Review october 2025

KARST GHOST-ROCK PROCESS

Karsts

What is a karst ? :

- Environment
- Process
- System

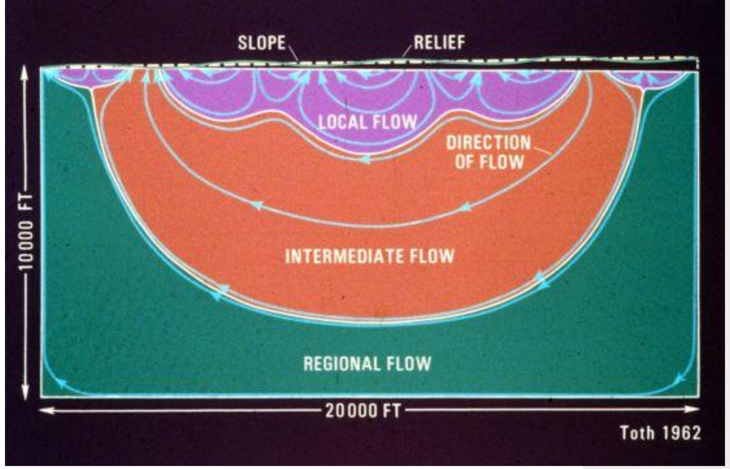
Erosion of the host rock through physical and chemical processes by a fluid

Broad variety of karsts :

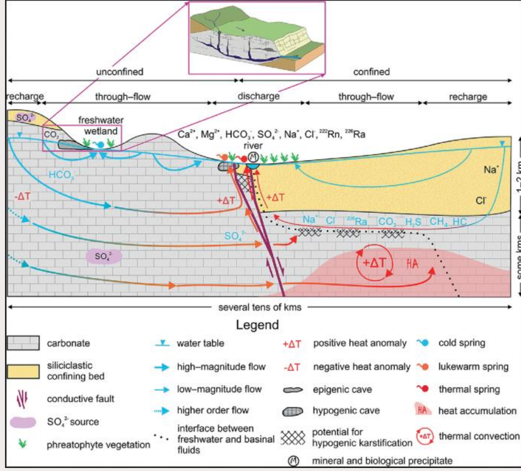
- Endokarsts
- Exokarsts
- (Cryokarsts, paleokarsts, perched karst, etc…)

- Flow induced by a difference in the gradient pressure --> inlet (recharge area) and outlet (discharge area)

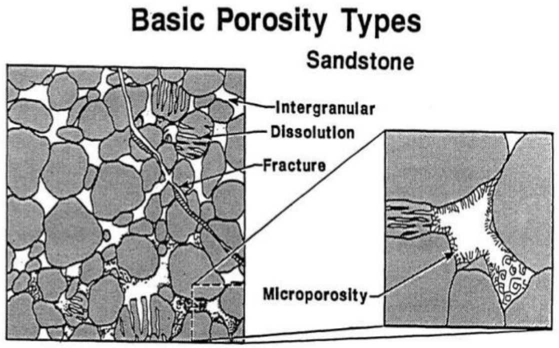
  or : thermal gradient --> thermal buoyancy effect
- Fluid driven into the soils through different types of porosity --> connection of those porosities enhance the permeability of the rock
- Acidification mