10. Nodal flows	IWNFLOW
Card 11. Time evolution of dependent variables at elements	LOUT, IELVOUT(1), ..., IELVOUT(10), INTERELEMENT
Card 12. Element numbers for time evolution of element-wise variables	NELOUT(1), ..., NELOUT(LOUT)

IV. CODE_BRIGHT. POSTPROCESS.

IV.1. POST-PROCESSING TOOLS: SHORT DESCRIPTION

The different results that the system allows to display are the following ones:

- **Geometry:** GiD displays the whole volumetric mesh, surface sets and boundary surfaces. It can also cut and divide them, in its original state as well as also in its deformed state, and switch them on and off. GiD displays how the meshes/sets will be deformed according to a certain vectorial variable. GiD provides two representations: on the first one all the results will then be drawn on these original or deformed meshes (Main Geometry); on the second one, a superimposed representation (Show Geometry) is provided, that can be also deformed, but the results will still be drawn on the main representation. The user can compare the main original/deformed meshes/sets with the second representation, which can also be deformed with the same or another vector deformation, or with no deformation at all. The scaling of all the displays can be modified interactively.
- **Show minimum and maximum:** The minimum and maximum values of the variable for the currently viewed meshes/sets can appear, pointing all the nodes where these limits are computed, in dark blue the minimum values and in red the maximum ones.
- **Vectors:** GiD presents a vector distribution according to the vectorial or matrix variables on each node, showing their magnitudes and directions. The scaling of the vectors can be modified interactively.
- **Contour fields:** GiD represents the variables through isosurfaces or contours that comprise all the values between two given values. GiD takes advantage of the graphical capabilities of the machine, allowing a smoothing of the results when a high number of colors is used.
- **Contour lines:** This representation is quite similar to the last one, but the uniform bands are substituted here by isolines, where each one ties several points with the same value.

IV.2. READ POST-PROCESSING

GiD displays a 'File Open Dialog Box' and asks the user for a file. Afterwards, it looks for the files `filename.msh`, `filename.bon` and `filename.res`. The description of what is found and being read, sorted (if necessary) and built appears on the message bar. Sometimes, it may be useful to use the visualization options to center and zoom the drawing on the screen, especially when the different scales affect the post-processing. All the post-processing facilities can be used for this new project, jump to the pre-processing, if desired, or go back to the previous or another project post-processings.

Other details on post-processing information are available from the GiD manual.

IV.3. POST PROCESS FILES FORMAT

In some cases the user needs to interact with the results given by the `CODE_BRIGHT` process in order to obtain different variables that are function of the variables considered as a result. The information needed to do that is stored in the post-process files, which are saved in the work directory. These files are:

- `root.post.res`
- `root.post.msh`

The file *root.post.msh* contains information about the mesh, like the coordinates of the nodes, and the coordinates of the elements, while the file *root.post.res* presents the information of the results and the variation in time of different variables in the nodes or Gauss points. To create the program it is important to take into account the format of these files, specially the *root.post.res* file. Note that with *root* we mean the root name of the project: for example, if our project is *DAM.gid* then the post process files will be *DAM.post.res* and *DAM.post.msh*.

The first lines of the file *root.post.res* are the header, which contains information about the Gauss points. Based on the type of element employed, this header may have 5 or 10 lines: 5 lines for triangular elements and 10 lines for quadrilateral elements. See Figure IV.3.1.

```

1 GiD Post Results File 1.0
- GaussPoints      EL_2DLQ ElemType  Quadrilateral      2DLQ
- Number of Gauss Points:      1
- Natural Coordinates:          Given
-   0.0000      0.0000
- End GaussPoints
- GaussPoints      GP_2DLQ ElemType  Quadrilateral      2DLQ
- Number of Gauss Points:      4
- Natural Coordinates:          Internal
10 End GaussPoints

```

Header for quadrilateral elements

```

- GiD Post Results File 1.0
- GaussPoints      GP_2DLT ElemType      Triangle      2DLT
- Number of Gauss Points:      1
- Natural Coordinates:          Internal
5 End GaussPoints

```

Header for triangular elements

Figure IV.3.1. Header format for quadrilateral and triangular elements

The results of the process appear in the next lines. The results are divided by time, which means that are presented for variable 1 in time 1, then variable 2 in time 1, until the last variable, and then start again for all the variables in time 2 and so on.

The line 6 –or 11, depending on the element employed– presents the header for the results of variable 1 in time 1, which has the following format:

Result “Variable” Isochrones “time” “type” “set”

Variable: Ex. Temperature, liquid pressure, stress

Type: Vector, scalar or matrix.

Set: Nodes (*onNodes*) or Gauss points (GP) depending of the variable.

For example: *Result Temperature Isochrones 0.549584E-06 Scalar onNodes*

The next line has the text “*Values*”. In the following lines 2 columns for scalar type variables appear, 3 columns for variable type vector or 6 columns for matrix type, as it is shown in Figure IV.3.2. The first column presents the number of the node or Gauss point, whose coordinates are presented in the file *root.post.msh*. After the last value, the line “end values” appears and in the succeeding line the header for the next variable appears.

```

Result Temperature      Isochrones      0.549584E-06 Scalar      onNodes
Values
      1      0.250000E+02
      2      0.250000E+02
      3      0.250000E+02
      4      0.250000E+02
      5      0.250000E+02
      6      0.250000E+02
      7      0.250000E+02
      8      0.250000E+02

```

Result format for a scalar variable.

```

Result qT              Isochrones      0.549584E-06 Vector      onGaussPoints GP_2DLT
Values
      1      0.240668E+01      0.290451E+02
      2      0.117073E+02      -0.266899E+02
      3      -0.229997E+02      0.179008E+02
      4      0.287474E+02      0.479733E+01
      5      -0.229995E+02      -0.179012E+02
      6      0.197391E+02      0.214426E+02

```

Result format for a vector variable.

```

Result Stresses        Isochrones      0.909091E-05 Matrix      onGaussPoints EL_2DLQ
Values
      1      -0.999896E-01      -0.100000E+00      -0.999896E-01      -0.173450E-10      0.000000E+00      0.000000E+00
      2      -0.999896E-01      -0.100000E+00      -0.999896E-01      -0.265378E-10      0.000000E+00      0.000000E+00
      3      -0.999896E-01      -0.100000E+00      -0.999896E-01      -0.238335E-10      0.000000E+00      0.000000E+00
      4      -0.999896E-01      -0.100000E+00      -0.999896E-01      -0.178791E-10      0.000000E+00      0.000000E+00
      5      -0.999896E-01      -0.100000E+00      -0.999896E-01      -0.138184E-10      0.000000E+00      0.000000E+00
      6      -0.999896E-01      -0.100000E+00      -0.999896E-01      -0.107282E-10      0.000000E+00      0.000000E+00
      7      -0.999896E-01      -0.100000E+00      -0.999896E-01      -0.782375E-11      0.000000E+00      0.000000E+00
      8      -0.999896E-01      -0.100000E+00      -0.999896E-01      -0.544043E-11      0.000000E+00      0.000000E+00

```

Result format for a matrix variable.

Figure IV.3.2. Results

If the user needs to create another file type *root.post.res* to visualize the results in the GID interface, it is important to consider the format presented before, and take into account that the header of the values has the following format:

```
'Result',1x,a15,1x,'Isochrones ',e12.6,1x,a15,1x,a30
```

V. CODE_BRIGHT. THEORETICAL ASPECTS

In porous media, subjected to thermal, hydraulic, and mechanical conditions, relevant thermo-hydro-mechanical (THM) phenomena takes place. In fact, there exist a number of mutual interactions that must be taken simultaneously into account in analyses. For instance, strains due to thermal loading will induce stress variations and changes in mass storage terms and hydraulic conductivity. The thermal expansion of the water in the pores itself causes changes in the degree of saturation or, if the material is saturated or quasi-saturated, increases of water pressure. Thermal induced vapor diffusion and the dependence of water viscosity on temperature also affect significantly the water transfer process.

On the other hand, changes in hydraulic conditions influence the temperature field via variations of thermal conductivity and affect the stress/strain field due to pore water pressure and pore gas pressure changes. Gas pressure is affected by the increase in vapour pressure with temperature. This may lead to further changes in the pattern of gas and water flow. Finally, porosity changes due to volumetric strain influence pore pressure distributions because of associated variations in storage terms and hydraulic conductivity. The effect on temperature is less important as the variations of thermal conductivity with porosity are relatively small. In APPENDIX V.A. the most significant interactions between the various phenomena are presented in a systematic manner.

An unavoidable consequence of all those phenomena interacting simultaneously is the need to carry out coupled THM analysis in which all the main aspects of the problem can be considered in an integrated way. Such a formulation and the numerical approach adopted to solve the governing equations are presented in the following sections.

V.1. BASIC FORMULATION FEATURES

A porous medium composed by solid grains, water and gas is considered. Thermal, hydraulic and mechanical aspects will be taken into account, including coupling between them in all possible directions. As illustrated in Figure V.1.1, the problem is formulated in a multiphase and multispecies approach.

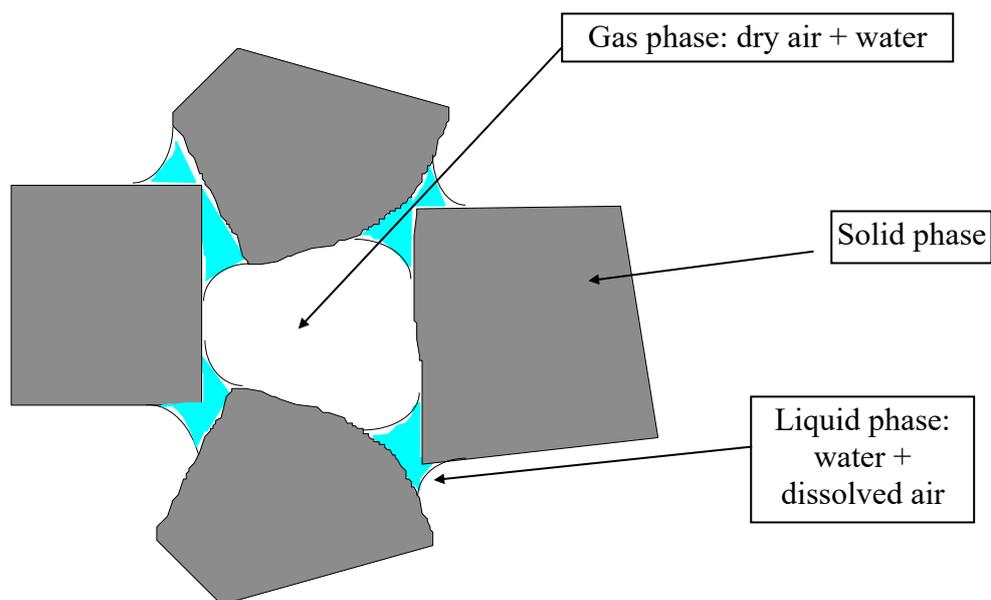


Figure V.1.1. Schematic representation of an unsaturated porous material

The three phases are:

- solid phase (s) : mineral
- liquid phase (l) : water + air dissolved
- gas phase (g) : mixture of dry air and water vapour

The three species are:

- solid (-) : the mineral is coincident with solid phase
- water (w) : as liquid or evaporated in the gas phase
- air (a) : dry air, as gas or dissolved in the liquid phase

The following assumptions and aspects are taken into account in the formulation of the problem:

- Dry air is considered a single species and it is the main component of the gaseous phase. Henry's law is used to express equilibrium of dissolved air.
- Thermal equilibrium between phases is assumed. This means that the three phases are at the same temperature
- Vapour concentration is in equilibrium with the liquid phase. Psychrometric law expresses its concentration.
- State variables (also called unknowns) are: solid displacements, \mathbf{u} (three spatial directions); liquid pressure, P_l ; gas pressure, P_g ; and temperature, T .
- Balance of momentum for the medium as a whole is reduced to the equation of stress equilibrium together with a mechanical constitutive model to relate stresses with strains. Strains are defined in terms of displacements.
- Small strains and small strain rates are assumed for solid deformation. Advective terms due to solid displacement are neglected after the formulation is transformed in terms of material derivatives (in fact, material derivatives are approximated as eulerian time derivatives). In this way, volumetric strain is properly considered.
- Balance of momentum for dissolved species and for fluid phases are reduced to constitutive equations (Fick's law and Darcy's law).
- Physical parameters in constitutive laws are function of pressure and temperature. For example: concentration of vapour under planar surface (in psychrometric law), surface tension (in retention curve), dynamic viscosity (in Darcy's law), strongly depend on temperature.

V.2. GOVERNING EQUATIONS

The governing equations for non-isothermal multiphase flow of water and gas through porous deformable saline media have been presented by Olivella et al. (1994). A detailed derivation is given there, and only a brief description is included here.

The equations that govern this problem can be categorised into four main groups. These are: balance equations, constitutive equations, equilibrium relationships and definition constraints. Equations for mass balance were established following the compositional approach. That is, mass balance is performed for water, air and salt species instead of using solid, liquid and gas phases. Equation for balance of energy is established for the medium as a whole. The equation of momentum balance for the porous medium is reduced to that of stress equilibrium.

The following notation will be used in writing balance equations:

ϕ : porosity	\mathbf{b} : body forces,
ρ : density	ω : mass fraction,
\mathbf{j} : total mass flux	ρ : mass content per unit volume of phase,
\mathbf{i} : non-advective mass flux	e : specific internal energy
\mathbf{q} : advective flux	\mathbf{i}_c : conductive heat flux
\mathbf{u} : solid displacements	\mathbf{j}_e : energy fluxes due to mass motion
$\boldsymbol{\sigma}$: stress tensor	
S_l, S_g : degree of saturation of liquid and gaseous phases i.e., fraction of pore volume occupied by each phase.	

Superscripts w and a refer to water and air, respectively

Subscripts s, l and g refer to solid, liquid and gas phase, respectively.

V.2.1. Balance Equations

The compositional approach is adopted to establish the mass balance equations. Volumetric mass of a species in a phase (e.g. water in gas phase ρ_g^w) is the product of the mass fraction of that species (ω_g^w) and the bulk density of the phase (ρ_g), i.e. $\rho_g^w = \omega_g^w \rho_g$.

The total mass flux of a species in a phase (e.g. flux of air present in gas phase \mathbf{j}_g^w) is, in general, the sum of three terms:

- the nonadvective flux: \mathbf{i}_g^w , i.e. diffusive/ dispersive,
- the advective flux caused by fluid motion: $\omega_g^w \rho_g \mathbf{q}_g$, where \mathbf{q}_g is the Darcy's flux,
- the advective flux caused by solid motion: $\omega_g^w \rho_g S_g \phi \frac{d\mathbf{u}}{dt}$ where $\frac{d\mathbf{u}}{dt}$ is the vector of solid velocities, S_g is the volumetric fraction of pores occupied by the gas phase and ϕ is porosity.

The sum of the nonadvective and fluid motion advective fluxes is separated from the total flux in order to simplify algebraic equations. This flux is relative to the solid phase and is denoted by \mathbf{j}'_g^w . It corresponds to the total flux minus the advective part caused by solid motion. When solid deformation is negligible, then $\mathbf{j}' = \mathbf{j}$. The relative contribution of each flux term to the total flux is not always the same. For instance, diffusion will become more important if advection is small.

Mass balance of solid

Mass balance of solid present in the medium is written as:

$$\frac{\partial(\rho_s(1 - \phi))}{\partial t} + \nabla \cdot (\mathbf{j}_s) = 0 \quad (1)$$

where θ_s is the mass of solid per unit volume of solid and \mathbf{j}_s is the flux of solid. From this equation, an expression for porosity variation was obtained as:

$$\frac{D_s \phi}{Dt} = \frac{(1 - \phi) D_s \rho_s}{\rho_s Dt} + (1 - \phi) \nabla \cdot \frac{d\mathbf{u}}{dt} \quad (2)$$

The material derivative with respect to the solid has been used and its definition is:

$$\frac{D_s(\blacksquare)}{Dt} = \frac{\partial(\blacksquare)}{\partial t} + \frac{d\mathbf{u}}{dt} \cdot \nabla(\blacksquare) \quad (3)$$

Equation (2) expresses the variation of porosity caused by volumetric deformation and solid density variation.

Mass balance of water

Water is present in liquid and gas phases. The total mass balance of water is expressed as:

$$\frac{\partial \left((\omega_g^w \rho_g S_g + \omega_l^w \rho_l S_l) \phi \right)}{\partial t} + \nabla \cdot (\mathbf{j}_g^w + \mathbf{j}_l^w) = f^w \quad (4)$$

where f^w is an external supply of water. An internal production term is not included because the total mass balance inside the medium is performed. The use of the material derivative leads to:

$$\begin{aligned} \phi \frac{D_s(\omega_l^w \rho_l S_l + \omega_g^w \rho_g S_g)}{Dt} + (\omega_l^w \rho_l S_l + \omega_g^w \rho_g S_g) \frac{D_s \phi}{Dt} + \\ + (\omega_l^w \rho_l S_l + \omega_g^w \rho_g S_g) \phi \nabla \cdot \frac{d\mathbf{u}}{dt} + \nabla \cdot (\mathbf{j}_l^w + \mathbf{j}_g^w) = f^w \end{aligned} \quad (5)$$

The final objective is to find the unknowns from the governing equations. Therefore, the dependent variables will have to be related to the unknowns in some way. For example, degree of saturation will be computed using a retention curve which should express it in terms of temperature, liquid pressure and gas pressure.

Porosity appears in this equation of water mass balance not only as a coefficient, but also in a term involving its variation caused by different processes. It is also hidden in variables that depend on porosity (e.g. intrinsic permeability). The way of expressing the derivative term as a function of the state variables is via the solid mass balance equation. This allows to take into account correctly the influence of porosity variation in the balance equation for water.

It should be noted that in the last equation the material derivatives can be approximated as eulerian if the assumption of small strain rate is performed while the volumetric change (porosity derivative and volumetric strain) is not neglected. This is the classical way of obtaining the coupled flow-deformation equations.

Mass balance of air

Once the other mass balance equations have been written it is straightforward to obtain the mass balance of air taking into account that air is the main component of the gas phase and that it may be also present as air dissolved in the liquid phase.

$$\begin{aligned} \phi \frac{D_s(\omega_l^a \rho_l S_l + \omega_g^a \rho_g S_g)}{Dt} + (\omega_l^a \rho_l S_l + \omega_g^a \rho_g S_g) \frac{D_s \phi}{Dt} + \\ + (\omega_l^a \rho_l S_l + \omega_g^a \rho_g S_g) \phi \nabla \cdot \frac{d\mathbf{u}}{dt} + \nabla \cdot (\mathbf{j}_l^a + \mathbf{j}_g^a) = f^a \end{aligned} \quad (6)$$

Momentum balance for the medium

The momentum balance reduces to the equilibrium of stresses if the inertial terms are neglected:

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0} \quad (7)$$

where $\boldsymbol{\sigma}$ is the stress tensor and \mathbf{b} is the vector of body forces.

Internal energy balance for the medium

The equation for internal energy balance for the porous medium is established taking into account the internal energy in each phase (e_s, e_l, e_g) or enthalpy (h_s, h_l, h_g):

$$\begin{aligned} \frac{\partial(e_g \rho_s (1 - \phi) + e_g \rho_g S_g \phi + e_l \rho_l S_l \phi)}{\partial t} - \frac{\phi S_g p_g}{\rho_g} \frac{\partial \rho_g}{\partial t} + \\ + \nabla \cdot (\mathbf{i}_c + \mathbf{j}_{es} + \mathbf{j}_{eg} + \mathbf{j}_{el}) = f^Q \end{aligned} \quad (8)$$

$$\begin{aligned} \frac{\partial(h_s \rho_s (1 - \phi) + h_g \rho_g S_g \phi + h_l \rho_l S_l \phi)}{\partial t} - \phi S_g \frac{\partial p_g}{\partial t} + \\ + \nabla \cdot (\mathbf{i}_c + \mathbf{j}_{hs} + \mathbf{j}_{hg} + \mathbf{j}_{hl}) = f^Q \end{aligned}$$

where \mathbf{i}_c is energy flux due to conduction through the porous medium, the other fluxes ($\mathbf{j}_{es}, \mathbf{j}_{el}, \mathbf{j}_{eg}, \mathbf{j}_{hs}, \mathbf{j}_{hl}, \mathbf{j}_{hg}$) are advective fluxes of energy or enthalpy caused by mass motions and f^Q is an internal/external energy supply (heat supply). In this case this term accounts, for instance, energy dissipation due to medium deformation which is not explicit because it is negligible in most cases. The use of the material derivative allows obtaining an equation formally similar to the mass balance of water. The reason for the similarity is that both water and internal energy, are considered present in the three phases.

Hence, only one equation is required which expresses the balance of internal energy in the porous medium as a whole. The enthalpy equation is obtained using the definition of enthalpy as $h = e + pv$. The density time derivative or the pressure time derivative terms in energy or enthalpy balance are sometimes neglected.

The fluxes in the divergence term include conduction of heat and advection of heat caused by the motion of every species in the medium. A non-advective mass flux causes an advective heat

flux because a species inside a phase moves and transports energy. Contrary to what happens with the movement of a contaminant in a groundwater system, the diffusive term for heat transport (conduction of heat) is much larger than the term concerning hydromechanical dispersion (non-advective flux caused by the velocity of fluids). For this reason, this term is sometimes neglected.

V.2.2. Constitutive equations and equilibrium restrictions

Associated with this formulation there is a set of necessary constitutive and equilibrium laws. Table V.2.1 is a summary of the constitutive laws and equilibrium restrictions that should be incorporated in the general formulation. The dependent variables that are computed using each of the laws are also included.

Table V.2.1. Constitutive equations and equilibrium restrictions

EQUATION	VARIABLE NAME	VARIABLE
<i>Constitutive equations</i>		
Darcy's law	liquid and gas advective flux	$\mathbf{q}_l, \mathbf{q}_g$
Fick's law	vapour and air non-advective fluxes	$\mathbf{i}_g^w, \mathbf{i}_l^a$
Fourier's law	conductive heat flux	\mathbf{i}_c
Retention curve	Liquid phase degree of saturation	S_l, S_g
Mechanical constitutive model	Stress tensor	$\boldsymbol{\sigma}$
Phase density	liquid density	ρ_l
Gases law	gas density	ρ_g
<i>Equilibrium restrictions</i>		
Henry's law	Air dissolved mass fraction	ω_l^a
Psychrometric law	Vapour mass fraction	ω_g^w

The constitutive equations establish the link between the independent variables (or unknowns) and the dependent variables. There are several categories of dependent variables depending on the complexity with which they are related to the unknowns. The governing equations are finally written in terms of the unknowns when the constitutive equations are substituted in the balance equations.

Another type of relationships that relate dependent variables with unknowns are the equilibrium restrictions. They are obtained assuming chemical equilibrium for dissolution of the different species (air and vapour) in phases (liquid, gas). This assumption is sufficiently adequate because these chemical processes are fast compared to the transport processes that take place in porous media and, for this reason, they are not rate controlling.

V.2.3. Boundary conditions

Application of the Green's theorem to the divergence term (both in the balance or equilibrium of stresses equations) produces terms which represent fluxes or stresses across or on the boundaries. These terms are substituted by nodal flow rates or forces in the discretized form of the equations. For the mechanical problem, the classical approach is followed to impose external forces. Imposing displacements is made by means of a Cauchy type boundary condition, i.e. a force computed as the stiffness of a spring times the displacement increment. The boundary conditions for balance equations are incorporated by means the simple addition of nodal flow rates. For instance, the mass flow rate of water as a component of gas phase (i.e. vapour) is:

$$j_g^w = (\omega_g^w)^0 j_g^0 + (\omega_g^w)^0 \gamma_g (P_g^0 - P_g) + \beta_g \left((\rho_g \omega_g^w)^0 - (\rho_g \omega_g^w) \right) \quad (9)$$

where the superscript $()^0$ stands for prescribed values. This general form of boundary condition, includes three terms. The first one is the mass inflow or outflow that takes place when a flow rate of gas (j_g^0) is prescribed. The second term is the mass inflow or outflow that takes place when the gas phase pressure (P_g^0) is prescribed at a node. The coefficient γ_g is a leakage coefficient, i.e., a parameter that allows a boundary condition of the Cauchy type. The third term is the mass inflow or outflow that takes place when vapour mass fraction is prescribed at the boundary. This term naturally comes from the nonadvective flux (Fick's law). Mass fraction and density prescribed values are only required when inflow takes place. For outflow, the values in the medium are considered. For the energy balance equation, the boundary condition has a similar form.

V.2.4. Summary of governing equations

As stated above the governing equations for non-isothermal multiphase flow of liquid and gas through porous deformable saline media have been established by Olivella et al. (1994). A detailed derivation is presented there. The theoretical work briefly presented above has been used as a basis for the development of the computer program CODE_BRIGHT, which stands for COupled DEformation, BRIne, Gas and Heat Transport problems.

Table V.2.2.: Equation and variable summary

EQUATION	VARIABLE NAME	VARIABLE
equilibrium of stresses	displacements	u
balance of water mass	liquid pressure	P_l
balance of air mass	gas pressure	P_g
balance of internal energy	temperature	T

V.3. NUMERICAL APPROACH

V.3.1. Introduction

The system of PDE's (Partial Differential Equations) is solved numerically. The numerical approach can be viewed as divided into two parts: spatial and temporal discretizations. Finite element method is used for the spatial discretization while finite differences are used for the temporal discretization. The discretization in time is linear and the implicit scheme uses two intermediate points, $t^{k+\varepsilon}$ and $t^{k+\theta}$ between the initial t^k and final t^{k+1} times. Finally, since the problem presented here is non-linear, the Newton-Raphson method was adopted to find an iterative scheme.

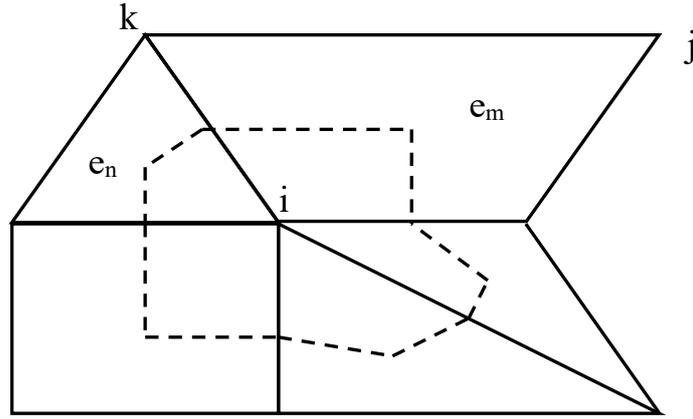


Figure V.3.1. Concept of cell in a finite element mesh.

Once the solid balance is substituted in the other balance equations, computation of porosity at an intermediate point is not necessary because its variation is expected to occur at slow rates. For this reason, porosity is integrated explicitly, that is, the values at t^k are used. Since the variation of porosity is expressed by the solid mass balance equation, this assumption leads also to some advantages for the iterative scheme. After the spatial discretization of the partial differential equations, the residuals that are obtained can be written (for one finite element) as:

$$\begin{pmatrix} \mathbf{r}_u \\ \mathbf{r}_{P_l} \\ \mathbf{r}_{P_g} \\ \mathbf{r}_T \end{pmatrix} = \frac{d}{dt} \begin{pmatrix} \mathbf{d}_u \\ \mathbf{d}_{P_l} \\ \mathbf{d}_{P_g} \\ \mathbf{d}_T \end{pmatrix} + \begin{pmatrix} \mathbf{a}_u \\ \mathbf{a}_{P_l} \\ \mathbf{a}_{P_g} \\ \mathbf{a}_T \end{pmatrix} + \begin{pmatrix} \mathbf{b}_u \\ \mathbf{b}_{P_l} \\ \mathbf{b}_{P_g} \\ \mathbf{b}_T \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix} \quad (10)$$

where \mathbf{r} are the residuals, $d\mathbf{d}/dt$ are the storage or accumulation terms, \mathbf{a} are the conductance terms, and \mathbf{b} are the sink/source terms and boundary conditions. After time discretization a more compact form can read as:

$$\mathbf{r}(\mathbf{X}^{k+1}) = \frac{\mathbf{d}^{k+1} - \mathbf{d}^k}{\Delta t^k} + \mathbf{A}(\mathbf{X}^{k+\varepsilon})\mathbf{X}^{k+\theta} + \mathbf{b}(\mathbf{X}^{k+\theta}) = \mathbf{0} \quad (11)$$

where k is the time step index, $\mathbf{X} = [(u_x, u_y, u_z, P_l, P_g, T)_{(1)}, \dots, (u_x, u_y, u_z, P_l, P_g, T)_{(n)}]$, is the vector of unknowns (i.e. a maximum of seven degrees of freedom per node), \mathbf{A} represents the conductance matrix. The Newton-Raphson scheme of solution for this non-linear system of AE's is:

$$\frac{\partial \mathbf{r}(\mathbf{X}^{k+1})}{\partial \mathbf{X}^{k+1}} (\mathbf{X}^{k+1,l+1} - \mathbf{X}^{k+1,l}) = -\mathbf{R}(\mathbf{X}^{k+1,l}) \quad (12)$$

where l indicates iteration.

In the present approach, the standard Galerkin method is used with some variations in order to facilitate computations. General aspects related to numerical solution of hydrogeological problems can be found in Huyakorn and Pinder (1983). As shown in the preceding section, in the mass and energy balance equations the following terms may be distinguished:

- Storage terms. These terms represent the variation of mass or energy content and therefore, they are calculated by means of variables such as degree of saturation, density, porosity, mass fraction and specific energy.
- Advective fluxes. The advective fluxes caused by motion of fluids computed using Darcy's law and, except for the coefficients, they are explicit in terms of pressure gradients.
- Nonadvective fluxes. These terms, computed through Fick's law, are proportional to gradients of mass fractions which do not belong to the set of unknowns. Fourier's law is used for the conductive heat flux and it expresses proportionality to temperature gradients.
- Volumetric strain terms. In fact, these terms are also storage terms. They are proportional to $\nabla \cdot d\mathbf{u}/dt$ which is equivalent to the volumetric strain rate.
- Sink/source terms.

Each of these terms requires specific treatment. This is described in detail in Olivella et al (1996).

In order to explain the treatment of the different terms and equations the following notation is introduced:

- node i : node in a finite element mesh
- e_1, e_2, \dots, e_m : elements that contain node i , i.e. a cell centered in node i is composed by a fraction of these elements. m is variable from node to node and it is not related to the number of nodes per element.
- n_{em} : number of nodes in element e_m . For example, $n_{em}=3$ for triangles, $n_{em}=4$ for quadrilaterals, $n_{em}=4$ for tetrahedrons, etc.
- $(\cdot)^k$: the quantity is computed at time t^k of the temporal discretization. The same for t^{k+1} , $t^{k+\varepsilon}$ or $t^{k+\theta}$
- $(\cdot)_{em}$: the quantity is computed in element e_m . This means at the center of the element or, in other words, using the average of nodal unknowns.
- $(\cdot)_i$: the quantity is computed in node i as a function of the unknowns in that node. \item--}
- $(\cdot)_{i,em}$: the quantity is computed in node i but with the material properties corresponding to element e_m .
- V_{em} : volume of element e_m .
- ξ_i : shape function for node i .

V.3.2. Treatment of different terms

Treatment of storage terms

In this sub-section we refer to terms not related to volumetric strain or porosity variation. The storage or accumulation terms are computed in a mass conservative approach (Allen and Murphy, 1986; Celia et al., 1990; Milly, 1984). The conservative approach discretizes directly the accumulation terms while the capacitative approach uses the chain rule to transform time derivatives in terms of the unknowns. Milly (1984) proposes modifications of the capacitative approach in order to conserve mass. It seems reasonable that the mass conservative approach should give a more accurate solution than the capacitative approach.

Mass conservation in time is achieved if the time derivatives are directly approximated by a finite difference in time. Finite element method for the space discretization conserves mass (Milly, 1984).

A typical storage term is (from Eq. 5) the variation of water in the gas phase:

$$\phi \frac{D_s(\omega_g^w \rho_g S_g)}{Dt} \cong \phi \frac{\partial(\omega_g^w \rho_g S_g)}{\partial t} \quad (13)$$

where the material derivative with respect to the solid is approximated as an eulerian derivative because the small strain rate assumption. The weighted residual method is applied to the governing equations and, for node i , (13) is transformed into:

$$\int_v N_i \phi \frac{\partial(\omega_g^w \rho_g S_g)}{\partial t} dv = \sum_{e_m} \int_{e_m} N_i \phi \frac{\partial(\omega_g^w \rho_g S_g)}{\partial t} dv \quad (14)$$

At this point of the development we assume that porosity is defined element-wise. An element-wise variable (Voss, 1984) is space-constant over every element, but different from element to element. We will use $\phi_{e_m}^k$ for porosity in element e_m at time t^k . Similarly, a cell-wise variable (Voss, 1984) is space constant over the cell centered in the node. It would be very easy to compute (14) if the time derivative could be computed in a cell-wise way, because one value would be sufficient for node i and (14) would be transformed into a very simplified form. However, the degree of saturation is not only a function of nodal unknowns but also of material properties such as porosity or retention parameters. To overcome this difficulty, the time derivative in (14) is computed from nodal unknowns but with material properties of every element in contact with the node. Hence m values are necessary in node i . Obviously if part of this time derivative is not material dependent (density and concentration are only function of temperature and pressure) then the corresponding variables are only computed in the node. This leads to a kind of modified cell-wise variables.

Making use of these approximations, we finally obtain, for example for any integral in (14):

$$\int_{e_m} N_i \phi \frac{\partial(\omega_g^w \rho_g S_g)}{\partial t} dv \cong \phi_{e_m}^k \left(\frac{(\omega_g^w \rho_g S_g)_{i,e_m}^{k+1} - (\omega_g^w \rho_g S_g)_{i,e_m}^k}{t^{k+1} - t^k} \right) \int_{e_m} N_i dv \quad (15)$$

where a simple finite difference is used for the time discretization. This approximation allows us to make the space integration independently of the physical variables. Therefore, computation of geometrical coefficients is necessary only once for a given finite element mesh. The integral of the shape function over an element is equal to V_{em}/n_{em} for the case of linear shape functions. These geometrical coefficients are also called influence coefficients. Without loss of generality, they can be computed either analytically or numerically. Finally, it should be

pointed out that this formulation gives rise to a concentrated scheme, which means that the storage term in node i is only a function of unknowns in node i . This is clearly advantageous from a computational point of view (Huyakorn and Pinder, 1983).

Treatment of advective terms

The weighted residual method is applied to each balance equation. Then Green's theorem allows one to reduce the order of the derivatives and the divergence of flows is transformed into two terms, one of them with the gradient of the shape function. Hence, after that, in the water balance equation of node i we find, the following advective term:

$$\begin{aligned} - \int_v (\nabla^t N_i) \omega_g^w \rho_g \mathbf{q}_g dv = & \left(\int_v (\nabla^t N_i) \omega_g^w \rho_g \frac{\mathbf{k} k_{rg}}{\mu_g} (\nabla N_j) dv \right) (p_g)_j - \\ & - \left(\int_v (\nabla^t N_i) \omega_g^w \rho_g \frac{\mathbf{k} k_{rg}}{\mu_g} \rho_g \mathbf{g} dv \right) \end{aligned} \quad (16)$$

where the subscript j indicates summation over element nodes. P_g is a node-wise (Voss, 1984) variable, which means that it is defined by its nodal values and interpolated on the elements using the shape functions. Generalised Darcy's law has been used to compute the flux of the gas phase:

$$\mathbf{q}_g = - \frac{\mathbf{k} k_{rg}}{\mu_g} (\nabla P_g - \rho_g \mathbf{g}) \quad (17)$$

where \mathbf{k} is the tensor of intrinsic permeability, k_{rg} is the relative permeability of the gas phase, μ_g is the dynamic viscosity of gas and \mathbf{g} is a vector of gravity forces. For node i the volume v over which the integrals in (16) have to be performed is composed by the elements e_1, e_2, \dots, e_m . In this way, the advective terms (16) represent the lateral mass fluxes to cell associated to node i from contiguous cells. The pressure term is considered first. The contribution of element e_m to the total lateral flux towards node i is approximated as:

$$\begin{aligned} & \left(\int_{e_m} (\nabla^t N_i) \omega_g^w \rho_g \frac{\mathbf{k} k_{rg}}{\mu_g} (\nabla N_j) dv \right) (p_g)_j \approx \\ & \approx \left(\omega_g^w \rho_g \frac{k_{rg}}{\mu_g} \right)_{e_m}^{k+\varepsilon} \left(\int_{e_m} (\nabla^t N_i) \mathbf{k}_{e_m}^k (\nabla N_j) dv \right) (p_g)_j^{k+\theta} \end{aligned} \quad (18)$$

where three different intermediate points may be used, one for the pressure ($t^{k+\theta}$), another for the intrinsic permeability (t^k) and yet another for the remaining coefficients ($t^{k+\varepsilon}$) including the relative permeability. The intrinsic permeability remains in the integral because it is a tensorial quantity, but if its product with the shape function gradients is split, then its coefficients can be taken off from the integral. It should be noticed that intrinsic permeability is handled explicitly (i.e. evaluated at time t^k) because it is a function of porosity structure, which we assume to vary slowly. Since all physical variables can appear outside the integral because they are considered element-wise, the integrals of products of shape function gradients are also considered influence coefficients (Huyakorn et al., 1986). They have to be computed for each element, but only once for a given mesh.

A similar approximation is used for the gravity term in (16). Evaluation of density element-wise is convenient in order to balance correctly pressure gradients with gravity forces at element level.

Treatment of nonadvective terms (diffusive/dispersiv)

In the balance equation of node i we find, typically, the following diffusive term:

$$-\int_v (\nabla^t N_i) \mathbf{i}_g dv = \left(\int_v (\nabla^t N_i) \phi \tau \rho_g S_g D_g^w \mathbf{I} (\nabla N_j) dv \right) (\omega_g^w)_j \quad (19)$$

where the subscript j indicates summation over the nodes. ω_g^w is considered a node-wise variable. Fick's law has been used to compute the diffusive flux:

$$\mathbf{i}_g = -\phi \tau \rho_g S_g D_g^w \mathbf{I} \nabla \omega_g^w \quad (20)$$

where τ is a tortuosity coefficient, D_g^w is the molecular diffusion coefficient which is a function of temperature and gas pressure and \mathbf{I} is the identity matrix. The contribution of element e_m to the total lateral diffusive flux towards node i is approximated as:

$$\begin{aligned} & \left(\int_{e_m} (\nabla^t N_i) \phi \tau \rho_g S_g D_g^w \mathbf{I} (\nabla N_j) dv \right) (\omega_g^w)_j \approx \\ & \approx (\phi \tau)_{e_m}^k (\rho_g S_g D_g^w)_{e_m}^{k+\varepsilon} \left(\int_{e_m} (\nabla^t N_i) \mathbf{I} (\nabla N_j) dv \right) (\omega_g^w)_j^{k+\theta} \end{aligned} \quad (21)$$

where various time intermediate points have been used similarly to what was explained for the advective terms. The treatment of these diffusive terms also takes advantage of the fact that the Newton-Raphson method is used to obtain the iterative scheme. We directly interpolate mass fractions (e.g. ω_g^w) and compute gradients.

The dispersive term is treated in a similar way as the diffusive. In this case dispersivities are element-wise dependent variables. In principle, the liquid and gas fluxes, used to compute the dispersion tensor, are also computed element-wise.

Treatment of volumetric strain terms

If equation of balance of solid (2) is substituted in all other balance equations, the variations of porosity are not explicit in them. In this way porosity only appears as parameter or coefficient and terms of volumetric strain remain in the balance equations. In equation for node i these terms are of the type:

$$\int_{e_m} N_i \alpha \nabla \cdot \frac{d\mathbf{u}}{dt} dv = \int_{e_m} N_i \alpha \mathbf{m}^t \mathbf{B} \frac{d\mathbf{u}}{dt} dv \quad (22)$$

where α is defined from de equations and $d\mathbf{u}/dt$ is the vector of solid velocities, $\mathbf{m}^t=(1,1,1,0,0,0)$ is an auxiliary vector and \mathbf{B} is the matrix used in the finite element approach for the mechanical problem. The coefficients of \mathbf{B} are gradients of shape functions (Zienkiewick and Zaylor, 1989). In (22), $d\mathbf{u}/dt$ is transformed from a continuous vectorial function to a nodal-discrete vectorial function, although the same symbol is kept (i.e. $u_x = N_j u_{xj}$), ..., where j indicates summation). Following the same methodology as for the other terms we have approximated the integral given above. The contribution of element e_m to cell i is:

$$\int_{e_m} N_i \alpha \mathbf{m}^t \mathbf{B} \frac{d\mathbf{u}}{dt} dv \approx \alpha_{e_m}^{k+\varepsilon} \left[\int_{e_m} N_i \mathbf{m}^t \mathbf{B}_j dv \right] \left(\frac{\mathbf{u}_j^{k+1} - \mathbf{u}_j^k}{t^{k+1} - t^k} \right) \quad (23)$$

where j indicates summation over element nodes, \mathbf{u} is the vector of nodal displacements and \mathbf{B}_j is the j -submatrix of \mathbf{B} .

Treatment of mechanical equilibrium equations

The weighted residual method is applied to the stress equilibrium equation [6] followed by the Green's theorem. This leads to the equation

$$\mathbf{r}(\boldsymbol{\sigma}^{k+1}) = \int_v \mathbf{B}^t \boldsymbol{\sigma}^{k+1} dv - \mathbf{f}^{k+1} = \mathbf{0} \quad (24)$$

where $\mathbf{r}(\boldsymbol{\sigma}^{k+1})$ represents the residual corresponding to the mechanical problem and $\boldsymbol{\sigma}^{k+1}$ is the stress vector. Matrix \mathbf{B} (composed by gradients of shape functions) is defined in such a way that stress is a vector and not a tensor. The body force terms and the boundary traction terms are represented together by \mathbf{f}^{k+1} . The constitutive model relates stresses with strains, with fluid pressures and with temperatures at a point in the medium. Only if elasticity is included, the total strain rate is decomposed in the following way:

$$\frac{d\boldsymbol{\varepsilon}}{dt} = \frac{d\boldsymbol{\varepsilon}^e}{dt} = (\mathbf{D}^e)^{-1} \frac{d\boldsymbol{\sigma}'}{dt} + \mathbf{I}a_s \frac{ds}{dt} + \mathbf{I}a_T \frac{dT}{dt}, \quad \mathbf{I} \text{ or } \mathbf{m} \quad (25)$$

where \mathbf{D}^e is the elasticity matrix, a_s and a_T are coefficients for elastic dilation. $\boldsymbol{\sigma}'$ is the net stress tensor defined as $\boldsymbol{\sigma}' = \boldsymbol{\sigma} + \mathbf{m} P_g$ (compression negative). On the other hand, strain will be written in terms of displacements because $\boldsymbol{\varepsilon} = \mathbf{B} \mathbf{u}$. The last equation (25) must satisfy at every point in the medium. Space and time discretization lead to:

$$\mathbf{h}^{k+1} = -\mathbf{D}^e \mathbf{B}(\mathbf{u}^{k+1} - \mathbf{u}^k) + (\boldsymbol{\sigma}^{k+1} - \boldsymbol{\sigma}^k) + \mathbf{I}(p_g^{k+1} - p_g^k) + \mathbf{D}^e \mathbf{I}a_s (s^{k+1} - s^k) + \mathbf{D}^e \mathbf{I}a_T (T^{k+1} - T^k) \quad (26)$$

where \mathbf{h} is the residual of stresses at every point. If stress can be obtained in an explicit way from (26), it is simply substituted in (24). However, when nonlinear models are introduced a substitution of the differential or incremental forms is necessary.

For the mechanical problem, the approximations that should be made are different from the ones used for flow problems. According to the numerical approximations proposed for the flow problems (hydraulic and thermal), we would tend to use element-wise matrices. However, the mechanical problem has some peculiarities which do not allow this kind of simplified treatment.

First, linear triangular elements (the simplest element in two dimensional analyses), which have been proven to be very adequate for flow problems, should be avoided for mechanical problems. This is because if the medium is nearly-incompressible (creep of rocks takes place with very small volumetric deformation), locking takes place (not all displacements are permitted due to element restrictions). Second, linear quadrilateral elements with element-wise variables (this is equivalent to one integration point) lead to hour-glassing (uncontrolled displacement modes appear).

In order to overcome these difficulties, the selective integration (**B**-bar) method is used. It consists in using a modified form of matrix **B** which implies that the volumetric part of deformation and the deviatoric part are integrated with different order of numerical integration (Hughes, 1980). For linear quadrilateral elements, four integration points are used to integrate the deviatoric part while one is used for volumetric strain terms. Although this approximation is different from what is proposed for the flow problem, element-wise variables or parameters are maintained (porosity, saturation,...). Stress is not element-wise and it must be computed at the integration points.

V.4. THEORETICAL APPROACH SUMMARY

The governing equations include: stress equilibrium equations (1, 2 or 3 according to the dimensions of the problem), mass balance equations (different species) and internal energy balance equation for the medium as a whole (thermal equilibrium is assumed).

The stress equilibrium equations are a simplified form of the balance of momentum for the porous medium. Mass balance of water, solid and air are established. Since the assumption of equilibrium is made, the mass of each species as present in any phase (solid, liquid or gas) is balanced for the porous medium as a whole. In this way, one equation for each species is obtained. The equilibrium assumption implies that partition functions are required to compute the fraction of each species in each phase.

Each partial differential equation is naturally associated to an unknown. These unknowns can be solved in a coupled way, i.e., allowing all possible cross coupling processes that have been implemented, or, on the contrary, any uncoupled problem to obtain a single unknown can be solved.

The balance equations that CODE_BRIGHT solves are compiled here:

Equation: mechanical equilibrium equations (1, 2 or 3 dimensions):

$$\text{divergence} \begin{pmatrix} \text{tensor of} \\ \text{total stress} \end{pmatrix} + \begin{pmatrix} \text{vector of} \\ \text{body forces} \end{pmatrix} = \text{vector} \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \quad \text{Unknown:} \\ \nabla \cdot \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0} \quad \text{displacements,} \\ \mathbf{u}=(u_x, u_y, u_z)$$

Equation: water mass balance:

$$\frac{\partial}{\partial t} \begin{pmatrix} \text{mass of water in} \\ \text{liquid and gas phase} \end{pmatrix} + \text{divergence} \begin{pmatrix} \text{total fluxes} \\ \text{of water} \end{pmatrix} = \begin{pmatrix} \text{external supply} \\ \text{of water} \end{pmatrix} \quad \text{Unknown:} \\ \frac{\partial \left((\omega_g^w \rho_g S_g + \omega_l^w \rho_l S_l) \phi \right)}{\partial t} + \nabla \cdot (\mathbf{j}_g^w + \mathbf{j}_l^w) = f^w \quad \text{liquid pressure,} \\ P_l \text{ (MPa)}$$

Equation: air mass balance:

$$\frac{\partial}{\partial t} \begin{pmatrix} \text{mass of air in} \\ \text{liquid and gas phase} \end{pmatrix} + \text{divergence} \begin{pmatrix} \text{total fluxes} \\ \text{of air} \end{pmatrix} = \begin{pmatrix} \text{external supply} \\ \text{of air} \end{pmatrix} \quad \text{Unknown:} \\ \frac{\partial \left((\omega_g^a \rho_g S_g + \omega_l^a \rho_l S_l) \phi \right)}{\partial t} + \nabla \cdot (\mathbf{j}_g^a + \mathbf{j}_l^a) = f^a \quad \text{gas pressure,} \\ P_g \text{ (MPa)}$$

Equation: internal energy balance:

$$\frac{\partial}{\partial t} \left(\begin{array}{l} \text{internal energy in solid,} \\ \text{liquid and gas phase} \end{array} \right) + \text{divergence} \left(\begin{array}{l} \text{total fluxes} \\ \text{of energy} \end{array} \right) = \left(\begin{array}{l} \text{external supply} \\ \text{of heat} \end{array} \right) \quad \text{Unknown:} \\ \text{tempera-} \\ \text{ture, } T (^{\circ})$$

$$\frac{\partial (e_g \rho_s (1 - \phi) + e_g \rho_g S_g \phi + e_l \rho_l S_l \phi)}{\partial t} - \frac{\phi S_g p_g}{\rho_g} \frac{\partial \rho_g}{\partial t} +$$

$$+ \nabla \cdot (\mathbf{i}_c + \mathbf{j}_{es} + \mathbf{j}_{eg} + \mathbf{j}_{el}) = f^Q$$

Equation: solid mass balance:

$$\frac{\partial (\text{mass of solid})}{\partial t} + \text{divergence}(\text{flux of solid}) = 0 \quad \text{Unknown:}$$

$$\frac{\partial (\rho_s (1 - \phi))}{\partial t} + \nabla \cdot (\mathbf{j}_s) = 0 \quad \text{porosity,}$$

$$\phi (-)$$

The definition of a problem (which of the above described equations should be solved) is achieved by means of a set of general options (IOPTDISPL, IOPTPL, IOPTPG, IOPTTEMP). These general options indicate whether one equation is included or not. For instance a mechanical problem would require IOPTDISPL=1 and the other indexes equal to 0. Other secondary options allows to include or not any of the possible processes. Specific indexes are used to decide if the solid is soluble (i.e. the medium is saline), if the air solubility in liquid phase is taken into account and if vapour is considered. Vapour transfer can only be considered if the thermal problem is solved.

V.5. FEATURES OF CODE-BRIGHT

The implementation of a coupled non-linear approach requires some specific developments and approximations. In this section the main aspects of the numerical approximation are reviewed. The program CODE_BRIGHT uses the finite element method to solve the coupled equations presented above. The main features of the numerical approach are:

- Linear interpolation functions on segments, triangles, quadrilaterals, tetrahedrons, triangular prisms and quadrilateral prisms (regular). Analytical integration is used for segments, triangles and tetrahedrons. Numerical integration is used for quadrilateral, arbitrary triangular prisms (6 points) and quadrilateral prisms (8 points). For the mechanical problem selective integration is used for quadrilateral and quadrilateral prisms (this means that the volumetric part is integrated with a reduced quadrature of 1 point). Finally, for all elements the flow equations are solved using element-wise and cell-wise approximations. This approximation is independent of the type of integration performed.
- Finite differences and implicit scheme are used for time integration. Two intermediate points are defined between the two ends of the time interval (t^k, t^{k+1}). One represents the point where the equation will be accomplished ($t^{k+\theta}$) and the other is the point where the non-linear functions are computed ($t^{k+\varepsilon}$). For instance $\varepsilon=0$ and $\theta=1$ states for a linearised problem with a fully implicit scheme of integration.
- Newton-Raphson method for solution of the non-linear system of algebraic equations that results once the space and time discretizations are applied.
- LU decomposition and backsubstitution (non-symmetric matrix) or conjugate gradients squared to solve the system of linear equations that result from the Newton-Raphson application.
- Automatic discretization of time. Increase or reduction of time increment according to convergence conditions or output requirements. Reduction of time increment may be caused by: excessive variation of unknowns per iteration, excessive number of iterations to reach convergence and correction larger than in the previous iteration.

The main features of the program CODE_BRIGHT are:

- Options that allow to solve uncoupled and coupled problems. For instance: Hydro-mechanical, Thermo-mechanical, Hydro-thermal problems can be solved if the physical situation requires one of these approaches.
- Types of analysis: One dimension (uni-axial confined strain and axi-symmetric). Two dimension (plane strain and axi-symmetric). Three dimensions.
- Several element types.
- Constitutive laws: each law defined as a set of parameters. Different types of relationships can be chosen in some cases.
- Boundary conditions:
 - Mechanical problem: forces and displacement rate in any spatial direction and at any node
 - Hydraulic problem: mass flow rate of water and air prescribed and liquid/gas pressure prescribed at any node
 - Thermal problem: heat flow rate prescribed and temperature prescribed at any node

- Convergence criteria: Tolerances for absolute and relative error independent for each unknown. Tolerance for residual convergence of each problem (mechanical, hydraulic, etc). The node under worse conditions is used to verify the convergence condition.
 - Forces/flows = $\varepsilon \rightarrow 0$
 - Absolute variable correction = $\delta x \rightarrow 0$
 - Variable correction / variable increment = $\delta x / \Delta x \rightarrow 0$
- Output options: Time evolution of variables in nodes or elements. The user should decide 'a priori' the nodal or element variables that will be output at all times (absolutely all computed times will be output for a few variables). Contour maps in the solution domain. Nodal or element variables can be used to draw contour maps. However, in the second case it is required to perform an interpolation that may be difficult due to the lack of continuity of the element variables.

V.6.2. Iterative solver for nonsymmetrical linear systems of equations.

There are several alternatives for solving linear systems in an iterative way. It should be taken into account that the matrix is non-symmetric. Perhaps one of the simplest algorithms that can be used is the conjugate gradients squared method (CGS) which has been proposed by Sonneveld, 1989 and van der Vorst, 1990. This CGS method is a modification of the conjugate gradients for non-symmetric matrices. Iterative methods require some extra space and a pre-conditioner. In order to facilitate parallelism the simplest pre-conditioner that can be used is the inverse of the diagonal of the matrix (diagonal scaling). Of course this is the less efficient pre-conditioner from the point of view of a scalar machine. However Pini and Gambolatti (1990) have shown that in vectorial machines, diagonal scaling was the most efficient pre-conditioner in the majority of the applications they compared. A block diagonal scaling consists in the inversion of the NDFxNDF block corresponding to each node (block in the matrix diagonal).

Using CRS storage mode plus CGS iterative method plus block-diagonal scaling produces a quite simple structure of the solver. In fact, only *vector-vector* products, *matrix-vector* products and inversion of NDFxNDF matrices have to be performed. The requirements of extra space are only $8*N*NDF$ where N is the number of nodes and NDF the number of degrees of freedom per node. It should be mentioned that the *matrix-vector* products are easily performed with the CRS storage mode because the matrix is stored by rows. The CGS algorithm is described as:

```

x := x0 (initial guess);
r := b - Ax;
 $\tilde{\mathbf{r}}$  is an arbitrary vector such that  $(\mathbf{r}, \tilde{\mathbf{r}}) \neq 0$  (e.g.  $\tilde{\mathbf{r}} = \mathbf{r}$ );
 $\rho_0 = (\mathbf{r}, \tilde{\mathbf{r}}); \beta_0 = \rho_0; \mathbf{p} = \mathbf{q} = \mathbf{0}$ ;
K is a preconditioner matrix;
for i = 0,1,2,...
    u := r +  $\beta_i$ q;
    p := u +  $\beta_i$ (q +  $\beta_i$ p);
    Solve q from Kq = p;
    v := Aq;
     $\alpha_i = \rho_i / (\tilde{\mathbf{r}}, \mathbf{v})$ ;
    q := u -  $\alpha_i$ v;
    Solve v from Kv = u + q;
    u := Av;
    x := x +  $\alpha_i$ v;
    r := r -  $\alpha_i$ u;
    if x close enough to A-1b then quit;
     $\rho_{i+1} = (\mathbf{r}, \tilde{\mathbf{r}})$ ;
     $\beta_{i+1} = \rho_{i+1} / \rho_i$ ;
end i

```

where it can be seen that two *matrix - vector* products should be performed per iteration, two *vector-vector* products (indicated by (,)), and the remaining operations are vector updates.

VI. CODE_BRIGHT. CONSTITUTIVE LAWS

This chapter contains the different models available and the corresponding parameters required by each model. The following constitutive laws are available

<p>HYDRAULIC AND THERMAL CONSTITUTIVE MODELS (a) RETENTION CURVE INTRINSIC PERMEABILITY LIQUID PHASE RELATIVE PERMEABILITY GAS PHASE RELATIVE PERMEABILITY DIFFUSIVE FLUXES OF MASS DISPERSIVE FLUXES OF MASS AND ENERGY CONDUCTIVE FLUX OF HEAT</p>	<p>MECHANICAL CONSTITUTIVE MODELS ELASTICITY (b) NONLINEAR ELASTICITY (b) VISCOPLASTICITY FOR SALINE MATERIALS (b) VISCOPLASTICITY FOR SATURATED SOILS AND ROCKS (b) VISCOPLASTICITY - GENERAL (b) DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS (c) THERMOELASTOPLASTIC MODEL FOR SOILS (d) BARCELONA EXPANSIVE MODEL FOR SOILS (e) CASM's FAMILY MODELS (f)</p>
<p>PHASE PROPERTIES (a) SOLID PHASE PROPERTIES LIQUID PHASE PROPERTIES GAS PHASE PROPERTIES</p>	<p>EXCAVATION PROCESS (g)</p>

VI.a HYDRAULIC AND THERMAL CONSTITUTIVE LAWS. PHASE PROPERTIES

HYDRAULIC AND THERMAL LAWS

ICL	NAME	ITYCL	DESCRIPTION
6	Retention curve	1 2 4 9 12 18	Van Genuchten model Linear model Square law Van Genuchten model with asymptotic branch to negative capillary pressures Van Genuchten model modified for FEBEX project Van Genuchten model modified for freezing model
66	Retention curve 2	12	Van Genuchten model modified for FEBEX project
7	Intrinsic permeability	1 2 4 5 15 16	Kozeny's model Exponential law Kozeny's model for matrix + cubic law for discontinuity (normal strain is used to calculate aperture) Kozeny's model for matrix + cubic law for discontinuity (volumetric strain is used to calculate aperture) Same as 5 but with different relative permeability for matrix and discontinuity Barton's law – Joint element
14	Liquid phase relative permeability	1 5 6 8 12	Van Genuchten model Liquid perfectly mobile Generalized power Power with initial cut off Van Genuchten model for freezing model
19	Gas phase relative permeability	1 5 6 12	Default law Gas perfectly mobile Generalized power Van Genuchten Mualem model
11	Diffusive flux of vapor	1 2	Molecular diffusion of vapour or air Molecular diffusion of vapour or air + tortuosity is variable with gas pressure (P_g)
12	Diffusive fluxes of dissolved salt and air	1	Molecular diffusion of dissolved salt and dissolved air
8	Dispersive fluxes of mass and energy	1	Fick's law (mass flux) and Fourier's law (heat flux)
9	Conductive flux of heat (1)	1 2 3	Thermal conductivity dependence on porosity (geometric weighted mean) Thermal conductivity dependence on porosity (weighted arithmetic mean) Thermal conductivity dependence on porosity (nonlinear function of porosity)
20	Conductive flux of heat (2)	1 2 4 5 6	Dependence on degree of saturation Dependence on degree of saturation Dependence on degree of saturation Dependence on water/ice content Dependence on degree of saturation (Chen & Ledesma, 2009)

PHASE PROPERTIES

ICL	NAME	ITYCL	DESCRIPTION
10	Solid phase properties	1 2	Solid specific heat, density and expansion coefficient Solid specific heat, density and expansion coeff. (variation of solid phase specific heat)
15	Liquid phase properties: density	1 2 4 5 6	Liquid density (exponential variation) Liquid density (linear variation) Liquid density (CO ₂) Liquid density (linear dependency of the thermal expansion coefficient with temperature) Liquid density adjustment for a wide temperature range (-30°C—300°C)
16	Liquid phase properties: viscosity	1	Liquid viscosity
17	Gas phase properties: density	1 2 3 4	Dry air density. Law of ideal gases and Henry's law for dry air Usually used to consider a second liquid phase instead of the gas phase Like ITYCL=1 but with user defined values for gas molecular mass and Henry's constant Gas density CO ₂
18	Gas phase properties: viscosity	1 2 4	Gas viscosity Gas viscosity (exponential law) Gas viscosity CO ₂

RETENTION CURVE

<p>CODES in <i>ROOT_gen.dat</i></p>	<p>ICL = 6 ITYCL = 1, 2, 4, 9, 12, 18 (See ICL = 66 for ITYCL = 1, 9, 12, 18)</p>
<p>DESCRIPTION</p>	<p>Curve capillary pressure versus degree of saturation.</p>
<p>EQUATIONS</p>	<p>ITYCL = 1: Van Genuchten model:</p> $S_e = \frac{S_l - S_{rl}}{S_{ls} - S_{rl}} = \left(1 + \left(\frac{P_g - P_l}{P} \right)^{\frac{1}{1-\lambda}} \right)^{-\lambda} \quad \text{with } P = P_o \frac{\sigma}{\sigma_o}$ <p>ITYCL = 2: Linear model: $S_e = \frac{S_l - S_{rl}}{S_{ls} - S_{rl}} = 1 - \frac{P_g - P_l}{P_o}$</p> <p>ITYCL = 4: Square law: $S_e = \frac{S_l - S_{rl}}{S_{ls} - S_{rl}} = \frac{1}{\sqrt{1 + \frac{P_g - P_l}{P_o}}}$</p> <p>ITYCL = 9: Van Genuchten model with asymptotic branch that goes to negative capillary pressures.</p> $S_e = \frac{S_l - S_{rl}}{S_{ls} - S_{rl}} = \left(1 + \left(\frac{P_g - P_l}{P} \right)^{\frac{1}{1-\lambda}} \right)^{-\lambda} \quad P_g - P_l > a = \frac{P_o}{f} \quad P = P_o \frac{\sigma}{\sigma_o}$ $S_l = S_{ls} - \frac{b}{(P_g - P_l - a - c)^2} \quad P_g - P_l < a$ <p>where b, c are internal smoothing functions.</p> <p>ITYCL = 12: FEBEX model:</p> $S_e = \frac{S_l - S_{rl}}{S_{ls} - S_{rl}} = \left(1 + \left(\frac{P_g - P_l}{P} \right)^{\frac{1}{1-\lambda}} \right)^{-\lambda} f_d$ $P = P_o \frac{\sigma}{\sigma_o} \quad f_d = \left(1 - \frac{P_g - P_l}{P_d} \right)^{\lambda_d}$

EQUATIONS	<p>ITYCL = 18: Freezing model:</p> $S_e = \frac{S_l - S_{rl}}{S_{ls} - S_{rl}} = \left(1 + \left(\frac{P_i - P_l}{P} \right)^{\frac{1}{1-\lambda}} \right)^{-\lambda} ;$ $P_i = \frac{\rho_i}{\rho_l} P_l - \rho_i l \frac{T}{T + 273} \quad \text{Clausius Clayperon}$ <p>where P_i is the ice pressure, $\rho_i/\rho_l = 0.91$, $\rho_i l = 306 \text{MPa}$, T temperature in K</p> <p>Ice volumetric fraction: $S_i = 1 - S_l$</p>
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RETENTION CURVE (ICL = 6). PARAMETERS FOR ITYCL = 1 (Van Genuchten model; see ICL=66 for additional parameters):

P1	P_o	MPa	Measured P at certain temperature
P2	σ_o	N m ⁻¹	Surface tension at temperature in which P_o was measured (usually $\sigma_o = 0.072$ N/m at 20°C)
P3	λ		Shape function for retention curve
P4	S_{rl}		Residual saturation
P5	S_{ls}		Maximum saturation
P6	a		Parameter for porosity influence on retention curve: $P_o(\phi) = P_o \exp(a(\phi_o - \phi))$
P7	b		Parameter for porosity influence on retention curve: $\lambda(\phi) = \lambda \exp(b(\phi_o - \phi))$
P8	Void		
P9	ϕ_o		Reference porosity for porosity influence on retention curve

RETENTION CURVE (ICL = 6). PARAMETERS FOR ITYCL = 2 (linear model):

P1	P_o	MPa	Measured P at certain temperature
P2	Void		
P3	Void		
P4	S_{rl}		Residual saturation
P5	S_{ls}		Maximum saturation

RETENTION CURVE (ICL = 6). PARAMETERS FOR ITYCL = 4 (square law):

P1	P_o	MPa	Measured P at certain temperature
P2	Void		
P3	Void		
P4	S_{rl}		Residual saturation
P5	S_{ls}		Maximum saturation

RETENTION CURVE (ICL = 6). PARAMETERS FOR ITYCL = 9 (Van Genuchten model with asymptotic branch that goes to negative capillary pressures; see ICL=66 for additional parameters):

P1	P_o	MPa	Measured P at certain temperature
P2	σ_o	N m ⁻¹	Surface tension at temperature in which P_o was measured (usually $\sigma_o=0.072$ N/m at 20°C)
P3	λ		Shape function for retention curve
P4	S_{rl}		Residual saturation
P5	S_{ls}		Maximum saturation
P6	f		Used for the asymptotic branch

RETENTION CURVE (ICL = 6). PARAMETERS FOR ITYCL = 12 (FEBEX model; see ICL=66 for additional parameters):

P1	P_o	MPa	Measured P at certain temperature
P2	σ_o	N m ⁻¹	Surface tension at temperature in which P_o was measured (usually $\sigma_o=0.072$ N/m at 20°C)
P3	λ		Shape function for retention curve
P4	S_{rl}		Residual saturation
P5	S_{ls}		Maximum saturation
P6	a		Parameter for porosity influence on retention curve: $P_o(\phi)=P_o \exp(a(\phi_o-\phi))$; $P_d(\phi)=P_d \exp(a(\phi_o-\phi))$ <i>See Retention curve 2 (ICL=66) for additional parameters.</i>
P7	b		Parameter for porosity influence on retention curve: $\lambda(\phi) = \lambda \exp(b(\phi_o-\phi))$; $\lambda_d(\phi) = \lambda_d \exp(b(\phi_o-\phi))$ <i>See Retention curve 2 (ICL=66) for additional parameters.</i>
P8	ϕ_o		Reference porosity for porosity influence on retention curve
P9	P_d	MPa	Pressure related with the suction at zero degree of saturation
P10	λ_d		Model parameter

RETENTION CURVE (ICL = 6). PARAMETERS FOR ITYCL = 18 (freezing model; see ICL=66 for additional parameters):

P1	P_o	MPa	Measured P at certain temperature
P2	σ_o	N m ⁻¹	Surface tension at temperature in which P_o was measured (usually $\sigma_o = 0.072$ N/m at 20°C)
P3	λ		Shape function for retention curve
P4	S_{rl}		Residual saturation
P5	S_{ls}		Maximum saturation
P6	a		Parameter for porosity influence on retention curve: $P_o(\phi) = P_o \exp(a(\phi_o - \phi))$
P7	b		Parameter for porosity influence on retention curve: $\lambda(\phi) = \lambda \exp(b(\phi_o - \phi))$
P8	Void		
P9	ϕ_o		Reference porosity for porosity influence on retention curve
P10	i_stress		Flag to indicate stress concept for use in the mechanical model: $i_stress = 0$: Net stress ($\sigma_n = \sigma - P_i$) $i_stress = -1$: Bishop's stress ($\sigma_b = \sigma - P_i + S_r (P_i - P_l)$)

S_{rl} and S_{ls} are lower and upper bounds of saturation. Effective saturation S_e is defined in such a way that ranges between 0 and 1.

RETENTION CURVE 2

CODES in <i>ROOT_gen.dat</i>	ICL = 66 ITYCL = 1, 9, 12, 18
DESCRIPTION	Curve capillary pressure versus degree of saturation. Additional parameters for retention curve ICL = 6.
EQUATIONS	<p>ITYCL = 1, 9, 12, 18: Temperature influence on capillary pressure parameter P:</p> $P = P_0 \frac{\sigma}{\sigma_0} \exp(A(T - T_0))$ <p>ITYCL = 12: FEBEX model:</p> $S_e = \frac{S_l - S_{rl}}{S_{ls} - S_{rl}} = \left(1 + \left(\frac{P_g - P_l}{P} \right)^{\frac{1}{1-\lambda}} \right)^{-\lambda} f_d$ $P = P_0 \frac{\sigma}{\sigma_0} \quad f_d = \left(1 - \frac{P_g - P_l}{P_d} \right)^{\lambda_d}$

RETENTION CURVE (ICL = 66). PARAMETERS FOR ITYCL = 1, 9, 12, 18

P1*	A	C ⁻¹	Parameter A for temperature influence on capillary pressure parameter P: $P = P_0 \frac{\sigma}{\sigma_0} \exp(A(T - T_0))$
P2*	T ₀	C	Parameter T ₀ for temperature influence on capillary pressure parameter P: $P = P_0 \frac{\sigma}{\sigma_0} \exp(A(T - T_0))$

* Note that to be able to use the function $P = P_0 \frac{\sigma}{\sigma_0} \exp(A(T - T_0))$, it is required to input a value for σ_0 (usually 0.072 N/m at 20°C) in ICL = 6 (retention curve).

RETENTION CURVE (ICL = 66). PARAMETERS FOR ITYCL = 12 (FEBEX model):

P6	a _d		Parameter for porosity influence on retention curve: $P_d(\phi) = P_d \exp(a_d(\phi_0 - \phi))$
P7	b _d		Parameter for porosity influence on retention curve: $\lambda_d(\phi) = \lambda_d \exp(b_d(\phi_0 - \phi))$

INTRINSIC PERMEABILITY

CODES in <i>ROOT_gen.dat</i>	ICL = 7 ITYCL = 1, 2, 4, 5, 6, 15, 16
DESCRIPTION	Intrinsic permeability
EQUATIONS	<p>ITYCL = 1: For a continuum medium (Kozeny's model):</p> $\mathbf{k} = \mathbf{k}_o \frac{\phi^3}{(1-\phi)^2} \frac{(1-\phi_o)^2}{\phi_o^3} \quad \phi_o : \text{reference porosity}$ <p>\mathbf{k}_o : intrinsic permeability for matrix ϕ_o</p> <p>which is used in Darcy's law: $\mathbf{q}_\alpha = -\frac{\mathbf{k}k_{r\alpha}}{\mu_\alpha} (\nabla P_\alpha - \rho_\alpha \mathbf{g})$</p> <p>where viscosity, density and relative permeability are defined in other laws.</p> <p>ITYCL = 2: Exponential law: $\mathbf{k} = \mathbf{k}_o \exp\{b(\phi - \phi_o)\}$</p> <p>ITYCL = 4, 5: Intrinsic permeability depending on an embedded aperture:</p> $\mathbf{k} = \mathbf{k}_{matrix} + \frac{b^3}{12a} \quad b = b_o + \Delta b \quad \Delta b = a\Delta\varepsilon = a(\varepsilon - \varepsilon_o) \quad \text{for } \varepsilon > \varepsilon_o$ <p>where \mathbf{k}_{matrix} : reference intrinsic permeability of the rock matrix or porous material (without fractures). a: spacing of the fracture. b: variable aperture as a function of normal or volumetric strains. b_o: minimum aperture.</p> <p>Using this option, the capillary pressure P of the retention curve (ICL=6) varies as:</p> $P = P_o \frac{\sqrt[3]{\mathbf{k}_o}}{\sqrt[3]{\mathbf{k}}}$ <p>where P_o is the capillary pressure for a reference permeability \mathbf{k}_o, which can be the initial permeability.</p> <p>ITYCL = 6: Postfailure model: $\mathbf{k} = \mathbf{k}_o$ (pre-failure)</p> $\mathbf{k} = \mathbf{k}_o + \mathbf{k}_c \exp\{-\gamma \cdot \sigma_3\} \left(1 - \exp\left\{ \frac{\varepsilon_v - \varepsilon_B}{\varepsilon_B} \right\} \right) \quad (\text{post-failure})$ <p>ITYCL = 15: This model is similar to option ITYCL=5 except that:</p> $\mathbf{k}k_{rg} = \mathbf{k}_{matrix}k_{rg}^{matrix} + \mathbf{k}_{fracture}k_{rg}^{discontinuity}$ <p>where relative permeability is split into two functions depending if the intrinsic permeability corresponds to the matrix or the discontinuity:</p> <p>k_{rg}^{matrix} is calculated normally, and $k_{rg}^{discontinuity} = S_g = (1 - S_l)$</p>

	<p>ITYCL = 16: Zero thickness element Barton's law: Longitudinal intrinsic permeability</p> $k_l = \frac{e^2}{12} = \left[\frac{a^2}{JRC^{2.5}} \right]^2 \frac{1}{12}$ <p style="text-align: right;">a: Opening of the joint JRC: Joint Roughness Coefficient</p> <p>Transversal intrinsic permeability k_t is considered to be equal to the continuum media.</p> <p>For the retention curve (ICL=6), air entry value depends on joint aperture, as: $P = P_0 \frac{\sqrt{k_{l0}}}{k_l} \frac{\sigma}{\sigma_0}$</p>
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INTRINSIC PERMEABILITY (ICL = 7). PARAMETERS FOR ITYCL = 1

P1	$(k_{11})_o$	m^2	Intrinsic permeability, 1 st principal direction.
P2	$(k_{22})_o$	m^2	Intrinsic permeability, 2 nd principal direction.
P3	$(k_{33})_o$	m^2	Intrinsic permeability, 3 rd principal direction.
P4	ϕ_o		Reference porosity for read intrinsic permeability. If $\phi_o=0$, permeability will be constant.
P5	ϕ_{min}		Minimum porosity (porosity will not be lower than this value).

To use ITYCL = 4, 5, 15, the reference porosity (P4) needs to be greater than zero.

INTRINSIC PERMEABILITY (ICL = 7). PARAMETERS FOR ITYCL = 2

P1-P5	<i>The same as in ITYCL=1</i>		
P6	b	-	Parameter.

INTRINSIC PERMEABILITY (ICL = 7). PARAMETERS FOR ITYCL = 4, 5

P1-P5	<i>The same as in ITYCL=1</i>		
P6	b	-	Parameter. If abs (b) > 0, exponential law is used for matrix permeability. Otherwise, Kozeny's law is used.
P7	b_o	m	Minimum aperture to calculate a variable aperture as: $b = b_o + \Delta b$
P8	a	m	Spacing of the fractures: $k = k_{matrix} + \frac{b^3}{12a}$ Permeability of the matrix is obtained as usual in porous media.
P9	ϵ_o	-	Reference strain to calculate aperture variations: $\Delta b = a\Delta\epsilon = a(\epsilon - \epsilon_o)$ for $\epsilon > \epsilon_o$ If this value is negative, the initial aperture is larger than the minimum aperture (discontinuity is open). If this value is zero or positive, the discontinuity cannot close.
P10	b_{max}	m	Maximum aperture. Upper bound of aperture.

For ITYCL = 4, the normal strain to the discontinuity is used.

For ITYCL = 5, 15 the volumetric strain is used.

INTRINSIC PERMEABILITY (ICL = 7). PARAMETERS FOR ITYCL = 15

P1-P5	<i>The same as in ITYCL=1</i>		
P6			Power for gas relative permeability that applies to cubic law
P7	b_o	m	Minimum aperture to calculate a variable aperture as: $b = b_o + \Delta b$
P8	a	m	Spacing of the fractures: $k = k_{matrix} + \frac{b^3}{12a}$ Permeability of the matrix is obtained as usual in porous media.
P9	ϵ_o	-	Reference strain to calculate aperture variations: $\Delta b = a\Delta\epsilon = a(\epsilon - \epsilon_o)$ for $\epsilon > \epsilon_o$ If this value is negative, the initial aperture is larger than the minimum aperture (discontinuity is open). If this value is zero or positive, the discontinuity cannot close.
P10	b_{max}	m	Maximum aperture. Upper bound of aperture.

INTRINSIC PERMEABILITY (ICL=7). PARAMETERS FOR ITYCL=6

P1-P5	<i>The same as in ITYCL = 1</i>		
P6	γ	MPa ⁻¹	Dilatibility
P7	ϵ_B	-	Maximum volumetric strain
P9	K_c	-	Permeability at zero minor principal stress

INTRINSIC PERMEABILITY (ICL=7). PARAMETERS FOR ITYCL=16

P1	$(k_{11})_o$	m ²	Longitudinal intrinsic permeability, 1 st principal direction. If $(k_{11})_o = 1$, the intrinsic permeability, k_l , is calculated with Barton's law. Permeability and air entry value depends on joint aperture.
P2	$(k_{22})_o$	m ²	Transversal intrinsic permeability, k_t , 2 nd principal direction.
P4-P5	<i>The same as in ITYCL = 1</i>		
P6	JRC	-	Joint Roughness Coefficient.

LIQUID PHASE RELATIVE PERMEABILITY

CODES in <i>ROOT_gen.dat</i>	ICL = 14 ITYCL = 1, 5, 6, 8, 12
DESCRIPTION	By default, the consistent form of relative permeability with van Genuchten model is used. In this case, this ICL=14 can be ignored.
EQUATIONS	<p>ITYCL = 1: Van Genuchten - Mualem model:</p> $k_{rl} = \sqrt{S_e} \left(1 - \left(1 - S_e^{1/\lambda} \right)^\lambda \right)^2$ <p>ITYCL = 5: Liquid perfectly mobile: $k_{rl} = 1$</p> <p>ITYCL = 6: Generalized power: $k_{rl} = AS_e^\lambda$</p> <p>ITYCL = 8: Power with initial cut off</p> $k_{rl} = A \left(\frac{S_e - S_{eo}}{1 - S_{eo}} \right)^\lambda \quad S_e \geq S_{eo}$ $k_{rl} = 0 \quad \text{otherwise}$ <p>ITYCL = 12: Van Genuchten model for freezing model</p> $k_{rl} = \sqrt{S_e} \left(1 - \left(1 - S_e^{1/\lambda} \right)^\lambda \right)^2$ <p>(S_e from ICL = 6; ITYCL = 18)</p> <p>The effective liquid saturation is calculated as:</p> $S_e = \frac{S_l - S_{rl}}{S_{ls} - S_{rl}}$

Liquid phase relative permeability (ICL = 14). Parameters for ITYCL = 1 (Van Genuchten model):

P1	Void		
P2	Void		
P3	λ		Power
P4	S_{rl}		Residual liquid saturation (default = same value as for retention curve)
P5	S_{ls}		Maximum liquid saturation (default = same value as for retention curve)

Liquid phase relative permeability (ICL = 14). Parameters for ITYCL = 5 (liquid perfectly mobile): None.

Liquid phase relative permeability (ICL = 14). Parameters for ITYCL=6 (generalized power):

P1	Void		
P2	A		Constant
P3	λ		Power (typically 3)
P4	S_{rl}		Residual liquid saturation (default = same value as for retention curve)
P5	S_{ls}		Maximum liquid saturation (default = same value as for retention curve)

Liquid phase relative permeability (ICL = 14). Parameters for ITYCL = 8 (power with initial cut off):

P1	S_{eo}		Parameter
P2	A		Constant
P3	λ		Power
P4	S_{rl}		Residual liquid saturation (default = same value as for retention curve)
P5	S_{ls}		Maximum liquid saturation (default = same value as for retention curve)

Liquid phase relative permeability (ICL = 14). Parameters for ITYCL = 12 (Van Genuchten model for freezing model):

P1	Void		
P2	Void		
P3	λ		Power
P4	S_{rl}		Residual liquid saturation (default = same value as for retention curve)
P5	S_{ls}		Maximum liquid saturation (default = same value as for retention curve)

S_{rl} and S_{ls} are lower and upper bounds of liquid saturation. Effective liquid saturation S_e is defined in such a way that ranges between 0 and 1. In principle, the same values S_{rl} and S_{ls} should be defined for liquid and gas relative permeability and for retention curve. However, different values can be used to define a maximum saturation of liquid with possibility of remnant gas flow or *vice-versa*.

GAS PHASE RELATIVE PERMEABILITY

CODES in <i>ROOT_gen.dat</i>	ICL = 19 ITYCL = 1, 5, 6, 12
DESCRIPTION	Relative permeability of the gas phase
EQUATIONS	<p>ITYCL = 1: Default law: $k_{rg} = 1 - k_{rl}$</p> <p>ITYCL = 5: Gas perfectly mobile: $k_{rg} = 1$</p> <p>ITYCL = 6: Generalized power: $k_{rg} = AS_{eg}^\lambda$</p> <p>The effective gas saturation is calculated as:</p> $S_{eg} = \frac{S_g - S_{rg}}{S_{gs} - S_{rg}}$ <p>ITYCL = 12: Van Genuchten-Mualem</p> $k_{rg} = (1 - S_{el})^\gamma \left(1 - S_{el}^{\frac{1}{\lambda}}\right)^{2\lambda}$ <p>The effective liquid saturation can be calculated as:</p> $S_{el} = 1 - S_{eg} = 1 - \frac{S_g - S_{rg}}{S_{gs} - S_{rg}}$

GAS PHASE RELATIVE PERMEABILITY (ICL = 19). PARAMETERS FOR ITYCL = 1 (default law):

P1-P3	Void		
P4	S_{rg}	-	Residual gas saturation (default = $1 - S_{ls}$ in retention curve)
P5	S_{gs}	-	Maximum gas saturation (default = $1 - S_{rl}$ in retention curve)

GAS PHASE RELATIVE PERMEABILITY (ICL = 19). PARAMETERS FOR ITYCL = 5 (gas perfectly mobile): None

GAS PHASE RELATIVE PERMEABILITY (ICL = 19). PARAMETERS FOR ITYCL = 6 (generalized power):

P1	Void		
P2	A		Constant
P3	λ		Power
P4 – P5	<i>The same as in ITYCL = 1</i>		

GAS PHASE RELATIVE PERMEABILITY (ICL = 19). PARAMETERS FOR ITYCL = 12:

P1	Void		
P2	γ		Power
P3 – P5	<i>The same as in ITYCL = 6</i>		

DIFFUSIVE FLUXES OF VAPOUR

CODES in <i>ROOT_gen.dat</i>	ICL = 11 ITYCL = 1, 2
DESCRIPTION	Diffusion coefficients
EQUATIONS	<p>Fick's law for molecular diffusion is written as:</p> $\mathbf{i}_\alpha^i = -(\tau\phi\rho_\alpha S_\alpha D_\alpha^i \mathbf{I}) \nabla \omega_\alpha^i$ <p>where ϕ is porosity, ρ_α is density, S_α is degree of saturation, ω is mass fraction and D_α^i is the diffusion coefficient of species i in phase α in m^2/s.</p> <p>The non-advective flux of a species in a phase is composed by molecular diffusion and mechanical dispersion (dispersion is defined in another set of parameters).</p> <p>ITYCL = 1: Molecular diffusion of vapour or air in the gas phase:</p> $D_\alpha^i = D \left(\frac{(273.15 + T)^n}{P_g} \right)$ <p>where P_g is the gas pressure in Pa, and D and n are parameters. Tortuosity coefficient is defined as a constant value in this case:</p> $\tau = \text{constant} = \tau_0$ <p>ITYCL = 2: Molecular diffusion of vapour or air in the gas phase:</p> $D_\alpha^i = D \left(\frac{(273.15 + T)^n}{P_g} \right)$ <p>where P_g is the gas pressure in Pa, and D and n are parameters. Tortuosity coefficient is defined in this case as:</p> $\tau = \tau_0 (S_g)^m$ <p>where τ_0 and m are parameters.</p>

DIFFUSIVE FLUXES OF VAPOUR (ICL = 11). PARAMETERS FOR ITYCL = 1:

P1	D	$\text{m}^2 \text{s}^{-1} \text{K}^{-n} \text{Pa}$	Default value = 5.9×10^{-6}
P2	n		Default value = 2.3
P3	τ_0		Coefficient of tortuosity; default = 1.0

DIFFUSIVE FLUXES OF VAPOUR (ICL = 11). PARAMETERS FOR ITYCL = 2:

P1 – P3	The same as in ITYCL = 1		
P4	m		Power for tortuosity function of saturation

DIFFUSIVE FLUXES OF DISSOLVED SALT AND AIR

CODES in <i>ROOT_gen.dat</i>	ICL = 12 ITYCL = 1
DESCRIPTION	Diffusion coefficients
EQUATIONS	<p>Fick's law for molecular diffusion is written as:</p> $\mathbf{i}_\alpha^i = -(\tau\phi\rho_\alpha S_\alpha D_\alpha^i \mathbf{I}) \nabla \omega_\alpha^i$ <p>where ϕ is porosity, ρ_α is density, S_α is degree of saturation, ω is mass fraction and D_m^i is the diffusion coefficient of species i in phase α in m²/s.</p> <p>ITYCL = 1: Molecular diffusion of dissolved salt and/or dissolved air in the liquid phase:</p> $D_\alpha^i = D \exp\left(\frac{-Q}{R(273.15+T)}\right)$ <p>where D and Q are parameters and τ is the coefficient of tortuosity.</p>

DIFFUSIVE FLUXES OF DISSOLVED SALT AND AIR (ICL = 12). PARAMETERS FOR ITYCL = 1:

P1	D	m ² s ⁻¹	Default value = 1.1×10 ⁻⁴
P2	Q	J mol ⁻¹	Default value = 24530
P3	τ		Coefficient of tortuosity; default=1.0
P4 – P10	Void		

DISPERSIVE FLUXES OF MASS AND ENERGY

CODES in <i>ROOT_gen.dat</i>	ICL = 8 ITYCL = 1
DESCRIPTION	Dispersivities for vapour, dissolved air and heat.
EQUATIONS	<p>Mechanical dispersion mass flux is computed by means Fick's law written as:</p> $\mathbf{i}'_{\alpha} = -(\rho_{\alpha} \mathbf{D}'_{\alpha}) \nabla \omega_{\alpha}^i$ <p>where the mechanical dispersion tensor is defined as:</p> $\mathbf{D}'_{\alpha} = d_l \mathbf{q}_{\alpha} \mathbf{I} + (d_l - d_t) \frac{\mathbf{q}_{\alpha} \mathbf{q}'_{\alpha}}{ \mathbf{q}_{\alpha} }$ <p>where d_l is longitudinal dispersivity and d_t is transversal dispersivity.</p> <p>Mechanical dispersion heat flux is computed by means Fourier's law written as:</p> $\mathbf{i}_h = -(c_{\alpha} \rho_{\alpha} \mathbf{D}'_{\alpha}) \nabla T$ <p>where c_{α} is the specific heat of the α phase, and the mechanical dispersion tensor is defined in the same way as before but using the corresponding dispersivities for heat dispersion (only the contribution due to liquid phase dispersion, i.e. $\alpha = l$ has been implemented). Heat conduction is defined in another set of variables.</p>

DISPERSIVE FLUXES OF MASS AND ENERGY (ICL=8). PARAMETERS FOR ITYCL=1:

P1	d_l	m	Longitudinal dispersivity for solutes in liquid phase
P2	d_t	m	Transverse dispersivity for solutes in liquid phase
P3	Void		
P4	d_l	m	Longitudinal dispersivity for heat
P5	d_t	m	Transverse dispersivity for heat
P6	d_l	m	Longitudinal dispersivity for vapour, default: P1
P7	d_t	m	Transverse dispersivity for vapour, default: P2

CONDUCTIVE FLUX OF HEAT (1)

<p>CODES in <i>ROOT_gen.dat</i></p>	<p>ICL = 9 ITYCL = 1, 2, 3</p>
<p>DESCRIPTION</p>	<p>Dependence on porosity and temperature.</p>
<p>EQUATIONS</p>	<p>Thermal conductivity is used in Fourier's law to compute conductive heat flux, i.e.:</p> $\mathbf{i}_c = -\lambda \nabla T$ <p>There are two possibilities to solve conductive flux of heat through this law:</p> <p>a) Giving directly λ_{dry} and λ_{sat}. These values can be measured in the laboratory. They will be used in law ICL=20.</p> <p>b) Giving the conductivity of the phases of the soil, i.e. $(\lambda_{solid})_o$, λ_{liquid}, λ_{gas} and a_1, a_2, a_3. In this case, λ_{dry} and λ_{sat} are calculated according to the laws given below.</p> <p>ITYCL = 1: Thermal conductivity dependence on porosity. Geometric weighted mean.</p> $\lambda_{dry} = \lambda_{solid}^{(1-\phi)} \lambda_{gas}^{\phi} \qquad \lambda_{sat} = \lambda_{solid}^{(1-\phi)} \lambda_{liq}^{\phi}$ $\lambda_{solid} = (\lambda_{solid})_o + a_1 T + a_2 T^2 + a_3 T^3$ $\lambda(T) = C \times (T + 273.15)^n \quad \text{if } C, n > 0$ <p>ITYCL = 2: Thermal conductivity dependence on porosity. Weighted arithmetic mean.</p> $\lambda_{dry} = (1 - \phi)^n \lambda_{solid} + \phi^n \lambda_{gas} \qquad \lambda_{sat} = (1 - \phi)^n \lambda_{solid} + \phi^n \lambda_{liq}$ <p>ITYCL = 3: Thermal conductivity dependence on porosity. Nonlinear function of porosity.</p> $\lambda_{dry} = \lambda_{solid} + (\lambda_{dryo} - \lambda_{solid}) \left(\frac{\phi}{\phi_o} \right)^n$ $\lambda_{sat} = \lambda_{solid} + (\lambda_{sato} - \lambda_{solid}) \left(\frac{\phi}{\phi_o} \right)^n$

CONDUCTIVE FLUX OF HEAT 1 (ICL = 9). PARAMETERS FOR ITYCL = 1 (geometric weighted mean):

P1	λ_{dry}	$W\ m^{-1}\ K^{-1}$	Thermal conductivity of the dry porous medium
P2	λ_{sat}	$W\ m^{-1}\ K^{-1}$	Thermal conductivity of the water saturated porous medium
P3	$(\lambda_{solid})_o$	$W\ m^{-1}\ K^{-1}$	Solid phase thermal conductivity (ignored if $\lambda_{dry}, \lambda_{sat} > 0$)
P4	λ_{gas}	$W\ m^{-1}\ K^{-1}$	Gas phase thermal conductivity (ignored if $\lambda_{dry}, \lambda_{sat} > 0$)
P5	λ_{liq}	$W\ m^{-1}\ K^{-1}$	Liquid phase thermal conductivity (ignored if $\lambda_{dry}, \lambda_{sat} > 0$)
P6	a_1		Ignored if $\lambda_{dry}, \lambda_{sat} > 0$
P7	a_2		Ignored if $\lambda_{dry}, \lambda_{sat} > 0$
P8	a_3		Ignored if $\lambda_{dry}, \lambda_{sat} > 0$
P9	C		Constant in $\lambda(T) = C \times (T + 273.15)^n$ (ignored if $C = 0$)
P10	n		Power in $\lambda(T) = C \times (T + 273.15)^n$ (ignored if $n = 0$)

CONDUCTIVE FLUX OF HEAT 1 (ICL = 9). PARAMETERS FOR ITYCL = 2 (weighted arithmetic mean):

P1 – P8	The same as in ITYCL = 1		
P9	Void		
P10	n		Power of porosity function (default value = 1, so linear dependence with porosity)

CONDUCTIVE FLUX OF HEAT 1 (ICL = 9). PARAMETERS FOR ITYCL = 3 (nonlinear function of porosity):

P1 – P2	Void		
P3	$(\lambda_{solid})_o$	$W\ m^{-1}\ K^{-1}$	Solid phase thermal conductivity
P4	$(\lambda_{dry})_o$	$W\ m^{-1}\ K^{-1}$	Dry thermal conductivity for reference porosity
P5	$(\lambda_{sat})_o$	$W\ m^{-1}\ K^{-1}$	Saturated thermal conductivity for reference porosity
P6 – P8	Void		
P9	ϕ_o		Reference porosity
P10	n		Power of porosity

Heat dispersion is defined in the constitutive law ICL = 8, ITYCL = 1 (Dispersive fluxes of mass and energy).

CONDUCTIVE FLUX OF HEAT (2)

CODES in <i>ROOT_gen.dat</i>	ICL = 20 ITYCL = 1, 2, 4, 5, 6, 7
DESCRIPTION	Dependence on water content.
EQUATIONS	<p>Thermal conductivity is used in Fourier's law to compute conductive heat flux, i.e.:</p> $\mathbf{i}_c = -\lambda \nabla T$ <p>Dependence of thermal conductivity on degree of saturation can be considered in the following ways:</p> <p>ITYCL = 1: Linear with the square root of saturation</p> $\lambda = \lambda_{sat} \sqrt{S_l} + \lambda_{dry} (1 - \sqrt{S_l})$ <p>ITYCL = 2: Geometric mean: $\lambda = \lambda_{sat}^{S_l} \lambda_{dry}^{(1-S_l)}$</p> <p>ITYCL = 4: Linear with saturation: $\lambda = \lambda_{dry} (1 - S_l) + \lambda_{sat} S_l$</p> <p>ITYCL = 5: Geometric mean for frozen soil</p> <p>Dependence on water/ice content. Activating this option permits to have different values for thermal conductivity depending if the soil is frozen or unfrozen.</p> $\lambda = \lambda_{unfrozen}^{S_l} \lambda_{frozen}^{(1-S_l)}$ <p>$\lambda_{frozen} = \lambda_{dry}$ and $\lambda_{unfrozen} = \lambda_{sat}$, are introduced in ICL = 9, ITYCL = 1.</p> <p>The thermal conductivity of phases can be introduced to determine the thermal conductivity of the frozen and unfrozen soil. In such case the solid and liquid water are input as usual, and the ice thermal conductivity should be input in the same place as the gas thermal conductivity</p> <p>ITYCL = 6: Dependence of thermal conductivity on degree of saturation (Chen & Ledesma, 2009):</p> $\lambda = \lambda_{sat} \sin^2\left(\frac{\pi S_l}{2}\right) + \lambda_{dry} \cos^2\left(\frac{\pi S_l}{2}\right)$ <p>ITYCL = 7: S-shaped function</p> $\lambda = \frac{A_1 - A_2}{1 + e^{[(Sr - Sr^*)/b]}} + A_2$ <p>Where A_1 represents the value of λ for $Sr = 1$, A_2 the value of λ for $Sr = 0$, Sr^* the degree of saturation for which thermal conductivity is the average of the two extreme values and b is a parameter. In some cases, A_1 and A_2 are equivalent to λ_{sat} and λ_{dry}, respectively. A_1 and A_2 are introduced as λ_{sat} and λ_{dry} in ICL = 9, ITYCL = 1: Conductive flux of heat (1).</p> <p>Parameters are not necessary for ICL = 20 and ITYCL = 1, 2, 4, 5, 6. λ_{dry} and λ_{sat} are introduced in ICL = 9: Conductive flux of heat (1).</p>

CONDUCTIVE FLUX OF HEAT 2 (ICL = 20). PARAMETERS FOR ITYCL = 7 (S-shaped function):

P1	b	-	Parameter (since $A_1 > A_2$, this parameter is negative for the equation written above, so it must be input as a negative value).
P2	Sr^*	-	Degree of saturation corresponding to a value of thermal conductivity that is the average between the extreme values

CONDUCTIVE FLUX WITH ANISOTROPY:

CONDUCTIVE FLUX OF HEAT 1 (ICL = 9): **leave all parameters void.**

CONDUCTIVE FLUX OF HEAT 2 (ICL = 20): ITYCL = 1:

P6	λ_{11}	W/(mK)	Thermal conductivity in 1 st principal direction
P7	λ_{22}	W/(mK)	Thermal conductivity in 2 nd principal direction
P8	λ_{33}	W/(mK)	Thermal conductivity in 3 rd principal direction

Note this option does not allow using porosity, degree of saturation or temperature dependencies.

PHASE PROPERTIES

SOLID PHASE PROPERTIES

CODES in <i>ROOT_gen.dat</i>	ICL = 10 ITYCL = 1, 2
DESCRIPTION	Solid specific heat, density and expansion coefficient

SOLID PHASE PROPERTIES (ICL = 10). PARAMETERS FOR ITYCL = 1:

P1	C_s	$\text{J kg}^{-1} \text{K}^{-1}$	Solid phase specific heat (default: 1000) (**)
P2	ρ_s	kg m^{-3}	Solid phase density (default: 2700)
P3	α_s	C^{-1}	Linear thermal expansion coefficient for grains (not volumetric) (positive value; default = 1E-5). This does not produce thermal expansion of the medium. (*)
P4	T_o	C	Reference temperature for thermal expansion (default: 40)
P5 – P6	void		
P7	$1/K_s$	MPa^{-1}	Compressibility of solid phase against mean stress changes (positive value; default = 3E-5)
P8	p_o	MPa	Reference pressure for solid compressibility (default: 0.1 MPa)

SOLID PHASE PROPERTIES (ICL = 10). PARAMETERS FOR ITYCL = 2:

P1	c_s	$\text{J kg}^{-1} \text{K}^{-1}$	Solid phase specific heat for $T = \theta$ (default: 1000)
P2 – P5	The same as in ITYCL = 1		
P6	dc_s/dt		Variation of solid phase specific heat
P7 – P8	The same as in ITYCL = 1		

(*) Thermal expansion coefficient for grains should be equal to the bulk value if thermal expansion of the porous medium does not produce porosity variations.

(**) Specific heat for water and air are internal values.

Note that, in the case of parameters with default values, when setting them to zero –or to a value lower than 10^{-25} – automatically takes the default value. Hence, if the user actually wants to set a parameter to zero, a low value but greater than 10^{-25} should be input.

LIQUID PHASE PROPERTIES. LIQUID DENSITY.

CODES in <i>ROOT_gen.dat</i>	ICL = 15 ITYCL = 1, 2, 3, 4, 5, 6
DESCRIPTION	Liquid density
EQUATIONS	<p>ITYCL = 1: Exponential variation (default): $\rho_l = \rho_{l0} \exp(\beta(P_l - P_{l0}) + \alpha T + \gamma \omega_l^h)$</p> <p>ITYCL = 2: Linear variation: $\rho_l = \rho_{l0}(1 + \beta(P_l - P_{l0}) + \alpha T + \gamma \omega_l^h)$</p> <p>ITYCL = 4: CO₂ $\rho_l = \rho_{l0} \exp(\beta(P_l - P_{l0}) + \alpha T + \gamma \omega_l^h) (1 + \delta \omega_l^{CO_2})$ $\delta = 1 - \rho_l \frac{V_\phi}{M_{CO_2}}$ $V_\phi = (37.51 - 9.585 \times 10^{-2} T + 8.740 \times 10^{-4} T^2 - 5.044 \times 10^{-7} T^3) \times 10^{-6} \text{ m}^3/\text{mol}$ (Garcia, 2003)</p> <p>ITYCL = 5: Linear dependency of the thermal expansion coefficient with temperature: $\rho_l = \rho_{l0} \exp(\beta(P_l - P_{l0}) + A(T)T + \gamma \omega_l^h)$ $A(T) = -3.5 \times 10^{-6} T - 7.49 \times 10^{-5}$</p> <p>ITYCL = 6: Liquid density adjustment for a wide temperature range (-30°C—300°C): $\rho_l = \rho_{l0}(1 + \beta(P_l - P_{l0}) + A(T) + \gamma \omega_l^h)$ $A(T) = -(T + 288.9414)(T - 3.9863)^2 / (508929.2(T + 68.12963))$ (McCutcheon et al., 1993). $\rho_{l0} = 1000 \text{ kg/m}^3$ (note that in this case ρ_{l0} is not user defined as it corresponds to the maximum density of water at 4°C).</p> <p>Note: the thermal expansion coefficient would be expressed by: $\alpha(T) = \frac{1}{\rho_l} \frac{\partial \rho_l}{\partial T}$</p>

LIQUID PHASE DENSITY (ICL = 15). PARAMETERS FOR ITYCL = 1, 2:

P1	ρ_{lo}	kg m ⁻³	Reference density (default* = 1002.6 kg m ⁻³)
P2	β	MPa ⁻¹	Compressibility (default* = 4.5×10 ⁻⁴)
P3	α	C ⁻¹	Volumetric thermal expansion coefficient for water (default* = -3.4×10 ⁻⁴)
P4	γ		Solute variation (default* = 0.6923)
P5	P_{lo}	MPa	Reference pressure (default* = 0.1)

LIQUID PHASE DENSITY (ICL = 15). PARAMETERS FOR ITYCL = 4 (CO₂):

P1 – P3	The same as in ITYCL = 1		
P4	void		
P5	The same as in ITYCL = 1		
P6	M_{CO_2}	kg mol ⁻¹	Molecular mass of CO ₂ (0.044 kg mol ⁻¹)

LIQUID PHASE DENSITY (ICL = 15). PARAMETERS FOR ITYCL = 5:

P1 – P2	The same as in ITYCL = 1		
P3	void		
P4 – P5	The same as in ITYCL = 1		

LIQUID PHASE DENSITY (ICL = 15). PARAMETERS FOR ITYCL = 6:

P1	void		
P2	The same as in ITYCL = 1		
P3	void		
P4 – P5	The same as in ITYCL = 1		

* Note that, in the case of parameters with default values, when setting them to zero –or to a value lower than 10⁻²⁵– automatically takes the default value. Hence, if the user actually wants to set a parameter to zero, a low value but greater than 10⁻²⁵ should be input.

In APPENDIX VI.A. , it is explained how to model a porous material under TM conditions to get realistic and comparable results with THM.

LIQUID PHASE PROPERTIES. LIQUID VISCOSITY.

CODES in <i>ROOT_gen.dat</i>	ICL = 16 ITYCL = 1
DESCRIPTION	Liquid viscosity
EQUATIONS	ITYCL = 1: $\mu_l = A \exp\left(\frac{B}{273.15 + T}\right)$

LIQUID PHASE VISCOSITY (ICL=16). PARAMETERS FOR ITYCL=1:

P1	<i>A</i>	MPa s	Pre-exponential parameter (default* = 2.1×10^{-12})
P2	<i>B</i>	K	Exponential parameter; default* = 1808.5 (only used if $A = B = 0$, but not used if $A > 0$ and $B = 0$)

Remark: liquid and gas density and viscosity are not material dependents. For this reason, values should be prescribed only once. If these are multiplied defined, the code will use the values it reads first.

* Note that, in the case of parameters with default values, when setting them to zero –or to a value lower than 10^{-25} – automatically takes the default value. Hence, if the user actually wants to set a parameter to zero, a low value but greater than 10^{-25} should be input.

GAS PHASE PROPERTIES. GAS DENSITY.

CODES in <i>ROOT_gen.dat</i>	ICL = 17 ITYCL = 1, 2, 3, 4
DESCRIPTION	Gas density.
EQUATIONS	<p>ITYCL = 1: law of ideal gases and Henry's law for dry air (as ITYCL = 3 with $M_a = 0.02895$ and $H = 10000$ MPa)</p> <p>ITYCL = 2: $\rho_g^a = (\rho_g^a)_o \exp(\beta(P_g - P_{go}) + \alpha T)$ Usually used to consider a second liquid phase instead of the gas phase (in that case do not consider vapour in gas phase)</p> <p>ITYCL = 3: law of ideal gases and Henry's law for any dry gas species (as ITYCL=1, but with user defined values for gas molecular mass and Henry's constant:</p> $\omega_l^{dgs} = \frac{P_{dgs}}{H} \frac{M_{dgs}}{M_w}$ <p>where P_{dgs} is dry gas species pressure (air pressure in the formulation), M_w is molecular mass of water and M_{dgs} is molecular mass of dry gas species.</p> <p>ITYCL = 4: law for CO₂ with the values adjusted by Spycher <i>et al.</i>, 2003.</p> $\rho_{CO_2} = \frac{M_{CO_2}}{v}$ $v^3 - \left(\frac{RT}{P}\right)v^2 - \left(\frac{RTb}{P} - \frac{a}{P\sqrt{T}} + b^2\right)v - \left(\frac{ab}{P\sqrt{T}}\right) = 0$ <p>$b = 2.78 \times 10^{-5} \text{ m}^3/\text{mol}$ $a = a_1 + a_2 \times T \text{ m}^6\text{PaK}^{0.5}/\text{mol}^2$ $a_1 = 7.54 \quad a_2 = -0.00413$ $R = 8.314 \text{ J/molK}$</p>

GAS PHASE PROPERTIES (ICL = 17). PARAMETERS FOR ITYCL = 2:

P1	$(\rho_g^a)_o$	kg m ⁻³	Reference density for $T = 0 \text{ C}$
P2	β	MPa ⁻¹	Compressibility (default = 0.0)
P3	α	C ⁻¹	Volumetric thermal expansion coefficient for water (default = 0.0)
P4	Void		
P5	P_{go}	MPa	Reference pressure (default = 0.0)

GAS PHASE PROPERTIES (ICL = 17). PARAMETERS FOR ITYCL = 3 (gases law with modified molecular mass and Henry's constant):

P1	M	kg mol ⁻¹	Molecular mass
P2	H	MPa	Henry's constant

GAS PHASE PROPERTIES (ICL = 17). PARAMETERS FOR ITYCL = 4 (law for CO₂ with the values adjusted by Spycher *et al.*, 2003):

P1	M_{CO_2}	kg mol ⁻¹	Molecular mass of CO ₂ (0.044 kg mol ⁻¹)
P2	H	MPa	Henry's constant
P8			Alternative CO ₂ density function at $T=320$ K adjusted from Span and Wagner (1996) tables. To use it write: -777

GAS PHASE PROPERTIES. GAS VISCOSITY.

CODES in <i>ROOT_gen.dat</i>	ICL = 18 ITYCL = 1, 2, 4
DESCRIPTION	Gas viscosity
EQUATIONS	<p>ITYCL = 1:</p> $\mu_g = \frac{A\sqrt{273+T}}{\left(1 + \frac{B}{273+T}\right)} \frac{1}{1 + \frac{b_k}{P_g}}$ $b_k = C - Dk$ <p>(<i>k</i> : intrinsic permeability)</p> <p>ITYCL = 2: $\mu_g = A \exp\left(\frac{B}{273.15 + T}\right)$</p> <p>ITYCL = 4: Viscosity function for CO₂ (Altunin and Sakhabetdinov, 1972)</p> $\mu_g = \mu_0 \exp\left(\sum_{i=1}^4 \sum_{j=0}^1 \frac{a_{ij} \rho_R^i}{T_R^j}\right)$ $\mu_0 = T_R^{0.5} \left(27.2246461 - \frac{16.6346068}{T_R} + \frac{4.66920556}{T_R^2} \right)$ $T_R = \frac{T}{T_c}, \quad T_c = 304 \text{ K} \quad \rho_R = \frac{\rho_{CO_2}}{\rho_c}, \quad \rho_c = 468 \text{ kg/m}^3$ $a_{10} = 0.248566120 \quad a_{11} = 0.004894942$ $a_{20} = -0.373300660 \quad a_{21} = 1.22753488$ $a_{30} = 0.363854523 \quad a_{31} = -0.774229021$ $a_{40} = -0.0639070755 \quad a_{41} = 0.142507049$

GAS PHASE VISCOSITY (ICL = 18). PARAMETERS FOR ITYCL = 1:

P1	<i>A</i>	MPa s	default* = 1.48×10^{-12}
P2	<i>B</i>	C	default* = 119.4 (only used if $A = B = 0$, but not used if $A > 0$ and $B = 0$)
P3	<i>C</i>		default* = 0.14
P4	<i>D</i>		default* = 1.2×10^{15}

GAS PHASE VISCOSITY (ICL = 18). PARAMETERS FOR ITYCL = 2:

P1	<i>A</i>	MPa s	Pre-exponential parameter
P2	<i>B</i>	C	Exponential parameter (only used if $A = B = 0$, but not used if $A > 0$ and $B = 0$)

GAS PHASE VISCOSITY (ICL = 18). PARAMETERS FOR ITYCL = 4: Not necessary

Gas phase properties can be used to consider a second liquid in the case of a two immiscible phase flow problem in a porous medium. In this case, water vapour and air dissolved must not be considered, hence, VAPOUR NOT PERMITTED and DISSOLVED AIR NOT PERMITTED should be used to avoid the species to be mixed.

* Note that, in the case of parameters with default values, when setting them to zero –or to a value lower than 10^{-25} – automatically takes the default value. Hence, if the user actually wants to set a parameter to zero, a low value but greater than 10^{-25} should be input.

CODE_BRIGHT. CONSTITUTIVE LAWS

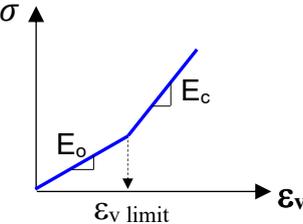
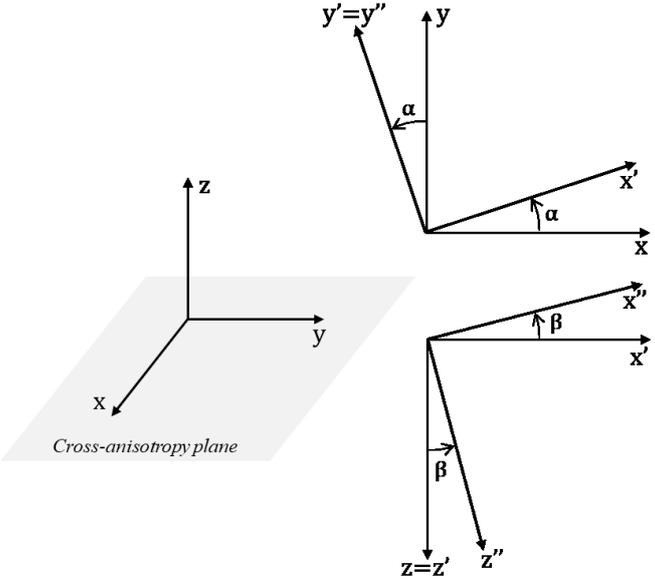
This chapter contains the different models available and the corresponding parameters required by each model. The following constitutive laws are available:

HYDRAULIC AND THERMAL CONSTITUTIVE MODELS (a) RETENTION CURVE INTRINSIC PERMEABILITY LIQUID PHASE RELATIVE PERMEABILITY GAS PHASE RELATIVE PERMEABILITY DIFFUSIVE FLUXES OF MASS DISPERSIVE FLUXES OF MASS AND ENERGY CONDUCTIVE FLUX OF HEAT	MECHANICAL CONSTITUTIVE MODELS ELASTICITY (b) NONLINEAR ELASTICITY (b) VISCOPLASTICITY FOR SALINE MATERIALS (b) VISCOPLASTICITY FOR SATURATED SOILS AND ROCKS (b) VISCOPLASTICITY - GENERAL (b) DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS (c) THERMO-ELASTOPLASTIC MODEL FOR SOILS (d) BARCELONA EXPANSIVE MODEL (e) CASM's FAMILY MODELS (f)
PHASE PROPERTIES (a) SOLID PHASE PROPERTIES LIQUID PHASE PROPERTIES GAS PHASE PROPERTIES	EXCAVATION PROCESS (g)

VI.b. ELASTIC AND VISCO-PLASTIC MODELS

ICL	NAME	ITYCL	DESCRIPTION
1	Linear Elasticity	1	Linear elasticity model
		2	Bi-linear elasticity model
5		5	Tri-linear elasticity model
		6	Anisotropic elastic model
		16	Elasticity – Zero thickness element
		1	Linear expansion coefficients induced by temperature and suction changes
4	Nonlinear Elasticity	1	Volumetric strain is calculated in a reversible way
		2	Nonlinear elasticity model with micro-macro interaction
		5	Volumetric strain is calculated in a reversible way with two independent coupling terms
2	Viscoelasticity - creep	1	Parameters for linear viscous deformation model
3	Viscoplasticity - creep	1	Creep of porous salt aggregates (nonlinear dependences on stresses)
33	Viscoplasticity for saturated soils and rocks (VPSSR)	1,2	Yield function and flow rule
		3	Cam-Clay
		4,5	Drucker-Prager –based on Mohr-Coulomb parameters
		9	For rock salt with dilatancy
		11	Mohr-Coulomb model with dilatancy
		12	Mohr-Coulomb model with dilatancy and strain-softening
		15	Mohr-Coulomb model with anisotropic behaviour
		20	Hoek-Brown model with dilatancy
21	Hoek-Brown model with dilatancy and strain-softening		
34		1	Viscoplasticity (general model based on Desai and Perzyna theory)
		16	Viscoplasticity – Zero thickness element
35	Viscoplasticity for unsaturated soils and rocks (VPUSR)	1	Parameters for yield function and plastic potential
		16	Viscoplasticity – Zero thickness element
36		1	Parameters for LC curve
		2,3	Parameters for LC curve for rockfill materials
		16	Viscoplasticity – Zero thickness element

LINEAR ELASTICITY 1 (Mechanical data 1)

<p>CODES in <i>ROOT_gen.dat</i></p>	<p>ICL = 1 ITYCL = 1, 2, 5, 6, 16</p>
<p>DESCRIPTION</p>	<p>Elastic parameters (linear elasticity model). Linear elasticity with parameters E and ν. Young modulus can be variable.</p>
<p>EQUATIONS</p>	<p>ITYCL = 1: Linear elasticity model</p> <p>This is the standard linear elasticity with Young's Modulus and Poisson's ratio.</p> <p>It is also possible to consider the variation of Young's Modulus with porosity, according to:</p> $E = E_o + (\phi - \phi_o) \frac{dE}{d\phi} \geq E_{\min}$ <p>ITYCL = 2: Bi-linear elasticity model</p>  <p style="text-align: center;">Compression is positive for this plot.</p> <p>ITYCL = 5: Tri-linear elasticity model</p> <p>ITYCL = 6: Anisotropic elastic model</p> 

CODES in <i>ROOT_gen.dat</i>	ICL = 1 ITYCL = 1, 2, 5, 6, 16
DESCRIPTION	Elastic parameters (linear elasticity model). Linear elasticity with parameters E and ν . Young modulus can be variable.
EQUATIONS	<p>ITYCL = 6: Anisotropic elastic model (continuation)</p> <p>The generalized Hooke's Law could be used to describe the elastic constitutive relationship of transversely isotropic rock in the local coordinate system (x'', y'', z'') according to: $\varepsilon'' = \mathbf{S}'' \sigma''$</p> <p>where: $\varepsilon'' = [\varepsilon''_x, \varepsilon''_y, \varepsilon''_z, \gamma''_{yz}, \gamma''_{zx}, \gamma''_{xy}]^T$, $\sigma'' = [\sigma''_x, \sigma''_y, \sigma''_z, \tau''_{yz}, \tau''_{zx}, \tau''_{xy}]^T$,</p> $\text{and } \mathbf{S}'' = \begin{bmatrix} 1/E_1 & -\nu_1/E_1 & -\nu_2/E_2 & 0 & 0 & 0 \\ -\nu_1/E_1 & 1/E_1 & -\nu_2/E_2 & 0 & 0 & 0 \\ -\nu_2/E_2 & -\nu_2/E_2 & 1/E_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2(1+\nu_1)/E_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/G & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/G \end{bmatrix}.$ <p>ITYCL = 16: Elasticity – Zero thickness element</p> <p>The elastic behaviour of the joint relates to the normal effective stress (σ') and the tangential stress (τ) to the normal (u_n) and the tangential (u_s) displacement of the joint element using normal (K_n) and tangential (K_s) stiffness, respectively, as:</p> $\begin{Bmatrix} \sigma' \\ \tau \end{Bmatrix} = \begin{bmatrix} K_n & 0 \\ 0 & K_s \end{bmatrix} \begin{Bmatrix} u_n \\ u_s \end{Bmatrix} \quad K_n = \frac{m}{a - a_{\min}}$

PARAMETERS LINEAR ELASTICITY 1 (Mechanical data 1; ICL=1)

LINEAR ELASTICITY 1 (Mechanical data 1). **ITYCL = 1** (Linear elasticity model)

P1	E	MPa	Young Modulus
P2	$dE/d\phi$	MPa	Variation of Young modulus with porosity
P3	ν	-	Poisson's Ratio
P4	ϕ_o	-	Reference porosity
P5	ϕ_{min}	-	Minimum porosity
P6	E_{min}	MPa	Minimum elastic modulus
P7	b	-	Biot coefficient (default value = 1)

Note: It is possible to uncouple the hydraulic effects on mechanics (H \rightarrow M) by using a very small value of Biot's coefficient (e.g. $b = 10^{-10}$; it cannot be exactly 0 because then CODE_BRIGHT uses the DEFAULT = 1.0).

LINEAR ELASTICITY 1 (Mechanical data 1). **ITYCL = 2** (Bi-linear elasticity model)

P1	E_c	MPa	Young Modulus for closed gap (if $\epsilon_v > \epsilon_v$ limit)
P2	E_o	MPa	Young Modulus for open gap (if $\epsilon_v < \epsilon_v$ limit)
P3	ν	-	Poisson's Ratio
P4	ϵ_v limit	-	Volumetric strain limit to change elastic modulus (positive value for an open gap)

LINEAR ELASTICITY 1 (Mechanical data 1). **ITYCL = 5** (Tri-linear elasticity model)

P1	E_3	MPa	Young Modulus if $\epsilon_v > \epsilon_v$ limit 2
P2	E_2	MPa	Young Modulus if $\epsilon_v < \epsilon_v$ limit 2
P3	E_1	MPa	Young Modulus if $\epsilon_v < \epsilon_v$ limit 1
P4	ν	-	Poisson's Ratio
P5	ϵ_v limit 1	-	First volumetric strain limit to change elastic modulus (positive value)
P6	ϵ_v limit 2	-	Second volumetric strain limit to change elastic modulus (positive value; ϵ_v limit 2 > ϵ_v limit 1)

LINEAR ELASTICITY 1. **ITYCL = 6** (Anisotropic elastic model)

P1	E_1	MPa	Young Modulus in the horizontal direction
P2	E_2	MPa	Young Modulus in the vertical direction
P3	ν_1	-	Poisson's Ratio for the effect of horizontal stress on the horizontal strain
P4	ν_2	-	Poisson's Ratio for the effect of vertical stress on the horizontal strain
P5	ϕ_{min}	-	Minimum porosity
P7	b	-	Biot coefficient (default value = 1)
P8	G	MPa	Shear modulus in the vertical plane

LINEAR ELASTICITY 1 (Mech. data 1). **ITYCL = 16** (Elasticity – Zero thickness element)

P1	m	MPa	Model parameter
P2	K_s	MPa m ⁻¹	Shear stiffness
P3	E	MPa m ⁻¹	Out of plane stiffness
P4	a_{min}	m	Minimum aperture
P5	a_0	m	Initial aperture of the joint

Note: Joint element should be created in GiD using the option: *Geometry/create/contact surface*.

Contact surfaces are defined as being between two lines that are physically in the same place, but which have different line and point entities. Choose the Contact surface option from the menu, and then select some lines on both bodies. Using contact surface entities is like a meshing specification. In this way, equal meshes will be generated for the two lines, ensuring a one-to-one relationship between nodes. You can also select no mesh for the contact entity. This makes it possible to have exactly the same mesh for both lines but without any additional element between them.

LINEAR ELASTICITY 2 (Mechanical data 1)

CODES in <i>ROOT_gen.dat</i>	ICL = 5 ITYCL = 1	
DESCRIPTION	Linear expansion coefficients induced by temperature and suction changes	
EQUATIONS	$\Delta\varepsilon_v = 3b_s\Delta T - 3a_s\Delta(P_g - P_l) \quad \Delta\varepsilon_v > 0, \text{ extension}$ $\Delta\varepsilon_v < 0, \text{ compression}$	

PARAMETERS LINEAR ELASTICITY 2 (Mechanical data 1; ICL=5)

LINEAR ELASTICITY 2. ITYCL = 1

P1	a_s	MPa ⁻¹	Swelling coefficient for changes in suction (positive value)
P2	void		
P3	b_s	C ⁻¹	Linear thermal expansion coefficient for the medium (positive value)
P4	Void		
P5	Void		

NONLINEAR ELASTICITY (Mechanical data 1)

CODES in <i>ROOT_gen.dat</i>	ICL = 4 ITYCL = 1, 2, 5
DESCRIPTION	Nonlinear elasticity model
EQUATIONS	<p>ITYCL = 1: Volumetric strain is calculated in a reversible way, according to:</p> $\frac{\Delta e}{1+e} = a_1 \Delta \ln(-p') + a_2 \Delta \ln\left(\frac{s+0.1}{0.1}\right) + a_3 \Delta \left[\ln(-p') \ln\left(\frac{s+0.1}{0.1}\right) \right]$ <p>where p' is the mean effective stress (mean stress plus maximum of liquid and gas pressure) and s is suction (gas pressure minus liquid pressure). Shear strain is linearly elastic with modulus G or, alternatively, a constant value of the Poisson's ratio can be used.</p> <p>ITYCL = 2: Nonlinear elasticity model with micro-macro interaction:</p> $\begin{aligned} \frac{\Delta e}{1+e} = & a_1 \Delta \ln(-p') + a_2 \Delta \ln\left(\frac{s+0.1}{0.1}\right) + a_3 \Delta \left[\ln(-p') \ln\left(\frac{s+0.1}{0.1}\right) \right] + \\ & + a_{1micro} \Delta \ln(-p') + a_{2micro} \Delta \ln\left(\frac{s_{micro}+0.1}{0.1}\right) + \\ & + a_{3micro} \Delta \left[\ln(-p') \ln\left(\frac{s_{micro}+0.1}{0.1}\right) \right] \end{aligned}$ <p>where s_{micro} is suction in the microstructure. A minimum bulk modulus $K_{min} = 10$ MPa is considered internally to avoid tractions.</p> <p>ITYCL = 5: Volumetric strain is calculated in a reversible way with two independent coupling terms:</p> $\begin{aligned} \frac{\Delta e}{1+e} = & a_1 \Delta \ln(p') + a_2 \Delta \ln\left(\frac{s+0.1}{0.1}\right) + \\ & + a_3 \ln(p'/p_{ref}) \Delta \ln\left(\frac{s+0.1}{0.1}\right) + a_4 s \Delta \ln(p') \end{aligned}$

For further reference, in [APPENDIX VI.B.1](#) it is explained the analogy between this nonlinear elastic model and the BBM model. And in [APPENDIX VI.B.2](#) the correspondence between nonlinear elasticity and linear elasticity parameters is described.

PARAMETERS NONLINEAR ELASTICITY (Mechanical data 1; ICL=4)

NONLINEAR ELASTICITY. **ITYCL = 1** (volumetric strain is calculated in a reversible way):

P1	a_1	-	= $-\kappa/(1+e)$, where κ is the slope of the unload/reload curve in the (e - ln p') diagram
P2	a_2	-	= $-\kappa_s/(1+e)$, where κ_s is the slope of the unload/reload curve in the (e - ln((s+0.1)/0.1)) diagram
P3	a_3	-	Coupling term
P4	G	MPa	Shear modulus (P4 > 0 requires P5 = 0)
P5	ν	-	Poisson's ratio (P5 > 0 requires P4 = 0)
P6	$tens$	MPa	Tension term to avoid tractions ($p' - tens \leq 0$)
P7	K_{min}	MPa	Minimum bulk modulus

NONLINEAR ELASTICITY. **ITYCL = 2** (nonlinear elasticity with micro-macro interaction)

P1 – P5	The same as in ITYCL = 1		
P6	a_{1micro}	-	Volumetric deformation associated to microstructure
P7	a_{2micro}	-	Volumetric deformation associated to microstructure
P8	a_{3micro}	-	Volumetric deformation associated to microstructure
P9	α		Term of interchange of water between micro and macro structures of deformation
P10	Initial s_{micro}	MPa	Initial suction of the micro structure

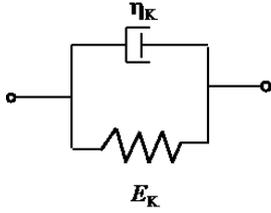
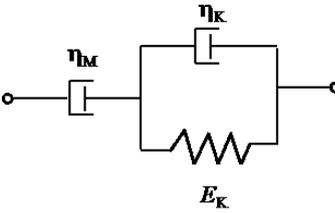
Suction micro is used as history variable and, therefore, the model cannot be combined with viscoplastic models.

NONLINEAR ELASTICITY. **ITYCL = 5** (with two independent coupling terms)

P1 – P7	The same as in ITYCL = 1		
P8	a_4	MPa ⁻¹	Coupling term
P9	p_{ref}	MPa	Reference pressure

VISCOELASTICITY - CREEP (Mechanical data 1)

CODES in <i>ROOT_gen.dat</i>	ICL = 2 ITYCL = 1, 2, 4, 6, 11, 12
DESCRIPTION	Parameters for linear viscous deformation model.
EQUATIONS	<p>ITYCL = 1: FADT for saline materials</p> <p>The deformation mechanism fluid assisted diffusional transfer (FADT) was applied to develop an equation for creep of salt under wet conditions.</p> <p>Strain rate for a linear viscoelasticity is computed as:</p> $\frac{d\boldsymbol{\varepsilon}^{FADT}}{dt} = \frac{1}{2\eta_{FADT}^d}(\boldsymbol{\sigma}' - p'\mathbf{I}) + \frac{1}{3\eta_{FADT}^v}p'\mathbf{I}$ <p>where $\boldsymbol{\sigma}'$ is the effective stress tensor ($\boldsymbol{\sigma}' = \boldsymbol{\sigma} + P_f$, where $P_f = \max(P_g, P_l)$), p' is the mean effective stress ($p' = p + P_f$), \mathbf{I} is the identity tensor.</p> <p>Volumetric and deviatoric viscosities are defined as:</p> $\frac{1}{\eta_{FADT}^v} = \frac{16B(T)\sqrt{S_l}}{d_0^3}g_{FADT}^v(e)$ $\frac{1}{2\eta_{FADT}^d} = \frac{16B(T)\sqrt{S_l}}{d_0^3}g_{FADT}^d(e)$ <p>where $g_{FADT}^d(e)$ and $g_{FADT}^v(e)$ are internal nonlinear functions of void ratio (e), and S_l is degree of saturation.</p> $B(T) = \frac{A_B}{RT} \exp\left(\frac{-Q_B}{RT}\right)$ $g_{FADT}^v(e) = \frac{3g^2e^{3/2}}{(1+e)} \quad g_{FADT}^d(e) = \frac{g^2}{(1+e)}$ $g = \frac{1}{(1-f)^2} \quad f = \sqrt{\frac{2e}{3(1-e^{3/2})(1+e)}}$ <p>ITYCL= 2, 4: Constant viscosity plus degree of saturation effect</p> <p>Strain rate for a linear viscoelasticity is computed as:</p> $\frac{d\boldsymbol{\varepsilon}}{dt} = \left(\frac{1}{2\eta_d}(\boldsymbol{\sigma}' - p'\mathbf{I}) + \frac{1}{3\eta_v}p'\mathbf{I}\right)f(S_l)$ <p>where $\boldsymbol{\sigma}'$ is the effective stress tensor ($\boldsymbol{\sigma}' = \boldsymbol{\sigma} + P_f$, where $P_f = \max(P_g, P_l)$), p' is the mean effective stress ($p' = p + P_f$), \mathbf{I} is the identity tensor. For ITYCL=2 the degree of saturation function is calculated as $f(S_l) = \sqrt{S_l}$ while for ITYCL=4 the degree of saturation is not considered, i.e. $f(S_l) = 1$.</p>

CODES in <i>ROOT_gen.dat</i>	ICL = 2 ITYCL = 1, 2, 4, 6, 11, 12
DESCRIPTION	Parameters for linear viscous deformation model.
EQUATIONS	<p>ITYCL = 6: Secondary consolidation for unsaturated soils Strain rate for a linear viscoelasticity is computed as:</p> $\frac{d\varepsilon}{dt} = \left(\frac{1}{2\eta_d} (\sigma' - p'\mathbf{I}) + \frac{1}{3\eta_v} p'\mathbf{I} \right)$ <p>where</p> $\frac{1}{\eta_v} = A \left(1 - \beta \log \left(\frac{s + 0.1}{0.1} \right) \right) \frac{1}{t - t_0} \eta_d = B\eta_v$ <p>where t is time in seconds, t_0 is a reference time and s is suction.</p> <p>ITYCL = 11: Kelvin model</p>  <p>The Kelvin viscoelastic model can simulate the primary creep stage of rocks. The strain rate for linear viscoelasticity using the Kelvin model is computed as:</p> $\frac{d\varepsilon}{dt} = \mathbf{C}^v (\sigma - \varepsilon)$ <p>where \mathbf{C}^v represents the compliance matrix of the viscous dashpot. The Kelvin model can be combined with the elastic model, to be the Generalized Kelvin model.</p> <p>ITYCL = 12: Viscous dashpot combined with Kelvin model</p>  <p>This model can simulate the primary and secondary creep stages of rocks. Strain rate this model is computed as:</p> $\frac{d\varepsilon}{dt} = \frac{\sigma}{\eta_M} + \mathbf{C}^v (\sigma - \varepsilon)$ <p>This model can be combined with the elastic model, to become the Burgers model.</p>

PARAMETERS FOR ITYCL = 1 (Mech. data 1 – Viscoelasticity - Creep – ICL=2)

P1	d_o	m	Grain size
P2	A_B	$\text{m}^3 \text{s}^{-1} \text{MPa}^{-1}$	Pre-exponential parameter
P3	Q_B	J mol^{-1}	Activation energy

If the pre-exponential parameter is set to zero ($A_B = 0.0$) the viscous counterpart of the model does not work. In this way the parameter acts as option because the value of these pre-exponential parameter is checked to decide if this mechanism is considered.

This viscoelastic model (corresponding to FADT mechanism of deformation) requires that the liquid pressures are computed or, alternatively, a value of PLCONS greather that -10^{-12} MPa. Otherwise, liquid is considered inexistent and the mechanism FADT remains inactive.

PARAMETERS FOR ITYCL = 2, 4 (Mech. data 1 – Viscoelasticity - Creep – ICL=2)

P1	η_v	MPa s	Volumetric viscosity
P2	η_d	MPa s	Deviatoric viscosity

Note that a linear creep equation with a constant parameter A can be considered using Viscoelasticity-Creep (see [APPENDIX VI.B.3](#) for the relation between deviatoric viscosity and A).

PARAMETERS FOR ITYCL = 6 (Mech. data 1 – Viscoelasticity - Creep – ICL=2)

P1	A	$\text{MPa}^{-1} \text{s}^{-1}$	Parameter for volumetric viscosity
P2	β	(-)	Parameter for suction dependence
P3	t_0	s	Reference time
P4	Void		
P5	B	(-)	Parameter for deviatoric viscosity (infinity for no deviatoric viscous deformation)

PARAMETERS FOR ITYCL = 11 (Mech. data 1 – Viscoelasticity - Creep – ICL=2)

P1	E_K	MPa	Elastic modulus of the elastic spring
P2	ν_K	(-)	Possion's ratio of the elastic spring
P3	η_K^v	MPa s	Volumetric viscosity of the viscous dashpot
P4	η_K^d	MPa s	Deviatoric viscosity of the viscous dashpot

PARAMETERS FOR ITYCL = 12 (Mech. data 1 – Viscoelasticity - Creep – ICL=2)

P1	η_M^v	MPa s	Volumetric viscosity of the viscous dashpot (η_M^v)
P2	η_M^d	MPa s	Deviatoric viscosity of the viscous dashpot (η_M^d)
P3	E_K	MPa	Same as P1 of ITYCL = 11
P4	ν_K	(-)	Same as P2 of ITYCL = 11
P5	η_K^v	MPa s	Same as P3 of ITYCL = 11
P6	η_K^d	MPa s	Same as P4 of ITYCL = 11

VISCOPLASTICITY - CREEP (Mechanical data 1)

CODES in <i>ROOT_gen.dat</i>	ICL = 3 ITYCL = 1
DESCRIPTION	The deformation mechanism referred as dislocation creep (DC) has been applied to develop an equation for creep of porous salt aggregates. This mechanism leads to nonlinear dependences on stresses.
EQUATIONS	<p>Strain rate for a nonlinear viscoelasticity is computed as:</p> $\frac{d \varepsilon^{DC}}{dt} = \frac{1}{\eta_{DC}^d} \Phi(F) \frac{\partial G}{\partial \sigma'}$ <p>where G is a flow rule, F is a stress function and Φ is a scalar function. These functions are defined as:</p> $F = G = \sqrt{q^2 + \left(\frac{-p}{\alpha_p}\right)^2} \quad \Phi(F) = F^n \quad \alpha_p = \left(\frac{\eta_{DC}^v}{\eta_{DC}^d}\right)^{\frac{1}{n+1}}$ $\frac{1}{\eta_{DC}^v} = A(T) g_{DC}^v(e) \quad \frac{1}{\eta_{DC}^d} = A(T) g_{DC}^d(e)$ <p>where n is the power that comes from the rock power law and $g_{DC}^d(e)$ and $g_{DC}^v(e)$ are internal nonlinear functions of void ratio (e) defined as follows:</p> $g_{DC}^v(e) = 3(g-1)^n f$ $g_{DC}^d(e) = \left(\sqrt{\frac{1+g+g^2}{3}}\right)^{n-1} \left(\frac{2g+1}{3}\right) f + \frac{1}{\sqrt{g}}$ <p>where f and g are functions of the void ratio (see expression in the constitutive law Viscoelasticity for saline materials). The temperature dependence is considered as:</p> $A(T) = A_A \exp\left(\frac{-Q_A}{RT}\right)$

PARAMETERS FOR ITYCL = 1 (Mech. data 1 – Viscoelasticity - Creep – ICL=3)

P1	A_A	$s^{-1} MPa^{-n}$	Pre-exponential parameter
P2	Q_A	$J m^{-1}$	Activation energy
P3	n	-	Stress power
P4 – P10	Void		

If the pre-exponential parameter is set to zero the viscous counterpart of the model does not work. In this way the parameter acts as option because the value of this pre-exponential parameter is checked to decide if this part of the model is operating.

CODES in <i>ROOT_gen.dat</i>	ICL = 3 ITYCL = 3
DESCRIPTION	Viscoplastic constitutive equation based on a single internal state variable which is a function of plastic work are used to calculate the response of copper to change of strain rate over a range of temperatures.
EQUATIONS	<p>Starting with the Prandtl-Reuss-Von Mises law of isotropic plasticity:</p> $\dot{\epsilon}_{ij}^p = \lambda S_{ij} \quad (1)$ <p>Where $\dot{\epsilon}_{ij}^p$ and S_{ij} are the deviatoric plastic strain rate and the stress, respectively. Squaring equation (1) gives:</p> $D_2^p = \lambda^2 J_2$ $D_2^p = D_0^2 \left\{ \exp \left[\left(-\frac{Z^2}{3J_2} \right)^n \left(\frac{n+1}{n} \right) \right] \right\} \quad (2)$ <p>Where D_2^p is the second invariant of the plastic strain rate, and J_2 is the second invariant of the stress deviator.</p> <p>Combining equation 1 and 2, the plastic strain takes the form:</p> $\dot{\epsilon}_{ij}^p = \left\{ \left(\frac{Z^2}{3J_2} \right)^n \left(\frac{n+1}{2n} \right) \right\} \frac{S_{ij}}{\sqrt{J_2}}$ $n = (835 + 5T(K))/T(K)$ $T(K) = T(C) + 273.15$ <p>The parameter Z in the equation can be interpreted as an internal state variable which provides a measure of the overall resistance to plastic flow, and n is a strain rate sensitivity parameter.</p> $Z = Z_1 - (Z_1 - Z_0) \exp(-mw_p) \quad m = m_0 + m_1 \exp(-\alpha w_p)$ <p>The corresponding form is then based on the concept that plastic work, w_p, controls the hardening process, and that the plastic work and its time derivative are function of σ_{ij} and $\dot{\epsilon}_{ij}^p$.</p> $\dot{w}_p = \sigma_{ij} \dot{\epsilon}_{ij}^p$

PARAMETERS FOR ITYCL = 3 (Mech. data 1 – Viscoplasticity - Creep – ICL=3)

P1	D_0	s^{-1}	Limiting strain rate (usually $D_0 = 10^4 s^{-1}$ for copper)
P2	Z_0	MPa	Initial value of the internal state variable Z (typically $Z_0 = 31$ MPa)
P3	Z_1	MPa	Saturated value of the internal state variable Z (typically $Z_0 = 237$ MPa for copper)
P4	m_0	$(MPa)^{-1}$	Initial value of hardening parameter (typically $m_0 = 0.15$ MPa for copper)
P5	m_1	$(MPa)^{-1}$	Saturated value of hardening parameter (typically $m_1 = 0.25$ MPa for copper)
P6	α	$(MPa)^{-1}$	A material constant (typically $\alpha = 0.5$ MPa for copper)

VISCOPLASTICITY FOR SATURATED SOILS AND ROCKS – VPSSR

CODES in <i>ROOT_gen.dat</i>	ICL = 33 ITYCL = 1, 2, 3
DESCRIPTION	Viscoplasticity (general model for saturated soils and rocks)
EQUATIONS	<p>Viscoplastic constitutive model: $\frac{d\varepsilon}{dt} = \Gamma \langle \Phi(F) \rangle \frac{\partial G}{\partial \sigma}$ and the stress function adopted is: $\Phi(F) = F^m$ where the yield function and the flow rule are defined as:</p> <p>ITYCL = 1: $G = F = q^2 - \delta(p')^n + \delta(p')^{n+1} / p_o$ ITYCL = 2: $G = F = q^2 - \delta p_o (p')^n + \delta(p')^{n+1}$ ITYCL = 3 (Cam-Clay): $G = F = q^2 - \delta^2 (p_o p' - p'^2)$</p> <p>The fluidity (invers of viscosity) can be written as a function of temperature as: $\Gamma = \Gamma_o \exp\left(\frac{-Q}{RT}\right)$</p> <p>The hardening laws are expressed in general as: $dp_o = Dd(\varepsilon_v^l) + p_o \frac{1+e}{\lambda-\kappa} d\varepsilon_v = \left(Dl\varepsilon_v^{l-1} + p_o \frac{1+e}{\chi} \right) d\varepsilon_v$ where $D \neq 0$ or $(\lambda-\kappa) \neq 0$ permit to use each one of the two possibilities. $d\delta = Ed(\varepsilon_v^l) = El\varepsilon_v^{l-1} d\varepsilon_v$ where p_o and δ are parameters in the yield surface and flow rule.</p> <p>Invariants used in the models are defined as: $p = \sigma_{oct} = \frac{1}{3} I_1 = \frac{1}{3} (\sigma_x + \sigma_y + \sigma_z)$ $q = \frac{3}{\sqrt{2}} \tau_{oct} = \frac{1}{\sqrt{2}} \sqrt{(\sigma_x - \sigma_y)^2 + (\sigma_y - \sigma_z)^2 + (\sigma_z - \sigma_x)^2 + 6(\tau_{xy}^2 + \tau_{yz}^2 + \tau_{zx}^2)}$</p>

PARAMETERS FOR ITYCL = 1 and 2 (Mech. data 1 – VPSSR – ICL=33)

P1	m		Power of the stress function (integer value; typical value = 3)
P2	$\Gamma_o = 1/\eta$	$s^{-1} MPa^{-m}$ (*)	Fluidity = 1/viscosity (for plasticity use a sufficiently large value) (*) Units valid for F and G in units of stress. For other cases (e.g. units of stress squared) then the units are different.
P3	Q	$J mol^{-1}$	Activation energy (= 0 for temperature independent model)
P4	D	MPa	Constant in hardening law
P5	p_o	MPa	Initial value of p_o (positive)
P6	l	-	Power of hardening laws
P7	χ	-	Parameter in hardening law
P8	n	-	Power in F and G
P9	E	-	Constant for hardening law
P10	δ	-	Initial value of δ

PARAMETERS FOR ITYCL = 3 (Mech. data 1 – VPSSR – ICL=33)

P1 – P7; P9 – P10	Same as in ITYCL = 1
P8	Void

CODES in <i>ROOT_gen.dat</i>	ICL = 33 ITYCL = 4, 5
DESCRIPTION	Viscoplasticity (general model for saturated soils and rocks)
EQUATIONS	<p>Viscoplastic constitutive model: $\frac{d\epsilon}{dt} = \Gamma \langle \Phi(F) \rangle \frac{\partial G}{\partial \sigma}$</p> <p>and the stress function adopted is: $\Phi(F) = F^m$</p> <p>where the yield function and the flow rule are defined as:</p> <p>ITYCL = 4, 5 (Drucker-Prager –based on Mohr-Coulomb parameters):</p> $F = q - \delta p' - c\beta \quad G = q - \delta \alpha p' - c\beta$ $\delta = M = \frac{6 \sin \phi'}{3 - \sin \phi'}$ $\beta = \frac{6 \cos \phi'}{3 - \sin \phi'}$ <p>For this model, equations are written assuming $p > 0$ compression, but the program uses the standard sign criteria for continuum mechanics).</p> <p>The fluidity (invers of viscosity) can be written as a function of temperature as: $\Gamma = \Gamma_o \exp\left(\frac{-Q}{RT}\right)$</p> <p>Invariants used in the models are defined as:</p> $p = \sigma_{oct} = \frac{1}{3} I_1 = \frac{1}{3} (\sigma_x + \sigma_y + \sigma_z)$ $q = \frac{3}{\sqrt{2}} \tau_{oct} = \frac{1}{\sqrt{2}} \sqrt{(\sigma_x - \sigma_y)^2 + (\sigma_y - \sigma_z)^2 + (\sigma_z - \sigma_x)^2 + 6(\tau_{xy}^2 + \tau_{yz}^2 + \tau_{zx}^2)}$

PARAMETERS FOR ITYCL = 4 (Mech. data 1 – VPSSR – ICL=33)

P1	m		Power of the stress function (integer value; typical value = 3)
P2	$\Gamma_o = 1/\eta$	$s^{-1}MPa^{-m}$ (*)	Fluidity = 1/viscosity (for plasticity use a sufficiently large value) (*) Units valid for F and G in units of stress. For other cases (e.g. units of stress squared) then the units are different.
P3	Q	$J mol^{-1}$	Activation energy (= 0 for temperature independent model)
P4	b	-	Cohesion: $c' = (a + bs)g(\phi)$; $g(\phi) = (f + f)/2$
P5	a	MPa	Cohesion: $c' = (a + bs)g(\phi)$; $g(\phi) = (f + f)/2$
P6	n		Porosity function: $f(\phi) = 1 - (\phi/\phi_{oo})^n$
P7	$\alpha (0 - 1)$		Parameter to reduce dilatancy. 0: no volumetric plastic strain; 1 (default*): associative plasticity.
P8	ϕ_{oo}	-	Reference porosity
P9	Void		
P10	δ	-	Equivalent to M

* Note that, in the case of parameters with default values, when setting them to zero –or to a value lower than 10^{-25} – automatically takes the default value. Hence, if the user actually wants to set a parameter to zero, a low value but greater than 10^{-25} should be input.

PARAMETERS FOR ITYCL = 5 (Mech. data 1 – VPSSR – ICL=33)

P1 – P3, P7, P10	Same as in ITYCL = 4		
P4, P6, P8, P9	Void		
P5	c	MPa	Cohesion

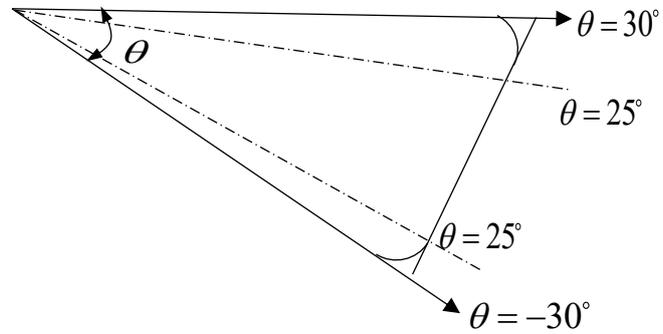
CODES in <i>ROOT_gen.dat</i>	ICL = 33 ITYCL = 9
DESCRIPTION	Viscoplasticity (general model for saturated soils and rocks)
EQUATIONS	<p>ITYCL = 9: For rock salt with dilatancy:</p> $F = a_1 q - bp \qquad G = a_1 q - \alpha bp$ $\Phi(F) = F^m \text{ for } F \geq 0 \qquad \Phi(F) = 0 \text{ for } F < 0$ $b = a_3 + a_2 (W_d)^{0.25} - a_4 \langle W_d - W_{d0} \rangle^{0.25}$ $\alpha = a_5 + a_6 W_d + a_7 \langle W_d - W_{d0} \rangle^2 \qquad dW_d = q d\varepsilon_d$ <p>From a numerical point of view, it is set $a_6 = a_7$</p>

PARAMETERS FOR ITYCL = 9 (Mech. data 1 – VPSSR – ICL=33)

P1	m		Power of the stress function (integer value; typical value = 3)
P2	$\Gamma_o = 1/\eta$	$s^{-1} MPa^{-m}$ (*)	Fluidity = 1/viscosity (for plasticity use a sufficiently large value) (*) Units valid for F and G in units of stress. For other cases (e.g. units of stress squared) then the units are different.
P3	Q	$J mol^{-1}$	Activation energy (= 0 for temperature independent model)
P4	a_6		
P5	W_{d0}		
P6	a_1		
P7	a_2		
P8	a_3		
P9	a_4		
P10	a_5		

CODES in <i>ROOT_gen.dat</i>	ICL = 33 ITYCL = 11, 12, 15, 20, 21, 22, 23, 24, 25
DESCRIPTION	Viscoplasticity (general model for saturated soils and rocks)
EQUATIONS	<p>ITYCL = 11: Mohr-Coulomb (MC) model with dilatancy:</p> $F = p \cdot \sin \varphi + \left(\cos \theta - \frac{1}{\sqrt{3}} \sin \theta \cdot \sin \varphi \right) \cdot \sqrt{J_2} - c \cdot \cos \varphi$ $G = \alpha \cdot p \cdot \sin \psi + \left(\cos \theta - \frac{1}{\sqrt{3}} \sin \theta \cdot \sin \psi \right) \cdot \sqrt{J_2} - c \cdot \cos \psi$ $\Phi(F) = F^m \quad \text{for } F \geq 0 \quad \Phi(F) = 0 \quad \text{for } F < 0$ <p>This model uses the standard sign criteria for continuum mechanics, and equations are written assuming $p > 0$ tension. ψ is the dilatancy angle and α is a parameter for the plastic potential.</p> <p>Invariants used in the models are defined as:</p> $p = \frac{1}{3} I_1 = \frac{1}{3} (\sigma_x + \sigma_y + \sigma_z)$ $J_2 = \frac{1}{2} S_{ij} S_{ij} = \frac{1}{6} \sqrt{(\sigma_x - \sigma_y)^2 + (\sigma_y - \sigma_z)^2 + (\sigma_z - \sigma_x)^2 + 6(\tau_{xy}^2 + \tau_{yz}^2 + \tau_{zx}^2)}$ $\theta = \frac{1}{3} \sin^{-1} \left(-\frac{3\sqrt{3}}{2} \frac{J_3}{\sqrt{J_2^3}} \right), \quad -30^\circ \leq \theta \leq 30^\circ$ <p>Where $J_3 = S_x S_y S_z + 2\tau_{xy} \tau_{yz} \tau_{zx} - S_x \tau_{yz}^2 - S_y \tau_{xz}^2 - S_z \tau_{xy}^2$.</p> <p>To avoid numerical issues, the corners of the MC yield surface are rounded by introducing θ_T. The rounded yield surface is as follows:</p> $F = p \cdot \sin \varphi + \sqrt{J_2} \cdot K_F(\theta) - c \cdot \cos \varphi$ $K_F(\theta) = \begin{cases} A + B \cdot \sin 3\theta, & \theta > \theta_T \\ \cos \theta - \frac{1}{\sqrt{3}} \cdot \sin \varphi \cdot \sin \theta, & \theta \leq \theta_T \end{cases}$ $A = \frac{1}{3} \cdot \cos \theta_T \left(3 + \tan \theta_T \cdot \tan 3\theta_T + \frac{1}{\sqrt{3}} \text{sign}(\theta) \cdot \left(\tan 3\theta_T - 3 \tan \theta_T \right) \sin \varphi \right)$ $B = -\frac{1}{3 \cdot \cos 3\theta_T} \left(\text{sign}(\theta) \sin \theta_T + \frac{1}{\sqrt{3}} \sin \varphi \cdot \cos \theta_T \right)$

$$\text{sign}(\theta) = \begin{cases} +1, & \theta \geq 0 \\ -1, & \theta < 0 \end{cases}$$

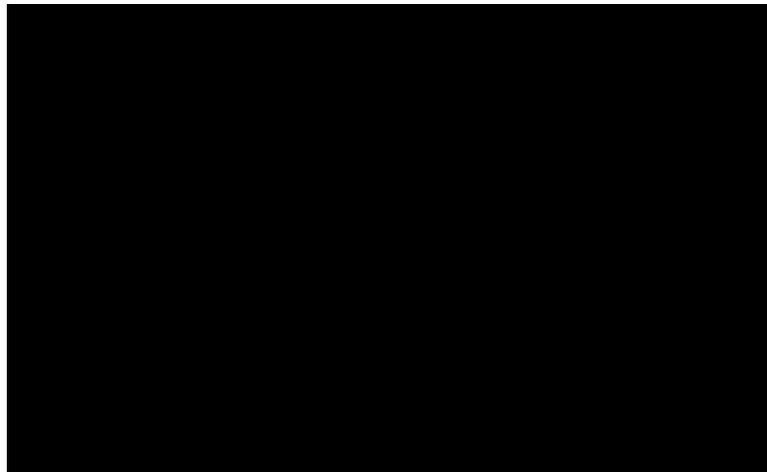


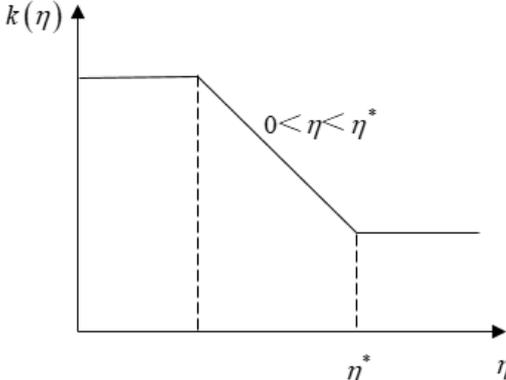
For the numerical calculation, a hyperbolic yield surface is adopted, as follows:

$$F = \sqrt{J_2 \cdot K_F^2(\theta) + a^2 \cdot \sin^2 \varphi} + p \cdot \sin \varphi - c \cdot \cos \varphi$$

Where: $a = m_{mc} \cdot c \cdot \cot \varphi$

The closer to 0 is the value of m_{mc} , the closer would be the hyperbolic surface to the actual MC surface, as shown in the following figure:



CODES in <i>ROOT_gen.dat</i>	ICL = 33 ITYCL = 11, 12, 15, 20, 21, 22, 23, 24, 25
DESCRIPTION	Viscoplasticity (general model for saturated soils and rocks)
EQUATIONS	<p>ITYCL = 12: MC model with dilatancy and strain-softening:</p> $F = p \cdot \sin \varphi(\eta) + \left[\cos \theta - \frac{1}{\sqrt{3}} \sin \theta \cdot \sin \varphi(\eta) \right] \cdot \sqrt{J_2} - c(\eta) \cdot \cos \varphi(\eta)$ $G = \alpha \cdot p \cdot \sin \psi + \left(\cos \theta - \frac{1}{\sqrt{3}} \sin \theta \cdot \sin \psi \right) \cdot \sqrt{J_2} - c(\eta) \cdot \cos \psi(\eta)$ $\Phi(F) = F^m \quad \text{for } F \geq 0 \quad \Phi(F) = 0 \quad \text{for } F < 0$ <p>Similar model to ITYCL=11, but in this case both the cohesion and the friction angle depend on the softening parameter η,</p> $k(\eta) = \begin{cases} k^{peak}, & \eta \leq 0 \\ k^{peak} + \left(\frac{k^{res} - k^{peak}}{\eta^*} \right) \cdot \eta, & 0 \leq \eta \leq \eta^* \\ k^{res}, & \eta^* \leq \eta \end{cases}$  <p>Where k^{peak} and k^{res} are peak and residual values of k, respectively; k represents both cohesion c and friction angle φ. η^* is defined as the value of the softening parameter controlling the transition between the softening and residual stages.</p> <p>The expression of the softening parameter is the following:</p> $\eta = \sqrt{\frac{3}{2} \cdot \left[\left(\varepsilon_x^p - \varepsilon_m^p \right)^2 + \left(\varepsilon_y^p - \varepsilon_m^p \right)^2 + \left(\varepsilon_z^p - \varepsilon_m^p \right)^2 + \left(\frac{1}{2} \gamma_{xy}^p \right)^2 + \left(\frac{1}{2} \gamma_{yz}^p \right)^2 + \left(\frac{1}{2} \gamma_{zx}^p \right)^2 \right]}$ <p>Where $\varepsilon_m^p = \frac{1}{3} (\varepsilon_x^p + \varepsilon_y^p + \varepsilon_z^p)$.</p> <p>The corners of MC yield surface are rounded by introducing θ_T. The rounded method is the same as in ITYCL=11, but the rounded parameters θ_T and m_{mc} are fixed at 25° and 0.25 in this model.</p>

CODES in <i>ROOT_gen.dat</i>	ICL = 33 ITYCL = 11, 12, 15, 20, 21, 22, 23, 24, 25
DESCRIPTION	Viscoplasticity (general model for saturated soils and rocks)

EQUATIONS	<p>ITYCL = 15: MC model with anisotropic behaviour:</p> <p>The stress space in the global coordinate system (σ^{global}) can be transferred to the local one (σ^{local}), using the transformation matrix \mathbf{a}. Moreover, the anisotropic stress space (σ^{ani}) can be obtained by introducing the stresses scaling factor (C_N and C_T):</p> $\sigma^{\text{local}} = \mathbf{a} \sigma^{\text{global}} \mathbf{a}^T$ $\sigma^{\text{ani}} = \begin{bmatrix} \sigma_{11}^{\text{local}}/C_N & \sigma_{12}^{\text{local}} & C_T \sigma_{13}^{\text{local}} \\ \sigma_{12}^{\text{local}} & \sigma_{22}^{\text{local}}/C_N & C_T \sigma_{23}^{\text{local}} \\ C_T \sigma_{13}^{\text{local}} & C_T \sigma_{23}^{\text{local}} & C_N \sigma_{33}^{\text{local}} \end{bmatrix}$ <p>where $\mathbf{a} = \begin{bmatrix} \cos \alpha \cdot \cos \beta & -\sin \alpha & \cos \alpha \cdot \sin \beta \\ \sin \alpha \cdot \cos \beta & \cos \alpha & \sin \alpha \cdot \sin \beta \\ -\sin \beta & 0 & \cos \beta \end{bmatrix}$</p> <p>with α [deg] rotating around z-axis, and then, β [deg] rotating around the y-axis.</p> <p>Then, the anisotropic Mohr-Coulomb failure behaviour model can be expressed in the anisotropic stress space (σ^{ani}):</p> $F_{\text{MC}}^{\text{ani}} = p^{\text{ani}} \sin \varphi + \sqrt{J_2^{\text{ani}}} \left[\cos \theta^{\text{ani}} - \frac{1}{\sqrt{3}} \cdot \sin \varphi \sin \theta^{\text{ani}} \right] - c \cos \varphi$ $G_{\text{MC}}^{\text{ani}} = \alpha p^{\text{ani}} \sin \psi + \sqrt{J_2^{\text{ani}}} \left[\cos \theta^{\text{ani}} - \frac{1}{\sqrt{3}} \sin \psi \sin \theta^{\text{ani}} \right]$ <p>No dilatation is considered (i.e. $\psi = 0$) because of the adopted perfectly-plastic post-failure behaviour model. α is a parameter for the plastic potential.</p> <p>Invariants used in the models are defined as:</p> $p^{\text{ani}} = \frac{1}{3} (\sigma_x^{\text{ani}} + \sigma_y^{\text{ani}} + \sigma_z^{\text{ani}})$ $J_2^{\text{ani}} = \frac{1}{2} S_{ij}^{\text{ani}} S_{ij}^{\text{ani}}$ $J_3^{\text{ani}} = S_x^{\text{ani}} S_y^{\text{ani}} S_z^{\text{ani}} + 2\tau_{xy}^{\text{ani}} \tau_{yz}^{\text{ani}} \tau_{zx}^{\text{ani}} - S_x^{\text{ani}} (\tau_{yz}^{\text{ani}})^2 - S_y^{\text{ani}} (\tau_{xz}^{\text{ani}})^2 - S_z^{\text{ani}} (\tau_{xy}^{\text{ani}})^2$ $\theta^{\text{ani}} = \frac{1}{3} \sin^{-1} \left(-\frac{3\sqrt{3}}{2} \frac{J_3^{\text{ani}}}{\sqrt{J_2^{\text{ani}}{}^3}} \right)$ <p>This model is based in Mánica M, Gens A, Vaunat J, et al. A cross-anisotropic formulation for elasto-plastic models. Géotechnique Letters, 2016, 6(2): 156-162.</p>
CODES in ROOT_gen.dat	ICL = 33 ITYCL = 11, 12, 15, 20, 21, 22, 23, 24, 25
DESCRIPTION	Viscoplasticity (general model for saturated soils and rocks)

EQUATIONS	<p>ITYCL = 20: Hoek-Brown (HB) model with dilatancy:</p> $F = \left[\frac{4}{\sigma_{ci}} \cos^2 \theta \cdot \sqrt{J_2} + \frac{2}{\sqrt{3}} \cdot m_{hb} \cdot \cos \left(\theta + \frac{\pi}{6} \right) \right] \cdot \sqrt{J_2} - m_{hb} \cdot \left(-p + \frac{s_{hb} \cdot \sigma_{ci}}{m_{hb}} \right)$ $G = \alpha \cdot p \cdot \sin \psi + \left(\cos \theta - \frac{1}{\sqrt{3}} \sin \theta \cdot \sin \psi \right) \cdot \sqrt{J_2}$ $\Phi(F) = F^m \quad \text{for } F \geq 0 \quad \Phi(F) = 0 \quad \text{for } F < 0$ <p>This model uses the standard sign criteria for continuum mechanics, and equations are written assuming $p > 0$ tension; m_{hb} and s_{hb} are parameters of HB failure criterion. σ_{ci} is the compressive strength of intact rock mass. ψ is the dilatancy angle and α is a parameter for the plastic potential.</p> <p>For this model, the corners of HB yield surface are rounded by introducing θ_T. The rounded yield surface is as follows:</p> $F = K_F(\theta) \cdot \sqrt{J_2} - m_{hb} \cdot \left(-p + \frac{s_{hb} \cdot \sigma_{ci}}{m_{hb}} \right)$ $K_F(\theta) = \begin{cases} A_+ + B_+ \sin 3\theta, & \theta_T \leq \theta \leq 3\theta_T \\ \frac{4}{\sigma_{ci}} \cos^2 \theta \cdot \sqrt{J_2} + \frac{2}{\sqrt{3}} \cdot m_{hb} \cdot \cos \left(\theta + \frac{\pi}{6} \right), & -\theta_T \leq \theta \leq \theta_T \\ A_- - B_- \sin 3\theta, & -3\theta_T \leq \theta \leq -\theta_T \end{cases}$ <p>where:</p> $A_+ = m_{hb} \cdot \left[\left(\cos \theta_T - \frac{\sin \theta_T}{\sqrt{3}} \right) + \left(\frac{\cos \theta_T}{3\sqrt{3}} + \frac{1}{3} \sin \theta_T \right) \tan 3\theta_T \right]$ $+ \sqrt{J_2} \cdot \left[\frac{4 \cdot \cos^2 \theta_T}{\sigma_{ci}} + \frac{8 \cdot \sin \theta_T \cos \theta_T \tan 3\theta_T}{3\sigma_{ci}} \right]$ $B_+ = \sqrt{J_2} \cdot \left(-\frac{8 \cdot \sin \theta_T \cos \theta_T}{3\sigma_{ci} \cos 3\theta_T} \right) - \frac{m_{hb}}{3 \cos 3\theta_T} \cdot \left(\sin \theta_T + \frac{\cos \theta_T}{\sqrt{3}} \right)$ $A_- = m_{hb} \cdot \left[\left(\cos \theta_T + \frac{\sin \theta_T}{\sqrt{3}} \right) - \left(\frac{\cos \theta_T}{3\sqrt{3}} - \frac{1}{3} \sin \theta_T \right) \tan 3\theta_T \right]$ $+ \sqrt{J_2} \cdot \left[\frac{4 \cdot \cos^2 \theta_T}{\sigma_{ci}} + \frac{8 \cdot \sin \theta_T \cos \theta_T \tan 3\theta_T}{3\sigma_{ci}} \right]$ $B_- = -\sqrt{J_2} \cdot \left(\frac{8 \cdot \sin \theta_T}{3\sigma_{ci} \cos 3\theta_T} \right) + \frac{m_{hb}}{3 \cos 3\theta_T} \cdot \left(\frac{\cos \theta_T}{\sqrt{3}} - \sin \theta_T \right)$
CODES in ROOT_gen.dat	ICL = 33 ITYCL = 11, 12, 15, 20, 21, 22, 23, 24, 25
DESCRIPTION	Viscoplasticity (general model for saturated soils and rocks)

EQUATIONS

ITYCL = 21: HB model with dilatancy and strain-softening:

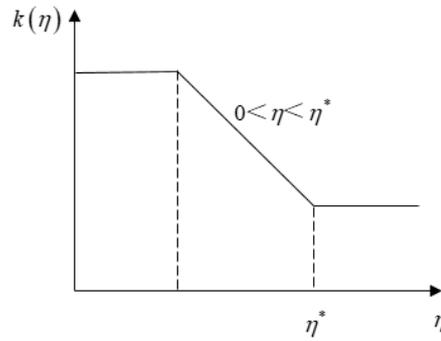
$$F = \left[\frac{4}{\sigma_{ci}} \cos^2 \theta \cdot \sqrt{J_2} + \frac{2}{\sqrt{3}} \cdot m_{hb}(\eta) \cdot \cos \left(\theta + \frac{\pi}{6} \right) \right] \cdot \sqrt{J_2} - m_{hb}(\eta) \cdot \left(-p + \frac{s_{hb}(\eta) \cdot \sigma_{ci}}{m_{hb}(\eta)} \right)$$

$$G = \alpha \cdot p \cdot \sin \psi + \left(\cos \theta - \frac{1}{\sqrt{3}} \sin \theta \cdot \sin \psi \right) \cdot \sqrt{J_2}$$

$$\Phi(F) = F^m \text{ for } F \geq 0 \quad \Phi(F) = 0 \text{ for } F < 0$$

Similar model to ITYCL=20, but in this case both the parameters of Hoek-Brown failure criterion, $m_{hb}(\eta)$ and $s_{hb}(\eta)$, are functions of the softening parameter η :

$$k(\eta) = \begin{cases} k^{peak}, \eta \leq 0 \\ k^{peak} + \left(\frac{k^{res} - k^{peak}}{\eta^*} \right) \cdot \eta, 0 \leq \eta \leq \eta^* \\ k^{res}, \eta^* \leq \eta \end{cases}$$



Where k^{peak} and k^{res} are peak and residual value of k , respectively; k represents both m_{hb} and s_{hb} . η^* is defined as the value of the softening parameter controlling the transition between the softening and residual stages. The expression for the softening parameter is:

$$\eta = \sqrt{\frac{3}{2} \cdot \left[\left(\varepsilon_x^p - \varepsilon_m^p \right)^2 + \left(\varepsilon_y^p - \varepsilon_m^p \right)^2 + \left(\varepsilon_z^p - \varepsilon_m^p \right)^2 + \left(\frac{1}{2} \gamma_{xy}^p \right)^2 + \left(\frac{1}{2} \gamma_{yz}^p \right)^2 + \left(\frac{1}{2} \gamma_{zx}^p \right)^2 \right]}$$

$$\text{Where } \varepsilon_m^p = \frac{1}{3} (\varepsilon_x^p + \varepsilon_y^p + \varepsilon_z^p).$$

The corners of strain-softening HB yield surface are rounded by introducing θ_T . The rounded method is the same as in ITYCL=20, but the rounded parameter θ_T is fixed at 25° in this model.

CODES in
ROOT_gen.dat

ICL = 33 ITYCL = 11, 12, 15, 20, 21, 22, 23, 24, 25

DESCRIPTION	Viscoplasticity (general model for saturated soils and rocks)
EQUATIONS	<p>ITYCL = 22: HB model with dilatancy:</p> $F = \left[\frac{4}{\sigma_{ci}} \cos^2 \theta \cdot \sqrt{J_2} + \frac{2}{\sqrt{3}} \cdot m_{hb} \cdot \cos \left(\theta + \frac{\pi}{6} \right) \right] \cdot \sqrt{J_2}$ $- m_{hb} \cdot \left(-p + \frac{s_{hb} \cdot \sigma_{ci}}{m_{hb}} \right)$ $G = \left[\frac{4}{\sigma_{ci}} \cos^2 \theta \cdot \sqrt{J_2} + \frac{2}{\sqrt{3}} \cdot m_{hb} \cdot \cos \left(\theta + \frac{\pi}{6} \right) \right] \cdot \sqrt{J_2}$ $- \alpha \cdot m_{hb} \cdot \left(-p + \frac{s_{hb} \cdot \sigma_{ci}}{m_{hb}} \right)$ $\Phi(F) = F^m \quad \text{for } F \geq 0 \quad \Phi(F) = 0 \quad \text{for } F < 0$ <p>Similar model to ITYCL=20, except for the form of the plastic potential G. In this model, the expression for the plastic potential is related to the yield surface. It is considered an associated flow rule, <i>i.e.</i> F=G, when α equal to 1.</p> <p>ITYCL = 23: HB model with dilatancy and strain-softening:</p> $F = \left[\frac{4}{\sigma_{ci}} \cos^2 \theta \cdot \sqrt{J_2} + \frac{2}{\sqrt{3}} \cdot m_{hb}(\eta) \cdot \cos \left(\theta + \frac{\pi}{6} \right) \right] \cdot \sqrt{J_2}$ $- m_{hb}(\eta) \cdot \left(-p + \frac{s_{hb}(\eta) \cdot \sigma_{ci}}{m_{hb}(\eta)} \right)$ $G = \left[\frac{4}{\sigma_{ci}} \cos^2 \theta \cdot \sqrt{J_2} + \frac{2}{\sqrt{3}} \cdot m_{hb}(\eta) \cdot \cos \left(\theta + \frac{\pi}{6} \right) \right] \cdot \sqrt{J_2}$ $- \alpha \cdot m_{hb}(\eta) \cdot \left(-p + \frac{s_{hb}(\eta) \cdot \sigma_{ci}}{m_{hb}(\eta)} \right)$ <p>Similar model to ITYCL=21, except for the form of the plastic potential G. In this model, the expression of the plastic potential is related to the yield surface. It is considered an associated flow rule, <i>i.e.</i> F=G, when α equal to 1. In this model, both the yield surface and the plastic potential depend on the softening parameter η.</p>

CODES in ROOT_gen.dat	ICL = 33 ITYCL = 1, 2, 3, 4, 5, 9, 11, 12, 15, 20, 21, 22, 23, 24, 25
DESCRIPTION	Viscoplasticity (general model for saturated soils and rocks)
EQUATIONS	<p>ITYCL = 24: 3D Pan-Hudson simplified HB model (Pan & Hudson, 1988):</p> $F = m_{hb} \cdot p + \frac{3}{\sigma_{ci}} \cdot \sqrt{J_2} + \frac{\sqrt{3}}{2} \cdot m_{hb} \cdot \sqrt{J_2} - s_{hb} \cdot \sigma_{ci}^2$ $G = \alpha \cdot m_{hb} \cdot p + \frac{3}{\sigma_{ci}} \cdot \sqrt{J_2} + \frac{\sqrt{3}}{2} \cdot m_{hb} \cdot \sqrt{J_2} - s_{hb} \cdot \sigma_{ci}^2$ $\Phi(F) = F^m \quad \text{for } F \geq 0 \quad \Phi(F) = 0 \quad \text{for } F < 0$ <p>This model uses the standard sign criteria for continuum mechanics, and equations are written assuming $p > 0$ tension; m_{hb} and s_{hb} are parameters of the HB failure criterion. σ_{ci} is the compressive strength of the intact rock mass. ψ is the dilatancy angle and α is a parameter for the plastic potential. It is considered associated flow rule, when α equal to 1.</p> <p>ITYCL = 25: 3D Pan-Hudson simplified HB model (Pan & Hudson, 1988) with strain-softening:</p> $F = m_{hb}(\eta) \cdot p + \frac{3}{\sigma_{ci}} \cdot \sqrt{J_2} + \frac{\sqrt{3}}{2} \cdot m_{hb}(\eta) \cdot \sqrt{J_2} - s_{hb}(\eta) \cdot \sigma_{ci}^2$ $G = \alpha \cdot m_{hb}(\eta) \cdot p + \frac{3}{\sigma_{ci}} \cdot \sqrt{J_2} + \frac{\sqrt{3}}{2} \cdot m_{hb}(\eta) \cdot \sqrt{J_2} - s_{hb}(\eta) \cdot \sigma_{ci}^2$ $\Phi(F) = F^m \quad \text{for } F \geq 0 \quad \Phi(F) = 0 \quad \text{for } F < 0$ <p>Similar model to ITYCL=24, but in this case both the parameters of 3D Pan-Hudson simplified Hoek-Brown failure criterion, $m_{hb}(\eta)$ and $s_{hb}(\eta)$, are dependent on the softening parameter η, following the same relationships as in ITYCL=21.</p>

PARAMETERS FOR ITYCL = 11 (Mech. data 1 – VPSSR – ICL=33)

P1	m		Power of the stress function (integer value; typical value = 3)
P2	$\Gamma_o = 1/\eta$	$s^{-1} MPa^{-m} (*)$	Fluidity = 1/Viscosity (for plasticity use a sufficiently large value) (*) Units valid for F and G in units of stress. For other cases (e.g. units of stress squared) then the units are different.
P3	Q	$J mol^{-1}$	Activation energy (= 0 for temperature independent model)
P4	Void		
P5	c	MPa	Cohesion
P6	φ	°	Friction angle
P7	θ_T	°	Lode angle value at which the corner smoothing function starts (typical value –default* – = 25°)
P8	m_{mc} (0-1)		Hyperbolic parameters for the yield surface. If $m_{mc} = 0$ then the failure surface would be the actual Mohr-Coulomb failure surface (typical value –default* – = 0.25)
P9	α (0 - 1)		Parameter for the plastic potential (default* = 1)
P10	ψ	°	Dilatancy angle (default* value = friction angle).

PARAMETERS FOR ITYCL = 12 (Mech. data 1 – VPSSR – ICL=33)

P1 – P3	Same as in ITYCL = 11		
P4	η^*		Critical value of the softening parameter (corresponding to the transition between softening and residual stages)
P5	c_{peak}	MPa	Peak cohesion
P6	φ_{peak}	°	Peak friction angle
P7	c_{res}	MPa	Residual cohesion (default* = peak cohesion)
P8	φ_{res}	°	Residual friction angle (default* = peak friction angle)
P9	α (0 - 1)		Parameter for the plastic potential (default* = 1)
P10	ψ	°	Dilatancy angle (default* value = peak friction angle)

* Note that, in the case of parameters with default values, when setting them to zero –or to a value lower than 10^{-25} – automatically takes the default value. Hence, if the user actually wants to set a parameter to zero, a low value but greater than 10^{-25} should be input.

PARAMETERS FOR ITYCL = 15 (Mech. data 1 – VPSSR – ICL=33)

P1 – P3	Same as in ITYCL = 11		
P4, P10	Void		
P5	c	MPa	Cohesion
P6	φ	°	Friction angle
P7	C_N		Stress scaling factor
P8	C_T		Stress scaling factor
P9	α (0 - 1)		Parameter for the plastic potential (default = 1)

PARAMETERS FOR ITYCL = 20 (Mech. data 1 – VPSSR – ICL=33)

P1 – P3	Same as in ITYCL = 11		
P4	Void		
P5	m_{hb}	MPa	Hoek-Brown parameter m
P6	s_{hb}		Hoek-Brown parameter s
P7	σ_{ci}	MPa	Compressive strength of the intact rock mass
P8	θ_T	°	Lode angle value at which the corner smoothing function starts (typical value –default– = 25°)
P9	α (0 - 1)		Parameter for the plastic potential (default = 1)
P10	ψ	°	Dilatancy angle

PARAMETERS FOR ITYCL = 21 (Mech. data 1 – VPSSR – ICL=33)

P1 – P3	Same as in ITYCL = 11		
P4	η^*		Critical value of the softening parameter (corresponding to the transition between softening and residual stages)
P5	m_{hb}^{peak}	MPa	Hoek-Brown parameter m (peak value)
P6	s_{hb}^{peak}		Hoek-Brown parameter s (peak value)
P7	m_{hb}^{res}	MPa	Hoek-Brown parameter m (residual value)
P8	s_{hb}^{res}		Hoek-Brown parameter s (residual value)
P9	σ_{ci}	MPa	Compressive strength of the intact rock mass
P10	ψ	°	Dilatancy angle

PARAMETERS FOR ITYCL = 22, 24 (Mech. data 1 – VPSSR – ICL=33)

P1 – P9	Same as in ITYCL = 20		
P10	Void		

PARAMETERS FOR ITYCL = 23, 25 (Mech. data 1 – VPSSR – ICL=33)

P1 – P9	Same as in ITYCL = 21		
P10	α (0 - 1)		Parameter for the plastic potential (default = 0)

HISTORY VARIABLES:

The VPSSR (ICL = 33) requires four history variables:

Hist_var 1	P_o	MPa	Evolution of preconsolidation mean stress
Hist_var 2	δ_0		Evolution of δ (parameter of the flow rule)
Hist_var 3	EDP		Plastic deviatoric strain
Hist_var 4	EVP		Plastic volumetric strain

The first two variables can be assigned as initial conditions on *surfaces/volumes* if an initial particular distribution on the geometry is required. The procedure is the same as followed by initial stresses as was described in chapter II. PREPROCESS, PROBLEM DATA, section II.2.3.5.

If no value is assigned for the first two variables in conditions, internally, the program sets the input parameters P5 (for P_o^*) and P10 (for δ_0) of the ICL = 33 (ITYCL = 1, 2 or 3), as initial values.

The evolution of the four history variables can be visualized as an output in Post-process GID interface.

VISCOPLASTICITY FOR UNSATURATED SOILS AND ROCKS - VPUSR

CODES in <i>ROOT_gen.dat</i>	ICL = 34, 35 and 36 ITYCL = 1, 16
DESCRIPTION	Viscoplasticity (general model based on Desai and Perzyna theory)
EQUATIONS	<p>ITYCL = 1: Viscoplastic constitutive model</p> $\frac{d\varepsilon}{dt} = \Gamma \langle \phi(F) \rangle \frac{\partial G}{\partial \sigma'} \quad \phi(F) = \left(\frac{F}{F_o} \right)^N$ <p>where the yield function is defined as: $F(J_1, J_{2D}, J_{3D}, s) = aJ_{2D} - \mu^2 F_b F_s$ with the following additional functions:</p> $F_b = \gamma \left[- (J_1^0(s) + k_2 s + k_4)^{2-n} (J_1 + k_1 s + k_4)^n + (J_1 + k_1 s + k_4)^2 - k_3 s J_1^0(s) \right]$ $F_s = (1 - \beta_s s)^m \quad S = \frac{\sqrt{27}}{2} J_{3D} (J_{2D})^{(-3/2)}$ <p>The viscoplastic potential is defined similarly as:</p> $G(J_1, J_{2D}, J_{3D}, s) = aJ_{2D} - b\mu^2 F_b F_s$ <p>where b is a non-associativity parameter.</p> <p>Hardening is described with the following function, which is equivalent to the BBM model:</p> $J_1^0(s) = 3p^c \left(\frac{J_1^{0*}}{3p^c} \right)^{\frac{\lambda(0)-\kappa}{\lambda(s)-\kappa}} \quad p_o(s) = J_1^0(s) / 3$ $\lambda(s) = \lambda(0) [(1-r) \exp(-\beta s) + r]$ <p>Suction and net stress are defined as:</p> $s = \max((P_g - P_l), 0) \quad \sigma_n = \sigma_n^{total} - \max(P_g, P_l)$ <p>And the invariants are:</p> $p' = \frac{1}{3} (\sigma'_x + \sigma'_y + \sigma'_z) = p - \max(p_g, p_l) = J_1 / 3 - \max(p_g, p_l)$ $J_{2D} = \frac{1}{2} \text{trace}(\mathbf{s} : \mathbf{s}) = \frac{1}{3} q^2 \quad \mathbf{s} = \sigma' - p' \mathbf{I}$ $J_{3D} = s_x s_y s_z + 2\tau_{xy} \tau_{yz} \tau_{zx} - s_x \tau_{yz}^2 - s_y \tau_{xz}^2 - s_z \tau_{xy}^2$ <p>Hardening depends on viscoplastic volumetric strains according to:</p> $dJ_1^{0*} = \frac{1+e}{(\lambda(0)-\kappa)} J_1^{0*} d\varepsilon_v^{vp} \Leftrightarrow dp_o^* = \frac{1+e}{(\lambda(0)-\kappa)} p_o^* d\varepsilon_v^{vp} \Leftrightarrow \frac{dp_o^*}{p_o^*} = \frac{1+e}{\chi(0)} d\varepsilon_v^{vp}$ <p>which is equivalent to BBM model as shown.</p> <p>Note that, using $k_1 = 3k$, $k_2 = 3k$, $k_3 = 0$, $k_4 = 0$, and $F_s = 1$:</p> $F(q, p, s) = a \frac{1}{3} q^2 - \mu^2 \gamma 3^2 \left[-(p_o(s) + ks)^{2-n} (p + ks)^n + (p + ks)^2 \right]$ <p>In the same way, the viscoplastic potential is described as:</p> $G(q, p, s) = a \frac{1}{3} q^2 - b\mu^2 \gamma 3^2 \left[-(p_o(s) + ks)^{2-n} (p + ks)^n + (p + ks)^2 \right]$ <p>which incorporates a parameter to allow for non-associativity conditions.</p> <p>Strength can be considered also a function of suction:</p> $\mu(s) = \mu_{dry} - (\mu_{dry} - \mu_{sat}) \left(\frac{\mu_{sat}}{\mu_{dry}} \right)^s \quad (\mu_{sat} < \mu_{dry})$

PARAMETERS FOR ITYCL=1

ICL = 34 (Mechanical data 1 → VPUSR 1) ITYCL = 1

P1	Γ_o	$s^{-1} MPa^{-1}$	Fluidity = 1/Viscosity (for plasticity use a sufficiently large value)
P2	N		Power of the stress function (integer value)
P3	F_o	MPa^2	$F_o = 1 MPa^2$
P4	δ		$\Gamma = \Gamma_o \exp(\delta s)$
P5	b		Non associativity parameter.

ICL = 35 (Mechanical data 1 → VPUSR 2) ITYCL = 1

P1	n	-	Power in F and G (integer value)
P2	γ	-	Parameter in F and G
P3	β_s	-	Typical value 0 (then $F_s = 1$, and J_{3D} is not considered)
P4	m	-	Typical value -0.5, only required if $\beta_s \neq 0$
P5	μ_{DRY}	-	For some cases, $\mu = M_{DRY}$ corresponding approximately to Cam-Clay model.
P6	-	-	
P7	$(J_1^{o*})_F$	MPa	Positive value, initial size of F (note that this is the 1s invariant)
P8	$(J_1^{o*})_G$	MPa	Positive value, initial size of G (note that this is the 1st invariant)
P9	a	-	Parameter in F and G
P10	μ_{SAT}	-	For some cases $\mu = M_{SAT}$ corresponding approximately to Cam-Clay model.

ICL = 36 (Mechanical data 1 → VPUSR 3) ITYCL = 1

P1	κ	-	Elastic compression parameter
P2	$\lambda(0)$	-	Viscoplastic compression parameter
P3	r	-	Parameter in LC curve
P4	β	-	Parameter in LC curve
P5	p^c	MPa	Parameter in LC curve
P6	k_1	-	
P7	k_2	-	
P8	k_3	-	
P9	k_4	-	

This model has the following case that can be used:

	Cam-Clay model	Cap models
a	3	3
n	1	3,5,7,9
γ	-1/9	+1/9
k_1	0	0
k_2	-3 <i>k</i>	?
k_3	3 <i>k</i>	?
k_4	3 <i>p</i> _{s0}	?
μ	<i>M</i>	<i>M</i>

Parameters *k*, *p*_{s0} (see BBM). *M*: slope of critical state line

VISCOPLASTICITY FOR UNSATURATED SOILS AND ROCKS - VPUSR

CODES in <i>ROOT_gen.dat</i>	ICL = 34, 35, 36 (continued)
DESCRIPTION	Viscoplasticity (general model for unsaturated soils based on Desai and Perzyna theory).
EQUATIONS	<p>ICL = 36 (VPUSR 3), ITYCL = 2: The LC curve is defined in the following way:</p> $J_1^o(s) = \frac{3p_y \lambda^d(s) + J_1^{o*} (\lambda^i - \kappa)}{\lambda^i + \lambda^d(s) - \kappa} = 3J_y + \left(\frac{\lambda(0) - \kappa}{\lambda(s) - \kappa} \right) (J_1^{o*} - 3J_y)$ <p>and the form of the compressibility is: $\lambda(s) = \lambda(0) [(1-r) \exp(-\beta s) + r]$ Hardening depends on viscoplastic volumetric strains according to:</p> $dJ_1^{o*} = 3 \left(\frac{1}{\lambda(0) - k_{io}} \right) d\varepsilon_v^{vp}$ <p>ICL = 36 (VPUSR 3), ITYCL = 3: The LC curve is defined in the following way:</p> $J_1^o(s) = \frac{3p_y \lambda^d(s) + J_1^{o*} (\lambda^i - \kappa)}{\lambda^i + \lambda^d(s) - \kappa} = 3p_y + \left(\frac{\lambda^i - \kappa}{\lambda^i + \lambda^d(s) - \kappa} \right) (J_1^{o*} - 3p_y)$ <p>and the form of the compressibility is: $\lambda(s) = \lambda_i + \lambda_d(s)$; $\lambda_d(s) = \lambda_d - \alpha_s \ln \left(\frac{s+0.1}{0.1} \right)$ Hardening depends on viscoplastic volumetric strains according to:</p> $dJ_1^{o*} = 3 \left(\frac{1}{\lambda_i - k_{io}} \right) d\varepsilon_v^{vp}$ <p>For more details see Oldecop & Alonso, 2001.</p>

ICL = 36 (Mechanical data 1 → VPUSR 3); ITYCL = 2

P1	void	-	
P2	$\lambda(0) - \kappa = \chi(0)$	-	Viscoplastic compression parameter
P3	r	-	Parameter in LC curve
P4	β	-	Parameter in LC curve
P5	J_y	MPa	Parameter in LC curve
P6	k_1	-	
P7	k_2	-	
P8	k_3	-	
P9	k_4	-	
P10	aa		-

ICL = 36 (Mechanical data 1 → VPUSR 3); ITYCL = 3

	void	-	
P2	$\lambda_{i-\kappa}$	-	Viscoplastic compression parameter
P3	λ_d	-	Viscoplastic compression parameter
P4	α_s	-	Parameter $\lambda(s)$ curve
P5	p_y	MPa	Parameter in LC curve
P6	k_1	-	
P7	k_2	-	
P8	k_3	-	
P9	k_4	-	

VISCOPLASTICITY FOR UNSATURATED SOILS AND ROCKS - VPUSR

CODES in <i>ROOT_gen.dat</i>	ICL = 34, 35, 36 (continued)
DESCRIPTION	Viscoplasticity – Zero thickness element
EQUATIONS	<p>ICL = 34, 35, 36; ITYCL = 16 Viscoplastic constitutive model:</p> $\frac{d\varepsilon}{dt} = \Gamma \langle \phi(F) \rangle \frac{\partial G}{\partial \sigma'} \quad \phi(F) = \left(\frac{F}{F_o} \right)^N$ <p>- The yield function is defined as: $F = \tau^2 - (c' - \sigma' \tan \phi')^2$, where τ is the shear stress; c' is the effective cohesion, σ' is the net normal stress, $\tan \phi'$ is the tangent or internal friction angle and χ is the tensile strength.</p> <p>- Evolution of strength parameters with suction:</p> $c'_{0(\psi, \alpha_a)} = (c_0 + c_1 \psi) + (b_0 + b_1 \psi) (1 - e^{-b_2 \tan \alpha_a})$ $\tan \phi'_{0(\psi, \alpha_a)} = (\tan \phi_0 + t_1 \psi) + (d_0 + d_1 \psi) \tan \alpha_a$ <p>where $c'_{0(\psi, \alpha_a)}$ is the effective initial cohesion that changes with suction (ψ) and the asperity roughness angle (α_a) (Figure VIb.1); c_0 is the value of cohesion for $\psi = 0^\circ$ and $\alpha_a = 0^\circ$, c_1 is the slope of the cohesion-suction fit line for $\alpha_a = 0^\circ$ (Figure VIb.2). b_0 is an average value of cohesion for $\alpha_a = 15^\circ, 30^\circ, 45^\circ$ and b_1 is a parameter of the model that controls the increment of cohesion with suction for $\alpha_a = 15^\circ, 30^\circ, 45^\circ$. The term $(1 - e^{-b_2 \tan \alpha_a})$ controls the sharp increment of cohesion with α_a and b_2 is a parameter that controls the shape of the cohesion-α_a curve. $\tan \phi'_{0(\psi, \alpha_a)}$ is the tangent of the internal friction effective initial angle that depends of ψ and α_a (Figure VIb.3); $\tan \phi_0$ is the value of $\tan \phi'_0$ for $\psi = 0$ and $\alpha_a = 0^\circ$; t_1 is the slope of the $\tan \phi'_0 - \psi$ fit line for $\alpha_a = 0^\circ$ (Figure VIb.4); d_0 and d_1 are model parameters that control the increment of $\tan \phi'_0$ with suction for $\alpha_a = 5^\circ, 15^\circ, 30^\circ, 45^\circ$ and $\tan \alpha_a$ is the geometric tangent of the asperity roughness angle.</p> <p>- The softening is defined as:</p> $c' = c'_0 \left(1 - \frac{u_s^{vp}}{u_c^*} \right) \tan \phi' = \tan \phi'_0 - \left(\tan \phi'_0 - \tan \phi'_{res} \right) \frac{u_s^{vp}}{u_\phi^*}$ <p>where u_s^{vp} is the visco-plastic shear displacement; u_c^* is the critical value for shear displacement when $c'=0$; $\tan \phi'_{res}$ is the tangent of internal friction effective residual angle and u_ϕ^* is the critical value of shear displacement when $\tan \phi' = \tan \phi'_{res}$.</p> <p>- The viscoplastic potential is defined as:</p> $\frac{\partial G}{\partial \sigma} = \left[2 \tan \phi' (c' - \sigma' \tan \phi') f_\sigma^{dil} f_c^{dil}, 2\tau \right]^T$ $f_\sigma^{dil} = \chi_d \sqrt{\tan \alpha_a} \left(1 - \frac{ \sigma' }{q_u} \right) \exp \left(-\beta_d \frac{\sigma'}{q_u} \right) f_c^{dil} = \frac{c'}{c'_0}$ <p>where, q_u is the compression strength at which dilatancy vanishes; χ_d and β_d are model parameters.</p>

See the [APPENDIX VI.B.4. ZERO THICKNESS](#) for more information.

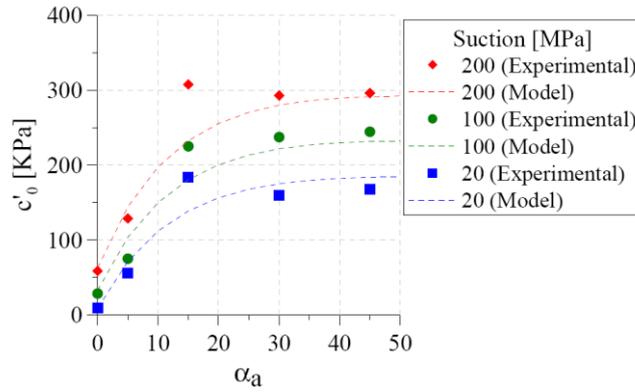


Figure VIb.1. Effective cohesion vs. α_a (Zandarin, 2010)

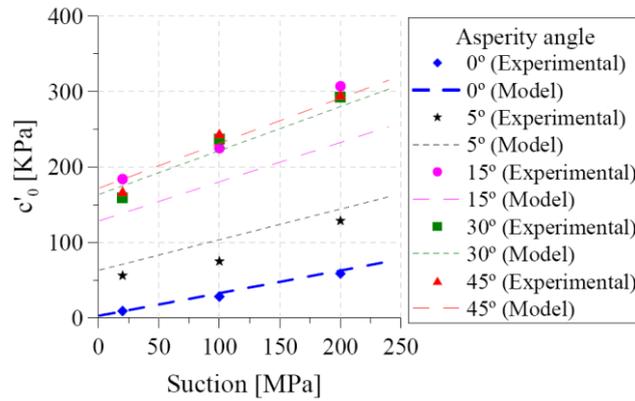


Figure VIb.2. Effective cohesion vs. suction (Zandarin, 2010)

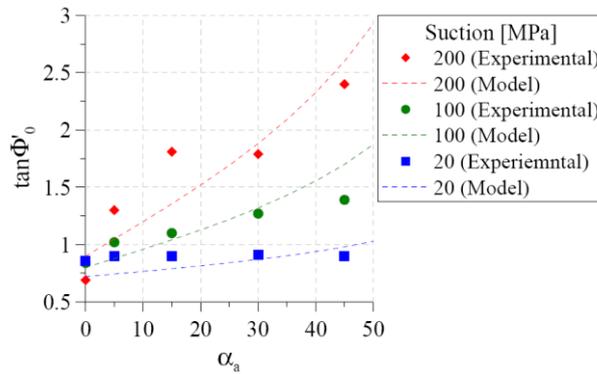


Figure VIb.3. Effective tangent of the internal friction angle vs. α_a (Zandarin, 2010)

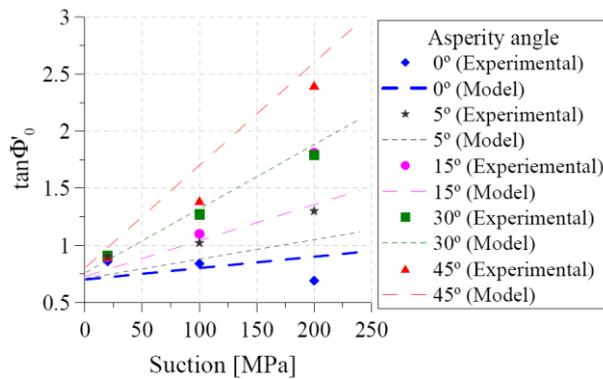


Figure VIb.4. Effective tangent of the internal friction angle vs. suction (Zandarin, 2010)

PARAMETERS FOR ITYCL=16

ICL = 34 (Mechanical data 1 → VPUSR 1); **ITYCL = 16**

P1	c_0	MPa	Initial cohesion
P2	ϕ_0	°	Initial friction angle
P3	-		
P4	ϕ_{res}	°	Residual friction angle
P5	u_c^*	m	Critical value of shear displacement for cohesion
P6	u_ϕ^*	m	Critical value of shear displacement for friction
P7	χ_d	-	Model parameter for dilatancy function
P8	β_d	-	Model parameter for dilatancy function
P9	α_a	°	Joint asperity angle
P10	q_u	MPa	Compression strength for which dilatancy vanishes

ICL = 35 (Mechanical data 1 → VPUSR 2); **ITYCL = 16**

P1-P2	-		
P3	Γ_o	1/s	Fluidity
P4	N		Power of the stress function (integer value)
P5	F_0	MPa	$F_0=1$ MPa (Default value)

ICL = 36 (Mechanical data 1 → VPUSR 3); **ITYCL = 16**

P1	c_1	MPa	Model parameter for evolution of cohesion with suction
P2	b_0	MPa	Model parameter for evolution of cohesion with suction
P3	b_1	-	Model parameter for evolution of cohesion with suction
P4	b_2	-	Model parameter for evolution of cohesion with suction
P5	t_1	-	Model parameter for evolution of friction angle with suction
P6	d_0	-	Model parameter for evolution of friction angle with suction
P7	d_1	-	Model parameter for evolution of friction angle with suction
P8	α_a	°	Joint asperity angle

HISTORY VARIABLES:

The VPUSR model (ICL = 34, 35, 36) requires four history variables:

Hist_var 1	$(J_1^{o*})_F$	MPa	Evolution of size of F (note that this is the 1s invariant)
Hist_var 2	$(J_1^{o*})_G$	MPa	Evolution of size of G (note that this is the 1st invariant)
Hist_var 3	EDP		Plastic deviatoric strain
Hist_var 4	EVP		Plastic volumetric strain

The first two variables can be assigned as initial conditions on *surfaces/volumes* if an initial particular distribution on the geometry is required. The procedure is the same followed by initial stresses as was described in chapter II. PREPROCESS, PROBLEM DATA, section II.2.3.5.

If no value is assigned for the first two variables in conditions, internally, the program sets the input parameters P7 (for $(J_1^{o*})_F$) and P8 (for $(J_1^{o*})_G$) of the ICL=35 (ITYCL=1), as initial values.

The evolution of the four history variables can be visualized as an output in Post-process GID interface.

Note: Effective stresses plotted in the Post-process GID interface correspond with net stresses for unsaturated conditions and Terzaghi's effective stresses for saturated conditions. Stress and strain invariants follow the soil mechanics notation (positive for compression).

An example of use of the elastic and viscoplastic models is presented in APPENDIX VI.B.5

CODE_BRIGHT. CONSTITUTIVE LAWS

This chapter contains the different models available and the corresponding parameters required by each model. The following constitutive laws are available:

<p>HYDRAULIC AND THERMAL CONSTITUTIVE MODELS (a) RETENTION CURVE INTRINSIC PERMEABILITY LIQUID PHASE RELATIVE PERMEABILITY GAS PHASE RELATIVE PERMEABILITY DIFFUSIVE FLUXES OF MASS DISPERSIVE FLUXES OF MASS AND ENERGY CONDUCTIVE FLUX OF HEAT</p>	<p>MECHANICAL CONSTITUTIVE MODELS ELASTICITY (b) NONLINEAR ELASTICITY (b) VISCOPLASTICITY FOR SALINE MATERIALS (b) VISCOPLASTICITY FOR SATURATED SOILS AND ROCKS (b) VISCOPLASTICITY - GENERAL (b) DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS (c) THERMO-ELASTOPLASTIC MODEL FOR SOILS (d) BARCELONA EXPANSIVE MODEL FOR SOILS (e) CASM's FAMILY MODELS (f)</p>
<p>PHASE PROPERTIES (a) SOLID PHASE PROPERTIES LIQUID PHASE PROPERTIES GAS PHASE PROPERTIES</p>	<p>EXCAVATION PROCESS (g)</p>

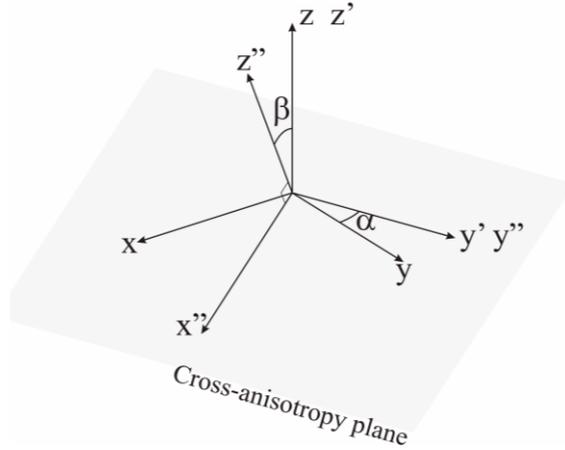
VI.c. DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS

MECHANICAL CONSTITUTIVE LAWS (part c)

ICL	NAME	ITYCL	DESCRIPTION
70	DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS	1,2,3	Damage orthotropic elastic model for the bonded material (1:linear damage law; 2:exponential damage law; 3:logarithmic damage law)
71	DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS	1,2,3	Linear Orthotropic elastic model parameters for the soil matrix. (1; MC; 2;HB, 3;Camclay)
72	DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS	1	Coupling behaviour. ITYCL = 0: bond behaviour is not activated
73	DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS	1,2,3	MC or HB or BBM for the clay matrix - shape in p-q diagram
74	DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS	1,2,3	MC or HB or BBM for the clay matrix - shape in deviatoric plane
75	DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS	1,2,3	MC or HB or BBM potential for the clay matrix - shape in p-q diagram
76	DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS	1,2,3	MC or HB or BBM plastic potential for the clay matrix - shape in the deviatoric plane
77	DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS	1,2,3	MC or HB or BBM Hardening law for clay matrix, used only if bond behaviour is not activated
78	DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS	1	Rate dependency parameters
79	DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS	1	Control parameters for SPA (Backward euler scheme)

DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS

CODES	ICL = 70 to 79 ITYCL = see below
DESCRIPTION	<p>Damage-elastoplastic model for argillaceous rock This model considers the argillaceous rock as a composite material made of a clay matrix interlocked by bond. Clay matrix behaviour is modeled through an elastoplastic constitutive law, typical of soils. Bonds are modeled through a damage elastic law (Carol <i>et al.</i>, 2001), typical of quasi-brittle materials. A coupling parameter gives the relative importance of clay and bond response for the composite material. This law applies to material having a response transitional between that of a soil and a rock.</p>
EQUATIONS	<p>For this model, equations are written assuming Soils Mechanics convention ($p > 0$, $\varepsilon_v > 0$, compression). p is the mean effective stress, J the square root of the second invariant of deviatoric stress tensor, θ the Lode' angle (-30° in triaxial compression, $+30^\circ$ in triaxial extension) (see ICL 21 to 27 for their definition).</p> <p>Clay matrix behaviour</p> <p>Elastic law: $d\sigma_{ij}^M = D_{ijkl}^{eM} \left(d\varepsilon_{kl}^M - \delta_{kl} \frac{ds}{K_s^M} - d\varepsilon_{kl}^p \right)$</p> <p>$\sigma_{ij}^M$ are the stresses prevailing at clay particles contact, D_{ijkl}^{eM} is the mechanical elastic stiffness matrix of the clay, $d\varepsilon_{kl}^M$ are the strains corresponding to the clay matrix deformation (equal to the external strains), K_s^M is the bulk modulus against suction changes (if any), $d\varepsilon_{kl}^p$ are the plastic strains of the clay matrix.</p> <p>2 elastic laws are considered:</p> <p><i>Orthotropic linear elasticity (ITYCL = 1, 2, 5, or 6):</i></p> <p>D_{ijkl}^{eM} is defined by clay matrix Young's moduli E^M_h and E^M_v and Poisson's ratio ν^M_h, ν^M_v, ν^M_{hv} and ν^M_{vh}. K_s^M is taken constant. Subscript h indicate value in the direction orthogonal to the orthotropy axis, subscript v along the orthotropy axis (and not necessarily along the horizontal plane and the vertical axis). The direction of orthotropy axis is indicated for each element in the file <root>_gri.dat by the two angles shown in the figure below.</p> <p>Value of E^M_h is computed as:</p> $E^M_h = \max(E^M_{h0}, E^M_{h1} p^M + E^M_{h2})$ <p>where E^M_{h0}, E^M_{h1} and E^M_{h2} are parameters of the model.</p>



Camclay type orthotropic elasticity (ITYCL = 3):

D_{ijkl}^{eM} is defined by clay matrix bulk modulus K_h^M and K_v^M and clay matrix Poisson's ratio ν_h^M , ν_v^M , ν_{hv}^M and ν_{vh}^M . Bulk modulus against stress changes is linearly dependent of the mean stress following the relationship:

$$K_h^M = \frac{(1+e)\sigma_h^M}{\kappa^M} \quad K_v^M = \frac{(1+e)\sigma_v^M}{\kappa^M}$$

Bulk modulus against suction changes is linearly dependent of the mean stress following the relationship:

$$K_s^M = \frac{(1+e)(s + p_{atm})}{\kappa_s^M}$$

e is the void ratio, κ^M and κ_s^M the slopes of the unloading/reloading and drying/wetting lines in the planes $e-\ln p^M$ and $e-\ln(s + p_{atm})$, respectively. p_{atm} is the atmospheric pressure and is taken equal to 0.1 MPa.

Yield function: 5 yield criteria are considered:

Mohr-Coulomb (ITYCL = 1):

$$F^p = \left(\cos \theta^M + \frac{1}{\sqrt{3}} \sin \theta^M \sin \phi^{iM} \right) J^M - \sin \phi^i (p^M + p_i^M) \geq 0$$

$p_i^M = c^{iM} \cot \phi^{iM}$ is clay matrix tensile strength, c^{iM} clay matrix cohesion, ϕ^{iM} clay matrix friction angle.

Cohesion depends on suction following the law:

$$c^{iM}(s) = c^{iM}(0) + s \tan \phi_b^M$$

Hoek & Brown (1980) (ITYCL = 2):

$$F^p = \frac{4 \sin^2 \left(\theta^M - \frac{\pi}{6} \right)}{R_c^M} J^{M2} - \frac{2 m^M \sin \theta^M}{\sqrt{3}} J^M - m^M (p^M + p_t^M) \geq 0$$

$p_t^M = R_c^M / m^M$ is clay matrix tensile strength, R_c^M clay matrix uniaxial compressive strength, m^M a parameter defining the shape of the parabolic yield criterion.

R_c^M depends on suction following the law:

$$R_c^M(s) = R_c^M(0) \left[(1 - r^M) \exp(-\beta^M s) + r^M \right]$$

BBM model (ITYCL = 3):

$$F^p = J^{M2} - \frac{M^{M2}}{3} (p^M + p_t^M)(p^M - p_0^M) \geq 0$$

where p_t^M is the clay matrix tensile strength, p_0^M the clay matrix isotropic yield locus and M the slope of the critical state line in the $p^M - vq^M$ diagram. The following dependencies on suction are considered:

$$p_t^M = k^M s$$

$$p_0^M = p_c^M \left(\frac{p_0^{*M}}{p_c^M} \right)^{\frac{\lambda^M(0) - \kappa^M}{\lambda^M(s) - \kappa^M}} \quad \text{with} \quad \lambda^M(s) = \lambda^M(0) \left[(1 - r^M) + r e^{-\beta^M s} \right]$$

Anisotropic Mohr-Coulomb (ITYCL = 5):

$$F^p = \left(\cos \theta^{*M} + \frac{1}{\sqrt{3}} \sin \theta^{*M} \sin \phi'^M \right) J^{*M} - \sin \phi'^M (p^{*M} + p_t^M) \geq 0$$

$p_t^M = c'^M \cot \phi'^M$ is clay matrix tensile strength, c'^M clay matrix cohesion, and ϕ'^M clay matrix friction angle.

In this case the invariants p^{*M} , J^{*M} , and θ^{*M} are computed from the rotated and scaled anisotropic stress tensor defined as:

$$\boldsymbol{\sigma}^* = \begin{bmatrix} \frac{\sigma_{11}^r}{c_N} & c_S \sigma_{12}^r & \sigma_{13}^r \\ c_S \sigma_{12}^r & c_N \sigma_{22}^r & c_S \sigma_{23}^r \\ \sigma_{13}^r & c_S \sigma_{23}^r & \frac{\sigma_{33}^r}{c_N} \end{bmatrix} \quad \boldsymbol{\sigma}^r = \mathbf{a} \boldsymbol{\sigma}^* \mathbf{a}^T \quad \mathbf{a} = \begin{bmatrix} \cos \beta & \sin \beta & 0 \\ -\sin \beta & \cos \beta & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos \alpha & 0 & -\sin \alpha \\ 0 & 1 & 0 \\ \sin \alpha & 0 & \cos \alpha \end{bmatrix}$$

where c_N and c_S are scaling factors and α and β the two angles defining the direction of the orthotropy axis.

Hyperbolic Mohr-Coulomb (*ITYCL* = 6):

$$F^p = \sqrt{\frac{J^M}{f_2(\theta^M)} + (c'^M + p_t^M \tan \phi'^M)^2} - (c'^M + p_t^M \tan \phi'^M) \geq 0$$

$$f_2(\theta^M) = \alpha^\theta (1 + \beta^\theta \sin 3\theta^M)^{n^\theta}$$

p_t^M is clay matrix tensile strength, c'^M clay matrix cohesion, and ϕ'^M clay matrix friction angle.

Strength anisotropy is included by assuming that c'^M and p_t^M depend on the relative orientation between bedding and principal effective stress (δ):

$$c'^M = \Omega(\delta) c'_0{}^M$$

$$p_t^M = \Omega(\delta) p_{t0}^M$$

where $c'_0{}^M$ and p_{t0}^M are the values measured with the major principal stress normal to bedding, and δ is the angle between the normal to bedding and the major principal stress. The function proposed by Conesa et al. (2018) is used for $\Omega(\delta)$, defined as (with Ω_{90} , Ω_m , δ_m , and \hat{n} material parameters):

$$\Omega = \frac{\hat{A}e^{(\delta_m - \delta)\hat{n}}}{[1 + e^{(\delta_m - \delta)\hat{n}}]^2} + \frac{\hat{B}}{1 + e^{(\delta_m - \delta)\hat{n}}} + \hat{C}$$

where:

$$\hat{A} = \frac{2(e_1 + 1)(e_2 + 1)(e_1 - e_2 + \Omega_{90} + e_1 e_2 + e_1 \Omega_{90} - e_2 \Omega_{90} - 2e_1 \Omega_m + 2e_2 \Omega_m - e_1 e_2 \Omega_{90} - 1)}{(e_1 - e_2)(e_1 - 1)(e_2 - 1)}$$

$$\hat{B} = \frac{\Omega_{90} - \frac{\hat{A}e_1}{(e_1 + 1)^2} + \frac{\hat{A}e_2}{(e_2 + 1)^2} - 1}{\frac{1}{e_1 + 1} - \frac{1}{e_2 + 1}}$$

$$\hat{C} = 1 - \frac{\hat{A}e_2}{(e_2 + 1)^2} - \frac{\hat{B}}{e_2 + 1}$$

$$e_1 = e^{(\delta_m - 90)\hat{n}}$$

$$e_2 = e^{\hat{n}\delta_m}$$

Deviatoric plane: Mohr Coulomb and Hoek & Brown yield criteria present corners in the deviatoric plane. They are smoothed using Sloan & Booker (1986) procedure. Lode's angle θ at which smoothing starts must be defined (see ICL = 74).

Rate dependency: Rate dependency is introduced as a visco-plastic mechanism. Plastic multiplier λ^p is expressed as a function of the distance between the current clay matrix stress point and the inviscid plastic locus:

$$d\lambda^p = \frac{dt}{\eta^M} \langle F^p \rangle$$

where dt is the time increment, η^M is the clay matrix viscosity and $\langle \rangle$ are the Macauley brackets. Inviscid plastic locus takes the form:

$$\bar{F}^p = F^p - \frac{\eta^M}{dt} d\lambda^p \leq 0$$

where F^p can be either the Mohr Coulomb or Hoek & Brown yield criterion.

Plastic potential: A non associated plastic potential in the p-q diagram is defined for each yield criterion. In the deviatoric plane, plastic potential is considered associated.

Mohr-Coulomb (ITYCL = 1):

$$G^p = \left(\cos \theta^M + \frac{1}{\sqrt{3}} \sin \theta^M \sin \phi'^M \right) J^M - \omega^M \sin \phi' (p^M + p_t^M)$$

p_t^M , c'^M and ϕ'^M are parameters defining the yield criterion. ω^M is a parameter defining the non associativity of the flow. It takes a value equal to 1 when associated and equal to 0 for null dilatancy.

Hoek & Brown (ITYCL = 2):

$$G^p = \frac{4 \sin^2 \left(\theta^M - \frac{\pi}{6} \right)}{R_c^M} J^{M2} - \frac{2 m^M \sin \theta^M}{\sqrt{3}} J^M - m^M (p^M + p_t^M)$$

p_t^M , R_c^M and m^M are parameters defining the yield criterion. ω^M is a parameter defining the non associativity of the flow. It takes a value equal to 1 when associated and equal to 0 for null dilatancy.

Barcelona Basic Model (ITYCL = 3):

$$G^p = J^{M^2} - \varpi^M \frac{M^{M^2}}{3} (p^M + p_t^M)(p^M - p_0^M)$$

p_t^M , p_0^M and M^M are parameters defining the yield criterion. ω^M is a parameter defining the non associativity of the flow. It takes a value equal to 1 when associated and equal to 0 for null dilatancy. To respect the condition of null lateral strain during K_0 -loading, ω^M must be set to:

$$\varpi^M = \frac{M^M (M^M - 9)(M^M - 3)}{9(6 - M^M)} \frac{1}{1 - \kappa^M / \lambda^M(0)}$$

Anisotropic Mohr-Coulomb (ITYCL = 5):

$$G^p = \left(\cos \theta^{*M} + \frac{1}{\sqrt{3}} \sin \theta^{*M} \sin \phi'^M \right) J^{*M} - \omega^M \sin \phi'^M (p^{*M} + p_t^M)$$

p_t^M , c'^M and ϕ'^M are parameters defining the yield criterion. ω^M is a parameter defining the non associativity of the flow. It takes a value equal to 1 when associated and equal to 0 for null dilatancy.

Hyperbolic Mohr-Coulomb (ITYCL = 6):

$$G^p = \sqrt{\frac{J^M}{f_2(\theta^M)} + (c'^M + p_t^M \tan \phi'^M)^2} - \omega^M (c'^M + p^M \tan \phi'^M)$$

p_t^M , c'^M and ϕ'^M are parameters defining the yield criterion. ω^M is a parameter defining the non associativity of the flow. It takes a value equal to 1 when associated and equal to 0 for null dilatancy.

Hardening law:

Mohr-Coulomb (ITYCL = 1):

A softening law is introduced through the following dependency of the tensile strength on the plastic strain:

$$p_t^M = c'^M \cotan \phi'^M$$

with

$$c'^M = c'_{\text{peak}}^M \quad \text{if } \varepsilon_{eq}^{pM} < \xi_{rc0}^M$$

$$c'^M = c'_{\text{peak}}^M + \frac{c'_{\text{peak}}^M (1 - \alpha^M)}{(\xi_{rc}^M - \xi_{rc0}^M)} (\varepsilon_{eq}^{pM} - \xi_{rc0}^M) \quad \text{if } \xi_{rc0}^M \leq \varepsilon_{eq}^{pM} \leq \xi_{rc}^M$$

$$c'^M = \alpha^M c'_{\text{peak}}^M \quad \text{if } \xi_{rc}^M < \varepsilon_{eq}^{pM}$$

and

$$\phi'^M = \phi'_{\text{peak}}^M \quad \text{if } \varepsilon_{eq}^{pM} < \xi_{r\phi0}^M$$

$$\phi'^M = \phi'_{\text{peak}}^M + \frac{\phi'_{\text{peak}}^M (1 - \beta^M)}{(\xi_{r\phi}^M - \xi_{r\phi 0}^M)} (\varepsilon_{eq}^{pM} - \xi_{r\phi 0}^M) \quad \text{if } \xi_{r\phi 0}^M \leq \varepsilon_{eq}^{pM} \leq \xi_{r\phi}^M$$

$$\phi'^M = \beta^M \phi'_{\text{peak}}^M \quad \text{if } \xi_{r\phi}^M < \varepsilon_{eq}^{pM}$$

$\alpha^M = c'_{\text{res}}{}^M / c'_{\text{peak}}{}^M$ is a brittleness parameter for the cohesive component, $\beta^M = \phi'_{\text{res}}{}^M / \phi'_{\text{peak}}{}^M$ is a brittleness parameter for the frictional component, ε_{eq}^{pM} is the equivalent plastic strain, ξ_{rc0}^M the accumulated equivalent plastic strain at which the cohesion starts to degrade, ξ_{rc}^M the accumulated equivalent plastic strain at which the residual cohesion $c_{\text{res}}{}^M$ is reached, $\xi_{r\phi 0}^M$ the accumulated equivalent plastic strain at which the friction angle starts to degrade, $\xi_{r\phi}^M$ the accumulated equivalent plastic strain at which the residual friction angle $\phi'_{\text{res}}{}^M$ is reached. $\alpha^M = \beta^M = 1$ means perfect plasticity, $\alpha^M = \beta^M = 0$, total strength degradation (residual cohesion and friction angle equal to 0).

Hoek & Brown (ITYCL = 2):

A softening law is introduced through the following dependency of the tensile strength on the plastic strain:

$$p_t^M = \frac{R_{c0}^M}{m^M} \left[1 - (1 - \alpha^M) \frac{\max(\varepsilon_1^{pM}, \xi_r^M)}{\xi_r^M} \right]^2$$

R_{c0}^M is the intact strength, α^M a brittleness parameter, ε_1^{pM} is the major principal plastic strain, ξ_r^M the accumulated major principal plastic strain at which the residual strength $\alpha^M R_{c0}^M$ is reached. α^M is related to the intact and residual uniaxial compressive strength R_{c0}^M and R_{cres}^M by the formula:

$$\alpha^M = \sqrt{\left(\frac{R_{cres}^M}{R_{c0}^M} \right)^2 + \frac{2}{3} m^M \frac{R_{cres}^M}{R_{c0}^M}}$$

$\alpha^M = 1$ means perfect plasticity, $\alpha^M = 0$, total degradation (residual strength equal to 0). $\alpha^M > 1$ means hardening plasticity while $\alpha^M < 1$ means softening plasticity.

Barcelona Basic Model (ITYCL = 3):

The hardening/softening law is introduced through the following dependency of the saturated isotropic yield locus on the plastic strain:

$$\frac{dp_0^*{}^M}{p_0^*{}^M} = \frac{(1+e)}{\lambda^M - \kappa^M} d\varepsilon_v^{pM}$$

Anisotropic Mohr-Coulomb (ITYCL = 5):

A hardening-softening law is introduced through the following dependency of cohesion and friction angle on the plastic strain:

$$\begin{aligned} \phi'^M &= \phi_i + \varepsilon_{eq}^{pM} \left[a_h + \frac{\varepsilon_{eq}^{pM}}{\xi_1} \left(\frac{\xi_1}{\phi_p - \phi_i} - a_h \right) \right]^{-1} & \text{if } \varepsilon_{eq}^{pM} \leq \xi_1 \\ \phi'^M &= \phi_p & \text{if } \xi_1 < \varepsilon_{eq}^{pM} \leq \xi_2 \\ \phi'^M &= \phi_p - (\varepsilon_{eq}^{pM} - \xi_2) \left[a_s + \frac{\varepsilon_{eq}^{pM} - \xi_2}{\xi_3 - \xi_2} \left(\frac{\xi_3 - \xi_2}{\phi_p - \phi_r} - a_s \right) \right]^{-1} & \text{if } \xi_2 < \varepsilon_{eq}^{pM} \leq \xi_3 \\ \phi'^M &= \phi_r & \text{if } \varepsilon_{eq}^{pM} > \xi_3 \end{aligned}$$

and

$$c'^M = c_p \frac{\tan \phi'^M}{\tan \phi_p}$$

where ϕ_i , ϕ_p , and ϕ_r are the initial, peak, and residual friction angles, c_p is the peak cohesion, ξ_1 , ξ_2 , and ξ_3 are the equivalent plastic strains at which the maximum strength is reached, the softening begins, and the residual strength is reached respectively, and a_h and a_s are parameters controlling the curvature of the hardening and softening branches.

Hyperbolic Mohr-Coulomb (ITYCL = 6):

A hardening-softening law is introduced through the following dependency of the strength parameters on the plastic strain:

$$\begin{aligned} \tan \phi'^M &= \tan \phi_i + \varepsilon_{eq}^{pM} \left[a_\phi + \frac{\varepsilon_{eq}^{pM}}{\xi_p} \left(\frac{\xi_p}{\tan \phi_p - \tan \phi_i} - a_\phi \right) \right]^{-1} & \text{if } \varepsilon_{eq}^{pM} \leq \xi_p \\ \tan \phi'^M &= \tan \phi_p - (\tan \phi_p - \tan \phi_r) \left[1 - e^{-b_\phi (\varepsilon_{eq}^{pM} - \xi_p)} \right] & \text{if } \varepsilon_{eq}^{pM} > \xi_p \\ c_0'^M &= c_{0\text{ ini}} & \text{if } \varepsilon_{eq}^{pM} \leq \xi_p \\ c_0'^M &= (c_{0\text{ ini}} - c_{0\text{ post}}) e^{-b_{\text{post}} (\varepsilon_{eq}^{pM} - \xi_p)} + c_{0\text{ post}} e^{-b_{\text{res}} (\varepsilon_{eq}^{pM} - \xi_p)} & \text{if } \varepsilon_{eq}^{pM} > \xi_p \\ p_{t0}'^M &= p_{t0\text{ ini}} & \text{if } \varepsilon_{eq}^{pM} \leq \xi_p \\ p_{t0}'^M &= (p_{t0\text{ ini}} - p_{t0\text{ post}}) e^{-b_{\text{post}} (\varepsilon_{eq}^{pM} - \xi_p)} + p_{t0\text{ post}} e^{-b_{\text{res}} (\varepsilon_{eq}^{pM} - \xi_p)} & \text{if } \varepsilon_{eq}^{pM} > \xi_p \end{aligned}$$

where ϕ_i , ϕ_p , and ϕ_r are the initial, peak, and residual friction angles, $c_{0\text{ ini}}$ and $c_{0\text{ post}}$ are the initial and post-rupture cohesion, $p_{t0\text{ ini}}$ and $p_{t0\text{ post}}$ are the initial and post-rupture tensile strength, ξ_p is the equivalent plastic strains at which the maximum strength is reached, and a_ϕ , b_ϕ , b_{post} , and b_{res} are parameters controlling the curvature of the hardening and softening branches.

A post-rupture ratio is defined so that the post-rupture parameters are a function of the initial ones:

$$r_{\text{post}} = \frac{c_{0\text{ post}}}{c_{0\text{ ini}}} = \frac{p_{t0\text{ post}}}{p_{t0\text{ ini}}}$$

A nonlocal regularization can be employed to simulate localised deformations. The local state variable ε_{eq}^{pM} is replaced by its nonlocal counterpart, computed as:

$$\widetilde{\varepsilon}_{eq}^{pM} = \int_V \omega(\mathbf{X}, \boldsymbol{\kappa}) \varepsilon_{eq}^{pM}(\boldsymbol{\kappa}) d\boldsymbol{\kappa}$$

where V stands for volume and ω is a weighting function controlling the importance of neighbouring points as a function of its position ($\boldsymbol{\kappa}$) relative to the position of the actual point under consideration (\mathbf{X}). The weighting function is defined in the following normalised form:

$$\omega(\mathbf{X}, \boldsymbol{\kappa}) = \frac{\omega_0(\|\mathbf{X} - \boldsymbol{\kappa}\|)}{\int_V \omega_0(\|\mathbf{X} - \boldsymbol{\Upsilon}\|) d\boldsymbol{\Upsilon}}$$

where ω_0 is characterized by the expression proposed by Galavi and Schweiger (2010):

$$\omega_0 = \frac{\|\mathbf{X} - \boldsymbol{\kappa}\|}{l_s} e^{-\left(\frac{\|\mathbf{X} - \boldsymbol{\kappa}\|}{l_s}\right)^2}$$

where l_s is a material parameter introducing an internal length scale to the material behaviour.

Creep deformations: 3 different additional time-dependent creep models can be defined in ICL = 77.

For ITYCL=1, or 2, creep strains are computed explicitly at the beginning of the time step and they are not coupled in the hardening-softening law. The additional creep model can be used with any of the yield criteria described before.

For ITYCL=3, creep strains are coupled with the plastic component, and can mobilise the strength. This is achieved by computing the equivalent plastic strain ε_{eq}^p as the sum of the plastic and creep strains. Only available for the Hyperbolic Mohr-Coulomb yield criteria

Creep model 1 (ITYCL = 1):

Creep strains increments are computed as:

$$d\boldsymbol{\varepsilon}^c = \dot{\boldsymbol{\varepsilon}}^c dt \quad \dot{\boldsymbol{\varepsilon}}^c = \frac{2}{3} \gamma_c \frac{\langle q - q_{thr} \rangle^{n_c}}{q} (1 - \varepsilon_{eq}^c)^{m_c} \mathbf{s}$$

where dt is the time increment, $\dot{\boldsymbol{\varepsilon}}^c$ is the creep strain rate tensor, \mathbf{s} is the deviatoric stress tensor, $q = \left(\frac{3}{2} \mathbf{s} : \mathbf{s}\right)^{1/2}$, ε_{eq}^c is the state variable for the creep component ($\varepsilon_{eq}^c = \left(\frac{2}{3} \boldsymbol{\varepsilon}^c : \boldsymbol{\varepsilon}^c\right)^{1/2}$), γ_c , n_c and m_c are material parameters, and q_{thr} is a deviatoric stress threshold at which creep strains are activated.

Creep model 2 (ITYCL = 2):

Creep strains increments are computed as:

$$d\boldsymbol{\varepsilon}^c = \dot{\boldsymbol{\varepsilon}}^c dt$$

$$\dot{\boldsymbol{\varepsilon}}^c = \begin{cases} 0 & \text{if } \varepsilon_{eq}^p \leq \varepsilon_{thr} \\ \gamma^c e^{-a^c \varepsilon_{eq}^c} (\mathbf{s} + \psi^c p^M \mathbf{I}) & \text{if } \varepsilon_{eq}^p > \varepsilon_{thr} \end{cases}$$

where dt is the time increment, $\dot{\boldsymbol{\varepsilon}}^c$ is the creep strain rate tensor, \mathbf{s} is the deviatoric stress tensor, ε_{eq}^c is the state variable for the creep component ($\varepsilon_{eq}^c = (\boldsymbol{\varepsilon}^c : \boldsymbol{\varepsilon}^c)^{1/2}$), γ^c , a^c and ψ^c are material parameters, and ε_{thr} is a threshold defining the level of non-elastic deformation at which creep deformations are activated.

Creep model coupled with Hyperbolic Mohr-Coulomb (ITYCL = 3):

Creep strains increments are computed as in ITYCL=2.

Bond behaviour

Elastic law:

$$d\sigma_{ij}^b = D_{ijkl}^{eb} (d\varepsilon_{kl}^b - d\varepsilon_{kl}^d)$$

D_{ijkl}^{eb} is the secant damaged elastic matrix. It is related to the secant undamaged elastic tensor D_{ijkl}^{eb0} by $D_{ijkl}^{eb} = e^{-L} D_{ijkl}^{eb0}$. L is the damage variable, related to the ratio of bond microcracks area over the whole bond area. D_{ijkl}^{eb0} is defined by the undamaged bond Young's modulus E_b and bond Poisson's ratio ν_b through the classical linear orthotropic elasticity.

Damage locus: Damage locus is defined as an energy threshold

$$F^d = \frac{1}{2} \sigma_{ij}^b \varepsilon_{ij}^b - r^b(s)$$

r^b is the value of energy threshold that depends on suction following:

$$r^b(s) = r^b + r_{0s}^b s$$

r_{0s}^b is a parameter which controls the change of bond damage locus with suction.

Rate dependency: Rate dependency is introduced as a delayed microcracking and use the visco-damage formalism. Damage variable is expressed as a function of the distance between the current bond stress point and the infinitely slow damage locus:

$$dL = \frac{dt}{\eta^b} \langle F^d \rangle$$

where dt is the time increment, η_b is the bond viscosity and $\langle \rangle$ are the Macauley brackets. Infinitely low damage locus takes the form:

$$\bar{F}^d = F^d - \frac{\eta^b}{dt} dL \leq 0$$

Damage rule: Damage rule gives the evolution of damage strain $d\varepsilon_{kl}^d$ with damage variable L . This relation is constrained by bond elastic moduli evolution and must take the form: $d\varepsilon_{kl}^d = \varepsilon_{kl}^b dL$

Damage evolution law: It gives the evolution of damage locus r_b with damage variable L . Three different expressions may be considered:

a) linear: $r^b = r_0^b + r_1^b L$

a) exponential: $r^b = r_0^b \exp^{r_1^b L}$

a) logarithm: $r^b = r_0^b + r_1^b \ln L$

r_0 is the damage of the intact material and r_1 a parameter giving the rate of evolution (higher value of r_1 gives lower damage rate). r_1 is taken function of suction following: $r_1^b = r_{10}^b + r_{1s}^b s$

r_{10}^b is a parameter which controls the damage evolution rate for the saturated bond material and r_{1s}^b is a parameter which controls the change of damage evolution rate with suction.

Coupling behaviour: Coupling comes from the restrictions that local strain ε_{ij}^M and ε_{ij}^b must be compatible with the external strain ε_{ij} and local stresses σ_{ij}^M and σ_{ij}^b must be in equilibrium with external stresses σ_{ij} .

These restrictions read: $d\varepsilon_{ij}^M = d\varepsilon_{ij} + d\varepsilon_{ij}^b$

$$\sigma_{ij} = (1 + \chi) \sigma_{ij}^M + \chi \sigma_{ij}^b \quad \text{with} \quad \chi = \chi_0 e^{-L/2}$$

L is the damage variable and χ_0 a coupling parameter that gives the relative importance of bond and clay matrix behaviour in the overall response of the composite material. $0 \leq \chi_0 \leq \infty$.

Since this model requires a substantial number of parameters, several ICL's are included in Mechanical Data 3:

Argillite Bonding (ICL = 70) contains elastic parameters for the bonding.

Argillite Matrix (ICL = 71) contains elastic parameters for the soil matrix.

Argillite – Coupling (ICL = 72) contains parameters for the coupling between bonding and soil matrix.

Argillite – Yield vol (ICL = 73) contains parameters for the shape of the yield function in the p - q plane (soil matrix).

Argillite – Yield dev (ICL = 74) contains parameters for the shape of the yield function in the deviatoric plane (soil matrix).

Argillite – Plastic vol (ICL = 75) contains parameters for the shape of the plastic potential in the p - q plane (soil matrix).

Argillite – Plastic dev (ICL = 76) contains parameters for the shape of the plastic potential in the deviatoric plane (soil matrix).

Argillite – Hardening (ICL = 77) contains parameters for the hardening law (soil matrix).

Argillite – Visco (ICL = 78) contains parameters for the viscoplastic model (bonding and soil matrix) and the additional time-dependent creep models (soil matrix).

Argillite – Control parameters (ICL = 79) contains parameters to control the integration of the constitutive law.

PARAMETERS FOR **ARGILLITE BONDING** ICL = 70 (Damage orthotropic elastic model for **the bond material**). ITYCL = 1: Linear damage evolution law. ITYCL = 2: exponential damage evolution law. ITYCL = 3: logarithm damage evolution law.

P1	E^b_h	MPa	Young's modulus for the bond material in the plane orthogonal to the direction of orthotropy If P6 = 0 or 1 (no anisotropy), isotropic Young's modulus
P2	ν^b_h	-	Poisson's ratio for the bond material in the plane orthogonal to the direction of orthotropy If P6 = 0 or 1 (no anisotropy), isotropic Poisson's ratio
P3	r^b_{I0}	MPa	Damage evolution rate for the saturated bond material
P4	r^b_{0s}	MPa	Change of bond damage locus with suction
P5	$r^b_{I_s}$	MPa	Change of bond damage evolution rate with suction
P6	$E^b_h / E^b_v = \nu^b_{hv} / \nu^b_{vh}$	-	Ratio of anisotropy (ratio between the value of Young's modulus for bond material in the direction perpendicular and parallel to the orthotropy axis). If P6 = 0, a default value equal to 1 (no anisotropy) is assigned to this parameter.
P7	ν^b_{hv}	-	Cross Poisson's ratio of the bond material ($\nu^b_{hv} = d\varepsilon^b_h / d\varepsilon^b_v$)
P8	G_v	MPa	Shear modulus of the bond material along the axis of orthotropy (ratio $d\varepsilon_h / d\varepsilon_v$)
P9	K^b_s	MPa	Bulk modulus against suction changes for the bond material (considered isotropic)

PARAMETERS FOR ARGILLITE MATRIX ICL = 71; ITYCL = 1, 2, 5, or 6 (Linear orthotropic elastic model for the soil matrix)

P1	E_h^M*	MPa	Young's modulus for the saturated matrix in the plane orthogonal to the direction of orthotropy. If P6 = 0 or 1 (no anisotropy), isotropic Young's modulus.
P2	ν_h^M	-	Poisson's ratio in the plane orthogonal to the direction of orthotropy. If P6 = 0 or 1 (no anisotropy), isotropic Poisson's ratio.
P3	K_s^M	MPa	Bulk modulus against suction changes (considered isotropic).
P4	E_s^M	-	Coefficient setting the change of E with suction according to the equation $E_h^M = E_h^M* + E_s^M s$
P5	-	-	Void
P6	$E_h^M / E_v^M = \nu_{hv}^M / \nu_{vh}^M$	-	Ratio of anisotropy (ratio between the value of Young's modulus in the direction perpendicular and parallel to the orthotropy axis). If P6 = 0, a default value equal to 1 (no anisotropy) is assigned to this parameter.
P7	ν_{hv}^M	-	Cross Poisson's ratio ($\nu_{hv}^M = d\varepsilon_h^M / d\varepsilon_v^M$)
P8	$G_{vh}^M = G_{hv}^M$	MPa	Cross shear modulus ($G_{vh}^M = d\tau_{vh} / d\gamma_{vh}$)
P9	E_{Ih}^M	-	Coefficient giving the change of the Young's modulus with the stress in the plane orthogonal to the direction of orthotropy.
P10	E_{2h}^M	MPa	Value of Young modulus in the plane orthogonal to the direction of orthotropy at null mean (net or effective) stress.

PARAMETERS FOR ARGILLITE MATRIX ICL = 71 (Elastic model for the soil matrix);
 ITYCL = 3 (Orthotropic Camclay type elastic model for the soil matrix)

P1	κ^M		Slope of the unloading-reloading line in the $e - \ln(\sigma_h)$ model If P6 = 0 or 1 (no anisotropy), Slope of the unloading-reloading line in the $e - \ln(p)$ model.
P2	ν^M_h	-	Poisson's ratio in the plane orthogonal to the direction of orthotropy. If P6 = 0 or 1 (no anisotropy), isotropic Poisson's ratio.
P3	κ^M_s	MPa	Slope of the wetting-redrying line in the $e - \ln(s + p_{atm})$ model (considered isotropic).
P4		-	Void
P5	-	-	Void
P6	$K^M_h / K^M_v = \nu^M_{hv} / \nu^M_{vh}$	-	Ratio of anisotropy (ratio between the value of bulk modulus in the direction perpendicular and parallel to the orthotropy axis). If P6 = 0, a default value equal to 1 (no anisotropy) is assigned to this parameter.
P7	ν^M_{hv}	-	Cross Poisson's ratio ($\nu^M_{hv} = d\varepsilon^M_h / d\varepsilon^M_v$)
P8	G_{vh}	MPa	Cross shear modulus $G^M_{vh} = d\tau_{vh} / d\gamma_{vh}$

PARAMETERS FOR ARGILLITE – COUPLING ICL = 72; ITYCL = 1 (Coupling behaviour).

P1	χ_0	-	Coupling parameter between bond and matrix.
P2	B	-	Biot coefficient
P3	-	-	void
P4	-	-	void
P5	iunsat	-	Flag to indicate stress concept in unsaturated conditions: 0 – Biot stress $p^b = p - B p^l$ 1 – Biot/Bishop stress $p^b = p - [1 - S_r + B S_r] p^l$
P6	b	-	Parameter to compute porosity as a function of damage multiplier (λ^d) as $\phi^b = \phi + \chi_0 \cdot b \cdot \sqrt{1 - \exp(-\lambda^d)}$ This porosity is then used to compute intrinsic permeability of Kozeny's model (ICL=7, ITYCL=1).
P7	α	-	Parameter to compute intrinsic permeability as a function of plastic multiplier (λ^p) as $k = k \exp[\alpha(\lambda^p - \lambda^p_{thr})]$ k : intrinsic permeability computed in ICL = 7
P8	λ^p_{thr}	-	Parameter to compute intrinsic permeability as a function of plastic multiplier (λ^p) as $k = k \exp[\alpha(\lambda^p - \lambda^p_{thr})]$ k : intrinsic permeability computed in ICL = 7

P9	$b_{s//}$	C^{-1}	Linear thermal expansion coefficient for the medium (isotropic or parallel, positive value).
P10	$b_{s\perp}$	C^{-1}	Linear thermal expansion coefficient for the medium (perpendicular, positive value).

PARAMETERS FOR ARGILLITE – COUPLING ICL = 72; ITYCL = 2 (Coupling behaviour).

P1 – P6	Same as in ICL = 72; ITYCL = 1		
P7	β^k	-	Parameter to compute intrinsic permeability as a function of equivalent plastic strains (ε_{eq}^p) as $\mathbf{k} = \mathbf{k} [1 + \beta^k (\varepsilon_{eq}^p - \varepsilon_{thr}^p)]$
P8	ε_{thr}^p	-	Parameter to compute intrinsic permeability as a function of equivalent plastic strains (ε_{eq}^p) as $\mathbf{k} = \mathbf{k} [1 + \beta^k (\varepsilon_{eq}^p - \varepsilon_{thr}^p)]$
P9 – P10	Same as in ICL = 72; ITYCL = 1		

PARAMETERS FOR ARGILLITE – YIELD VOL ICL = 73; ITYCL = 1 (Mohr Coulomb criterion **for the soil matrix** – shape in p^M - q^M diagram).

P1	ϕ'^M	°	Friction angle
P2	c'^M	MPa	Cohesion
P3	ϕ^{bM}	°	Coefficient setting the change in cohesion with suction following: $c'^M = s \tan(\phi^{bM})$
P4	β^M	MPa ⁻¹	Coefficient setting the change in friction angle with suction.

PARAMETERS FOR ARGILLITE – YIELD VOL ICL = 73; ITYCL = 2 (Hoek & Brown criterion **for the soil matrix** – shape in p^M - q^M diagram).

P1	m^M	-	Ratio of uniaxial compressive strength divided by tensile strength.
P2	R_c^M	MPa	Uniaxial compressive strength at the reference temperature (P8 field).
P3	r^M	-	Coefficient setting the change in cohesion with suction.
P4	β^M	MPa ⁻¹	Coefficient setting the change in cohesion with suction.
P5	-	-	Void
P6	-	-	Void
P7	k_T^M		Coefficient setting the decrease of uniaxial compressive strength with temperature.
P8	T_0		Reference temperature.

PARAMETERS FOR ARGILLITE – YIELD VOL ICL = 73; ITYCL = 3 (Basic Barcelona model criterion **for the soil matrix** – shape in p^M - q^M diagram).

P1	M^M	-	Slope of the critical state line.
P2	-	-	Void
P3	r^M	-	Coefficient setting the change in cohesion with suction.
P4	β^M	MPa ⁻¹	Coefficient setting the change in cohesion with suction
P5	p_c^M	MPa	Reference pressure
P6	k_s^M	-	Coefficient setting the increase of tensile strength with suction.

PARAMETERS FOR ARGILLITE – YIELD VOL ICL = 73; ITYCL = 5 (Anisotropic Mohr Coulomb criterion **for the soil matrix** – shape in p^M - q^M diagram).

P1	ϕ_p	°	Friction angle (peak)
P2	c_p	MPa	Cohesion (peak)
P3	-	-	Void
P4	-	-	Void
P5	c_N	-	Stress tensor scaling factor
P6	c_S	-	Stress tensor scaling factor

PARAMETERS FOR ARGILLITE – YIELD VOL ICL = 73; ITYCL = 6 (Hyperbolic Mohr Coulomb criterion **for the soil matrix** – shape in p^M - q^M diagram).

P1	ϕ_i	°	Friction angle (initial)
P2	ϕ_p	°	Friction angle (peak)
P3	ϕ_r	°	Friction angle (residual)
P4	$c_{0\ ini}$	MPa	Cohesion (initial)
P5	$p_{t0\ ini}$	MPa	Tensile strength (initial)
P6	-	-	Void
P7	Ω_{90}	-	Strength anisotropy parameter
P8	Ω_m	-	Strength anisotropy parameter
P9	\hat{n}	-	Strength anisotropy parameter
P10	δ_m	°	Strength anisotropy parameter

PARAMETERS FOR ARGILLITE – YIELD DEV ICL = 74; ITYCL = 1, 2, 3, 5 (Mohr Coulomb, Hoek & Brown, Basic Barcelona model, Anisotropic Mohr Coulomb, or Hyperbolic Mohr Coulomb criteria **for the soil matrix** – shape in deviatoric plane).

P1	θ^M	o	Lode angle value at which corner smoothing function is tangent to Mohr Coulomb envelope (typical value – not default – 25°).
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PARAMETERS FOR ARGILLITE – YIELD DEV ICL = 74; ITYCL = 6 (Hyperbolic Mohr Coulomb criterion **for the soil matrix** – shape in deviatoric plane).

P1	α^θ	-	Parameter to compute $f_2(\theta^M)$
P2	β^θ	-	Parameter to compute $f_2(\theta^M)$
P3	n^θ	-	Parameter to compute $f_2(\theta^M)$

PARAMETERS FOR ARGILLITE – PLASTIC VOL ICL = 75; ITYCL = 1, 2, 3, 5, 6 (Mohr Coulomb, Hoek & Brown, Basic Barcelona model, Anisotropic Mohr Coulomb, or Hyperbolic Mohr Coulomb plastic potential **for the soil matrix** – shape in p^M - q^M diagram).

P1	ω^M	-	Coefficient of non associativity (0: no volumetric plastic strain, 1: full volumetric plastic strain –associative plasticity).
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PARAMETERS FOR ARGILLITE – PLASTIC DEV ICL = 76; ITYCL = 1, 2, 3, 5, 6 (Mohr Coulomb, Hoek & Brown, Basic Barcelona model, Anisotropic Mohr Coulomb, or Hyperbolic Mohr Coulomb plastic potential **for the soil matrix** – considered associated in the deviatoric plane).

P1 - P10	Void
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PARAMETERS FOR ARGILLITE – HARDENING ICL = 77; ITYCL = 1 (Mohr Coulomb hardening law for clay matrix).

P1	α^M	-	Cohesion brittleness index: $\alpha^M = \frac{c_{res}^M}{c_{peak}^M}$
P2	ξ_{rc}^M	-	Equivalent plastic strain at which c^M starts to degrade.
P3	ξ_{rc}^M	-	Equivalent plastic strain at which c'_{res}^M is reached.
P4	β^M	-	Friction angle brittleness index: $\beta^M = \frac{\phi_{res}^M}{\phi_{peak}^M}$
P5	$\xi_{r\phi}^M$	-	Equivalent plastic strain at which ϕ^M starts to degrade.
P6	$\xi_{r\phi}^M$	-	Equivalent plastic strain at which ϕ'_{res}^M is reached.

PARAMETERS FOR ARGILLITE – HARDENING ICL = 77; ITYCL = 2 (Hoek & Brown hardening law **for the soil matrix**).

P1	α^M	-	Brittleness index: $\alpha^M = \sqrt{\left(\frac{R_{cres}^M}{R_{c0}^M}\right)^2 + \frac{2}{3} m^M \frac{R_{cres}^M}{R_{c0}^M}}$
P2	ξ^{rM}	-	Brittleness interval: ξ^{rM} is the major compressive plastic strain value ($ \epsilon ^{pM}$) at which R_{cres}^M is reached.

PARAMETERS FOR ARGILLITE – HARDENING ICL = 77; ITYCL = 3 (Basic Barcelona model does not need additional parameter for the hardening law for clay matrix).

P1	$\lambda^M(0)$	-	Slope of the virgin loading line in the e-ln(pM) diagram.
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PARAMETERS FOR ARGILLITE – HARDENING ICL = 77; ITYCL = 5 (Anisotropic Mohr Coulomb hardening law for clay matrix).

P1	β_{ini}	-	Initial to peak friction angle ratio: $\beta_{ini} = \frac{\phi_i}{\phi_p}$
P1	β_{res}	-	Residual to peak friction angle ratio: $\beta_{res} = \frac{\phi_r}{\phi_p}$
P3	a_h	-	Parameter controlling the curvature of the hardening branche.
P4	a_s	-	Parameter controlling the curvature of the softening branche.
P5	ξ_1	-	Equivalent plastic strain at which the maximum strength is reached.
P6	ξ_2	-	Equivalent plastic strain at which the softening begins.
P7	ξ_3	-	Equivalent plastic strain at which the residual strength is reached.

PARAMETERS FOR ARGILLITE – HARDENING ICL = 77; ITYCL = 6 (Hyperbolic Mohr Coulomb hardening law for clay matrix).

P1	ξ_p	-	Equivalent plastic strain at which the maximum strength is reached.
P1	a_ϕ	-	Parameter controlling the curvature of the hardening branche.
P3	b_ϕ	-	Parameter controlling the curvature of the softening branche.
P4	b_{res}	-	Parameter controlling the curvature of the softening branche.
P5	b_{post}	-	Parameter controlling the curvature of the softening branche.
P6	r_{post}	-	Post-rupture ratio: $r_{post} = \frac{c_{0\ post}}{c_{0\ ini}} = \frac{p_{to\ post}}{p_{to\ ini}}$
P7-P9	-	-	Void
P10	l_s	m	Non-local internal length (if = 0, non-local model deactivated)

PARAMETERS FOR ARGILLITE – VISCO ICL = 78; ITYCL = 1 (Rate dependency parameters – Creep model 1).

P1	η^b	MPa.s	Bond viscosity
P2	η^M	MPa.s	Matrix viscosity
P3	q_{thr}	MPa	Deviatoric stress threshold at which creep strains are activated.
P4	γ_c	day ⁻¹	Creep strain rate parameter
P5	n_c	-	Creep strain rate parameter
P6	m_c	-	Creep strain rate parameter

PARAMETERS FOR ARGILLITE – VISCO ICL = 78; ITYCL = 2 (Rate dependency parameters – Creep model 2).

P1	η^b	MPa.s	Bond viscosity
P2	η^M	MPa.s	Matrix viscosity
P3	ϵ_{thr}	-	Threshold defining the level of non-elastic deformation at which creep deformations are activated.
P4	γ_c	MPa ⁻¹ s ⁻¹	Creep strain rate parameter
P5	a^c	-	Creep strain rate parameter
P6	ψ^c	-	Creep strain rate parameter

PARAMETERS FOR ARGILLITE – VISCO ICL = 78; ITYCL = 3 (Rate dependency parameters – Creep model 2 coupled with Hyperbolic Mohr Coulomb).

P1 – P6	Same as in ICL = 78; ITYCL = 2		
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PARAMETERS FOR ARGILLITE – CONTROL PARAMETERS ICL = 79; ITYCL = 1 (Control parameter for the Stress Point Algorithm – Backward-Euler scheme is used).

P1	tol	-	Tolerance over SPA residual (typical value – not default – 1.e-8)
P2	$itmax$	-	Number of SPA Newton Raphson iterations at which local subincrementation is performed (typical value – not default – 30)
P3	$isubmax$	-	Maximum number of local (SPA) subincrementations by global iteration (typical value – not default – 500)
P4	$iJac$	-	Flag to define the type of F.E. elementary tangent matrix to use: 1 – elastic matrix -1 – elastoplastic tangent matrix (typical value –not default)

Important notes:

1. Damage only, elasticity only, elastoplasticity only or coupled damage-elastoplasticity can be defined depending on the combinations of ITYCL used. They are:

	ICL = 70	ICL = 71	ICL = 73
Damage only	ITYCL = 1, 2, or 3	ITYCL = 0	ITYCL = 0
Elasticity only	ITYCL = 0	ITYCL = 1, 2, 3, 5, or 6	ITYCL = 0
Plasticity only	ITYCL = 0	ITYCL = 1, 2, 3, 5, or 6	ITYCL = 1 for Mohr Coulomb ITYCL = 2 for Hoek & Brown ITYCL = 3 for Basic Barcelona model ITYCL = 5 for Anisotropic Mohr Coulomb ITYCL = 6 for Hyperbolic Mohr Coulomb
Coupled damage-elasto-plasticity	ITYCL = 1, 2, or 3	ITYCL = 1, 2, 3, 5, or 6	ITYCL = 1 for Mohr Coulomb ITYCL = 2 for Hoek & Brown ITYCL = 3 for Basic Barcelona model ITYCL = 5 for Anisotropic Mohr Coulomb ITYCL = 6 for Hyperbolic Mohr Coulomb

2. Inviscid damage or elastoplasticity can be defined by setting $\eta^b = 0$ and $\eta^M = 0$ (or ITYCL = 0 for ICL = 78)
3. ITYCL for ICL = 74 to 77 are automatically set to the value of ITYCL for ICL = 73.

HISTORY VARIABLES

Argillite model requires in total 35 history variables. They are listed in the following table.

Variable 1 is the history variable of the elastoplastic model for the matrix. In the most general case, value for this variable need to be specified in the input file (see format in the Part III).

In the case of Mohr Coulomb model ($ITYCL(73) = 1$), variable 1 corresponds to the tensile strength of the material p_t . If a null value is specified in the input file for this variable, the program will compute the value of the tensile strength for each element from the cohesion and the friction angle of the material assigned to the element. The expression used to compute the default value is: $p_t = c' \cotan\phi'$.

In the case of Hoek & Brown model ($ITYCL(73) = 2$), variable 1 corresponds to the tensile strength of the material p_t . If a null value is specified in the input file from this variable, the program will compute the value of the tensile strength for each element from the uniaxial compressive strength R_c and the parameter m of the material assigned to the element. The expression used to compute the default value is: $p_t = R_c / m$.

In the case of Cam clay model ($ITYCL(73) = 3$), variable 1 corresponds to the preconsolidation pressure of the material p_0^* . IF A NULL VALUE IS SPECIFIED IN THE INPUT FILE FOR THIS VALUE, THE PROGRAM WILL ABORT DUE TO A MATH ERROR (this ellipse of Cam clay model degenerates into a point).

Variable 2 is the history variable of the damage model for the bond. In the most general case, value for this variable need to be specified in the input file (see format in the Part III). However, in many cases, this value can be set to 0. It means that damage will start for any stress changes.

Variable 3 is used internally to keep memory of the type of constitutive matrix (elastic, tangent elastoplastic, tangent damage or tangent damage elastoplastic) used to build the global tangent stiffness. No input from the user is associated to this variable.

Variable 4 is the plastic multiplier of the matrix. This variable measures the amount of plastic strain. It is usually set to 0 at the beginning of the computation and updated within the argillite subroutine. This variable is used only by the user for output visualization purposes (it provides the spatial distribution of plastic strain intensity within the mesh at any output time).

Variable 5 is the damage multiplier of the bonds. This variable measures the amount of damage. It is usually set to 0 at the beginning of the computation and updated within the argillite subroutine. This variable is used by the user for output visualization purposes only (it provides the spatial distribution of damage intensity within the mesh at any output time).

Variables 6 to 11 are the current stresses within the bonds. **Variables 12 to 17** are the stresses within the matrix at time of bond formation. In the most general case, all these variables have to be specified in the input file*. However, from a practical point of view, most of the problems can be run setting these values to 0 at the beginning of the computation (in this case, the damage locus is centered on the initial stress state at the beginning of the computation).

Variables 18 to 35 contain the total, plastic and damage strain tensor components. They are usually set to 0 at the beginning of the computation and updated within the argillite subroutine. These variables are used by the user for output visualization purposes only (they provides the spatial distribution of the total, plastic and damage strain within the mesh at any output time).

Hist var	Symbol	Unit	Description	Type
1	p_t p_0^*	MPa	Matrix Tensile strength (Mohr Coulomb or Hoek & Brown models, ITCL(73)=1,2). Isotropic yield point (Camclay model, ITYCL(73)=3)	Input
2	r_0	MPa	Bond damage locus	Input
3	$flag$	–	Type of tangent matrix	Internal
4	λ^p	–	Plastic multiplier	Output
5	λ^d	–	Damage multiplier	Output
6 to 11	σ^b	MPa	Initial bond stress vector ($\sigma_{xy}^b, \sigma_{yz}^b, \tau_{xy}^b, \tau_{xz}^b, \tau_{yz}^b$)	Input
12 to 17	σ^0	MPa	Matrix stress vector at time of bond formation ($\sigma_{xy}^0, \sigma_{yz}^0, \tau_{xy}^0, \tau_{xz}^0, \tau_{yz}^0$)	Input
18 to 23	ϵ		Strain vector ($\epsilon_{xy}, \epsilon_{yz}, \gamma_{xy}, \gamma_{xz}, \gamma_{yz}$)	Output
24 to 29	ϵ^p		Plastic strain vector ($\epsilon_{xy}^p, \epsilon_{yz}^p, \gamma_{xy}^p, \gamma_{xz}^p, \gamma_{yz}^p$)	Output
30 to 35	ϵ^d		Damage strain vector ($\epsilon_{xy}^d, \epsilon_{yz}^d, \gamma_{xy}^d, \gamma_{xz}^d, \gamma_{yz}^d$)	Output

A summary of the different options for history variables input is summarized in the following table.

Type of input of history variables	Characteristics of the problem		
All variables = 0	Mohr Coulomb ITYCL(73) = 1 Tensile strength is constant within each material and computed from cohesion and friction angle	Hoek & Brown ITYCL(73) = 2 Tensile strength is constant within each material and computed from uniaxial compressive strength and parameter m	Cam clay model ITYCL(73) = 3 NOT POSSIBLE
	Damage locus is centred on the initial stress state of the problem. Material is not damaged at time 0 of the computation. From $t=0$, damage occurs for any stress changes		
Variable 1 \neq 0 Variable 2 = 0 Variable 6 to 17 = 0	Mohr Coulomb ITYCL(73) = 1 Tensile strength can vary from element to element and is equal to the specified value for Variable 1	Hoek & Brown ITYCL(73) = 2 Tensile strength can vary from element to element and is equal to the specified value for Variable 1	Cam clay model ITYCL(73) = 3 Preconsolidation pressure can vary from element to element and is equal to the specified value for Variable 1
	Damage locus is centred on the initial stress state of the problem. Material is not damaged at time 0 of the computation. Damage occurs for any stress changes		

	Mohr Coulomb	Hoek & Brown	Cam clay model
Variable 1 \neq 0	ITYCL(73) = 1	ITYCL(73) = 2	ITYCL(73) = 3
Variable 2 \neq 0	Tensile strength can vary from element to element and is equal to the specified value for Variable 1	Tensile strength can vary from element to element and is equal to the specified value for Variable 1	Preconsolidation pressure can vary from element to element and is equal to the specified value for Variable 1
Variable 6 to 17 \neq 0	<p>Damage locus is centred on the stress state at time of bond stress state of the problem. It reflects the history of damage previous to time 0 of the computations.</p> <p>Damage occurs only when the energy input to the material is equal to the specified value for Variable 2</p>		

Variables 3, 4 and 18 to 35 can be specified in the input file when the history of plastic and damage strain previous to the current computations is wanted to be reproduced (particularly in case of restart).

CODE_BRIGHT. CONSTITUTIVE LAWS

This chapter contains the different models available and the corresponding parameters required by each model. The following constitutive laws are available:

<p>HYDRAULIC AND THERMAL CONSTITUTIVE MODELS (a) RETENTION CURVE INTRINSIC PERMEABILITY LIQUID PHASE RELATIVE PERMEABILITY GAS PHASE RELATIVE PERMEABILITY DIFFUSIVE FLUXES OF MASS DISPERSIVE FLUXES OF MASS AND ENERGY CONDUCTIVE FLUX OF HEAT</p>	<p>MECHANICAL CONSTITUTIVE MODELS ELASTICITY (b) NONLINEAR ELASTICITY (b) VISCOPLASTICITY FOR SALINE MATERIALS (b) VISCOPLASTICITY FOR SATURATED SOILS AND ROCKS (b) VISCOPLASTICITY - GENERAL (b) DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS (c) THERMO-ELASTOPLASTIC MODEL FOR SOILS (d) BARCELONA EXPANSIVE MODEL FOR SOILS (e) CASM's FAMILY MODELS (f)</p>
<p>PHASE PROPERTIES (a) SOLID PHASE PROPERTIES LIQUID PHASE PROPERTIES GAS PHASE PROPERTIES</p>	<p>EXCAVATION PROCESS (g)</p>

VI.d. THERMO-ELASTOPLASTIC MODEL

MECHANICAL CONSTITUTIVE LAWS (part d)

ICL	NAME	ITYCL	DESCRIPTION
21	THERMOELASTOPLASTIC MODEL FOR UNSATURATED SOILS	1	Contain elastic parameters
22	THERMOELASTOPLASTIC MODEL FOR UNSATURATED SOILS	1	Contain parameters for the thermal terms
23	THERMOELASTOPLASTIC MODEL FOR UNSATURATED SOILS	1	Contain plastic parameters
24	THERMOELASTOPLASTIC MODEL FOR UNSATURATED SOILS	1	Contain plastic parameters (2)
25	THERMOELASTOPLASTIC MODEL FOR UNSATURATED SOILS	1,2,3	Contain parameters for the function gy (Mohr-Coulomb function, van Eeckelen function, Von mises)
26	THERMOELASTOPLASTIC MODEL FOR UNSATURATED SOILS	1,2,3	Contain parameters for the function gp (Mohr-Coulomb function, van Eeckelen function, Von mises)
27	THERMOELASTOPLASTIC MODEL FOR UNSATURATED SOILS	1	Contain parameters for the integration of the model

THERMO-ELASTOPLASTIC MODEL FOR SOILS

CODES in <i>ROOT_gen.dat</i>	ICL = 21 to 27 ITYCL = see below
DESCRIPTION	Thermo-elastoplastic model for unsaturated soils
EQUATIONS	<p>For this model, equations are written assuming Soils Mechancis compression ($p > 0$, $\varepsilon_v > 0$, compression).</p> <p>The mechanical constitutive equation takes the incremental general form:</p> $d\boldsymbol{\sigma}' = \mathbf{D}d\boldsymbol{\varepsilon} + \mathbf{h}ds$ <p>This equation is derived from: $d\boldsymbol{\varepsilon} = d\boldsymbol{\varepsilon}^e + d\boldsymbol{\varepsilon}^p = (\mathbf{D}^e)^{-1}d\boldsymbol{\sigma}' + \alpha\mathbf{I}ds + \Lambda \frac{\partial G}{\partial \boldsymbol{\sigma}'}$</p> <p>where an elasto-plastic constitutive law has been selected that is based on a generalized yield surface that depends not only on stresses but on suction as well: $F = F(\boldsymbol{\sigma}', \varepsilon_v^p, s)$</p> <p>Volumetric strain is defined as: $\varepsilon_v = \varepsilon_x + \varepsilon_y + \varepsilon_z$</p> <p>and ε_v^p is the plastic volumetric strain.</p> <p>Using stress invariants this equation depends on: $F = F(p', J, \theta, \varepsilon_v^p, s)$</p> <div style="margin-left: 20px;"> <p>where</p> $\begin{cases} p' = \frac{1}{3}(\sigma'_x + \sigma'_y + \sigma'_z) = p - \max(p_g, p_l) \\ J = \sqrt{\frac{1}{2} \text{trace}(\mathbf{s} : \mathbf{s})} & \mathbf{s} = \boldsymbol{\sigma}' - p'\mathbf{I} \\ \theta = -\frac{1}{3} \sin^{-1}(1.5\sqrt{3} \det \mathbf{s} / J^3) \quad (\text{Lode's angle}) \end{cases}$ </div> <p>where \mathbf{I} is the identity tensor.</p> <p>For simplicity, a form of the classical Modified Cam-Clay model is taken as the reference isothermal saturated constitutive law:</p> $F = \frac{3J^2}{g_y} - L_y^2 (p' + p_s)(p_o - p') = 0$ <p>where g_y is a function of the Lode angle and $L_y = M / g_y _{\theta=-\pi/6}$</p> <p>$P_o$, is considered dependent on suction:</p> $p_o = p^c \left(\frac{p_o^*(T)}{p^c} \right)^{\frac{\lambda(o)-k_{io}}{\lambda(s)-k_{io}}}$ $p_o^*(T) = p_o^* + 2(\alpha_1 \Delta T + \alpha_3 \Delta T \Delta T)$ $\lambda(s) = \lambda(o) \left[(1-r) \exp(-\beta s) + r \right]$ $p_s = p_{s0} + k s \exp(-\rho \Delta T), \quad \Delta T = T - T_{ref}$ <p>Hardening depends on plastic volumetric strain according to:</p> $dp_o^* = \frac{1+e}{\lambda(0) - k_{io}} p_o^* d\varepsilon_v^p$

EQUATIONS
(continuation)

The plastic potential is taken as:

$$G = \alpha \frac{3J^2}{g_p} - L_p^2 (p' + p_s)(p_o - p')$$

where g_p is a function of the Lode angle and

$$L_p = M / g_p \Big|_{\theta = -\pi/6}$$

α is a non-associativity parameter.

The variation of stress-stiffness with suction and, especially, the variation of swelling potential with stress and suction have been considered. Elastic component of the model (volumetric strains):

$$d\varepsilon_v^e = \frac{k_i(s)}{1+e} \frac{dp'}{p'} + \frac{k_s(p',s)}{1+e} \frac{ds}{s+0.1} + (\alpha_o + 2\alpha_2 \Delta T) dT$$

where:

$$k_i(s) = k_{io} \left(1 + \alpha_{is} s + \alpha_{il} \ln \left(\frac{s+0.1}{0.1} \right) \right)$$

$$k_s(p',s) = k_{so} \left(1 + \alpha_{sp} \ln p'/p_{ref} \right) \exp(\alpha_{ss} s)$$

Moreover, if $\alpha_{sp} = 777$ (flag), then:

$$\kappa_s = k_{s0} \exp(\alpha_{ss} s) \ln \left(\frac{p}{p_{ref}} \right) / \ln \left(\frac{p_{swell}}{p_{ref}} \right)$$

$$p_{swell}(\text{MPa}) = \frac{10^{c_0 + c_1 \rho_{dry} + c_2 \rho_{dry}^2}}{1000}$$

For deviatoric elastic strains, a constant Poisson's ratio is used.

Strain-dependent shear modulus model (for small strains)

Evolution of the small-strain shear stiffness G with shear strain:

$$G(\gamma) = \frac{G_0}{1 + \alpha \frac{\gamma}{\gamma_{0.7}}} \quad G_0 = G_0^{ref} \left(\frac{p}{0.1} \right)^n$$

Where G_0^{ref} is the initial shear modulus at a reference mean stress (p) of 0.1 MPa (default = 0), γ is the invariant of the deviatoric strain tensor and $\gamma_{0.7}$ is the shear strain at which the modulus G is $0.722 \cdot G_0$ (approximately $0.7 \cdot G_0$).

In order to “activate” this model, then G_0^{ref} (ICL=22; ITYCL=1; P7) and $\gamma_{0.7}$ (ICL=22; ITYCL=1; P8) must be greater than 0.

Since this model requires a substantial number of parameters, several ICL's are included:

TEP – Elastic parameters (ICL = 21) contains elastic parameters (ITYCL = 1).

TEP – Thermal and other parameters (ICL = 22) contains other parameters (ITYCL = 1).

TEP – Plastic parameters 1 (ICL = 23) contains plastic parameters (ITYCL = 1).

TEP – Plastic parameters 2 (ICL = 24) contains parameters for different aspects (ITYCL = 1).

TEP – Parameters Shape Yield Surf. (ICL = 25) contains parameters for the function g_y (ITYCL = 1, 2, 3).

TEP – Parameters Shape Plastic Pot. (ICL = 26) contains parameters for the function g_p (ITYCL = 1, 2, 3).

TEP – Integration Control Parameters (ICL = 27) contains parameters for the integration of the model (ITYCL = 1).

PARAMETERS FOR ICL = 21 (TEP Elastic Parameters); ITYCL = 1

P1	κ_{io}	-	Initial (zero suction) elastic slope for specific volume-mean stress.
P2	κ_{so}	-	Initial (zero suction) elastic slope for specific volume-suction.
P3	K_{min}	MPa	Minimum bulk module.
P4	-	-	
P5	ν	-	Poisson's ratio ($-1 < \nu < 0.5$).
P6	α_{ss}	-	Parameter for κ_s (only for expansive material).
P7	α_{il}	-	Parameter for κ_i (only for expansive material).
P8	α_i	-	Parameter for κ_i (only for expansive material).
P9	α_{sp}	-	Parameter for κ_s (only for expansive material).
P10	p_{ref}	MPa	Reference mean stress (only for expansive material).

PARAMETERS FOR ICL = 22 (TEP Thermal and Other Parameters); ITYCL = 1

P1	α_o	C^{-1}	Parameter for elastic thermal strain
P2	α_l	$MPa C^{-1}$	Parameter for plastic thermal strain
P3	α_2	C^{-2}	Parameter for elastic thermal strain
P4	α_3	$MPa C^{-2}$	Parameter for plastic thermal strain
P5	T_{ref}	C	Reference temperature
P6	b	-	Biot coefficient (default value = 1)
P7	G_0^{ref}	MPa	Initial shear modulus at a reference mean stress (p) of 0.1 MPa (default = 0). If $P7 = 0 \Rightarrow G$ obtained from bulk modulus and Poisson's ratio. If $P8 = 0 \Rightarrow G = G_0^{ref}$ (default = 0). If $P8 > 0 \Rightarrow$ Strain-dependent shear modulus model is used.
P8	$\gamma_{0.7}$	-	Shear strain at which the modulus G is $0.722 \cdot G_0$
P9	a	-	Parameter (default value = 0.385)
P10	n	-	Parameter (default value = 0.2)

PARAMETERS FOR ICL = 23 (TEP Plastic Parameters 1); ITYCL = 1

P1	$\lambda(\theta)$		Slope of void ratio - mean stress curve at zero suction
P2	r		Parameter defining the maximum soil stiffness
P3	β	MPa ⁻¹	Parameter controlling the rate of increase of soil stiffness with suction
P4	ρ	C ⁻¹	Parameter that takes into account decrease of tensile strength due to temperature
P5	k		Parameter that takes into account increase of tensile strength due to suction
P6	p_{s0}	MPa	Tensile strength in saturated conditions

PARAMETERS FOR ICL = 24 (TEP Plastic Parameters 2); ITYCL = 1

P1	p^c	MPa	Reference pressure
P2	M		Critical state line parameter
P3	α		Non-associativity parameter
P4	e_o		Initial void ratio
P5	p_o^*	MPa	Initial preconsolidation mean stress for saturated soil
P8	c_0		Parameter in the swelling pressure function
P9	c_1		Parameter in the swelling pressure function
P10	c_2		Parameter in the swelling pressure function

Note P8-P9-P10 are taken into account only if $\alpha_{sp} = 777$ (ICL = 21; ITYCL = 1; P9)

PARAMETERS FOR ICL = 25 (TEP Parameters Shape Yield Surf.); ITYCL = 1

Mohr Coulomb function: $g_y(\theta) = \sin\phi / (\cos\phi + 0.577\sin\theta \sin\phi)$

P1	ϕ	deg	
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PARAMETERS FOR ICL = 25 (TEP Parameters Shape Yield Surf.); ITYCL = 2

van Eeckelen function: $g_y(\theta) = X/Y \sin 3\theta^Z$

P1	X		
P2	Y		
P3	Z		

PARAMETERS FOR ICL = 25 (TEP Parameters Shape Yield Surf.); ITYCL = 3

Von Mises (default option): $g_y(\theta) = 1$

PARAMETERS FOR ICL = 26 (TEP Parameters Shape Plastic Pot.); ITYCL = 1

Mohr Coulomb function: $g_p(\theta) = \sin\phi / (\cos\phi + 0.577\sin\theta \sin\phi)$

P1	ϕ	deg	
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PARAMETERS FOR ICL = 26 (TEP Parameters Shape Plastic Pot.); ITYCL = 2
 van Eeckelen function: $g_p(\theta) = X/Y \sin 3\theta^{-Z}$

P1	X		
P2	Y		
P3	Z		

PARAMETERS FOR ICL = 26 (TEP Parameters Shape Plastic Pot.); ITYCL = 3
 Von Mises (default option): $g_p(\theta) = 1$

PARAMETERS FOR ICL = 27 (TEP Integration Control Parameters); ITYCL = 1

P1	<i>Tole1</i>	Yield surface tolerance (typically 1.e-8).
P2	<i>Tole2</i>	Elastic integration tolerance (typically between 1.e-4 and 1.e-6).
P3	<i>Tole3</i>	Plastic integration tolerance (typically between 1.e-4 and 1.e-2).
P4	μ	Integration weight (ranges from 0 to 1) (typically 1).
P5	<i>Index</i>	-1 elastoplastic matrix (typical value). +1 elastic matrix.
P6	<i>Itermaxc</i>	Maximum allowed subincrementations. When this value is reached, the execution continues even if stress errors are large. Default=100. Note that if $Itermaxc > Itermaxs$ this condition is not used.
P7	<i>Itermaxs</i>	Maximum allowed subincrementations. When this value is reached, the stress and stiffness matrices calculation stops and the time step is reduced. A message about the type of problem encountered appears. Default=10.
P10	<i>Index2</i>	Indicator of stress option: (0: net stress; 1: Bishop's stress)

The integration procedure is based on an incremental scheme. A second-order integration procedure is used in order to obtain an integration error estimation. μ is considered as a weight in the evaluation of second-order integration matrix and vectors.

HISTORY VARIABLES:

The Thermo-elastoplastic (ICL = 21 to 27) model requires two history variables:

Hist_var 1	P_o^*	MPa	Evolution of preconsolidation mean stress for saturated soil
Hist_var 2	e_o		Evolution of void ratio

These variables can be assigned as initial conditions on *surfaces/volumes* if an initial particular distribution on the geometry is required. The procedure is the same as followed by initial stresses as was described in chapter II. PREPROCESS, PROBLEM DATA, section II.2.3.5. If no value is assigned for these variables in conditions, internally, the program sets the input parameters P4 (for e_o) and P5 (for P_o^*) of the ICL=24, as initial values.

The evolution of P_o^* can be visualized as an output in Post-process GID interface.

Note: Effective stresses plotted in the Post-process GID interface correspond with net stresses for unsaturated conditions and Terzaghi's effective stresses for saturated conditions. Stress and strain invariants follow the soil mechanics notation (positive for compression).

CODE_BRIGHT. CONSTITUTIVE LAWS

This chapter contains the different models available and the corresponding parameters required by each model. The following constitutive laws are available:

HYDRAULIC AND THERMAL CONSTITUTIVE MODELS (a) RETENTION CURVE INTRINSIC PERMEABILITY LIQUID PHASE RELATIVE PERMEABILITY GAS PHASE RELATIVE PERMEABILITY DIFFUSIVE FLUXES OF MASS DISPERSIVE FLUXES OF MASS AND ENERGY CONDUCTIVE FLUX OF HEAT	MECHANICAL CONSTITUTIVE MODELS ELASTICITY (b) NONLINEAR ELASTICITY (b) VISCOPLASTICITY FOR SALINE MATERIALS (b) VISCOPLASTICITY FOR SATURATED SOILS AND ROCKS (b) VISCOPLASTICITY - GENERAL (b) DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS (c) THERMO-ELASTOPLASTIC MODEL FOR SOILS (d) BARCELONA EXPANSIVE MODEL FOR SOILS (e) CASM's FAMILY MODELS (f)
PHASE PROPERTIES (a) SOLID PHASE PROPERTIES LIQUID PHASE PROPERTIES GAS PHASE PROPERTIES	EXCAVATION PROCESS (g)

VI.e. BARCELONA EXPANSIVE MODEL

MECHANICAL CONSTITUTIVE LAWS (part e) – Mechanical data 4

ICL	NAME	ITYCL	DESCRIPTION
80	Barcelona Expansive Model BExM - Inactive	1	Inactive
81	Barcelona Expansive Model BExM - Elastic	1	Elastic model
82	Barcelona Expansive Model BExM - Coupling	1	Coupling behavior – Interaction functions
83	Barcelona Expansive Model BExM - Yield surface	1	BBM – shape in p-q diagram
84	Barcelona Expansive Model BExM - Inactive2	1	Inactive
85	Barcelona Expansive Model BExM - Plastic potential	1	BBM plastic potential – shape in p-q diagram
86	Barcelona Expansive Model BExM - Inactive3	1	Inactive
87	Barcelona Expansive Model BExM - Hardening	1	BBM Hardening law
88	Barcelona Expansive Model BExM - Convergence	1	Control parameters for the integration of the model

BARCELONA EXPANSIVE MODEL FOR SOILS (BExM)

CODES	ICL = 80 to 88 (Mechanical data 4) ITYCL = 1
DESCRIPTION	Elastoplastic constitutive law for expansive soils (BExM by Alonso et al., 1999).
EQUATIONS	<p>For this model, equations are written assuming Soils Mechanics convention ($p > 0$, $\varepsilon_v > 0$, compression). p is the mean effective stress, J the square root of the second invariant of deviatoric stress tensor, θ the Lode' angle (-30° in triaxial compression, $+30^\circ$ in triaxial extension) (see ICL 21 to 27 for their definition).</p> <p>Two levels of soil structure are defined: macrostructural level (Macro) and microstructural level (micro) (see APPENDIX VI.E):</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="border: 1px solid black; padding: 10px; width: 15%;"> V_T </div> <div style="border: 1px solid black; padding: 10px; width: 15%;"> V_p^M V_p^m V_s </div> <div style="border: 1px solid black; padding: 10px; width: 15%;"> V_p^M V_{ag} </div> <div style="border: 1px solid black; padding: 10px; width: 15%;"> V_p V_s </div> </div> <p>where:</p> <p>V_T = Total volume</p> <p>V_p^M = Volume of macropores</p> <p>V_p^m = Volume of micropores</p> <p>V_p = Total volume of pores ($=V_p^M + V_p^m$)</p> <p>V_s = Volume of solid particles</p> <p>V_{ag} = Volume of aggregates ($=V_s + V_p^m$)</p> <p>Micropores are assumed saturated.</p> <p>The following definitions are established:</p> <p>Total porosity over total volume: $n = \frac{V_p}{V_T}$</p> <p>Macro porosity over total volume: $n^M = \frac{V_p^M}{V_T}$</p> <p>Micro porosity over total volume: $n^m = \frac{V_p^m}{V_T}$</p> <p>Micro porosity over volume of aggregates: $\bar{n}^m = \frac{V_p^m}{V_{ag}} = \frac{V_p^m}{V_s + V_p^m}$</p>

$$\text{Total void ratio: } e = \frac{V_p}{V_s}$$

$$\text{Macro void ratio: } e^M = \frac{V_p^M}{V_{ag}}$$

$$\text{Micro void ratio: } \bar{e}^m = \frac{V_p^m}{V_s}$$

These definitions lead to the following relationships:

$$\begin{aligned} e &= \frac{n}{1-n} & n &= \frac{e}{1+e} \\ e^M &= \frac{n^M}{1-n^M} & n^M &= \frac{e^M}{1+e^M} \\ \bar{e}^m &= \frac{\bar{n}^m}{1-\bar{n}^m} & \bar{n}^m &= \frac{\bar{e}^m}{1+\bar{e}^m} \\ e &= \bar{e}^m + e^M(1+\bar{e}^m) & n &= n^M + n^m \\ n^m &= \bar{n}^m(1-n^M) & n &= n^M + \bar{n}^m(1-n^M) \end{aligned}$$

The following additive equation for the total strain rate holds:

$$d\boldsymbol{\varepsilon}_{kl} = d\boldsymbol{\varepsilon}_{kl}^{Macro} + d\boldsymbol{\varepsilon}_{kl}^{micro}$$

where

$$d\boldsymbol{\varepsilon}_{kl} \text{ is the total strain rate: } tr(\boldsymbol{\varepsilon}_{kl}) = \frac{de}{1+e};$$

$d\boldsymbol{\varepsilon}_{kl}^{Macro}$ is the macrostructural strain rate, associated to the macroskeleton: $tr(\boldsymbol{\varepsilon}_{kl}^{Macro}) = \frac{de^M}{1+e^M};$

$d\boldsymbol{\varepsilon}_{kl}^{micro}$ is the microstructural strain rate (only volumetric behaviour is considered at this level): $tr(\boldsymbol{\varepsilon}_{kl}^{Micro}) = \frac{de^m}{1+e^m}$

Elastic law:

$$d\sigma_{ij} = D_{ijkl}^{Macro} \left(d\boldsymbol{\varepsilon}_{kl}^{Macro} - \delta_{kl} \frac{ds^{Macro}}{3K_s^{Macro}} - d\boldsymbol{\varepsilon}_{kl}^{LC} - d\boldsymbol{\varepsilon}_{kl}^{SD} - d\boldsymbol{\varepsilon}_{kl}^{SI} \right)$$

$$d\sigma_{ij} = D_{ijkl}^{micro} \left(d\boldsymbol{\varepsilon}_{kl}^{micro} - \delta_{kl} \frac{ds^{micro}}{3K_s^{micro}} \right)$$

D_{ijkl}^{Macro} is the mechanical elastic stiffness matrix which relates stress and elastic deformation at macro level ($d\boldsymbol{\varepsilon}_{kl}^{Macro}$);

D_{ijkl}^{micro} is the mechanical elastic stiffness which relates stress and elastic deformation at micro level ($d\boldsymbol{\varepsilon}_{kl}^{micro}$).

K_s^{Macro} is the bulk modulus against macro suction changes and K_s^{micro} the bulk modulus against micro suction changes.

$d\boldsymbol{\varepsilon}_{kl}^{LC}$ are the macro plastic strains if LC is activated.

$d\varepsilon_{kl}^{SD}$ and $d\varepsilon_{kl}^{SI}$ are the macro plastic strains if SD and SI are activated, respectively.

Linear elasticity (Camclay type elasticity):

D_{ijkl}^{Macro} is defined by the bulk modulus K^{Macro} and Poisson's ratio at macro level ν_M .

D_{ijkl}^{micro} is defined by the bulk modulus K^{micro} .

Macro bulk modulus against net stress changes is linearly dependent of the logarithmic mean net stress (p) following the relationship:

$$K^{Macro} = \frac{(1 + e^M) p}{\kappa^{Macro}}$$

Micro bulk modulus against effective stress changes is linearly dependent of the logarithmic effective net stress ($p+s$) following the relationship:

$$K^{micro} = \frac{(1 + e^m)(p + s)}{\kappa^{micro}}$$

where κ^{Macro} and κ^{micro} the slopes of the unloading/reloading lines in the plane $e^{Macro}-\ln p$ and $e^{micro}-\ln(p+s)$, respectively. Note that the behaviour of the microstructure is formalized by means of an effective stress concept generalized for unsaturated conditions (effective stress is recovered).

Bulk modulus against suction changes is linearly dependent of the logarithmic suction following the relationship:

$$K_s^{Macro} = \frac{(1 + e^M)(s + p_{atm})}{\kappa_s}$$

where κ_s is the slope of the drying/wetting line in the plane $e^M-\ln(s+p_{atm})$. p_{atm} is the atmospheric pressure and is taken equal to 0.1 MPa by default.

Yield function

$$F^{LC} = J^2 - \frac{M^2}{3} (p + p_t)(p_0 - p) \leq 0$$

where p_t is the clay tensile strength, p_0 the clay matrix isotropic yield locus and M the slope of the critical state line in the p - q diagram. The following dependencies on suction are considered:

$$p_t = k_s s$$

$$p_0 = p_c \left(\frac{p_0^*}{p_c} \right)^{\frac{\lambda(0) - \kappa^{Macro}}{\lambda(s) - \kappa^{Macro}}} \quad \text{with} \quad \lambda(s) = \lambda(0) [(1-r)e^{-\beta s} + r]$$

$$F^{SD} = \gamma^{SD} - p - s$$

$$F^{SI} = p + s - \gamma^{SI}$$

Rate dependency

Rate dependency is introduced as a visco-plastic mechanism. Plastic multiplier λ^p is expressed as a function of the distance between the current stress point and the inviscid plastic locus:

$$d\lambda^p = \frac{dt}{\eta} \langle F \rangle$$

where dt is the time increment, η is the clay viscosity and $\langle \rangle$ are the Macauley brackets. Inviscid plastic locus takes the form:

$$\bar{F} = F - \frac{\eta}{dt} d\lambda^p \leq 0$$

where F can be either the LC, SD or SI yield criterion

Plastic potential

$$G^p = J^2 - \omega \frac{M^2}{3} (p + p_t)(p - p_0)$$

p_t , p_0 and M are parameters defining the yield criterion. ω is a parameter defining the non associativity of the flow. It takes a value equal to 1 when associated and equal to 0 for null dilatancy. To respect the condition of null lateral strain during K_0 -loading, ω must be set to:

$$\omega = \frac{M(M-9)(M-3)}{9(6-M)} \frac{1}{1 - \kappa/\lambda(0)}$$

In the deviatoric plane, plastic potentials are considered associated.

An associated plastic potential in the $p - q$ diagram is defined for SD and SI.

Hardening law:

The hardening/softening law is introduced through the following dependency of the saturated isotropic yield locus on the plastic strain:

$$\frac{dp_0^*}{p_0^*} = \frac{(1+e)}{\lambda - \kappa} (d\varepsilon_{vol}^{LC} + d\varepsilon_{vol}^{SD} + d\varepsilon_{vol}^{SI})$$

$$d\gamma^{SD} = \frac{K^{micro}}{f^{SD}} d\varepsilon_{vol}^{SD} + \frac{K^{micro}}{f^{SI}} d\varepsilon_{vol}^{SI}$$

$$d\gamma^{SI} = \frac{K^{micro}}{f^{SD}} d\varepsilon_{vol}^{SD} + \frac{K^{micro}}{f^{SI}} d\varepsilon_{vol}^{SI}$$

where f^{SD} and f^{SI} are the micro-macro interaction functions defined as follow:

$$f^{SD} = f_{SD0} + f_{SD1} \left(1 - \frac{p}{p_0}\right)^{n_{SD}} \quad \text{and} \quad f^{SI} = f_{SI0} + f_{SI1} \left(\frac{p}{p_0}\right)^{n_{SI}}$$

Model parameters should be introduced in the following ICL:

BExM – Inactive (ICL = 80) VOID

BExM – Elastic (ICL = 81) contains parameters of elastic model

BExM – Coupling (ICL = 82) contains parameters of coupling

BExM – Yield surface (ICL = 83) contains parameters for the shape of the yield function in the p-q plane

BExM – Inactive2 (ICL = 84) VOID

BExM – Plastic potential (ICL = 85) contains parameters for the shape of the plastic potential in the p-q plane

BExM – Inactive3 (ICL = 86) VOID

BExM – Hardening (ICL = 87) contains parameters for the hardening law

BExM – Convergence (ICL = 88) contains parameters to control the integration of the constitutive law

PARAMETERS FOR BEXM – INACTIVE ICL = 80; ITYCL = 1 (INACTIVE)

PARAMETERS FOR BEXM – ELASTIC ICL = 81; ITYCL = 1 (Elastic model)

P1	κ^{Macro}	-	Matrix elastic stiffness parameter at macro level for changes in mean stress (p)
P2	κ^{micro}	-	Matrix elastic stiffness parameter at micro level for changes in mean effective stress ($p + s^{micro}$)
P3	void	-	
P4	void	-	
P5	κ_s	-	Elastic macro stiffness parameter for changes in macro suction (s^{Macro})
P6	ν^M	-	Poisson's ratio
P7	K_{min}^{Macro}	MPa	Minimum bulk modulus at macro level
P8	K_{min}^{micro}	MPa	Minimum bulk modulus at micro level
P10	If P10 \neq 0 \Rightarrow total porosity is used instead of macroporosity		

PARAMETERS FOR BEXM – COUPLING ICL = 82; ITYCL = 1 (Coupling behaviour).

P1	void	-	
P2	void	-	
P3	f_{sd0}	-	Parameter micro-macro coupling functions when SD is active
P4	f_{sd1}	-	Parameter micro-macro coupling functions when SD is active
P5	n_{sd}	-	Parameter micro-macro coupling functions when SD is active
P6	f_{si0}	-	Parameter micro-macro coupling functions when SI is active
P7	f_{si1}	-	Parameter micro-macro coupling functions when SI is active
P8	n_{si}	-	Parameter micro-macro coupling functions when SI is active

PARAMETERS FOR BEXM – YIELD SURFACE ICL = 83; ITYCL = 1 (Basic Barcelona model criterion for the clay – shape in p - q diagram).

P1	M	-	Slope of the critical state line
P2	void	-	-
P3	r	-	Coefficient setting the change in cohesion with suction
P4	β	MPa ⁻¹	Coefficient setting the change in cohesion with suction
P5	p_c	MPa	Reference pressure
P6	k_s	-	Coefficient setting the increase of tensile strength with suction
P7	p_{t0}	MPa	Cohesion corresponding to suction equal to zero

PARAMETERS FOR BEXM – INACTIVE2 ICL = 84; ITYCL = 1 (INACTIVE)

PARAMETERS FOR BEXM – PLASTIC POTENTIAL ICL = 85; ITYCL = 1 (Basic Barcelona model plastic potential for the clay– shape in p - q diagram).

P1	ω	-	Coefficient of non associativity (0: no volumetric plastic strain, 1: full volumetric plastic strain –associative plasticity)
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PARAMETERS FOR BEXM – MACRO-MICRO INTERACTION ICL = 86; ITYCL = 1

P6	ϕ_{mic}	-	Micro-porosity
P7	β		Retention curve parameter for micro
P8	P_0		Retention curve parameter for micro
P9	α	kg MPa ⁻¹ m ⁻³	Interchange of water coefficient
P10	s_{mic}	MPa	Initial suction micro

PARAMETERS FOR BEXM – HARDENING ICL = 87; ITYCL = 1 (Basic Barcelona model does not need additional parameter for the hardening law for clay).

P1	$\lambda(0)$	-	Slope of the virgin loading line in the e - $\ln(p)$ diagram
P2	η	MPa.s	Clay viscosity parameter

PARAMETERS FOR BEXM – CONVERGENCE ICL = 88; ITYCL = 1 (Control parameter for the Stress Point Algorithm – Backward-Euler scheme is used).

P1	tol	-	Tolerance over SPA residual (typical value – not default – 1.e-8)
P2	tol_for_subin	-	Tolerance over the elastic subincrementation (typical value 1e-4)
P3	void	-	
P4	$toler_ini_SI_SD$	MPa	Initial separation between SI and SD (typical value 1.e-4)

HISTORY VARIABLES:

The Barcelona Expansive Model (BExM) (ICL = 80 to 88) model requires the following history variables:

Hist_var 1	P_0^*	MPa	Initial preconsolidation mean stress for saturated soil
Hist_var 2	γ^{SD}	MPa	Initial value of the parameter that defines the position of SD yield surface
Hist_var 3	γ^{SI}	MPa	Initial value of the parameter that defines the position of SI yield surface
Hist_var 4	n^m		Initial microstructural porosity (micropore volume V_p^m / total volume V_T)

These variables can be assigned as initial conditions on *surfaces/volumes* if an initial particular distribution on the geometry is required. The procedure is the same as followed by initial stresses as was described in chapter II. PREPROCESS, PROBLEM DATA, section II.2.3.5.

Initial values of P_0^* defining the initial position of LC surface are required.

By default, initial position of the surfaces γ^{SD} and γ^{SI} is fixed using the initial stress state involving no elastic region between SD and SI surface. To do this, first γ^{SI} is computed as $\gamma^{SI} = p + s^{\text{micro}}$, then, the position of γ^{SD} is computed using an initial separation between SI and SD surfaces which is prescribed as an input parameter in P4 of the ICL=88. If user wants to control the initial position of γ^{SD} and γ^{SI} , then, specific values should be introduced as initial conditions on *surfaces/volumes*, otherwise, these values should be keep as zero.

The evolution of history variables can be visualized as an output in Post-process GID interface.

Note: Effective stresses plotted in the Post-process GID interface correspond with net stresses for unsaturated conditions and Terzaghi's effective stresses for saturated conditions. Stress and strain invariants follow the soil mechanics notation (positive for compression).

CODE_BRIGHT. CONSTITUTIVE LAWS

This chapter contains the different models available and the corresponding parameters required by each model. The following constitutive laws are available:

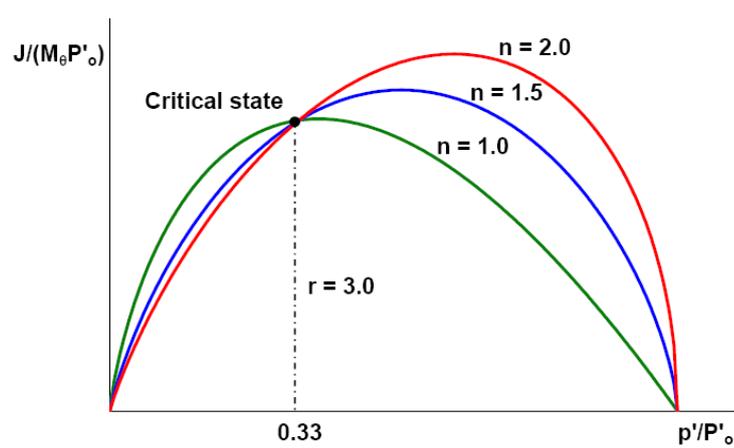
HYDRAULIC AND THERMAL CONSTITUTIVE MODELS (a) RETENTION CURVE INTRINSIC PERMEABILITY LIQUID PHASE RELATIVE PERMEABILITY GAS PHASE RELATIVE PERMEABILITY DIFFUSIVE FLUXES OF MASS DISPERSIVE FLUXES OF MASS AND ENERGY CONDUCTIVE FLUX OF HEAT	MECHANICAL CONSTITUTIVE MODELS ELASTICITY (b) NONLINEAR ELASTICITY (b) VISCOPLASTICITY FOR SALINE MATERIALS (b) VISCOPLASTICITY FOR SATURATED SOILS AND ROCKS (b) VISCOPLASTICITY - GENERAL (b) DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS (c) THERMO-ELASTOPLASTIC MODEL FOR SOILS (d) BARCELONA EXPANSIVE MODEL FOR SOILS (e) CASM's FAMILY MODELS (f)
PHASE PROPERTIES (a) SOLID PHASE PROPERTIES LIQUID PHASE PROPERTIES GAS PHASE PROPERTIES	EXCAVATION PROCESS (g)

VI.f. CASM's FAMILY MODELS

MECHANICAL CONSTITUTIVE LAWS (part f)

ICL	NAME	ITYCL	DESCRIPTION
90	Clay and Sand model (CASM): GENERAL	1	Contain general parameters for CASM (saturated)
91	Clay and Sand model (CASM):SPECIFIC	2	Contain parameters for Unsaturated CASM model
		3	Contain parameters for Cemented CASM model
		4	Contain parameters for Doble hardening CASM model

CASM's FAMILY MODELS

CODES in <i>ROOT_gen.dat</i>	ICL = 90, 91 (Mechanical data 3) ITYCL = 1, 2, 3, 4
DESCRIPTION	Clay and Sand model for soils (CASM)
EQUATIONS	<p>ICL = 90 (CASM – General); ITYCL = 1: Saturated CASM model</p> <p><u>Yield function:</u> The yield function for CASM (Yu, 1998) expressed for a general stress state is:</p> $f = \left(\frac{\sqrt{3}J}{M_\theta p'} \right)^n + \frac{1}{\ln r} \ln \frac{p'}{P'_0}$ <p>where: p' is the mean effective stress</p> $J = \left(\frac{1}{2} \text{trace}(\sigma_{ij} - p' \delta_{ij}) \right)^{1/2} \quad (\text{for axi-symmetric conditions: } q = \sqrt{3}J)$ <p>P'_0 is the preconsolidation pressure M_θ is the slope of the critical state line n is a constant used to specify the shape of the yield surface r is a spacing ratio introduced to control the location of the intersection of the critical state line with the yield surface.</p>  <p>M_θ is expressed as a function of Lode's angle θ, and determines the shape of the failure surface in the deviatoric plane. The relationship proposed by Sheng et al (2000), to approximate a hexagonal Mohr-Coulomb failure surface is adopted:</p> $M_\theta = M \left(\frac{2\alpha^4}{1 + \alpha^4 + (1 - \alpha^4) \sin 3\theta} \right)^{1/4}$ <p>where M is the slope of the CSL under triaxial compression ($\theta = -30^\circ$). The parameter α controls the difference of the strengths between the triaxial compression and extension. Often, α is taken as: $\alpha = \frac{3 - \sin \phi_{cs}}{3 + \sin \phi_{cs}}$ where ϕ_{cs} denotes the friction angle of the soil at the critical state.</p>

EQUATIONS

ICL = 90 (CASM – General); ITYCL = 1: Saturated CASM model (continued)Hardening parameter:

Similar to the Cam-clay models, in CASM the change in size of the yield surface (dP'_0) is assumed to be related to the incremental plastic volumetric by:

$$dP'_0 = \frac{P'_0}{\lambda^* - \kappa^*} d\varepsilon_v^p$$

where: $\lambda^* = \frac{\lambda}{1+e_0}$ and $\kappa^* = \frac{\kappa}{1+e_0}$ are the modified compression index and modified elastic swelling index.

Plastic potential:

The plastic potential for CASM follows the stress-dilatancy relation of Rowe (1962).

$$g = 3M_\theta \ln \frac{p'}{\zeta} + (3 + 2M_\theta) \ln \left(\frac{2\sqrt{3}J}{p'} + 3 \right) - (3 - M_\theta) \ln \left(3 - \frac{\sqrt{3}J}{p'} \right)$$

Where ζ is a size parameter, which can be determinate easily for any given stress state (p', J) by solving the above equation and it is internally computed.

Elastic behaviour:

The elastic behaviour of this critical state model is the same as in the Cam-clay models with the tangent modulus (K) and shear modulus (G) being defined by the following expressions (a constant Poisson's ratio (ν) is assumed):

$$K = \frac{p'}{\kappa^*} \quad G = \frac{3(1-2\nu)K}{2(1+\nu)}$$

Undrained analysis in terms of the undrained shear strength parameter (S_u) (Optional case):

When this option is activated, the desired undrained shear strength S_u of the material will be fitted and is not more a result of the constitutive model. To do this, the spacing ratio r is calculated as a function of the undrained shear strength S_u (which is a input parameter in this case) to obtain a yield surface shape that will result in the desired S_u , as,

$$r = \left(\frac{M_\theta \cos \theta}{\sqrt{3}} \frac{P'_e}{S_u} \right)^{\frac{1}{\lambda}} \quad P'_e = p' \left(\frac{p'}{P'_0} \right)^{\frac{\kappa}{\lambda}}$$

This expression links a total stress characteristic of the soils, the undrained shear strength, with effective stress parameters and the consolidation history of the soil.

EQUATIONS

ICL = 91 (CASM – Specific); ITYCL = 2: Unsaturated CASM model

This model require P1 to P9 parameters of the ICL=90 and ICL=91.

Model follows the Barcelona Basic Model (BBM) characteristics. The model is formulated using two alternative options for the constitutive stresses variables: Net stress and Bishop's or average stress, which can be selected using an indicator parameter.

$$\text{- Bishop's stress: } \sigma'_{ij} = \sigma_{ij} - P_g \delta_{ij} + S_r s \delta_{ij}$$

$$\text{- Net stress: } \bar{\sigma}_{ij} = \sigma_{ij} - \max(P_g, P_l) \delta_{ij}$$

$$\text{- Suction: } s = \sigma_{ij} - \max((P_g - P_l), 0)$$

σ_{ij} is the total stresses, P_g the gas pressure, P_l the liquid pressure, S_r the degree of saturation and δ_{ij} the Kroneckers's delta.

Yield function:

In terms of *Bishop's* stress:

$$f = \left(\frac{\sqrt{3}J}{M_\theta p'} \right)^n + \frac{1}{\ln r} \ln \frac{p'}{P_c}$$

In terms of *Net* stress:

$$f = \left(\frac{\sqrt{3}J}{M_\theta (\bar{p} + p_s)} \right)^n + \frac{1}{\ln r} \ln \left(\frac{\bar{p} + p_s}{P_c + p_s} \right)$$

p' is the mean *Bishop* stress, \bar{p} is the mean net stress, p_s is a tensile strength due to suction, J is the square root of the second stress invariant of deviatoric stress tensor and M_θ is the slope of the critical state line expressed as a function of Lode's angle (see ICL=90).

Preconsolidation pressure P_c is assumed to vary with suction and define the yield curve denoted as LC (loading-collapse),

$$P_c = p_r \left(\frac{P_0}{p_r} \right)^{\frac{\lambda_0 - \kappa}{\lambda_s - \kappa}}$$

P_0 is the yield surface location at zero suction and is also the hardening parameter, p_r is a reference mean stress, λ_0 is the slope of the saturated virgin consolidation line, λ_s is the slope of the virgin consolidation line for an specific value of suction and κ is the slope of the unloading-reloading line (assumed independent of suction). λ_s is assumed to vary with the suction according to,

$$\lambda_s = \lambda_o \left[(1 - r^*) \exp(-\beta s) + r^* \right]$$

where, r^* and β are material parameters. The first is related to the maximum stiffness of the soil (for an infinite suction): $r^* = \lambda_s(s \rightarrow \infty) / \lambda_o$ and the second controls the rate of increase of soil stiffness with suction.

Net stress formulation requires an explicit variation of apparent cohesion with suction. The increase in cohesion follows a linear relationship with suction,

$$p_s = k_s s$$

where k_s is a scalar variable.

Plastic potential:

Three options are available for the flow rule. An scalar variable is introduced to select a particular option as follow,

Flow_rule = 1. Non associated flow rule following the stress-dilatancy relation of Rowe (see ICL=90 ITYCL=1)

Flow_rule = 2. Non associated flow rule to fit an one-dimensional consolidation stress path (K_0)

$$g = \left(\frac{\alpha \sqrt{3} J}{M_\theta p'} \right)^n + \frac{1}{\ln r} \ln \frac{p'}{P'_c}$$

$$\text{with } \alpha = \frac{2}{3} \frac{[M_\theta (6 - M_\theta)]^n - (3M_\theta)^n}{(6 - M_\theta)(3M_\theta)^{n-1}} \frac{\lambda^*}{\lambda^* - \kappa^*}$$

Flow_rule = 3. Associated flow rule ($f=g$)

Hardening parameter:

Isotropic hardening is controlled by the plastic volumetric strains ($d\varepsilon_v^p$) through,

$$dP_o = \frac{P_o (1+e)}{\lambda_o - \kappa} d\varepsilon_v^p$$

Elastic behaviour:

Elastic behaviour is the same as defined in ICL=90 ITYCL=1. However, net stress formulation requires an explicit relation to consider the effect of suction on volumetric elastic strains, through the incorporation of the elastic compressibility parameter for changes in suction, K_s ,

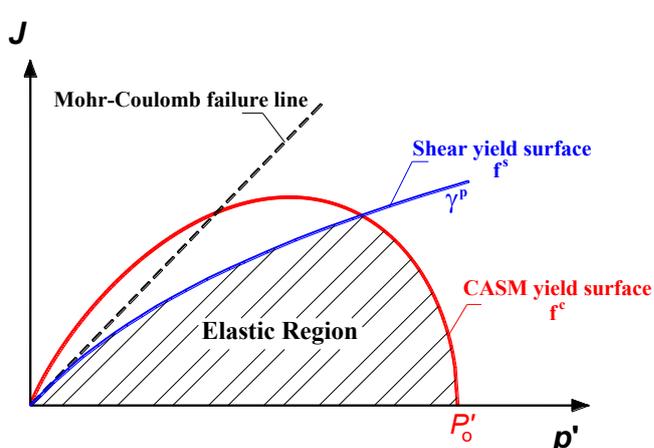
$$d\varepsilon_{ij}^{e,s} = \frac{K_s}{(1+e)(s + p_{atm})} ds \delta_{ij} = \frac{1}{3K_s} ds \delta_{ij}$$

Where K_s is the Bulk modulus for changes in suction. If Bishop's stress is configured, the effect of suction on volumetric elastic strains is accounted for via the variation in Bishop's stress with suction. Elastic strain increments are computed using the following equations for Net stress approach and Bishop's stress approach, respectively.

$$d\varepsilon_{ij}^e = \frac{2G - 3K}{6KG} d\bar{p} \delta_{ij} + \frac{1}{2G} d\bar{\sigma}_{ij} + \frac{1}{3K_s} ds \delta_{ij}$$

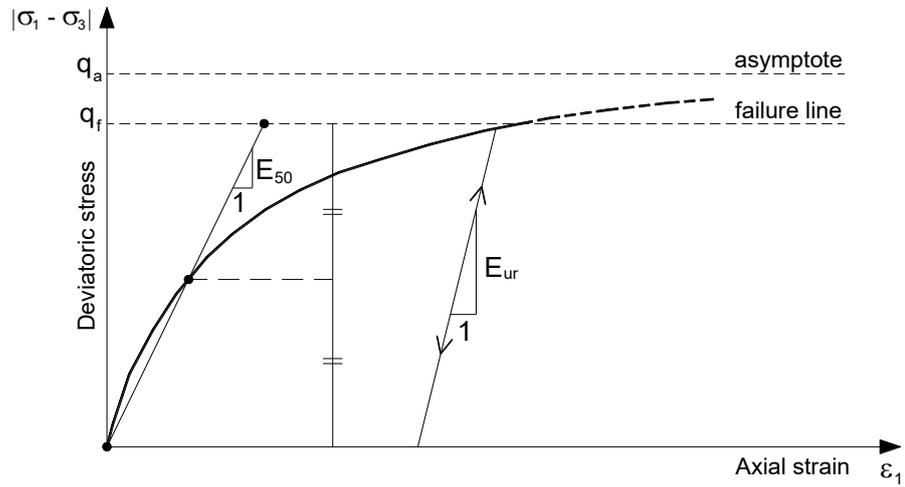
$$d\varepsilon_{ij}^e = \frac{2G - 3K}{6KG} d(\bar{p} + Sr \cdot s) \delta_{ij} + \frac{1}{2G} d\sigma'_{ij}$$

CODES in <i>ROOT_gen.dat</i>	ICL = 90, 91 (Mechanical data 3) ITYCL = 1, 2, 3, 4
DESCRIPTION	Clay and Sand model for soils (CASM)
EQUATIONS	<p>ICL = 91 (CASM – Specific); ITYCL = 3: Cemented CASM model</p> <p>This model require P1 to P9 of ICL = 90 and P1 to P7 of ICL = 91 Cemented CASM model is based on the formulation for cemented soils proposed by Gens & Nova (1993), in which a new state variable denoted as ‘bonding’ b is incorporated.</p> <p><u>Yield function:</u></p> $f = \left(\frac{\sqrt{3}J}{M_o(p' + p_t)} \right)^n + \frac{1}{\ln r} \ln \frac{(p' + p_t)}{(P'_c + p_t)} \quad \begin{matrix} P'_c = P'_o(1+b) \\ p_t = P'_o(\alpha_t b) \end{matrix}$ <p>Where, b is a non-dimensional variable that represents the degree of bonding. P'_o is the preconsolidation pressure of the unbonded material. P'_c controls the yielding of the bonded soil in isotropic compression and p_t is related to the cohesion and tensile strength of the material; α_t is a parameter. Both P'_c and p_t increase with the magnitude of bonding. The unbonded behaviour is recovered when b goes to zero.</p> <p>The function defining the reduction of bonding (b) with increased degradation and the relationship controlling the evolution of degradation in response to plastic strains, are:</p> $b = b_0 e^{-(h-h_0)}$ $dh = h_1 d\varepsilon_v^p + h_2 d\varepsilon_q^p $ <p>The above expressions ensure that degradation increases monotonically, independently of the sign of the plastic strains. h_1 y h_2 are material parameters (greater than zero) defining the rate of degradation. $d\varepsilon_v^p$ and $d\varepsilon_q^p$ are the plastic volumetric strain increment and plastic deviatoric strain increment, respectively.</p> <p>The three options for the plastic potential used in the ICL = 91 ITYCL = 2 (Unsaturated model) are also available for this model.</p> <p><u>Hardening parameter:</u></p> <p>Either a volumetric hardening law or a combined volumetric and shear hardening law can be used for this propose. If a combined hardening is adopted, then:</p> $\frac{dP'_o}{P'_o} = \frac{1}{\lambda^* - \kappa^*} [d\varepsilon_v^p + \omega d\varepsilon_q^p]$ <p>which reduces to the usual volumetric hardening law if it set $\omega = 0$. ω is a new constant introduced to control the relative contribution of the incremental plastic deviatoric strain ($d\varepsilon_q^p$) to the rate of change of the hardening parameter (P'_o).</p> <p>Elastic behaviour is the same as defined in ICL = 90; ITYCL = 1.</p>

CODES in <i>ROOT_gen.dat</i>	ICL = 90, 91 (Mechanical data 3) ITYCL = 1, 2 ,3, 4
DESCRIPTION	Clay and Sand model for soils (CASM)
EQUATIONS	<p>ICL = 91 (CASM – Specific); ITYCL = 4: Double hardening soil model (DHSM)</p> <p>This model require P1 to P9 of ICL = 90 and P1 to P8 of ICL = 91</p> <p>The model involves two plastic mechanisms: a plastic volumetric-driven mechanism with isotropic hardening, by means of the use of the CASM yield surface (ICL=90), and a plastic shear-driven mechanism that gives rise to a nonlinear stress-strain relationship of a hyperbolic type, by the use of a shear yield surface based on the Hardening Soil Model (HSM) (Schanz et al., 1999).</p> <p><u>Yield functions:</u></p> <ul style="list-style-type: none"> - Volumetric yield surface: CASM surface (see ICL = 1; ITYCL = 1) - Shear yield surface: $f^s = \frac{1}{E_{50}} \frac{J}{\left(1 - \frac{J}{J_a}\right)} - \frac{2J}{E_{ur}} - \gamma^p$ <p>with:</p> $J_a = \frac{J_f}{R_f} = \frac{(p' + c' \cot \phi') g(\theta)}{R_f} \quad \text{and} \quad g(\theta) = \frac{\sin \phi'}{\cos \theta + \frac{\sin \theta \sin \phi'}{\sqrt{3}}}$ <p>J_a is the asymptotic value of the shear strength, R_f stands for the relation between the ultimate deviatoric stress, J_f, and the asymptotic stress, a standard setting is $R_f = 0.9$. γ^p is the hardening parameter of the shear yield surface and corresponds to the plastic deviatoric strain (ε_d^p), as is described in the next section.</p> 

E_{50} is a secant stiffness modulus for primary loading and E_{ur} is a secant stiffness modulus for elastic unloading and reloading, these modulus are computed as,

$$E_{50} = E_{50}^{ref} \left(\frac{p' + c' \cot \phi'}{p^{ref} + c' \cot \phi'} \right)^m \quad \text{and} \quad E_{ur} = E_{ur}^{ref} \left(\frac{p' + c' \cot \phi'}{p^{ref} + c' \cot \phi'} \right)^m$$



E_{50}^{ref} is a reference stiffness modulus corresponding to a reference confining pressure p^{ref} , usually taken equal to the atmospheric pressure (100 kPa) and E_{ur}^{ref} is the secant reference modulus for unloading and reloading. The amount of stress dependency is given by the power m , for soft clays m usually is taken equal to 1.0 and for sand, m lies in the range between 0.35 and 0.65.

Plastic potentials:

A non-associative flow rule is used for the shear yield surface which has the following form,

$$d\varepsilon_v^p = g(\psi_m) d\gamma^p$$

where $g(\psi_m)$ is a function of mobilized dilatancy angle, ψ_m , and Lode's angle, θ , as,

$$g(\psi_m) = \frac{\sin \psi_m}{\cos \theta + \frac{\sin \theta \sin \psi_m}{\sqrt{3}}}$$

The mobilized dilatancy angle, ψ_m , is defined as,

$$\sin \psi_m = \frac{\sin \phi_m - \sin \phi_{cs}}{1 - \sin \phi_m \sin \phi_{cs}}$$

ϕ_{cs} is the friction angle at the critical state and ϕ_m is the mobilized friction angle. Material contracts for small stress ratios $\phi_m < \phi_{cs}$, while dilatancy occurs for high stress ratios $\phi_m > \phi_{cs}$. Considering dense materials contraction is excluded by taking $\psi_m = 0$ for a mobilized friction angle $\phi_m < \phi_{cs}$.

The volumetric surface uses a non-associated flow rule, the plastic potential is defined in the ICL = 90; ITYCL = 1.

Hardening parameters:

The hardening parameter of the shear surface, γ^p , is the plastic deviatoric strain $\gamma^p = \varepsilon_d^p$. The plastic deviatoric strain rate is calculated as,

$$d\varepsilon_d^p = 2\sqrt{dJ_2^\varepsilon}$$

$$d\varepsilon_d^p = \left\{ \frac{2}{3} \left[(d\varepsilon_x^p - d\varepsilon_y^p)^2 + (d\varepsilon_x^p - d\varepsilon_z^p)^2 + (d\varepsilon_y^p - d\varepsilon_z^p)^2 \right] + [d\gamma_{xy}^2 + d\gamma_{xz}^2 + d\gamma_{yz}^2] \right\}^{1/2}$$

where, J_2^ε is the second strain invariant of deviatoric strain tensor, γ^p is the integral of plastic deviatoric strain rates.

The hardening parameter of the volumetric yield surface is the so-called preconsolidation pressure (P_0^i) defined in the ICL = 90; ITYCL = 1.

The two surfaces can be activated simultaneously and move together as in a multi-surface plasticity problem, if the stress path reaches the intersection between both surfaces.

Elastic behaviour of the DHSM is the same as in basic CASM model defined in the ICL = 90; ITYCL = 1.

Enhanced model (E-DHSM):

For stiff materials an enhanced model (E-DHSM) can be used, which allows the evolution of the shear yield surface until the volumetric yield surface is engaged on the dry side of the critical state, providing the simulation of softening controlled by the hardening/softening law of the CASM. In this case, a simple linear variation of the strength parameters with plastic deviatoric strain, ε_d^p , is employed, as,

$$\phi' = A_\phi \varepsilon_d^p + \phi'_{cs} \quad c' = A_c \varepsilon_d^p + c'_{res}$$

where, A_ϕ and A_c are two input parameters. If these parameters are zero the basic DHSM is recovered.

PARAMETERS FOR CASM – GENERAL ICL = 90; ITYCL = 1 (General: required for ICL = 91, ITYCL = 2, 3, 4)

P1	ν	-	Poisson ratio
P2	κ	-	Slope of unload/reload compression curve
P3	λ	-	Slope of the normal compression curve
P4	r	-	Spacing ratio
P5	n	-	Shape parameter
P6	M	-	Slope of Critical State Line
P7	ϕ_{cs}	°	Friction angle at CS (computed as a function of M). If $\phi_{cs}=0$, the shape of the YS plots as a circle in the deviatoric plane)
P8-P9	-	-	
P10	S_u	MPa	Undrained shear strength (<u>optional</u>). By default = 0

PARAMETERS FOR CASM – SPECIFIC ICL = 91; ITYCL = 2 (Unsaturated)

P1	P_r	MPa	Reference mean stress (LC curve)
P2	r		Parameter to control infinite suction (LC curve)
P3	β	MPa ⁻¹	Parameter to control stiffness (LC curve)
P4	κ_s		Elastic stiffness due to suction
P5	k_s	-	Parameter to account tensile strength due to suction
P6	iunsat	-	Indicator of stress option: (0: net stress; 1: Bishop's stress)
P7	p_t	MPa	Tensile strength for saturated conditions
P8	<i>flow_rule</i>	-	Flow rule indicator: 1: Non-associated: Rowe 2: Non-associated: K ₀ fit. Parameter α is required 3: Associated
P9	α	-	Non-associated parameter in case of <i>flow_rule</i> option equal to 2.

PARAMETERS FOR CASM – SPECIFIC ICL = 91; ITYCL = 3 (Cemented)

P1	b_0	-	Initial bonding. Evolution of bonding is stored as a history variable
P2	h_0	-	Degradation threshold
P3	h_1	-	Degradation rate for compression
P4	h_2	-	Degradation rate for shear
P5	α	-	Parameter for tensile strength
P6	ω	-	Contribution of the plastic deviatoric strain to hardening parameter
P7	$Flow_rule$	-	Flow rule indicator: 1: Non-associated: Rowe 2: Non-associated: K_0 fit. Parameter α is required 3: Associated
P8	α	-	Non-associated parameter in case of $flow_rule$ option equal to 2.

PARAMETERS FOR CASM – SPECIFIC ICL = 91; ITYCL = 4 (Double hardening)

P1	ϕ	°	Peak friction angle
P2	c	MPa	Cohesion
P3	ψ	°	Peak dilatancy angle
P4	E_ref_50	MPa	Reference secant stiffness
P5	m	-	Power stress-level dependency of stiffness
P6	R_f	-	Failure ratio
P7	p_{ref}	MPa	Reference stress for stiffness
P8	E_ref_ur	MPa	Unloading/reloading stiffness
P9	A_ϕ	-	Rate of evolution of friction angle with ε_d^p . Required by E-DSHM
P10	A_c	-	Rate of evolution of cohesion with ε_d^p . Required by E-DSHM

HISTORY VARIABLES:

The CASM's family of constitutive models (ICL = 90, 91) use the following history variables. Output variables can be visualized in the Post-process interface of GID.

Model	Hist_var	Description	Type
ICL = 90 (ITYCL 1) General CASM model	1	P_0 (MPa): Evolution of preconsolidation pressure	Input/Output
	2	F: Value of the yield function	Internal
	3	e: Void ratio	Internal
	4	Id_F1: Indicator of plasticity	Internal
ICL = 91 (ITYCL 2) Unsaturated CASM model	1	P_0 (MPa): Evolution of preconsolidation pressure	Input/Output
	2	s: Suction	Output
	3	e: Void ratio	Internal
	4	P_c (MPa): Evolution of preconsolidation pressure due to suction	Output
	5	p_s (MPa): Evolution of tensile strength due to suction	Output
	5	F: Value of the yield function	Internal
ICL = 91 (ITYCL 3) Cemented CASM model	6	Id_F1: Indicator of plasticity	Internal
	1	P_0 (MPa): Evolution of preconsolidation pressure	Input/Output
	2	P_c (MPa): Evolution of preconsolidation pressure due to bond	Internal
	3	p_t (MPa): Evolution of tensile strength due to bond	Output
	4	b: Evolution of bonding	Input/Output
	5	h: Evolution of degradation rate	Output
	6	F: Value of the yield function	Internal
	7	e: Void ratio	Internal
ICL = 91 (ITYCL 4) Double hardening CASM model	8	Id_F1: Indicator of plasticity	Internal
	1	P_0 (MPa): Evolution of preconsolidation pressure (volumetric surface)	Input/Output
	2	γ^p : Evolution of plastic shear strain (deviatoric surface)	Output
	3	F1: Value of the volumetric yield function	Internal
	4	F2: Value of the shear yield function	Internal
	5	c: Evolution of cohesion with plastic strain	Internal
	6	ϕ : Evolution of friction angle with plastic strain	Internal
	7	e: Void ratio	Internal
	8	Id_F1: Indicator of plasticity (volumetric surface)	Internal
9	Id_F2: Indicator of plasticity (deviatoric surface)	Internal	

The input variable (P_0) is introduced as initial condition on *surfaces/volumes* in the *conditions* window of GiD. Void ratio (e) is computed internally as a function of porosity.

Hist_var 1	P_0	MPa	Evolution of preconsolidation mean stress for saturated soil
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The evolution of some history variables can be visualized as an output in Post-process GiD interface.

Note: Effective stresses plotted in the Post-process GiD interface correspond with Terzaghi's effective stresses for saturated conditions (ITYCL = 1, 3, 4). For ITYCL = 2 (Unsaturated CASM model) if the indicator *iunsat* (P6 of ICL = 91; ITYCL = 2) is equal to 0, net stress are plotted, if *iunsat* = 1, Bishop's effective stresses are plotted. Stress and strain invariants follow the soil mechanics notation (positive for compression).

CODE_BRIGHT. CONSTITUTIVE LAWS

This chapter contains the different models available and the corresponding parameters required by each model. The following constitutive laws are available:

<p>HYDRAULIC AND THERMAL CONSTITUTIVE MODELS (a)</p> <p>RETENTION CURVE INTRINSIC PERMEABILITY LIQUID PHASE RELATIVE PERMEABILITY GAS PHASE RELATIVE PERMEABILITY DIFFUSIVE FLUXES OF MASS DISPERSIVE FLUXES OF MASS AND ENERGY CONDUCTIVE FLUX OF HEAT</p>	<p>MECHANICAL CONSTITUTIVE MODELS</p> <p>ELASTICITY (b) NONLINEAR ELASTICITY (b) VISCOPLASTICITY FOR SALINE MATERIALS (b) VISCOPLASTICITY FOR SATURATED SOILS AND ROCKS (b) VISCOPLASTICITY - GENERAL (b) DAMAGE-ELASTOPLASTIC MODEL FOR ARGILLACEOUS ROCKS (c) THERMOELASTOPLASTIC MODEL FOR SOILS (d) BARCELONA EXPANSIVE MODEL FOR SOILS (e) CASM's FAMILY MODELS (f)</p>
<p>PHASE PROPERTIES (a)</p> <p>SOLID PHASE PROPERTIES LIQUID PHASE PROPERTIES GAS PHASE PROPERTIES</p>	<p>EXCAVATION PROCESS (g)</p>

VI.g. EXCAVATION/CONSTRUCTION PROCESS

EXCAVATION/CONSTRUCTION

CODES	ICL = 50 ITYCL = 1
DESCRIPTION	Flag for excavation and construction process
EQUATIONS	<p>Options:</p> <ul style="list-style-type: none"> - Active material (default option) → P1 = 0 - Inactive material: material that has not yet been constructed or material that has been excavated → P1 = -1 - Construction: the material is constructed with its gravity increased linearly during the interval → P1 = 1 <p>After the construction interval is finished, the constructed material automatically will be considered active in the next interval → P1 = 0</p> <ul style="list-style-type: none"> - Smooth excavation (P1 = 2): the material excavated becomes elastic and its stress is relaxed smoothly according to the following equation: $\sigma^t = \sigma^{timei} \left(A - B \left[\frac{t - timei}{timef - timei} \right]^n \right)$ <p>where: <i>timei</i> = interval initial time <i>timef</i> = interval final time <i>t</i> = current time σ^t = stress in time <i>t</i> σ^{timei} = stress at the initial time of the interval <i>A</i> is a user-defined parameter taking values between 0 and 1 <i>B</i> is a user-defined parameter taking values between 0 and 1 <i>n</i> is a user-defined exponent</p> <p>If A = 1 (default value), then the excavated material is relaxed from its current stress (recommended). If A < 1, then the excavated material is relaxed from a lower stress level.</p> <p>If B = 1 (default value), then the excavated material is relaxed until zero (usual case). If B < 1, then the excavated material is relaxed until a stress level higher than zero (useful in some cases, like e.g. installing support in a 2D model after a given relaxation).</p> <p>If n = 1 (default value), then the excavated material is relaxed linearly (recommended), but it could also be relaxed in an accelerated (n > 1) or decelerated manner (n < 1) during the interval.</p> <p>After the excavation interval is finished, the excavated material automatically will be considered inactive in the next interval, and thus will not be considered in the calculation process.</p> <p>Finally, if P7 = 1, then volumetric deformation effects on hydraulics are neglected. As a consequence, the numerical performance of the model is better, especially during excavation.</p>

PARAMETERS FOR ITYCL = 1

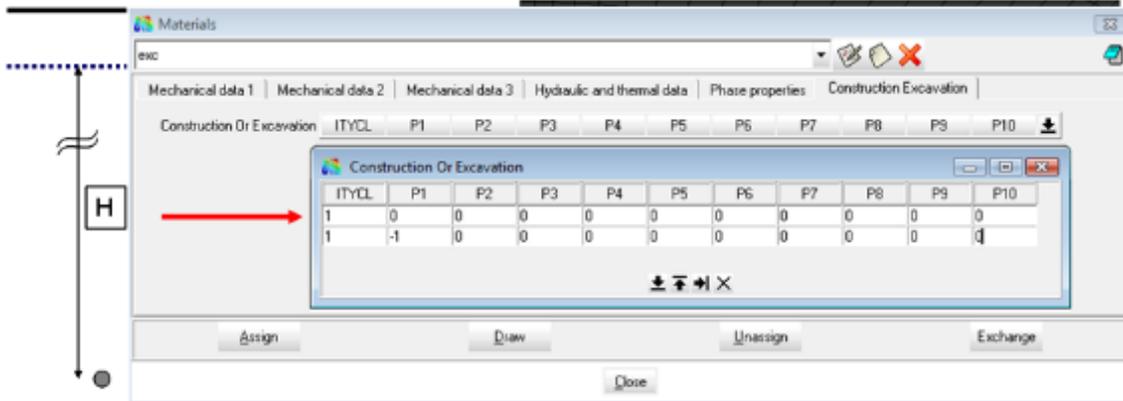
P1	<i>Option</i>	-1: material is inactive. 0: material is active (default option). 1: material is constructed (during the current time interval with gravity increasing linearly with time). After construction interval, P1 is set to 0 internally. 2: material is excavated smoothly (during the current time interval). After excavation interval, P1 is set to -1 internally.
P2	<i>Properties</i>	IMATEQ: Material index (integer) of the material (previously defined) that has the same properties as the current one. Normally, some construction or excavation layers may have the same properties. P2 = 0, properties should be given for the current material. P2 = IMATEQ, properties from the material IMAT = IMATEQ will be copied for this material.
P3	<i>Smoothing exponent n</i>	May be used when P1 = 2. Default value = 1
P4	<i>Smoothing parameter A</i>	May be used when P1 = 2. Default value = 1
P5	<i>Smoothing parameter B</i>	May be used when P1 = 2. Default value = 1
P7	<i>M→H uncoupled</i>	If P7=1, then volumetric deformation effects on hydraulics are neglected.

By default (P1 = 0), the material is active and all the parameters read are used by the programme. When P1 = -1, elements having the material number are not assembled.

As an example, Figure VIg.1 show the two main steps followed in an excavation problem (tunnel). In the first interval time is necessary to impose the initial conditions before excavation. In this time interval, the material is active (P1 = 0). In the second interval time, the relaxation of stresses occurs due to excavation of the material, parameter P1 is equal to -1 (or alternatively P1=2 using the smooth excavation feature).

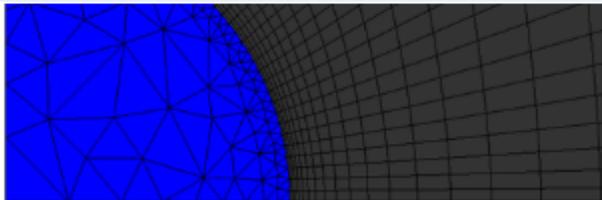
During the excavation interval, it is necessary to impose the ambient conditions in the tunnel, namely, pore water pressure in equilibrium with atmospheric pressure, pore air phase in equilibrium with the relative humidity and temperature equilibrium. When setting these ambient conditions during excavation, it is recommended to use a ramp and/or a small value of the corresponding gamma parameter, to avoid numerical issues.

First time interval: Initial conditions



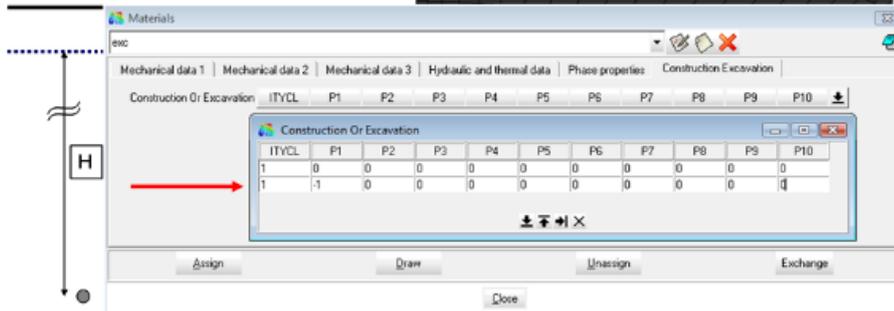
$\sigma = \text{constant} = 4 \text{ MPa}$

$p_w = \text{constant} = 2.25 \text{ MPa}$



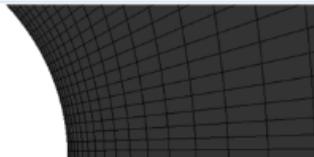
Stress relaxation

Second time interval: Excavation



$\sigma = \text{constant} = 4 \text{ MPa}$

$p_w = \text{constant} = 2.25 \text{ MPa}$



Ambient condition

Second time interval: Excavation

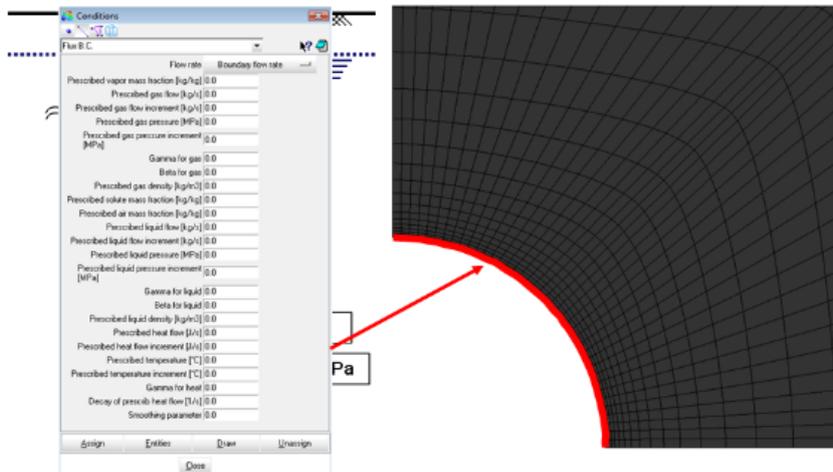


Figure VI.g.1. Illustration of the two main steps followed during excavation problem

VI.h. THM DISCONTINUITIES

Equivalent parameters for discontinuities discretized as thin elements of thickness t

Conditions	Equation for elastic parameters	Other
Normal and shear stiffness of the rock are known	$\nu_d = \frac{k_n - 2k_s}{2k_n - 2k_s}$ $E_d = \frac{(1 + \nu_d)(1 - 2\nu_d)}{(1 - \nu_d)} k_n t$	<p>Normal and shear stiffness of the rock are defined as:</p> $\Delta\sigma_n = k_n \Delta u_n$ $\Delta\tau = k_s \Delta u_s$ <p>t is the element thickness</p>
Shear stiffness of the rock (G) is known and fracture does not deform in volume	$G_d = R^2 G$ $\nu_d = 0.45$ $E_d = 2(1 + \nu_d) G_d$	<p>R is a parameter for reduction of strength (see below)</p> <p>Bulk modulus can be calculated as well:</p> $K_d = \frac{2G_d(1 + \nu_d)}{3(1 - 2\nu_d)}$
Discontinuity assumed like clay without swelling	$K_d = K = \frac{p'(1 + e)}{\kappa}$ $G_d = R^2 G$ <p>Where κ is the elastic compression index in CamClay model</p>	<p>Young and Poisson can be calculated as well:</p> $\nu_d = \frac{3K_d - 2G_d}{2(3K_d + G_d)}$ $E_d = \frac{9K_d G_d}{3K_d + G_d}$
Discontinuity assumed like clay without swelling	$K_d = K = \frac{p'(1 + e)}{\kappa}$ $\nu_d = \frac{1 + \nu - R^2(1 - 2\nu)}{2(1 + \nu + R^2(1 - 2\nu))}$	<p>Young and shear modulus can be calculated as:</p> $E_d = 3K_d(1 - 2\nu_d)$ $G_d = \frac{E_d}{2(1 + \nu_d)}$

Conditions	Equation for plastic parameters	
Cohesion and friction angle are known	$c'_d = Rc'_{soil}$ $\phi'_d = \text{atan}(R \tan \phi'_{soil})$	R is a reduction factor for strength properties
Slope of critical state and cohesion term are known	$M_d = RM$ $p_{s_d} = R(p_{s0} + ks)$	

In general, the corresponding intrinsic permeability is easy to calculate from transmissivity, if this later is known.

For soils, both intrinsic permeability and retention curve depend on porosity. If permeability and retention curve depend on porosity, it is sufficient to consider a larger porosity for the interface in order to increase permeability and reduce air entry value. The following options can be used:

- Exponential equation. In the case presented here, increasing porosity of the interface zone by 50% may be sufficient to produce this effect.
- Kozeny equation. It is also a function of porosity but it does not include parameters except a value of permeability for a given porosity.

Other alternatives can be considered if variation should be larger (cubic law) and more information of the discontinuity.

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APPENDIX II.A. ATMOSPHERIC SUBROUTINES DESCRIPTION

Subroutine `atmosferic_boundary_condition`

General description

This subroutine is the core of the atmospheric boundary condition module. It computes atmospheric boundary conditions, including evaporation, rain, radiation, advective and convective energy fluxes. Those are expressed in terms of fluxes of water, air and energy as functions of the state variables (liquid pressure, gas pressure and temperature of the soil). Moreover, the subroutine calculates the derivatives of these three fluxes with respect to the state variables. Positive values always mean entering the system. Negative values always mean leaving the system *e.g.* evaporation is negative.

It first calls `get_atm_data` to read atmospheric data which is stored in a matrix named `atmosferic`⁹ (see subroutine `get_atm_data` for more information on the format of this file). Some general parameters (like for instance dry and wet albedos) are read from `FLUX`, an argument passed to the main subroutine (which corresponds to CardGroup 20 of the problem data file `root_gen.dat`).

It then computes water flux (through gas and liquid phases, due to evaporation and rain), air flux and energy flux (radiation, advective and convective energy fluxes). Optionally, it can write these fluxes to files depending upon the presence of surveyed nodes or not. The general equations for calculating these fluxes are now presented.

Fluxes of mass

- Flux of gas: The flux of the gas phase q_g is given by the following equation, in which P_{ga} is the atmospheric pressure and γ_g is a leakage coefficient:

$$q_g = \gamma_g (P_g - P_{ga}) \quad (1)$$

- Flux of air: For the flux of air j_a only the advective part is considered:

$$j_a = \omega_g^a q_g = (1 - \omega_g^w) q_g \quad (2)$$

- Flux of water: Evaporation E is given by an aerodynamic diffusion relation:

$$E = \frac{k^2 v_a \phi}{\left(\ln \frac{z_a}{z_0} \right)^2} (\rho_{va} - \rho_v) \quad (3)$$

where ρ_{va} and ρ_v respectively are the absolute humidity (mass of vapour per volume of gas, which can be calculated from relative humidity H_r and temperature) of the atmosphere and at the node of the boundary condition, k is the von Karman's constant (often taken as 0.4), ϕ is a stability factor, v_a the wind velocity, z_0 is the roughness length, z_a is the screen height at which v_a and ρ_{va} are measured. In theory, ρ_v must be the value at roughness length (z_0). Instead, it is

⁹Matrix `atmosferic` is stored in `bb` (n74).

calculated from the state variables at the node of the boundary condition. Hence, a constant profile for ρ_v is assumed between this node and height z_0 .

The advective flux of vapour by the gas phase j_g^w is given by:

$$\begin{cases} j_g^w = \omega_g^w q_g & \text{if } P_g > P_{ga} \\ j_g^w = \frac{\rho_{va}}{\rho_{ga}} q_g & \text{if } P_g \leq P_{ga} \end{cases} \quad (4)$$

where ρ_{ga} is the atmospheric gas density and q_g is the flux of the gas phase given by equation (1).

Surface runoff j_{sr} (which corresponds to the flow rate of water through the liquid phase j_l^w) is written as:

$$\begin{cases} j_{sr} = \gamma_w (P_l - P_{ga}) & \text{if } P_l > P_{ga} \\ j_{sr} = 0 & \text{if } P_l \leq P_{ga} \end{cases} \quad (5)$$

where γ_w is another leakage coefficient. It must be said that ponding is not explicitly simulated, that is, CODE_BRIGHT does not have a special element representing storage of water in a pond. When one assumes no ponding, a very high value for γ_w can be used (but not too high to avoid numerical instabilities). Then, if the soil is saturated ($P_l > P_{ga}$) all rainfall that cannot infiltrate will runoff.

The flux of water j_w is the sum of rainfall P , evaporation E and advective flux of vapour gas phase j_g^w and of surface runoff j_{sr} :

$$j_w = k_{rain} P + k_{evap} E + j_g^w + j_{sr} \quad (6)$$

where coefficients k_{rain} and k_{evap} are input data passed through FLUX and may be used to disable their respective flux.

Flux of energy

- Radiation

Several options are available to evaluate radiation –using ISUN which is passed to the subroutine by FLUX (19) –: 0 for horizontal plane, 1 for vertical cylinder, 2 for measured sun radiation (only short wave radiation is considered), 3 for measured net radiation (short + long wavelength radiations), 4 for measured atmospheric and solar radiation and 5 for measured sun radiation (long and short wave radiations are considered). SUN subroutine is called only¹⁰ if ISUN is lower or equal to 1.

¹⁰ For other cases (ISUN = 2, 3, 4 or 5), RAD_DIR is set to values read from *root_atm.dat* by

The radiation R_n can be given as a measured data or it can be calculated, depending on the value of ISUN:

$$\begin{cases} R_n = (1 - A_l)R_s + R_a - \varepsilon\sigma T^4 & \text{If ISUN} \leq 1 \\ R_n = R_m & \text{If ISUN} = 2 \text{ or } 3 \\ R_n = (1 - A_l)R_m + R_l - \varepsilon\sigma T^4 & \text{If ISUN} = 4 \\ R_n = (1 - A_l)R_m + R_a - \varepsilon\sigma T^4 & \text{If ISUN} = 5 \end{cases} \quad (7)$$

where R_s is the direct solar short wave radiation, R_a is the long wave atmospheric radiation, A_l is the albedo, ε is the atmospheric emissivity, σ is the Stefan-Boltzman constant ($5.67 \times 10^{-8} \text{ J s}^{-1} \text{ m}^{-2} \text{ K}^{-4}$) R_m represents the values of measured radiation (net or solar according to the radiation type) and R_l represents the values of measured atmospheric radiation (long wave). R_m and R_l are read from file *root_atm.dat* by subroutine *get_atm_data*.

Both the albedo and emissivity are considered function of the liquid saturation S_l :

$$A_l = A_d + (A_d - A_w)(S_l^2 - 2S_l) \quad (8)$$

$$\varepsilon = 0.9 + 0.05S_l \quad (9)$$

where A_d and A_w are the dry and wet albedos.

The long wave atmospheric radiation R_a depends on the atmospheric temperature and absolute humidity according to an empirical relation:

$$R_a = \sigma T_a^4 (0.605 + 0.048 \sqrt{1370 \rho_{va}}) \quad (10)$$

The calculation of the solar radiation R_s depends on the value of ISUN. Only the case of a horizontal surface (ISUN=0) will be presented here. R_s for horizontal surface is simplified by:

$$\begin{cases} R_{s,hor} = S_0 f_e \tau_a (\cos \delta \cos \lambda \cos \theta + \sin \delta \sin \lambda) & \text{if } S_{up} > 0 \\ R_{s,hor} = 0 & \text{otherwise} \end{cases} \quad (11)$$

Where, τ_a is the atmospheric transmissivity, λ the latitude, S_0 the sun constant ($=1367 \text{ J m}^{-2} \text{ S}^{-1}$), f_e the correction factor related to the eccentricity of the earth's orbit, δ the earth declination and θ the solar angle.

f_e can be calculated from (Allen et al., 1998) as:

$$f_e = 1 + 0.033 \cos\left(\frac{t-t_{ph}}{d_a}\right) \quad (12)$$

where, d_a is the year duration ($= 365.241 \text{ days} = 3.15568 \times 10^7 \text{ s}$), t_{ph} is the time at perihelion (January 3^d)

The sun declination (δ) is the angle between the direction of the sun and the equator. It can be calculated by a yearly sinusoidal function:

$$\delta = \delta_{max} \sin\left(2\pi \frac{t-t_s}{d_a}\right) \quad (13)$$

where δ_{max} is the maximum sun declination ($= 0.4119 \text{ rad} = 23.26^\circ$), t_s is time at September equinox (September 21st for the northern hemisphere).

subroutine *get_atm_data*.

The solar angle (θ) describes the circular movement of the sun during a day. It equals 0, when the sun is at its zenith and can be estimated as:

$$\theta = \frac{t-t_m-t_c}{d_d} 2\pi \quad (14)$$

where, t_m is the time at noon for an arbitrary day, d_d is the day duration (= 86400 s) and t_c is the equation of time, used to correct the variations on the hour of zenith during the year, and defined as:

$$t_c = \frac{\delta_{max} d_d}{8\pi} \sin\left(\frac{t-t_s}{d_a} 4\pi\right) - \frac{e d_d}{\pi} \sin\left(\frac{t-t_{ph}}{d_a} 2\pi\right) \quad (15)$$

where, e is the eccentricity to the earth's orbit (=0.0167)

Subequations 2 to 5 in Eq. (7) use data read from *root_atm.dat* file. ISUN=2 suppose that only radiation considered is measured solar radiation (short wave), ISUN=3, assumes that measured data corresponds to net radiation (short + long wave length i.e. solar + atmospheric – surface), ISUN=4, considers that data available are solar radiation (R_m in *root_atm.data* file) and atmospheric radiation (R_l in *root_atm.data* file), while ISUN=5 considers that only data available are solar radiation (short wave length, R_m in *root_atm.data* file)

Solar radiation (short wave) is measured or calculate on a horizontal surface, when an inclined surface is considered this value must be corrected. The atmosphere scatters the sunlight, so the surface receives part of the sun radiation directly from the sun and another part in a diffusive form. An inclined surface in the shade does not receive the direct part but only the diffusive solar radiation.

Therefore, for an inclined surface the real solar radiation perceived can be obtained by the next expression:

$$R_s = R_{s,hor} \left[(1 - f_{dif}) \frac{\max(P^T S, 0)}{S_{up}} + f_{dif} \right] \quad (16)$$

where, $R_{s,hor}$ is the solar radiation on a horizontal surface (measured or calculated), f_{dif} the fraction of diffusive solar radiation over the total solar radiation, defined as:

$$f_{dif} = \frac{1}{1 + \exp(8.6\tau_a - 5)} \quad (17)$$

Vectors P and S, are unitary length vectors that define the position of Sun and Zenith. P is orthogonal to the earth surface pointing outwards and S points to the Sun, they are defined as follows:

$$P = \begin{pmatrix} P_{east} \\ P_{north} \\ P_{up} \end{pmatrix} = \begin{pmatrix} \cos \alpha \sin \beta \\ -\sin \alpha \sin \beta \\ \cos \beta \end{pmatrix} \quad (18)$$

$$S = \begin{pmatrix} S_{east} \\ S_{north} \\ S_{up} \end{pmatrix} = \begin{pmatrix} \cos \delta \sin \theta \\ \sin \delta \cos \lambda - \cos \theta \cos \delta \sin \lambda \\ \cos \delta \cos \lambda \cos \theta + \sin \delta \sin \lambda \end{pmatrix} \quad (19)$$

where, α and β are the surface strike and dip, respectively. The product of both vectors ($P^T S$) equals the cosine of the angle between them. For horizontal surface ($\beta = 0$) the vector $P^T = (0, 0, 1)$ and $P^T S = S_{up}$. At night $S_{up} < 0$, at daylight $S_{up} > 0$ and during the sunrise and sunset $S_{up} = 0$.

- Advective energy flux

The sensible heat flux H_s is, like evaporation, calculated through an aerodynamic diffusion relation:

$$H_s = \frac{k^2 v_a \rho}{\left(\ln \frac{z_0}{z_a} \right)^2} \rho_{ga} C_a (T_a - T) \quad (20)$$

where C_a is the specific heat of the gas.

- Convective energy flux

The convective or latent heat flux H_c is calculated taking into account the internal energy of liquid water, vapour and air:

$$H_c = h_v (E + j_w^g) + h_{la} (P + j_w^l) + h_{a0} j_a \quad (21)$$

where h_v , h_{la} and h_{a0} are the free energy of vapour, liquid water and air, respectively. These three properties depend on the temperature: temperatures used are the temperature at the node of the boundary for h_v , and h_{a0} and the dew point temperature, which depends on the atmospheric vapour pressure, for h_{la} .

- Total energy flux

The total energy flux j_e thus writes as follows:

$$j_e = k_{rad} R_n + H_s + H_c \quad (22)$$

where k_{rad} is an input parameter passed through FLUX and may be used to disable radiation flux.

Results output

If values are surveyed at a given node, the following variables are written to files 200+nodout: $t+\Delta t$, P , E , j_w^g , j_w^l , j_w , j_a , R_n , H_s , H_c , j_e .

Subroutine get_atm_data

This subroutine computes atmospheric data at time $t+dt$ either by simulation or by interpolation of input data. In both cases, returned values are summarized in Table II.2.8. This table also mentions implemented names for these variables and columns concerned in the matrix `atmosferic`, where all data needed for simulations or interpolations are stored.

Two options can be used to compute atmospheric data: interpolation and simulation. Interpolation uses a simple linear interpolation of the specified parameters versus time. Simulation uses the following sinusoidal expression:

$$x(t) = x_m + x_a \sin\left(2\pi \frac{t-t_a}{d_a}\right) + x_d \sin\left(2\pi \frac{t-t_d}{d_d}\right) \quad (23)$$

where x is the value of the parameter, x_m is its mean value, a_a is its annual amplitude, a_d its daily amplitude, t_a is the start of the annual variation, t_d is the start of the daily variation, d_a is the duration of a year and d_d is the duration of a day (= 86400 s).

Table II.2.8: Atmospheric data taken into account in the boundary conditions module.

<i>Atmospheric variable</i>	<i>Unit</i>	<i>Implemented name</i>	<i>Columns used</i>
Atmospheric temperature, T_a	°C	TEMP_ATM	1 – 2
Atmospheric gas pressure, P_{ga}	MPa	PG_ATM	3 – 4
Relative humidity, H_r	–	RELHUM	5 – 6
Solar radiation, R_n	J/m ² /s	RAD_DIR	7 – 8
Insolation fractions, I_n	–	FRACINS	9 – 10
Rain, P	kg/m ² /s	RAIN	11 – 12
Wind velocity, v_a	m/s	WIND	13 – 14

Matrix `atmosferic` is read from file `root_atm.dat` (or `root_atm.inp`) which index is `iin3` =103. This file is opened by `read_assign_files` subroutine (`read_grid.f`) and read by `read_atm_bc` (`read_general.f`) subroutine which assigns `atmosferic` its values and is called by `main_initialize` (`code_bright_main.f`).

Note that `atmosferic` dimensions also are read from `iin3` and that this instruction is present in `read_assign_dim_opt_2` (`code_bright_main.f`).

Data simulation

If a simulation is performed, a sinus shape function with annual and daily variations is used. The daily variation is only taken into account if the time increment is lower than one day. Input data (for each variable) needed for each variable is (Unit represents the unit given in Table II.2.8):

- annual mean (Unit), x_m ,
- annual amplitude (Unit), x_a ,
- annual gap (s), t_a ,
- daily amplitude (Unit), x_d ,
- daily gap (s), t_d .

For a given variable, the simulated value a time $t+dt$ is obtained according to the following relation¹¹:

¹¹ This expression cancels out daily variations if the time increment dt is higher than d_d , duration of one day.

$$x(t+dt) = x_m + \frac{1}{\pi dt} \left[x_a d_a \sin\left(\frac{2\pi(t+0.5dt-t_a)}{d_a}\right) \sin\left(\frac{\pi dt}{d_a}\right) + x_d d_d \sin\left(\frac{2\pi(t+0.5dt-t_d)}{d_d}\right) \sin\left(\frac{\pi dt}{d_d}\right) \right] \quad (24)$$

Figure II.2.6 and Figure II.2.7 show the simulation of the annual variation of an atmospheric variable (case of temperature).

Data interpolation

Interpolation concerns all available data for discrete times t_i satisfying $t < t_{i+1}$ and $t + dt > t_i$ until condition $t + dt < t_{i+1}$ is satisfied. If code time t is lower (resp. bigger) than lowest (resp. highest) discrete time, the subroutine is stopped.

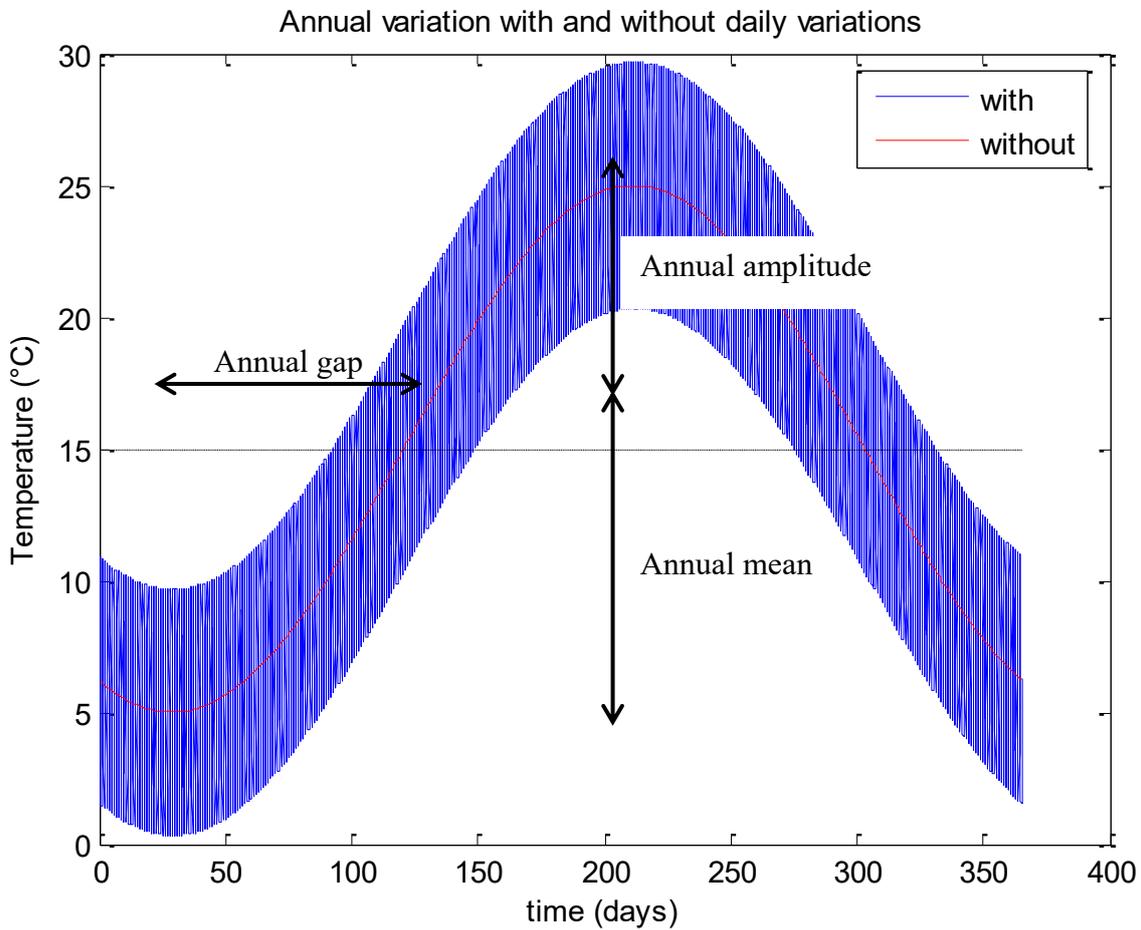


Figure II.2.6: Simulation of annual variation of an atmospheric variable (case of temperature).

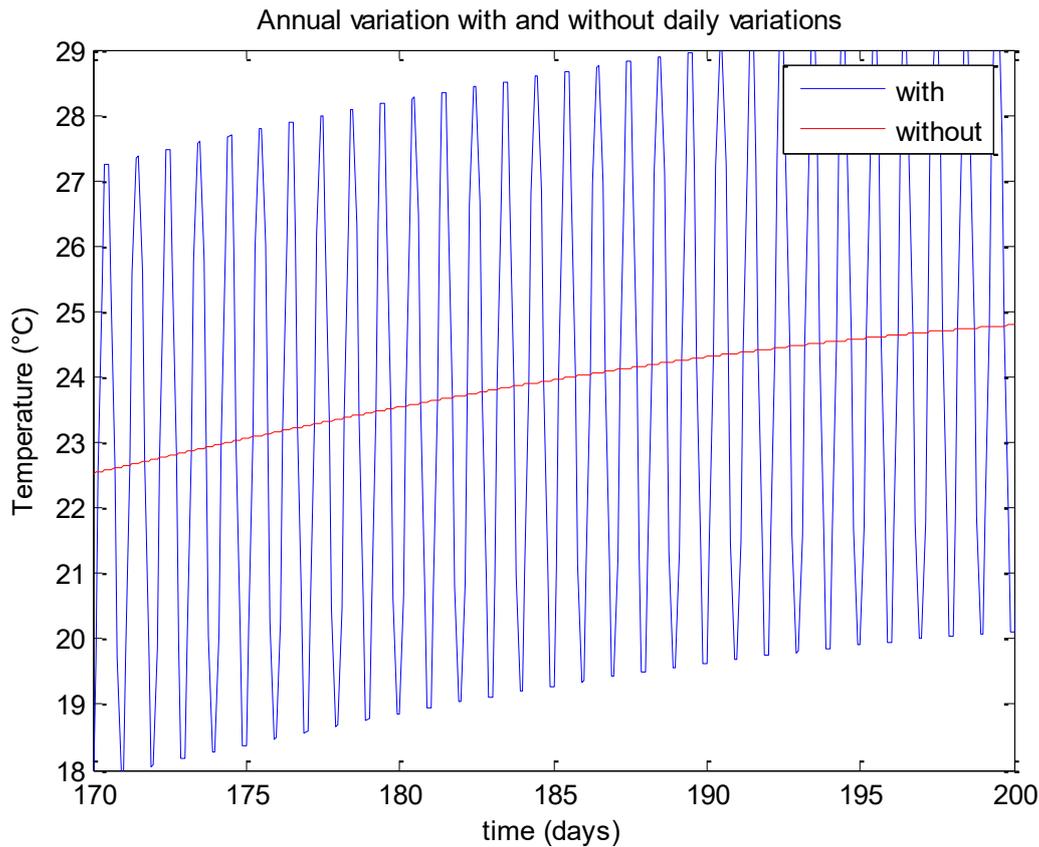


Figure II.2.7: Simulation of annual variation of an atmospheric variable (case of temperature; close view).

Subroutine SUN

This routine calculates the direct solar radiation. Calculation type (ISUN) is passed through FLUX vector in atmospheric_boundary_condition. The different values for ISUN that imply a call to SUN subroutine are:

- 0 - horizontal plane,
- 1 - vertical cylinder.

However, ISUN=0 is the unique option proposed in the manual of Retraso.

This calculation takes into account sun distance and declination (function of date from 1st January), solar day duration (function of latitude and declination). All this data together with insolation fraction allow computing daily radiation (equations where presented in section 0).

If time increment is bigger than a day, direct radiation directly uses daily radiation. Otherwise, time with respect to night is taken into account and the direct radiation is calculated.

Figure II.2.8 shows the simulated daily radiation versus time in both cases.

Case ISUN=1

$$R_A = S_0 r_s \frac{d_s}{2} \left(1 + \sqrt{1 - (\cos \lambda \cos \delta + \sin \lambda \sin \delta)^2} \right) \quad (25)$$

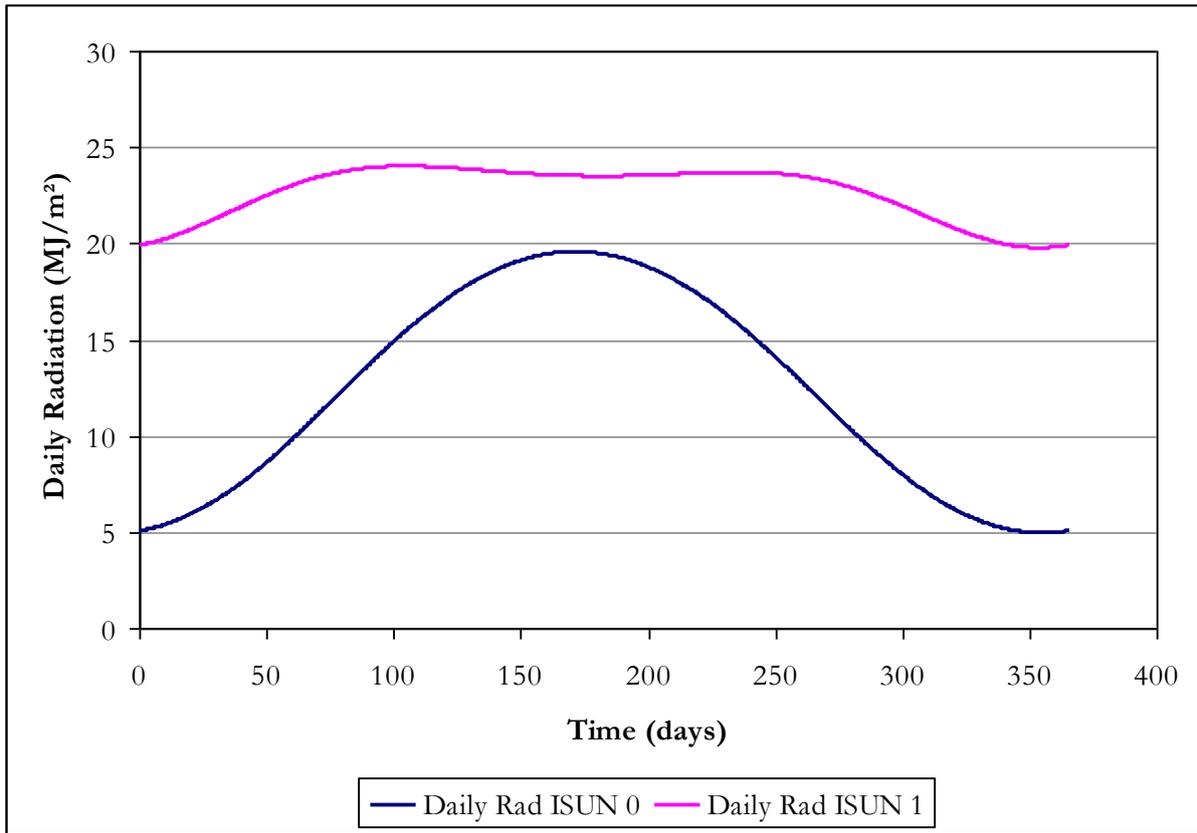


Figure II.2.8: Daily radiation as a function of time according to ISUN option.

Reference

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APPENDIX III.A. GENERAL INFORMATION FILE: ROOT_GEN.DAT

Card 1. Problem

Variables: HEAD

Format: (A40): Fixed format

-999: Free format

Card 2. Dimensions and options

Variables: NUMNP, NUMEL, NDIM, IAXISYM, NUMMAT, NHV

Format: (10I5). It is not required if free format is used

NUMNP: Number of nodes

NUMEL: Number of elements

NDIM: Space dimensions (1,2,3)

IAXISYM: Axisymmetric option: 0-no axisymmetry, 1-yes (around y-axis),

- NDIM=2. The principal stresses are: σ_r (radial), σ_y (axial), σ_θ (circumferential)

- NDIM=1. The principal stresses are: σ_r (radial), σ_θ (circumferential), σ_z (axial)

NUMMAT: Number of materials

NHV: Number of history variables (depends on the type of mechanical constitutive model used). This variable is checked internally.

Card 3. Dimensions and options

Variables: NZ1, NZ2, MFRONTH, NDF, MNVAL, ISOLVE

Format: (10I5). It is not required if free format is used

NZ1: = MXDIFN: maximum difference between connected nodes, this variable is read for dimensioning purposes. The node numeration of the grid is assumed to have been optimised in order to reduce the matrix band width. If $\theta = \varepsilon = 0$ are used in a non-mechanical problem, then MXDIFN can be 0 because a quasi-explicit approximation will be used, i.e. only a NDF-diagonal matrix is solved which contains derivatives of the storage terms. (See below for $NZ = NZ1 * NZ2$).

NZ2: = MBANDT: total band width (geometrical for 1 variable), ($MBANDT = 2 (MXDIFN+1) - 1$), the user should provide a value but the code checks this value. So this entry is redundant.

NZ=
NZ1*NZ2: Used only for ISOLVE = 5. It is the number of nonzero-blocks in the jacobian (i.e. the number of nonzeros for NDF = 1). This variable is computed as $NZ = NZ1 * NZ2$. Since this variable is checked internally, if the number of nonzeros is not known a priori, a guess can be used and the code automatically checks its validity. Otherwise, the required value is output.

MFRONTH: void

NDF: Number of degrees of freedom per node. For instance a 2-dimension thermomechanical analysis requires NDF = 3.

MNVAL: Maximum number of integration points in an element (default = 1). For a two-dimensional analysis with some (not necessarily all) quadrilateral elements, MNVAL = 4. For a three-dimensional analysis with some (not necessarily all) quadrilateral prism elements, MNVAL = 8.

ISOLVE: Solve the system of equations according to different algorithms.
ISOLVE = 3: LU decomposition + backsubstitution (NAG subroutines, fonts available). Recommended option for direct solution.
ISOLVE = 5: Sparse storage + CGS (conjugate gradients squared).

Card 4. Dimension boundary conditions

Variables: NFDTYPE, NFLUXTYPE

Format: (5I5). It is not required if free format is used

NFDTYPE: Number of prescribed force/displacement boundary condition types. NFDTYPE \leq NUMNP because the maximum types that can be defined is limited by one per node. If IOPTDISPL $>$ 0 then NFDTYPE \geq 1.

NFLUXTYPE: Number of flux boundary condition types. NFLUXTYPE \leq NUMNP. Boundary conditions for mass and energy balance problems are grouped in a single type due to practical reasons. See **Cards 17 to 20** for information about the form of boundary conditions.

Boundary conditions can be applied at all nodes, even in the internal nodes.

Card 5. Options. Unknowns to be calculated.

Variables: IOPTDISPL, IOPTPL, IOPTPG, IOPTTEMP, IOPTXWS

Format: (10I5). It is not required if free format is used

IOPTDISPL: = 1, solving for NDIM displacements (u_x, u_y, u_z)

IOPTPL: = 1, solving for liquid pressure (P_l) (see IOPTPC)

IOPTPG: = 1, solving for gas pressure (P_g)

IOPTTEMP: = 1, solving for temperature (T)

IOPTXWS: = 2, solving for a solute in liquid phase (c)

Card 6. Other options.

Variables: IOPTXHL, IUPDPOR, IOPTXWG, IOPTXAL, IOPTPC, IOPHTHS, IUPDC

Format: (10I5). It is not required if free format is used

IOPTXHL: = 1, halite is soluble in liquid phase. ω^h (the mass fraction of salt in liquid) is non-zero and considered a dependent variable on temperature. For isothermal problems this option is not very relevant because solubility has only been considered a function of temperature and not on pressure, however IOPTXHL = 1 can still be used in order that the liquid phase is considered a saturated brine instead of pure water. In this case, properties of liquid phase are computed according to the concentration obtained as a function of TCONS (**Card 8**)

IUPDPOR: = 1, porosity is updated including not only volumetric strain, but also dissolution/precipitation (see IOPTXHL).

If IUPDPOR = 0 and IOPTXHL is non zero a warning message is given because variations of porosity caused by other than deformation will be neglected. IUPDPOR = 1 only makes sense for IOPTXHL = 1.

- IOPTXWG: = 1, water vapour is NOT permitted even if the problem is non-isothermal and unsaturated. If IOPTXWG = 0, water vapour is permitted and its concentration computed through psychrometric law, vapour pressure and gases law.
Using IOPTXWG = 1 (i.e. vapour concentration is not computed) is convenient when the problem is nonisothermal but the whole medium will remain saturated during the entire simulation.
- IOPTXAL: = 1, air dissolved is NOT permitted even if the problem is two phase (liquid and gas) flow. If IOPTXAL = 0, air dissolved is permitted and its concentration computed through Henry's law.
- IOPTPC: index to modify some aspects related to capillary pressure, saturation and relative permeability.
IOPTPC = 0, S_l -element is computed as a function of the capillary pressure $P_g - P_l$ -element. (Consistent approximation, not recommended).
IOPTPC = -1, S_l -element is computed by averaging S_l -nodal values. k_{rl} -element and k_{rg} -element are computed as a function of S_l -element (recommended option).
IOPTPC = -2, k_{rl} -element and k_{rg} -element are computed by averaging nodal values of relative permeabilities.
IOPTPC = -3, k_{rl} -element and k_{rg} -element are computed by averaging nodal values. Derivatives of relative permeabilities are also averaged.
IOPTPC = -4, k_{rl} -element and k_{rg} -element are set equal to the maximum nodal value.
IOPTPC = 1: capillary pressure is used ($P_c = P_g - P_l$) as state variable instead of P_l . If IOPTPC = 1 then it is necessary to use IOPTXAL = 1 and IOPTXWG = 1, and IOPTDISPL = 0 and IOPTTEMP = 0. That is, IOPTPC = 1 is only available for two phase immiscible fluids.
- IOPTHYS: = 1: option for hysteretic behaviour of retention curve (currently not available).
- IUPDC: = 1: updated lagrangian method, i.e., co-ordinates are modified after each time increment is solved. If deformations are very large, some elements may distort. If distortion is very large the volume of an element may become negative and the execution would terminate immediately.

Remarks: vapour and air dissolved are considered automatically depending on options in Card 5. However, if for any reason they want not to be considered, then the auxiliary indexes IOPTXWG = 1 or IOPTXAL = 1 can be used.

Card 7. Flags. Auxiliary options.

Variables: IFLAG1, IFLAG2, IFLAG3, IFLAG4, IFLAG5

Format: (10I5). It is not required if free format is used

IFLAG1: 0
IFLAG2: 0
IFLAG3: 0
IFLAG4: 0
IFLAG5: 0

These options have been introduced for programming purposes. In general users should not use them.

Card 8. Constants.

Variables: EPSILON, THETA, PGCONS, TCONS, PLCONS

Format: (6F10.0). It is not required if free format is used

- EPSILON: Position of intermediate time $t^{k+\epsilon}$ for matrix evaluation, i.e. the point where the non-linear functions are computed. (frequent values: 0.5, 1)
- THETA: Position of intermediate time $t^{k+\theta}$ for vector evaluation, i.e. the point where the equation is accomplished. (frequent values: 0.5, 1)
- PGCONS: Constant gas phase pressure for solving with IOPTPG = 0, otherwise ignored. (frequent value: 0.1 MPa = atmospheric pressure).
- TCONS: Constant temperature for solving with IOPTTEMP = 0, otherwise this value is ignored.
- PLCONS: Constant liquid phase pressure for solving with IOPTPL = 0, otherwise ignored. (if PLCONS is greater than -1.0×10^{10} then wet conditions are assumed for computing viscous coefficients in creep laws. (Otherwise the medium is considered dry.)

Card 9. Void.

This line should be left blank.

Card 10. Options.

Variables: IOWIT, INTER, ITERMAX, IOWCONTOURS, ITERMAXS, ITIME, IMBACKUP, IWRALL, IPOLYFILES

Format: (10I5). It is not required if free format is used

- IOWIT: Iteration information is written in file *ROOT_GEN.OUT* according to:
- IOWIT = 0, no information about convergence is written. This option should be used if the user is very confident with the time discretization and not interested in details at every time step or problems with time increment reductions. Usually this happens when previous runs have shown that convergence and time discretization work very well.
 - IOWIT = 1, partial information is written. Time intervals and time-values, number of iterations, CPU-time values, etc. are written. Convergence information is only written if time increment reductions take place.
 - IOWIT = 2, all iteration information is written. Convergence information is written for all iterations and all time increments. This option may result in a very large file *ROOT_GEN.OUT*
- INTER: Writing results frequency in *ROOT_OUT.OUT* or in *ROOT.FLAVIA.RES*. For instance, if INTER = 20 results will be

written only every 20 time increments, results at intermediate points will be lost, except the values at few nodes or elements that may be requested in the *ROOT_GRI.DAT* file (see below).

ITERMAX: Maximum number of iterations per time increment

IOWCONTOURS: Option for writing results in files GiD post processor.

IOWCONTOURS = 2 then files of nodal values for GiD are generated. These are *ROOT.flavia.dat* and *ROOT.flavia.res*.

IOWCONTOURS = 5 or 6 then files for new GiD output (nodal variables at nodes, Gauss point variables at Gauss points without smoothing) are generated. These are *ROOT.post.msh* and *ROOT.post.res*. If IOWCONTOURS = 5, only one Gauss point of each element is printed (average value). If IOWCONTOURS = 6, all Gauss points are printed for all elements.

ITERMAXS: Maximum number of iterations for the solver, i.e. for Conjugate Gradients Squared solution (this variable is only required for ISOLVE = 5).

ITIME (see table):

- 0 No time step prediction
- 1 Time step prediction according to a limit of 4 iterations.
- 2 Time step prediction according to a limit of 3 iterations.
- 3 Time step prediction according to a limit of 2 iterations.
- 4 Time step prediction according to a limit of 1 iteration.
- 6 A new time step is predicted from the relative error in variables of the previous time increment. If this relative error is lower than $dtol = 0.01$, time increment is reduced according to error deviation.
- 7 The same as 6, but with $dtol = 0.001$.
- 8 The same as 6, but with $dtol = 0.0001$.
- 9 The same as 6, but with $dtol = 0.00001$.

ITIME = 0	TIME STEP FACTOR IS 1.4 ALWAYS DTIMEC is the upper bound of time step
NUMBER OF NR ITERATIONS AS A MEASURE OF ERROR	
ITIME = 1	$f = \left(\frac{4}{iter}\right)^{0.25} \geq 0.5$
ITIME = 2	$f = \left(\frac{3}{iter}\right)^{0.25} \geq 0.5$
ITIME = 3	$f = \left(\frac{2}{iter}\right)^{0.25} \geq 0.5$
ITIME = 4	$f = 1.05 \left(\frac{1}{iter}\right)^{0.25} \geq 0.5$

RELATIVE ERROR CONTROL	
First Order Approach $0.1 \leq f = 0.8 \left(\frac{DTOL}{error} \right)^{0.5} \leq pdfmax$	
ITIME = 6	DTOL = 0.01
ITIME = 7	DTOL = 0.001
ITIME = 8	DTOL = 0.0001
ITIME = 9	DTOL = 0.00001

In the upper Table, f is the factor for time step reduction and $pdfmax$ is set to 1.4.

- IMBACKUP: 0 No Backup.
 1 Backup only for the last time step.
 2 Backup for all time steps.
- IWRALL: 1 Write all information for output.
 0 Write partial information for output.
- IPLOYFILES: 1 Write in separated output files (select variables in output window). Two files are generated by each variable selected:
 ROOT_variable.post.msh and *ROOT_variable.post.res*
 0 If IWRALL = 1

CardGroup 11. Convergence parameters

Variables:

- Displacements: DELMXU, FACU, DELFMX, DUMX
 (Omit this line if IOPTDISPL = 0)
- Liquid pressure: DELMXPL, FACPL, DELQWMX, DPLMX
 (Omit this line if IOPTPL = 0)
- Gas pressure: DELMXPG, FACPG, DELQAMX, DPGMX
 (Omit this line if IOPTPG = 0)
- Temperature: DELMXT, FACT, DELQMX, DTMX
 (Omit this line if IOPTTEMP = 0)
- Inclusions conc.: DELMXI, FACI, DELIMX, DIMX
 (Omit this line if IOPTXWS = 0)

Format: (5F10.0). It is not required if free format is used

Each computed unknown requires a line with its associated parameters. In this way each equation has different tolerances. If IOPTDISPL = 1, only one line with DELMXU, FACU, DELFMX, DUMX should be read regardless whether the problem is one, two or three dimensional.

DELMXU: Maximum (absolute) displacement error tolerance (m). When correction of displacements (displacement difference between two iterations) is lower than DELMXU, convergence has been achieved.

FACU: Maximum (relative) displacement error tolerance (-).When correction of displacements (displacement difference between two iterations) divided by

displacement variation during the time interval is lower than FACU, convergence has been achieved.

These two conditions (DELMXU and FACU should be satisfied simultaneously. If one of them is not desired, a large value of DELMXU or FACU can be used.

- DELFMX: Maximum nodal force balance error tolerance (MN). If the residual of forces in all nodes is lower than DELFMX, convergence has been achieved.
- DUMX: Maximum displacement correction per iteration (m) (time increment is reduced if necessary). If correction of displacements (displacement difference between two iterations) is greater than DUMX then, time increment will be reduced until this condition is satisfied. For lower values of DUMX the time step used for the calculations will be small. For larger values of DUMX time step may be larger but errors will increase and convergence problems may appear.
- DELMXPL: Maximum (absolute) liquid pressure error tolerance (Mpa)
- FACPL: Maximum (relative) liquid pressure error tolerance (-)
- DELQWMX: Maximum nodal water mass balance error tolerance (kg/s)
- DPLMX: Maximum liquid pressure correction per iteration (MPa) (time increment is reduced if necessary)
- DELMXPG: Maximum (absolute) gas pressure error tolerance (MPa)
- FACPG: Maximum (relative) gas pressure error tolerance (-)
- DELQAMX: Maximum nodal air mass balance error tolerance (kg/s)
- DPGMX: Maximum gas pressure correction per iteration (MPa) (time increment is reduced if necessary).
- DELMXT: Maximum (absolute) temperature error tolerance (°C)
- FACT: Maximum (relative) temperature error tolerance (-)
- DELEMX: Maximum nodal energy balance error tolerance (J/s)
- DTMX: Maximum temperature correction per iteration (°C) (time increment is reduced if necessary).
- DELMXI: Maximum (absolute) water in inclusion mass fraction error tolerance (-)
- FACI: Maximum (relative) water in inclusion mass fraction error tolerance (-)
- DELIMX: Maximum nodal inclusions balance error tolerance (kg/s)
- DIMX: Maximum mass fraction in solid correction per iteration (-) (time increment is reduced if necessary)

Relative error is defined as the ratio between variable correction (δx) and variable increment (Δx).

Convergence criteria are as follows (only convergence on the equation of energy balance is illustrated, but the same applies for the other equations):

If ($\delta T < \text{DELMXT} + \text{FACT} \cdot T$) for all nodes, then convergence has been achieved (condition A). T is the value of the variable temperature.

If ($q_h < \text{DELEMX}$) for all nodes (q_h represents here the energy balance or residual in a node), then convergence has been achieved (condition B).

It should be mentioned that convergence in terms of δT and convergence in terms of q_h should be reached simultaneously because the Newton - Raphson is used. For this reason the program stops the iteration process and looks for another time step when one of the two conditions (A or B) is achieved. For instance if the user decides that convergence should be imposed because the residual has reached a tolerance then, DELMXT and FACT should be set to very low values.

When more than one degree of freedom is solved per node and the last option is used, convergence in terms of variable or residual should be achieved by all the variables simultaneously. In other words, it is not possible that the mechanical problem converges by residual and the thermal converges by the variable.

If ($\delta T > DTMX$), time increment will be reduced. This parameter controls the accuracy of the solution in terms of how large can be the time increments. A low value of DTMX will force to small time increments when large variations of temperature take place.

Usually, it is difficult to guess the values of the tolerances that should be used in a problem. The convergence criterion in terms of absolute terms is linked with the unknowns, and hence it also depends on the range of variation of the variable. In this case the user decides the degree of accuracy that is needed for each variable. The tolerances in relative terms are usually larger than the values for absolute.

Finally, the tolerance values for residual convergence are more difficult to guess because 'a priori' it is difficult to know the values of forces or flows equilibrating at nodes. Again the user should reach a compromise between a very strict value and a less severe condition.

Convergence parameters for **Conjugate Gradients Squared method** of solution (Omit this CARD if ISOLVE is not equal to 5).

Variables: DXS,DRS,DRSREL

Format: (5F10.0). It is not required if free format is used

This **Card** is only required for ISOLVE=5.

DXS: Maximum abs. correction for solver (usually a very low value)

DRS: Maximum abs. residual for solver ($< \min(\text{DELFMX}, \text{DELQWMX}, \text{DELQAMX}, \text{DTMX}, \text{DELIMX})$) assuming all them > 0

DRSREL: Maximum relative residual for solver. The solver residual is normalised with the RHS of the system of equations to be solved.

This group of **Cards** ends with ' -1' (forma I5).

Card 12. Gravity

Variables: GRAVITY(1), ..., GRAVITY(NDIM)

Format: (3F10.0). It is not required if free format is used.

GRAVITY(NDIM): gravity vector (m/s^2), usually (0,0,-9.81) for three dimensions, (0,-9.81) for two dimensions and (-9.81) for one dimension.

The following group of **Cards**, beginning with time interval definition can be repeated several times to define intervals with different material properties and/or boundary conditions. For the first interval all information should be read and for the subsequent intervals only modifications are required.

Card 13. Interval time variables

Variables: TIMEI, DTIME, TIME1, DTIMEC, TIMEF, FACTTIME

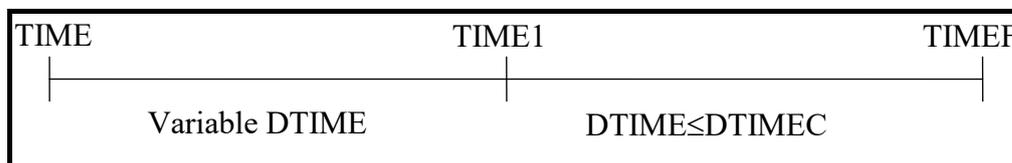
Format: (5F10.0), It is not required if free format is used

- TIMEI: Initial time. If TIMEI is not equal to final time of the last increment (TIME), then it is assumed $\text{TIMEI} = \text{TIME}$. Exception is made if $\text{TIMEI} = 0.0$, in which case, 0.0 is kept as a new origin of times.
- DTIME: Initial time increment for each time interval. If $\text{DTIME} = 0$, last DTIME value is used or, if it is the first time increment of the calculation, a small value is considered.
- TIME1: Time from which an upper bound is prescribed for the time increment. If $\text{TIME1} = 0$, then TIME1 is considered equal to TIMEI (the upper bound is prescribed during all the time step).
- DTIMEC: Upper bound value for the time increment used from TIME1 to TIMEF. If found to be equal to zero, no maximum time increment value is prescribed.
- TIMEF: Final time.
- FACTTIME: Factor for converting seconds (input time units) into another output time units. (Example: $\text{FACTTIME} = 86400$. for output in days).

Time increments during time step [TIMEI1, TIMEF] are adapted by the code according to flag control ITIME (see **Card 10**). This may cause inconveniences if the user desires the results at precisely fixed times (for instance: 6 months, 1 year, 2 year, etc.). However, this could be solved using a negative 'writing frequency' (see section II.2.1).

Moreover, if something changes between two runs (e.g. boundary conditions) and any time increment should be modified, the value of the times in which results are output will not be identical between the two runs. In this case, it would be difficult to make a comparison of the two analyses because we would not have the same times for output.

A first way to overcome this inconvenience is to prescribe an upper bound for the time increment, reflected in the variable DTIMEC. If convergence requires time increments smaller than DTIMEC, time increment is reduced. But, if convergence is easy and the current time increment becomes higher than DTIMEC, it is fixed to DTIMEC. Variable TIME1 allows for setting an intermediate time between TIMEI and TIMEF from which the upper bound for the increment becomes active, as represented below:



Another way to set fixed times for output results is to use a sequence of **Cards** number 13 separated by two (only flow or only mechanical problem) or three (flow and mechanical problem) lines with '-1' (format I5) indicating that nothing changes in the new time interval, except the time discretization. In this way, results will be output for all TIMEF's, and if the user is only interested in these fixed times a very large value may be used for INTER (see **Card 10**) to avoid output at other times.

Example:

-1 indicates no change in material properties
-1 indicates no change in mechanical boundary conditions
-1 indicates no change in flow boundary conditions
350000. 0.0 0.0 10000. 360000. 86400.
-1 indicates no change in material properties
-1 indicates no change in mechanical boundary conditions
-1 indicates no change in flow boundary conditions
360000. 0.0 0.0 10000. 370000. 86400.
-1 indicates no change in material properties
-1 indicates no change in mechanical boundary conditions
-1 indicates no change in flow boundary conditions

In this case for the times 350000, 360000 and 370000 the results would be written. Time step in this case would be lesser or equal than 10000.

It is possible to define at the beginning of the calculation a step for equilibration of the initial stress state. This is done by defining a time step starting from a negative value (TIMEI < 0) and ending at 0 (TIMEF = 0). During this step, gravity is applied as a ramp. Greater is time step (TIMEF – TIMEMAX), smoother is the gravity ramp.

Card 14. Number of material

Variables: IMAT

Format: (I5). It is not required if free format is used

IMAT: index of material (\leq NUMMAT)

(if '-1' (format I5) is read, no more materials are read, and hence, parameters will be zero (or default values when defined) or the value read in a former time interval)

Card 15. Number and name of constitutive law

Variables: ICL, TIT, ITYCL

Format: (I5, A20; I5). It is not required if free format is used

ICL: index of constitutive law (if '-1' (format I5) is read, no more constitutive laws are read for this material). Each process considered needs one or more ICL's.

TIT: text to identify (by the user) the constitutive law (ex: Retention curve), this text will be reproduced on output only for the user reference but will not be used by the program.

ITYCL: type of constitutive law. For each value of ICL several relationships (different values of ITYCL) may be available.

CardGroup 16. Parameters constitutive law

Variables: TIT, PARCL(1,ICL,IMAT)=P1, TIT, PARCL(6,ICL,IMAT)=P6
TIT, PARCL(2,ICL,IMAT)=P2, TIT, PARCL(7,ICL,IMAT)=P7
TIT, PARCL(3,ICL,IMAT)=P3, TIT, PARCL(8,ICL,IMAT)=P8
TIT, PARCL(4,ICL,IMAT)=P4, TIT, PARCL(9,ICL,IMAT)=P9
TIT, PARCL(5,ICL,IMAT)=P5, TIT, PARCL(10,ICL,IMAT)=P10

Format: (A20, F10.0, A20, F10.0) . It is not required if free format is used

TIT: text to identify (by the user) the parameter (ex: Young modulus (E)), this text will be reproduced on output only for user reference but will not be used by the program

PARCL(MNP,NCL,NUMM parameters of constitutive laws (MNP=10, NCL is the AT): maximum number of existing constitutive laws)

The matrix PARCL(MNP,NCL,NUMMAT) contains all information of parameters for the constitutive laws. A maximum of 10 parameters for each constitutive law is considered. These parameters are read in 2 columns, i.e., 5 lines are required to read each PARCL as indicated above. This is represented as:

Text Parameter 1	Value for P1	Text Parameter 6	Value for P6
Text Parameter 2	Value for P2	Text Parameter 7	Value for P7
Text Parameter 3	Value for P3	Text Parameter 8	Value for P8
Text Parameter 4	Value for P4	Text Parameter 9	Value for P9
Text Parameter 5	Value for P5	Text Parameter 10	Value for P10

A20 F10.0 A20 F10.0

Card 17. Type of Boundary Condition (Mechanical Problem)

Variables: IF

Format: (I5) . It is not required if free format is used

(Omit **Card 17** if IOPTDISPL=0)

IF: index of boundary condition (IF <= NFDTYPE)

(if ' -1' (format I5) is read, no more boundary condition types are expected)

CardGroup 18. Force/displacement prescribed

Variables: TIT, FORDISP(1,IF)=FD1, TIT, FORDISP(NPFD/2+1,IF)=FD\$,
TIT, FORDISP(2,IF)=FD2, TIT, FORDISP(NPFD/2+2,IF)=FD\$,
TIT, FORDISP(3,IF)=FD3, TIT, FORDISP(NPFD/2+3,IF)=FD\$,
etc. according to NPFD=2*(NDIM*(NDIM+2)+1).

Format: (A20, F10.0, A20, F10.0) . It is not required if free format is used

(Omit **CardGroup** 18 if IOPTDISPL=0)

TIT: title for each value

FORDISP(NPFD,NFDT array containing prescribed forces or prescribed
YPE): displacements. NPFD=2*(NDIM*(NDIM+2)+1). This is read
by means of two columns.

TIT for FD1	Value for FD1	TIT for FD\$	Value for FD\$
TIT for FD2	Value for FD2	TIT for FD\$	Value for FD\$
TIT for FD3	Value for FD3	TIT for FD\$	Value for FD\$
TIT for FD4	Value for FD4	TIT for FD\$	Value for FD\$
... etc. according to NPFD=2*(NDIM*(NDIM+2)+1).			
A20	F10.0	A20	F10.0

For NDIM=3 these columns are composed by:

FD1:	x direction force applied f_x^o	FD17	Δf_x^o obtained as ramp loading during TIMEI and TIMEF
FD2	y direction force applied f_y^o	FD18	Δf_y^o obtained as ramp loading during TIMEI and TIMEF
FD3	z direction force applied f_z^o	FD19	Δf_z^o obtained as ramp loading during TIMEI and TIMEF
FD4	displacement rate, first direction u_1^o	FD20	
FD5	displacement rate, second direction u_2^o	FD21	
FD6	displacement rate, third direction u_3^o	FD22	
FD7	$\cos(\alpha_1)$, first direction	FD23	
FD8	$\cos(\beta_1)$, first direction	FD24	
FD9	$\cos(\gamma_1)$, first direction	FD25	
FD10	$\cos(\alpha_2)$, second direction	FD26	
FD11	$\cos(\beta_2)$, second direction	FD27	
FD12	$\cos(\gamma_2)$, second direction	FD28	
FD13	$\cos(\alpha_3)$, third direction	FD29	
FD14	$\cos(\beta_3)$, third direction	FD30	
FD15	$\cos(\gamma_3)$, third direction	FD31	
FD16	γ	FD32	<i>index</i>

For a one dimensional problem the general boundary condition is applied by means a force computed as:

$$f_x = f_x^o + \gamma \cos(\alpha_1) (\dot{u}_1^o - \dot{u}_x) \Delta t$$

where u_1 is the computed displacement along the first direction. Obviously, for a one-dimensional problem $\cos\alpha_1$ can only be equal to zero or one.

For a two dimensional problem the general boundary condition is applied by means a force computed as:

$$f_x = f_x^o + \gamma \cos(\alpha_1)(\dot{u}_1^0 - \dot{u}_1)\Delta t + \gamma \cos(\alpha_2)(\dot{u}_2^0 - \dot{u}_2)\Delta t$$

$$f_y = f_y^o + \gamma \cos(\beta_1)(\dot{u}_1^0 - \dot{u}_1)\Delta t + \gamma \cos(\beta_2)(\dot{u}_2^0 - \dot{u}_2)\Delta t$$

where:

$$\dot{u}_1 = \dot{u}_x \cos(\alpha_1) + \dot{u}_y \cos(\beta_1)$$

$$\dot{u}_2 = \dot{u}_x \cos(\alpha_2) + \dot{u}_y \cos(\beta_2)$$

A very large value of γ can be used to impose a fixed displacement rate. If γ is insufficiently large, the prescription of the displacement will be inaccurate. On the contrary, extremely large values can cause matrix ill conditioning. Each specific problem requires an adjusted value.

If *index* is equal to 0, the values of forces calculated above are directly incorporated at the nodal force balance. If *index* is equal to 1 then, the forces are considered stresses on the boundary, and therefore the forces to be applied at nodes are internally obtained by the product with the lateral areas of elements.

For three dimensional problems, for instance, it is possible to prescribe displacement rate for three different directions, without any other restriction. In this way, any kind of displacement boundary condition (ex: displacement zero along a direction 45 degrees with respect to the vertical, etc) can be imposed. For a constant force applied on the boundary, the three components along x,y,z axes should be given.

This is a loop for IF=1, NFDTYPE. For each IF, I=1, NPFDD. This variable is (NPFDD=5 NDIM+1) the number of parameters for mechanical boundary condition.

The last **Card** of this group must be always ' -1' (format I5) regardless of the number of types read.

This group of **Cards** (**Card** 17 and **CardGroup** 18) (mechanical boundary conditions) only exists if the mechanical problem is solved. For each time interval, only the types that change need to be read.

Card 19. Type of Boundary Condition. Mass or heat transport problems.

Variables: IF

Format: (I5). It is not required if free format is used

(Omit **Card** 19 if IOPTPL + IOPTPG + IOPTTEMP = 0)

IF: index of flux boundary condition (<= NFLUXTYPE)

(if ' -1' (format I5) is read, no more boundary condition types are expected.)

CardGroup 20. Flux problem boundary condition

Variables: TIT, FLUX(1,IF), TIT, FLUX(21,IF),
TIT, FLUX(2,IF), TIT, FLUX(22,IF),
TIT, FLUX(3,IF), TIT, FLUX(23,IF),
TIT, FLUX(4,IF), TIT, FLUX(24,IF),
...
TIT, FLUX(20,IF), TIT, FLUX(40,IF),

Format: (A20, F10.0, A20, F10.0). It is not required if free format is used
(Omit **CardGroup 20** if IOPTPL + IOPTPG + IOPTTEMP =0)

TIT: title for each value (ex: *liquid pressure*)
FLUX(20,IF): array containing parameters for boundary conditions

TIT for FL1	Value for FL1	TIT for FL1	Value for FL1
TIT for FL2	Value for FL2	TIT for FL2	Value for FL2
...		...	
TIT for FL20	Value for FL20	TIT for FL20	Value for FL20

A20 F10.0 A20 F10.0

FL1	ω_g^w prescribed mass fraction (kg/kg)	FL21	
FL2	j_g prescribed gas flow rate (units in Table II.2.1)	FL22	increment of j_g during time step (units in Table II.2.1)
FL3	P_g prescribed gas pressure (MPa)	FL23	increment of P_g during time step (MPa)
FL4	γ_g (units in Table II.2.1)	FL24	
FL5	β_g (units in Table II.2.1)	FL25	
FL6	ρ_g prescribed gas density (kg/m ³)	FL26	
FL7	ω_l^w prescribed mass fraction of solute (kg/kg)	FL27	
FL8	ω_l^a prescribed mass fraction of air (kg/kg)	FL28	
FL9	j_l prescribed liquid flow rate (units in Table II.2.1)	FL29	increment of j_l during time step (units in Table II.2.1)
FL10	P_l prescribed liquid pressure (MPa)	FL30	increment of P_l during time step (MPa)
FL11	γ_l (see comments for negative value; units in Table II.2.1)	FL31	
FL12	β_l (units in Table II.2.1)	FL32	
FL13	ρ_l prescribed liquid density (kg/m ³)	FL33	
FL14	j_e prescribed heat flow rate (units in Table II.2.1)	FL34	increment of j_e during time step (units in Table II.2.1)
FL15	T prescribed temperature (C)	FL35	increment of T during time step (C)

FL16	γ_e (units in Table II.2.1)	FL36	
FL17	λ_e (positive values): [$j_e = j_e * \exp(-\text{abs}(\lambda_e)t)$] (units: 1/s) λ_e (negative values): [$j_e = j_e t^{-\text{abs}(\lambda_e)}$]	FL37	
FL18		FL38	
FL19	δ : parameter for smoothing curve the seepage (outflow of water only) boundary condition. For a positive value a parabolic curve is used; for a negative value an exponentially decaying curve is used. δ is the distance from the reference pressure to the point of change	FL39	
FL20	<i>index</i> : auxiliary index. <i>index</i> = +1.0 means that all flow rates are nodal values <i>index</i> = -1.0 means that all flow rates are per unit volume (3-D), area (2-D) or length (1-D) of medium (internal source or sink) <i>index</i> = +2.0 means that all flow rates are per unit area (3-D) or length (2-D) (lateral fluxes).	FL40	

The boundary condition is incorporated by adding a flux. The mass flux of species $i=w$ as a component of phase $\alpha=g$ (i.e. the inflow or outflow of vapour) is:

$$j_g^w = (\omega_g^w)^0 \left(j_g^0 + \Delta j_g^0 \frac{dt}{\Delta t} \right) + (\omega_g^w)^0 \gamma_g \left(\left(P_g^0 + \Delta P_g^0 \frac{dt}{\Delta t} \right) - P_g \right) + \beta_g \left((\rho_g \omega_g^w)^0 - (\rho_g \omega_g^w) \right)$$

where the superscript $()^0$ stands for the prescribed values, dt is the current time increment and Δt the current time step. Terms $\Delta(.) dt/\Delta t$ allow for imposing a linear variation of the variable $(.)$ during the time step. Mass fraction and density prescribed are only required for inflow because for outflow the values in the medium are automatically considered.

Positive values of mass flow rate indicate injection to the medium.

This general form of boundary condition, includes three terms. The first one is the mass inflow or outflow that takes place when a flow rate is prescribed at a node. The second term is the mass inflow or outflow that takes place when a phase pressure is prescribed at a node. The coefficient γ is a leakage coefficient, that is, a constant that allows to prescribe a pressure with more or less strength. If γ is large pressure will tend to reach the prescribed value. However, an extremely large value can produce matrix ill conditioning and a lower one can produce inaccuracy in prescribing the pressure. However, it is not difficult to guess adequate values for a given problem simply by trial. The third term is the mass inflow or outflow that takes place when species mass fraction is prescribed at a node.

A surface where seepage (only outflow for liquid phase is permitted) is possible has a boundary condition of prescribed liquid pressure. However, only liquid outflow is permitted. To recognize this fact, γ_l must be negative. This negative sign only indicates that nodes with this kind of boundary condition allow seepage.

Another situation occurs when an internal source or sink should be imposed. In this case it is preferable to use *index* = -1.0 and the program automatically considers that the nodal flows are per unit volume and will be multiplied by the volume associated to the cell centered in the node.

If there is inflow of gas or liquid phase, it is very important to give values of the following variables: ω_l^h , ω_g^w , ω_l^a , ρ_l , ρ_g and T . Otherwise they are assumed zero which is not correct because they will be far from the equilibrium. If outflow takes place, this is not relevant because the values of the medium are used.

For energy the boundary condition has the general form:

$$j_e = \left(j_e^0 + \Delta j_e^0 \frac{dt}{\Delta t} \right) + \gamma_e \left(T^0 + \Delta T^0 \frac{dt}{\Delta t} - T \right) + E_g^w (j_g^w) + \dots$$

In other words, the last terms imply that mass inflow and outflow through the boundary induces energy transfer.

In general, this is a loop for IF=1, NFLUXTYPE. For each IF, I=1, NPFLUX.

The last **Card** of this group must be always ' -1' (format I5).

This group of **Cards** (**Card** 19 and **CardGroup** 20) only exists if any balance (water, air, energy flow) problem is solved. For each time interval, only the types that change need to be read.

APPENDIX III.B. GEOMETRICAL DESCRIPTION FILE: ROOT_GRI.DAT

Card 1. Grid writing index

Variables: IOWGRI, IOFILE, IFMT

Format: (5I5). It is not required if free format is used

IOWGRI: =1, a *ROOTMSH.DAT* file is created on output

IOFILE: =1, four (4) names are read in the following four lines for files containing, respectively,

FILE1: nodes (**Card 2**),

FILE2: connectivities (**Card 3**),

FILE3: initial conditions (**Card 4**) and

FILE4: element-wise variables (stresses and porosities) (**Card 5**).

IFMT: =1, to read connectivities according to old format

CardGroup 2. Node co-ordinates and boundary condition type

Variables: N,COORD(1,N),..., COORD(NDIM,N), IFORDISP(1,N), IFORDISP(2,N), IFORDISP(3,N), IFLUXTYPE(1,N), IFLUXTYPE(2,N), IFLUXTYPE(3,N), WIDTH(N)

Format: (I5, (NDIM)F10.0, 3I3, 3I3, F10.0). It is not required if free format is used

N: Node number

COORD(NDIM,NUMNP): Nodal coordinates

IFORDISP(I,NUMNP): Integer matrix containing prescribed Force/displacement Boundary Condition code (0=no boundary condition; IFORDISP(1,12)=17, node 12 has, as first boundary condition, the Force/displacement condition numbered 17 in file *ROOT_GEN.DAT*. Up to 3 force/displacement conditions can be assigned to each node (typically used for corner nodes).

FLUXTYPE(NUMNP): Integer matrix containing prescribed Flux Boundary Condition code (0 = no boundary condition; FLUXTYPE(2,40)=8, node 40 has, as second boundary condition, the Flux Condition numbered 8 in file *ROOT_GEN.DAT*. Up to 3 Flux Boundary Conditions can be assigned to each node (typically used for corner nodes).

WIDTH(NUMNP): Initial nodal joint width (it is only necessary if node belongs to a joint element).

CardGroup 3. Node connectivities, material, element type, ...

Variables: L, MTYPE, LTYPE, KXX(1,L), ..., KXX(MNNEL,L)

Format: ((3+MNNEL)I5). It is not required if free format is used

L: Element number
MTYPE(L): Material type
LTYPE(L): Element type
KXX(MNNEL,L): Global connectivities (the maximum number of connectivities is 2 (ndim=1), 6 (ndim=2), and 8 (ndim=3),

MNNEL is the maximum number of nodes that may have a possible element in the finite element grid that is used in a problem. With the elements that are implemented at present the following values are internally assigned to MNNEL: for NDIM=1 is MNNEL=2, for NDIM=2 is MNNEL=6, and for NDIM=3 is MNNEL=8.

CardGroup 4. Initial values of unknowns

Variables: N, X(1,N), ..., X(NDF, N)

Format: (I5, 10F15.0). It is not required if free format is used

N: Node number
X: Array containing old values of unknowns

Here, the initial values of the unknowns are read and stored as the OLD values to begin time marching calculations.

In general, the following variables should be read:

n	u_x	u_y	u_z	P_l	P_g	T
I5	F15.0	F15.0	F15.0	F15.0	F15.0	F15.0

CardGroup 5. Initial values of stresses

Variables: L, STRESS(1,L), ..., STRESS(6,L), HISTVAR(1,L), HISTVAR(2,L)

Format: (I5, 10F15.0). It is not required if free format is used

(Omit if IOPTDISPL = 0)

L: Element number
STRESS: Array containing the stress tensor at integration points (if the element uses several integration points, only 1 value per element is read and assumed initially the same in all integration points)
HISTVAR: Array containing history variables for elastoplastic and viscoplastic models

CardGroup 6. Other element wise properties.

Variables: L, POROSITY(L), (FK(I,L),I=1,NDIM), ANISOTPER(1, L), ..., ANISOTPER(NISOT, L), THICKNESS (L), (FK(I, L), I=NDIM+1,NDIM+3)

Format: (I5, 10F15.0). It is not required if free format is used

L: Element number.
POROSITY(L): Initial porosity of element L
FK(I,L): Element-wise multiplying factor for intrinsic permeability
ANISOTPER(1,L): Angle of direction of anisotropy
ANISOTPER(NISOT,L): (NISOT =1 for NDIM=1 OR 2 ; NISOT =3 for NDIM=3)
THICKNESS (L): (only for segment in 2-D or 3-D, LTYPE=8)
FK(I,L): Element-wise multiplying factor for retention curve parameters

Card 7. Time evolution of state or dependent variables at nodes

Variables: NOUTOT, IVOU(1), ..., IVOU(10), INTERNODE

Format: (16I5). It is not required if free format is used

NOUTOT: Number of nodes for which time evolution is required
IVOU: Variable required at these nodes. IVOU can range from 1 (first unknown) to NDF (last unknown), and from NDF+1 (first nodal dependent variable (DEPVARN vector)) to NDF+NDVN (last nodal dependent variable).
INTERNODE: Frequency for output (=1 implies all time steps).

Card 8. Nodes for time evolution

Variables: NODOUT(1), ..., NODOUT(NOUTOT)

Format: (16I5). It is not required if free format is used

NODOUT(1,...,10): Node number of nodes for which time evolution is required. Time evolution is written at file 'FOR050.DAT' for time steps according to INTERNODE.

Card 9. Piezometric head map

Variables: IWHEAD, NWHEAD

Format: (16I5). It is not required if free format is used

IWHEAD: =1, Piezometric heads are written at file 'FOR060.DAT' or 'FOR061.DAT', depending whether liquid and/or gas phase is considered. Values for all nodes are written at times according to INTER frequency.

NWHEAD: Number of head contours that will be necessary in a plot. This value can be changed when drawing them.

The use of this option is restricted to problems of constant density for liquid and/or gas phases.

Card 10. Nodal flows

Variables: IWNFLOW

Format: (16I5). It is not required if free format is used.

IWNFLOW: =1, Different flow values at boundary nodes are written at file 'FOR070.DAT'. Values are written at times according to INTER frequency. The nodal flows have units of kg/s for mass and J/s for energy.
=2, the same, but values for all time steps are written.
=3, the same, but values for times according to INTERNODE frequency (see **Card 7**).

Card 11. Time evolution of dependent variables at elements

Variables: LOUT, IELVOUT(1), ..., IELVOUT(10), INTERELEM

Format: (16I5). It is not required if free format is used.

LOUT: Number of elements for which time evolution is required.

IELVOUT: Variable required at these elements. IELVOUT can range from 1 to 2 (DEPVARE vector, i.e. degree of saturation and/or porosity), or, from -1 to -6 (stress vector) and from -7 to (-7 - nhv/2) (history variables).

INTERELEM: Frequency for output (=1 implies all time steps).

Card 12. Element numbers for time evolution of element-wise variables}

Variables: NELOUT(1), ..., NELOUT(LOUT)

Format: (16I5). It is not required if free format is used

NELOUT(10): Element number of elements for which time evolution is required. Time evolution is written in file 'FOR080.DAT' for time steps according to INTERELEMENT

APPENDIX V.A. THERMO-HYDRO-MECHANICAL INTERACTIONS

In this Appendix the main interactions between the various thermo-hydro-mechanical processes are presented in a synthetic and systematic manner.

THERMAL PHENOMENA

Heat storage

Effects from:

- *Thermal phenomena*
 - Heat storage proportional to temperature
- *Hydraulic phenomena*
 - Liquid flow modifies the amount of water and air present
 - Gas flow modifies the amount of air and water present
 - Phase changes modifies heat storage through the latent heat of vapour
- *Mechanical phenomena*
 - Porosity changes modify the amount of space left for fluids

Heat conduction

Effects from:

- *Thermal phenomena*
 - Heat conduction driven by temperature gradients (Fourier's law)
- *Hydraulic phenomena*
 - Liquid flow modifies thermal conductivity
 - Gas flow modifies thermal conductivity
- *Mechanical phenomena*
 - Porosity changes modifies thermal conductivity

Heat advection by liquid flow

Effects from:

- *Hydraulic phenomena*
 - Heat transport by liquid flow

Heat advection by air flow

Effects from:

- *Hydraulic phenomena*
 - Heat transport by gas flow

Heat advection by vapour flow

Effects from:

- *Hydraulic phenomena*
 - Heat transport by vapour diffusion
 - Heat transport by gas flow

Phase changes

Effects from:

- *Thermal phenomena*
 - Vapour pressure affected by temperature (water phase diagram and psychrometric law)
- *Hydraulic phenomena*
 - Vapour pressure affected by liquid flow through suction changes (psychrometric law)
 - Vapour pressure affected by gas flow through suction changes (psychrometric law)

HYDRAULIC PHENOMENA

Water storage

Effects from:

- *Thermal phenomena*
 - Liquid density changes with temperature
 - Vapour density changes with temperature
 - Phase change modifies the amount of water in liquid and gas phases
- *Hydraulic phenomena*
 - Liquid density changes with liquid pressure
 - Vapour density changes with suction and gas pressure
- *Mechanical phenomena*
 - Porosity changes affect the space available for liquid and gas

Air storage

Effects from:

- *Thermal phenomena*
 - Gas density changes with temperature
 - Amount of dissolved air changes with temperature
- *Hydraulic phenomena*
 - Gas density changes with gas pressure
 - Amount of dissolved air depends on gas pressure
- *Mechanical phenomena*
 - Porosity changes affect the space available for liquid and gas

Liquid water transfer

Effects from:

- *Thermal phenomena*
 - Hydraulic conductivity affected by liquid viscosity that diminishes with temperature.
 - Degree of saturation varies with temperature in unsaturated conditions (thermal expansion and phase changes)
 - Pore water pressure increases with temperature in saturated and quasi-saturated conditions
 - Liquid density variation with temperature gives rise to convective flow
- *Hydraulic phenomena*
 - Liquid flow controlled by liquid pressure gradients (Darcy's law)
 - Hydraulic conductivity affected by degree of saturation, in turn controlled by the value of suction (retention curve)
- *Mechanical phenomena*
 - Porosity changes modifies the value of hydraulic conductivity

Gaseous air transfer

Effects from:

- *Thermal phenomena*
 - Hydraulic conductivity affected by gas viscosity that increases with temperature.
 - Degree of saturation varies with temperature (thermal expansion and phase changes)
 - Temperature variations influence gas density
- *Hydraulic phenomena*
 - Gas flow controlled by gas pressure gradients (Darcy's law)
 - Hydraulic conductivity affected by degree of saturation, in turn controlled by the value of suction (retention curve)
- *Mechanical phenomena*
 - Porosity changes affect the value of hydraulic conductivity
 - Porosity changes vary the pore space volume available for gas

Water vapour transfer

Effects from:

- *Thermal phenomena*
 - Vapour pressure is affected by temperature (water phase diagram and psychrometric law)
 - Degree of saturation varies with temperature. Vapour diffusion depends on degree of saturation.
- *Hydraulic phenomena*
 - Vapour diffusion controlled by gradients of vapour concentration (Fick's law)
 - Vapour advection controlled by gas flow
 - Vapour pressure affected by liquid flow through suction changes (psychrometric law)
 - Vapour pressure affected by gas flow through suction changes (psychrometric law)
- *Mechanical phenomena*
 - Porosity changes affect the vapour diffusion coefficient

Dissolved air transfer

- *Thermal phenomena*
 - Diffusion coefficient affected by temperature
- *Hydraulic phenomena*
 - Dissolved air transfer controlled by diffusion (Fick's law)
 - Advection of dissolved air by liquid flow
- *Mechanical phenomena*
 - Diffusion coefficient affected by porosity

MECHANICAL PHENOMENA

Stress/strain field

Effects from:

- *Thermal phenomena*
 - Thermal expansion of materials
 - Dependence of constitutive laws on temperature
 - *Hydraulic phenomena*
 - Dependence of constitutive laws on suction
 - *Mechanical phenomena*
 - Stress/strain constitutive laws
-

For the representation of a metal canister, in the following table some specific properties are recommended for numerical efficiency to solve THM problems:

Canister: specific properties to solve THM problems		
Initial Porosity	0.01	Initial condition applied on surface or volume
Initial Liquid Pressure	-100 MPa	Initial condition applied on surface or volume
Solid density	kg m ⁻³	Calibrate to obtain realistic canister weight
Specific heat	450 J kg ⁻¹ K ⁻¹	
Elastic Modulus	21000 MPa	
Thermal expansion of medium	0.0 K ⁻¹	P3 in Linear Elasticity 2
Thermal expansion of solid	0.0 K ⁻¹	P3 in Solid Phase Properties
Intrinsic permeability	10 ⁻²⁷ m ²	P1, P2, P3 in Intrinsic Permeability
Tortuosity for diffusion of vapour	10 ⁻¹⁰ (-)	P3 in Diffusion for Vapour
Retention curve parameter P0	30 MPa	P1 in Retention curve
Thermal conductivity	390 W m ⁻¹ K ⁻¹	
Biot Coefficient (coupling H to M)	10 ⁻¹⁰ (-)	P7 in Linear Elasticity 1
Coupling option (coupling M to H)	UNCOUPLED	P7=1 in Construction and Excavation

Note that, in the case of the thermal expansion of the solid, if zero –or a value lower than 10⁻²⁵– is input, then automatically takes the default value. Hence, if the user actually wants to set it to zero, a low value but greater than 10⁻²⁵ should be input (e.g. 10⁻²⁰).

APPENDIX VI.A. EQUIVALENT DENSITY AND SPECIFIC HEAT FOR A TM PROBLEM.

Temperature distribution and evolution in a porous medium is strongly affected by the specific heat of the water. When a porous material is modelled under TM conditions, equivalent parameters should be used in order to get realistic and comparable results with THM. Hence, it is explained here how to calculate those equivalent parameters.

Heat capacity of porous medium for a THM problem in a saturated porous medium:

$$\rho_s c_s (1 - \phi) + \rho_l c_l \phi$$

Where phase densities, phase specific heats and porosity can be used with their realistic value.

Heat capacity for a TM problem in an equivalent medium: $(\rho_s)_{eq} (c_s)_{eq} (1 - \phi)$

To obtain the same stresses induced by weight, an equivalent density for a TM problem in a saturated porous medium can be calculated as:

$$(\rho_s)_{eq} = \frac{\rho_s (1 - \phi) + \rho_l \phi}{(1 - \phi)}$$

And to obtain the same temperature, an equivalent specific heat for a TM problem in a saturated porous medium can be calculated as:

$$(c_s)_{eq} = \frac{\rho_s c_s (1 - \phi) + \rho_l c_l \phi}{(\rho_s)_{eq} (1 - \phi)}$$

APPENDIX VI.B.1. ANALOGY BETWEEN NONLINEAR ELASTICITY AND BBM

Elastic part of BBM (isothermal):

$$d\varepsilon_v^e = \frac{\kappa_i(s)}{1+e} \frac{dp'}{p'} + \frac{\kappa_s(p',s)}{1+e} \left(\frac{ds}{s+0.1} \right)$$

where:

$$\kappa_i(s) = \kappa_{i0} (1 + \alpha_{i,s} s) \quad \kappa_s(p',s) = \kappa_{s0} (1 + \alpha_{s,p} \ln(p'/p_{ref})) \exp(\alpha_{s,s} s)$$

For $a_3 = 0$, the model (ITYCL=1) coincides with the elastic part of BBM for constant coefficients:

$$\frac{\Delta e}{1+e} = a_1 \Delta \ln(-p') + a_2 \Delta \ln\left(\frac{s+0.1}{0.1}\right) = \left(\frac{-\kappa_{i0}}{1+e}\right) \Delta \ln(-p') + \left(\frac{-\kappa_{s0}}{1+e}\right) \Delta \ln\left(\frac{s+0.1}{0.1}\right)$$

For a_3 different from zero the equation (ITYCL=1) can be expanded in the following way.

$$\begin{aligned} \frac{\Delta e}{1+e} &= a_1 \Delta \ln(-p') + a_2 \Delta \ln\left(\frac{s+0.1}{0.1}\right) + a_3 \Delta \left[\ln(-p') \ln\left(\frac{s+0.1}{0.1}\right) \right] = \\ &= \left[a_1 + a_3 \ln\left(\frac{s+0.1}{0.1}\right) \right] \Delta \ln(-p') + \left[a_2 + a_3 \ln(-p') \right] \Delta \ln\left(\frac{s+0.1}{0.1}\right) = \\ &= a_1 \left[1 + \frac{a_3}{a_1} \ln\left(\frac{s+0.1}{0.1}\right) \right] \Delta \ln(-p') + a_2 \left[1 + \frac{a_3}{a_2} \ln(-p') \right] \Delta \ln\left(\frac{s+0.1}{0.1}\right) \end{aligned}$$

Depending on the values of the parameters, negative compressibility can be obtained. This can be limited with the K_{min} indicated above.

For a_3 and a_4 different from zero the equation (ITYCL=5) can be transformed in the following way.

$$\begin{aligned} \frac{\Delta e}{1+e} &= a_1 \Delta \ln(p') + a_2 \Delta \ln\left(\frac{s+0.1}{0.1}\right) + a_3 \ln(p'/p_{ref}) \Delta \left[\ln\left(\frac{s+0.1}{0.1}\right) \right] + a_4 s \Delta [\ln(p')] = \\ &= [a_1 + a_4 s] \Delta \ln(p') + [a_2 + a_3 \ln(p')] \Delta \ln\left(\frac{s+0.1}{0.1}\right) \\ &= a_1 \left[1 + \frac{a_4}{a_1} s \right] \Delta \ln(p') + a_2 \left[1 + \frac{a_3}{a_2} \ln(p'/p_{ref}) \right] \Delta \ln\left(\frac{s+0.1}{0.1}\right) \\ & \quad a_1 = -\frac{\kappa_{i0}}{1+e} \quad a_2 = -\frac{\kappa_{s0}}{1+e} \quad a_4 = a_1 \alpha_i \quad a_3 = a_2 \alpha_{sp} \end{aligned}$$

APPENDIX VI.B.2. CORRESPONDENCE BETWEEN NONLINEAR ELASTICITY AND LINEAR ELASTICITY PARAMETERS

Linear elasticity using volumetric and shear moduli:

$$d\varepsilon_v = \frac{dp'}{K} \quad d\varepsilon_d = \frac{dq}{2G}$$

Bulk and shear elastic parameters as a function of Young and Poisson parameters:

$$K = \frac{E}{3(1-2\nu)} \quad G = \frac{E}{1+\nu}$$

A typical non-linear elasticity model proportional to mean effective stress, can be compared with linear elasticity if the tangent moduli are calculated (for compression negative):

$$\frac{d\varepsilon_v}{dp'} = \frac{a_1 + a_3 \ln(s)}{p'} = \frac{1}{K} \quad \Rightarrow \quad K = \frac{p'}{a_1 + a_3 \ln(s)} > K_{min}$$

For constant Poisson ratio ν the following equivalences can be used:

$$E = 3K(1-2\nu) = 3(1-2\nu) \frac{p'}{a_1 + a_3 \ln(s)} > 3(1-2\nu)K_{min}$$

$$G = \frac{3(1-2\nu)}{1+\nu} \frac{p'}{a_1 + a_3 \ln(s)} > \frac{3(1-2\nu)}{1+\nu} K_{min}$$

In case that a constant shear modulus G is given instead of ν , then:

$$\nu = \frac{3K - 2G}{2(3K + G)} = \frac{3 \frac{p'}{a_1 + a_3 \ln(s)} - 2G}{2(3 \frac{p'}{a_1 + a_3 \ln(s)} + G)} > \frac{3K_{min} - 2G}{2(3K_{min} + G)}$$

$$E = \frac{9KG}{3K + G} = \frac{9 \frac{p'}{a_1 + a_3 \ln(s)} G}{3 \frac{p'}{a_1 + a_3 \ln(s)} + G} > \frac{9K_{min}G}{3K_{min} + G}$$

In case that a material with a **Young's Modulus changing with stress** has to be modelled, the following equation can be used (without suction effects):

$$E = \frac{3(1-2\nu)p'}{a_1} \quad \text{and} \quad E_{min} = 3K_{min}(1-2\nu)$$

Note that in this model implementation, a_1 must be input as a negative value.

APPENDIX VI.B.3. ANALOGY BETWEEN LINEAR CREEP AND VISCOELASTICITY

Linear viscoelasticity can be expressed as (in analogy with linear elasticity):

$$\frac{d\boldsymbol{\varepsilon}}{dt} = \frac{1}{2\eta_d}(\boldsymbol{\sigma} - \mathbf{I}p) + \frac{1}{3\eta_v}\mathbf{I}p$$

In absence of volumetric deformations ($\eta_v \rightarrow \infty$), it leads to:

$$\frac{d\boldsymbol{\varepsilon}}{dt} = \frac{1}{2\eta_d}(\boldsymbol{\sigma} - \mathbf{I}p)$$

And for uniaxial compression ($\sigma_1 > 0$ and $\sigma_2 = \sigma_3 = 0$), it is:

$$\frac{d\varepsilon_1}{dt} = \frac{1}{2\eta_d}\left(\sigma_1 - \frac{1}{3}\sigma_1\right) = \frac{1}{3\eta_d}\sigma_1$$

This equation can be compared with the simple linear creep equation:

$$\frac{d\varepsilon_1}{dt} = A\sigma_1$$

And therefore:

$$\eta_d = \frac{1}{3A}$$

Where A is the creep constant in $\text{MPa}^{-1}\text{s}^{-1}$ and η_d is the deviatoric viscosity in $\text{MPa}\cdot\text{s}$

How this can be compared with elasticity? Elasticity can be written as (total, increments or rates):

$$\boldsymbol{\varepsilon} = \frac{1}{2G}(\boldsymbol{\sigma} - \mathbf{I}p) + \frac{1}{3K}\mathbf{I}p$$

Then, for incompressible:

$$\boldsymbol{\varepsilon} = \frac{1}{2G}(\boldsymbol{\sigma} - \mathbf{I}p)$$

Then, for uniaxial compression:

$$\varepsilon_1 = \frac{1}{2G}\left(\sigma_1 - \frac{1}{3}\sigma_1\right) = \frac{1}{3G}\sigma_1$$

Then, comparing with Young modulus definition:

$$\varepsilon_1 = \frac{\sigma_1}{E}$$

It results in:

$$G = \frac{E}{3}$$

And this is consistent with the definition of G because for incompressible conditions ($\nu = 0.5$):

$$G = \frac{E}{2(1 + \nu)} = \frac{E}{2(1 + 0.5)} = \frac{E}{3}$$

Where E is the Young modulus MPa and G is the shear modulus in MPa

APPENDIX VI.B.4. ZERO THICKNESS

MECHANICAL PROBLEM

The mechanical behaviour of the joint elements is defined by the relation between stress and relative displacements of the joint element (Figure VIb.5) calculated on the mid-plane. The mid-plane relative displacements are interpolated using the nodal displacements and the shape functions.

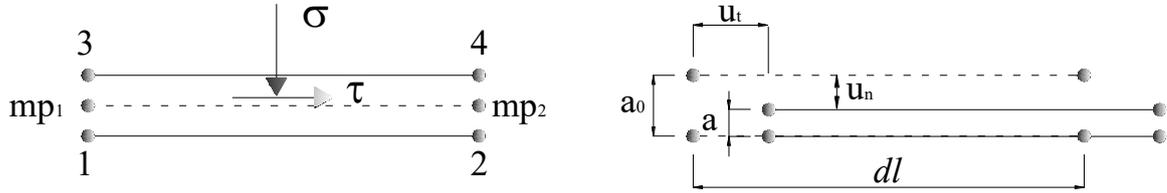


Figure VIb.5. Joint element with double nodes. a) Stress state on the mid-plane of the joint element. b) Relative displacement defined at mid plane.

The normal and shear displacement increment calculated on the midplane is defined as:

$$\mathbf{w}_{mp} = \begin{bmatrix} u_n \\ u_s \end{bmatrix}_{mp} = \mathbf{r} \mathbf{N}_{mp}^u [-\mathbf{I}_4 \quad \mathbf{I}_4] \mathbf{u}_j$$

where u_n and u_s are the normal and tangential relative displacements, \mathbf{r} is a rotation matrix, \mathbf{N}_{mp}^u is a matrix of shape functions, \mathbf{I}_4 is an identity matrix of 4th order, \mathbf{u}_j is the vector of nodal displacements.

The stress tensor on the mid-plane is calculated as a function of displacement components, normal and shear:

$$\boldsymbol{\sigma}'_{mp} = \begin{bmatrix} \sigma' \\ \tau \end{bmatrix}_{mp} = \mathbf{D} \mathbf{w}_{mp}$$

where σ'_{mp} is the net effective stress on the mid-plane of the element and it is defined as $\sigma'_{mp} = \sigma_{mp} - \max(Pg; Pl)_{mp}$; (σ is total mean stress; Pg is the gas pressure and Pl is the liquid pressure, both interpolated to the mid-plane of the element); τ is the tangential stress on the mid-plane; \mathbf{D} is the stiffness matrix which relate relative displacements with the stress state.

MECHANICAL MODEL BASED ON ELASTO-VISCOPLASTIC FORMULATION

An elasto-viscoplastic formulation is proposed to model the mechanical behaviour of joints. This formulation based on the development done by Perzyna (1963), Zienkiewicz et al. (1974), Loreface et al., (2007) allows the treatment of non-associated plasticity and strain softening behaviour of joints subjected to shear displacements. More over, using the viscoplasticity it is possible considered the variation of the strain rate with time.

The total displacements \mathbf{w} are calculated by addition of reversible elastic displacements, \mathbf{w}^e , and viscoplastic displacements \mathbf{w}^{vp} , which are zero when stresses are below a threshold value (the failure surface): $\mathbf{w} = \mathbf{w}^e + \mathbf{w}^{vp}$

The displacements are represented by a vector of two quantities in two-dimensional case and have the following components:

$$\mathbf{w}^T = [u_n, u_s] \tag{3.22}$$

ELASTIC BEHAVIOUR

The elastic behaviour of the joint is established as a relationship between the normal-tangential effective (σ', τ) and the normal-tangential (u_n, u_s) relative displacement of the joint element. This is established using a normal (K_n) and a tangential stiffness (K_s) coefficients. The normal stiffness depends on the opening of the joint.

$$\begin{Bmatrix} \sigma' \\ \tau \end{Bmatrix} = \begin{bmatrix} K_n & 0 \\ 0 & K_s \end{bmatrix} \begin{Bmatrix} u_n \\ u_s \end{Bmatrix} \quad K_n = \frac{m}{a - a_{\min}}, \quad K_s = \text{constant}$$

where m is a parameter of the model; a is the opening or aperture of the element and a_{\min} is the minimum opening or aperture of the element.

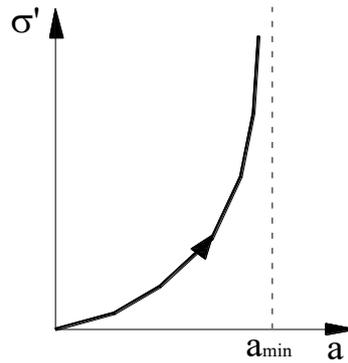


Figure VIb.6. Elastic constitutive law of the joint element. Normal stiffness depends on joint opening.

VISCO-PLASTIC BEHAVIOUR

The constitutive behaviour for the mechanical of rough rock joint was developed based on the formulations proposed by Gens, et al. (1985) and Carol, et al, (1997). According to these theories, it is necessary to define a yield surface, a plastic potential and a softening law to mathematical model the shear behaviour of a joint.

The visco-plastic displacements occur when the stress state of the joint reaches a failure condition. The failure surface can be defined linearly (the one implemented in CODE_BRIGHT):

$$F \equiv \tau^2 - (c' - \sigma' \tan \phi')^2$$

Or with hyperbolic shape (based on work done by Gens et al., (1990)):

$$F = \tau^2 - (c' - \sigma' \tan \phi')^2 + (c' - \chi \tan \phi')^2$$

where τ is the shear stress; c' is the effective cohesion; σ' is the net normal stress and $\tan \phi'$ is the tangent of effective angle of internal friction. χ is a parameter.

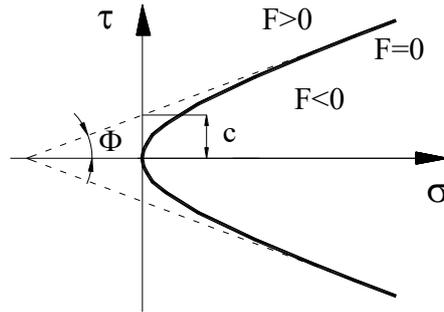


Figure VIb.7. Hyperbolic (continuous) and linear (dashed) failure surface and strength parameters

SOFTENING LAW

The strain-softening behaviour of the joint subjected to shear stress is modelled considering the degradation of the strength parameters $\tan\phi'$ and c' .

The degradation of the parameters $\tan\phi'$ and c' is considered dependent on the accumulated viscoplastic shear displacement. This is based on the slip weakening model introduced by Palmer & Rice (1973). In this way the tangent of the friction angle decays from the peak (intact material) to the residual value and the cohesion from the value c to zero. Two different values u^* permit to define the decrease of cohesion (u^*c') and friction angle ($u^*\tan\phi'$). The mathematical expressions are:

$$c' = c'_0 \left(1 - \frac{u_s^{vp}}{u_c^*} \right)$$

where c' is the effective cohesion that corresponds to the visco-plastic shear displacement u_s^{vp} ; c'_0 is the initial value of the effective cohesion; u_c^* is a parameter.

$$\tan\phi' = \tan\phi'_0 - (\tan\phi'_0 - \tan\phi'_{res}) \frac{u_s^{vp}}{u_\phi^*}$$

$\tan\phi'$ is the tangent of effective angle of internal friction that corresponds to the visco-plastic shear displacement u_s^{vp} ; $\tan\phi'_0$, $\tan\phi'_{res}$ and u_ϕ^* are parameters.

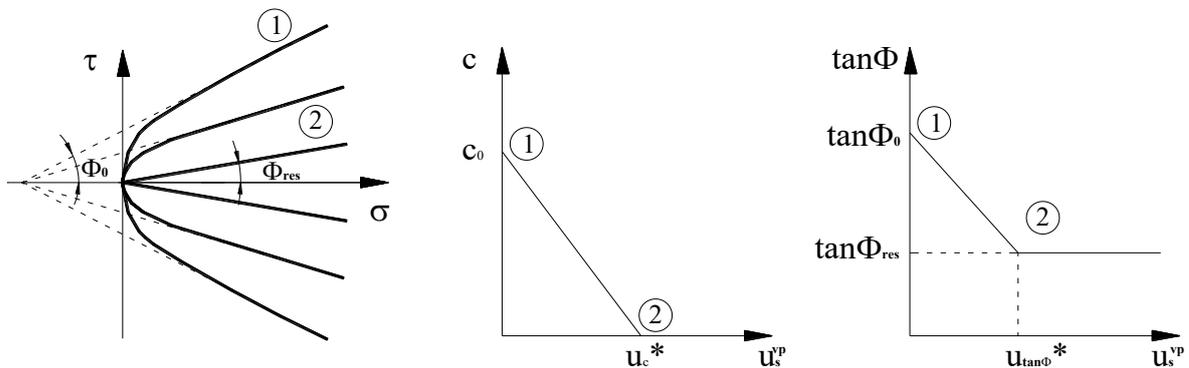


Figure VIb.8 a) Evolution of the failure surface during softening. b) Softening law of cohesion. c) Softening law of $\tan\phi$.

VISCO-PLASTIC DISPLACEMENTS

A viscoplastic yield surface implies that when $F < 0$ the stress state of the element falls inside of the elastic region. In contrast, if $F \geq 0$ the displacements of the element undergo a viscoplastic component. The viscoplastic displacements are calculated as:

$$\frac{d\mathbf{i}}{dt} = \Gamma \left\langle \phi \left(\frac{F}{F_0} \right) \right\rangle \frac{\partial G}{\partial \boldsymbol{\sigma}}$$

where Γ is a fluidity parameter. The visco-plastic displacement rate is given by a power of law considered for the function ϕ :

$$\Delta u_n^{vp} = \Gamma F^N \frac{\partial G}{\partial \sigma} \Delta t \quad \Delta u_s^{vp} = \Gamma F^N \frac{\partial G}{\partial \tau} \Delta t$$

PLASTIC POTENTIAL SURFACE AND DILATANCY

To calculate the direction of displacements it is necessary to define the derivatives of G with respect to stresses:

$$\frac{\partial G}{\partial \boldsymbol{\sigma}} = \left[2 \tan \phi' (c' - \sigma' \tan \phi') f_\sigma^{dil} f_c^{dil} \quad , \quad 2\tau \right]^T$$

This is a non-associated flow rule, because of the inclusion of both parameters f_σ^{dil} and f_c^{dil} which consider the dilatant behaviour of the joint with shear stresses (Lopez, et al. 1999). The amount of dilatancy depends on the level of the normal stress and on the degradation of the joint surface.

The following expressions describe these effects:

$$f_\sigma^{dil} = \left(1 - \frac{|\sigma'|}{q_u} \right) \exp \left(-\beta_d \frac{|\sigma'|}{q_u} \right) \quad f_c^{dil} = \frac{c'}{c_0'}$$

Where q_u , β_d are model parameters, c' is the cohesion value that correspond to the visco-plastic shear displacement u_s^{vp} ; and c_0' is the initial value of the cohesion.

Then, the tangent visco-plastic compliance matrix is calculated as:

$$C^{vp} = \begin{bmatrix} \frac{\partial \Delta u_n^{vp}}{\partial \sigma} & \frac{\partial \Delta u_n^{vp}}{\partial \tau} \\ \frac{\partial \Delta u_s^{vp}}{\partial \sigma} & \frac{\partial \Delta u_s^{vp}}{\partial \tau} \end{bmatrix}$$

$$\begin{aligned} \frac{\partial \Delta u_n^{vp}}{\partial \sigma} &= \Gamma N F^{N-1} f_\sigma^{dil} f_c^{dil} \left[2 \tan \phi' (c' - \sigma' \tan \phi') \right]^2 \Delta t + \\ &+ \Gamma F^N \left[-2 \tan^2 \phi' f_\sigma^{dil} f_c^{dil} \right] \Delta t \end{aligned}$$

$$\frac{\partial \Delta u_s^{vp}}{\partial \tau} = \Gamma N F^{N-1} 2\tau f_\sigma^{dil} f_c^{dil} \left[2 \tan \phi' (c' - \sigma' \tan \phi') \right] \Delta t$$

$$\frac{\partial \Delta u_s^{vp}}{\partial \sigma} = \Gamma N F^{N-1} 2\tau \left[2 \tan \phi' (c' - \sigma' \tan \phi') \right] \Delta t$$

$$\frac{\partial \Delta u_s^{vp}}{\partial \tau} = \Gamma N F^{N-1} 2\tau \Delta t + \Gamma F^N 2\Delta t$$

Finally, the elasto-viscoplastic mechanical model of the joint is expressed by the tangent stiffness matrix:

$$\mathbf{D}^{evp} = \left[\mathbf{C}^e + \mathbf{C}^{vp} \right]^{-1}$$

More information about this joint element can be found in Zandarin (2010) –see References.

APPENDIX VI.B.5. EXAMPLE OF USE OF THE ELASTIC AND VISCO-PLASTIC MODELS

The use of the BBM model can be achieved by combination of the non-linear elasticity and the viscoplasticity for unsaturated soils.

$$\boldsymbol{\varepsilon}^{total} = \boldsymbol{\varepsilon}^{elastic} + \boldsymbol{\varepsilon}^{viscoplastic}$$

The elastic part can be linear or nonlinear and may depend on suction and temperature. The viscoplastic part can also be a function of suction.

The following parameters are required and example values are given:

NONLINEAR ELASTICITY. ITYCL = 1

P1	a_1	-	= $-\kappa/(1+e)$, where κ is the slope of the unload/reload curve in the $(e - \ln p')$ diagram.	-0.05
P2	a_2	-	= $-\kappa_s/(1+e)$, where κ_s is the slope of the unload/reload curve in the $(e - \ln((s+0.1)/0.1))$ diagram.	-0.05
P3	a_3	-	Coupling term	+0.01
P4	G	MPa	Shear modulus (P4>0 requires P5=0)	10
P5	ν	-	Poisson's ratio (P5>0 requires P4=0)	-
P6	$tens$	MPa	Tension term to avoid tractions ($p' - tens \leq 0$)	0.1 MPa
P7	K_{min}	MPa	Minimum bulk modulus	1 MPa

The parameter P7 limits the stiffness coefficient, so it cannot go beyond a certain value. A value in the range of 1 MPa to 20 MPa is normally required. The parameter P6 limits the possibility of tensions. The model may use Poisson (P5) or shear stiffness (P4) alternatively. The use of one of them implies the other is variable as they are related.

The so-called state surface is an old model for unsaturated soils is based on reversibility. The volumetric strain is calculated in a reversible way according to:

$$\frac{\Delta e}{1+e} = a_1 \Delta \ln(p') + a_2 \Delta \ln\left(\frac{s+0.1}{0.1}\right) + a_3 \Delta \left[\ln(p') \ln\left(\frac{s+0.1}{0.1}\right) \right]$$

where p' is mean effective stress (mean stress plus maximum of liquid and gas pressure) and s is suction (gas pressure minus liquid pressure). Shear strain is linearly elastic with modulus G or, alternatively, a constant value of the Poisson's ratio can be used.

For $a_3 = 0$, the model coincides exactly with the elastic part of BBM for constant coefficients:

$$\frac{\Delta e}{1+e} = a_1 \Delta \ln(p') + a_2 \Delta \ln\left(\frac{s+0.1}{0.1}\right) = \left(\frac{-\kappa_{i0}}{1+e}\right) \Delta \ln(p') + \left(\frac{-\kappa_{s0}}{1+e}\right) \Delta \ln\left(\frac{s+0.1}{0.1}\right)$$

For a_3 different from zero the equation can be expanded in the following way:

$$\begin{aligned}
\frac{\Delta e}{1+e} &= a_1 \Delta \ln(p') + a_2 \Delta \ln\left(\frac{s+0.1}{0.1}\right) + a_3 \Delta \left[\ln(p') \ln\left(\frac{s+0.1}{0.1}\right) \right] = \\
&= \left[a_1 + a_3 \ln\left(\frac{s+0.1}{0.1}\right) \right] \Delta \ln(p') + \left[a_2 + a_3 \ln(p') \right] \Delta \ln\left(\frac{s+0.1}{0.1}\right) = \\
&= a_1 \left[1 + \frac{a_3}{a_1} \ln\left(\frac{s+0.1}{0.1}\right) \right] \Delta \ln(p') + a_2 \left[1 + \frac{a_3}{a_2} \ln(p') \right] \Delta \ln\left(\frac{s+0.1}{0.1}\right)
\end{aligned}$$

Depending on the values of the parameters, negative compressibility can be obtained. This can be limited with the K_{min} indicated above.

NONLINEAR ELASTICITY. ITYCL = 5

P1	a_1	-	= $-\kappa/(1+e)$, where κ is the slope of the unload/reload curve in the (e - $\ln p'$) diagram.	-0.05
P2	a_2	-	= $-\kappa_s/(1+e)$, where κ_s is the slope of the unload/reload curve in the (e - $\ln((s+0.1)/0.1)$) diagram.	-0.05
P3	a_3	-	Coupling term	+0.01
P4	G	MPa	Shear modulus (P4 > 0 requires P5 = 0)	10
P5	ν	-	Poisson's ratio (P5 > 0 requires P4 = 0)	-
P6	$tens$	MPa	Tension term to avoid tractions ($p' - tens \leq 0$)	0.1 MPa
P7	K_{min}	MPa	Minimum bulk modulus	1 MPa
P8	a_4	MPa ⁻¹	Coupling term	0.01
P9	p_{ref}	MPa	Reference pressure	1.0

Which correspond to (ITYCL = 5):

$$\begin{aligned}
\frac{\Delta e}{1+e} &= a_1 \Delta \ln(p') + a_2 \Delta \ln\left(\frac{s+0.1}{0.1}\right) + a_3 \ln(p' / p_{ref}) \Delta \left[\ln\left(\frac{s+0.1}{0.1}\right) \right] + a_4 s \Delta [\ln(p')] = \\
&= a_1 \left[1 + \frac{a_4}{a_1} s \right] \Delta \ln(p') + a_2 \left[1 + \frac{a_3}{a_2} \ln(p' / p_{ref}) \right] \Delta \ln\left(\frac{s+0.1}{0.1}\right)
\end{aligned}$$

With the following equivalence with BBM original parameters:

$$a_1 = -\frac{\kappa_{t0}}{1+e} \quad a_2 = -\frac{\kappa_{s0}}{1+e} \quad a_4 = a_1 \alpha_i \quad a_3 = a_2 \alpha_{sp}$$

VPUSR 1 (ICL = 34). ITYCL = 1

P1	Γ_o	1/s	Fluidity	1
P2	N		Power of the stress function (integer value)	5
P3	F_o	MPa	$F_o=1$ MPa	1.0
P4	δ		$\Gamma=\Gamma_o \exp(\delta s)$	-
P5	b		Non associativity parameter.	0.3

VPUSR 2 (ICL = 35). ITYCL = 1

P1	n	-	Power in F and G (integer value)	1
P2	γ	-	Parameter in F and G	-1/9 = -0.1111111
P3	β_s	-	0 (then $F_s=1$, and J_{3D} is not considered)	-
P4	m	-	Typical value -0.5, only required if $\beta_s \neq 0$	-
P5	μ_{DRY}	-	$\mu = M_{DRY}$	1.2
P6	-	-		-
P7	$(J_1^{o*})_F$	MPa	Positive value, initial size of F	1.2 (=3*0.4)
P8	$(J_1^{o*})_G$	MPa	Positive value, initial size of G	1.2 (=3*0.4)
P9	a	-	Parameter in F and G	3
P10	μ_{SAT}	-	$\mu = M_{SAT}$	1.2

P7 and P8 describe the size of F and G. This parameter is 3 times the preconsolidation mean stress for saturated conditions. P10 is the slope of the critical state line. This parameter can be related to the friction angle of the material $M = \frac{6 \sin \phi'}{3 - \sin \phi'}$.

VPUSR 3 (ICL = 36). ITYCL = 1

P1	κ	-	Elastic compression parameter	0.07
P2	$\lambda(0)$	-	Viscoplastic compression parameter	0.19
P3	r	-	Parameter in LC curve	0.5
P4	β	-	Parameter in LC curve	1
P5	p^c	MPa	Parameter in LC curve	0.1
P6	k_1	-		-
P7	k_2	-		-0.03 = -3*0.01
P8	k_3	-		+0.03 = + 3*0.01
P9	k_4	-		0.12 = 3*0.04
P10	-			-

The viscoplastic part is independent on the elastic part. What produces irreversible deformations is the plastic or viscoplastic part of the model. P2 is the viscoplastic compression parameter. P3, P4 and P5 describe the LC curve.

APPENDIX VI.E. ABOUT THE NOTIONS OF MICRO- AND MACRO-STRUCTURES IN THE DOUBLE-STRUCTURE MODEL IMPLEMENTED IN CODE_BRIGHT

The double structure models have been historically developed in order to reproduce the behavior of unsaturated expansive clays (Gens & Alonso, 1992; Alonso et al., 1999). In this seminal model, two levels of structure are considered (see Figure):

1. The microstructure, corresponding to the clay particles made of active minerals take place. As such, the microstructure is provided with a reversible strain-stress relationship derived from considerations about double-layer theory:

$$d\epsilon_v = \beta_m e^{\alpha_m p} dp$$

2. Macrostructure: Responsible of the structural rearrangements. At this level the response of collapse and loading occur. The relation of stress and strains is defined by the BBM model (Alonso et al. 1990).

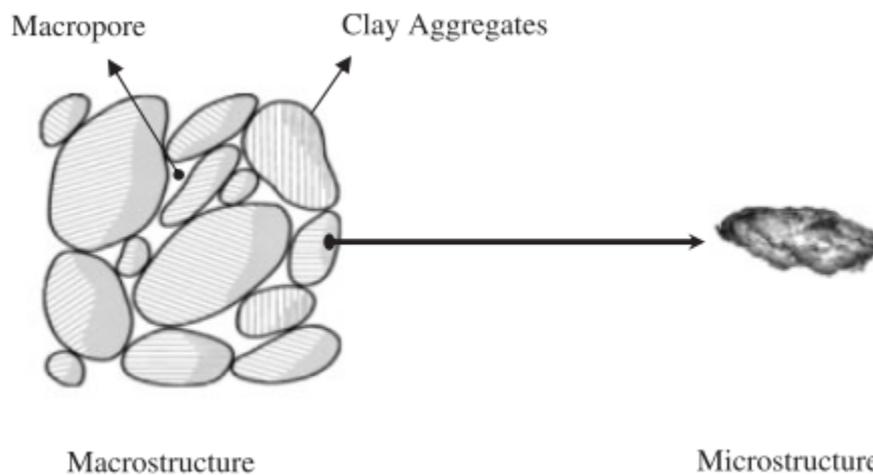


Figure VIe.1. Structural levels considered (Sánchez et al. 2005)

A clear picture of what is the micro and macro-structure can be illustrated by looking at the pore size distribution obtained in FEBEX bentonite (Figure VIe.2). Macropores corresponds in this case to voids with entrance radii close to $30 \mu\text{m}$ while the microstructure has radii around 70 \AA .

Even so, this model does not refer to unique process, or size of pores. The model is able to reproduce other types of problems. The mathematical formulation for double structure soils presented by Sánchez et al. 2005, is referred to the FEBEX bentonite, which present a clear double structure evidenced by the pore size distribution test presented in Figure VIe.2.

Formulation can be also used to model types of materials, provided two main pores families can be observed in the pore size distribution curve. An example is for example provided by the work on compacted silty clay. In this case, the macrostructure refers to the arrangement of silt particles and the large pores between them with entrance radii of order of $10 \mu\text{m}$. The microstructure refers to the clay particles and with entrance radii close to 1 mm .

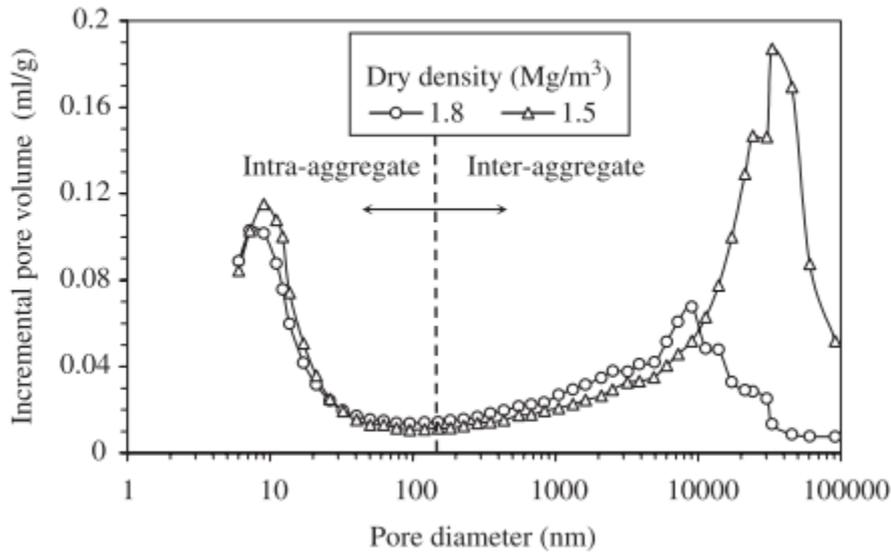


Figure VIe.2 Pore Size Distribution of FEBEX Bentonite (*Sánchez et al. 2005*)

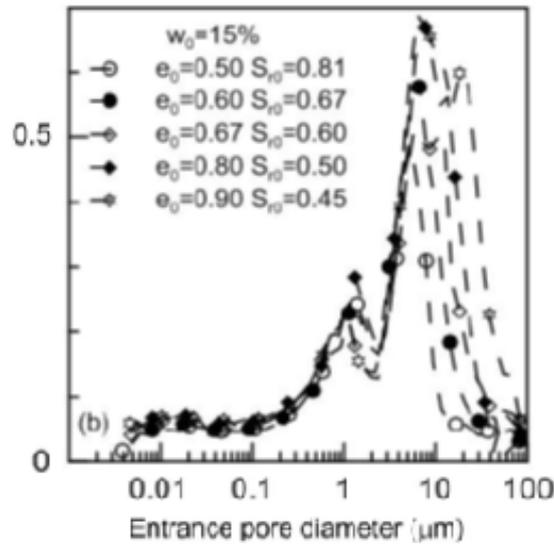


Figure VIe.3 Pore Size Distribution of compacted Jossigny silt (*Casini et al. 2012*)

Double-structure model can be used in this case to reproduce the fact that the stress dependency of microstructure is much lower than that of macrostructure. In this case, as the scale of the microstructure corresponds to the size of clay particles, the phenomenological law considered is taken from classical expression for soils:

$$d\epsilon_v = \frac{(1 + e_m)dp}{\kappa_m}$$

Model can be also used to model three-level structures materials as, for example, a mixture of bentonite powder with high density bentonite pellets. Three main pore families have been detected in these types of materials, as shown in Figure VIe.4.

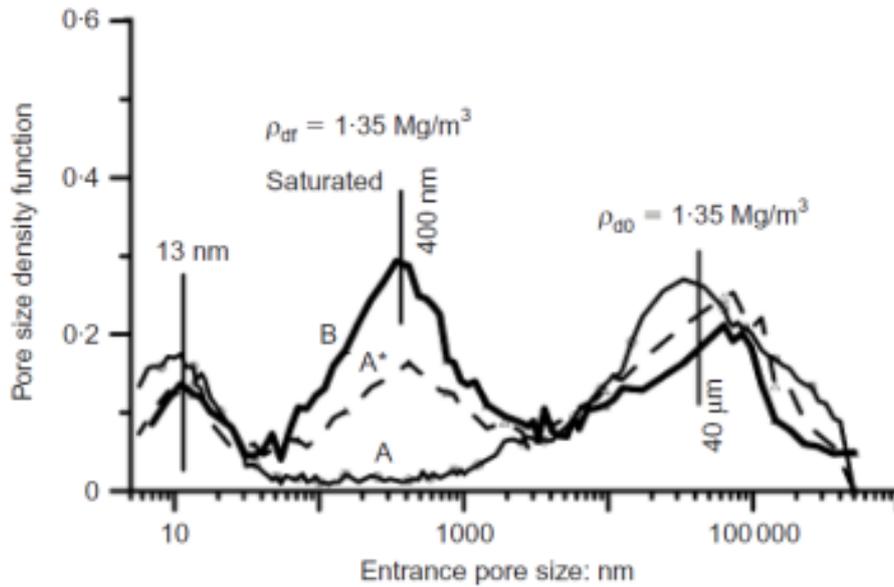


Figure VIe.4. Pore Size Distribution of mixture Bentonite powder/high density bentonite pellets (Alonso *et al.*, 2011)

In this case, the use of the double structure model needs an arbitrary split of the pore size distribution into two pore family, according to the requirements of the modelling (compressibility, permeability changes, ...).

As a conclusion, concepts of micro and macro-structure define essentially two different levels of scale within the material, not related to absolute value of pore size. For this reason, this type of models can also be used to model fissured materials when the upper scale corresponds to fissures and the lower scale to matrix.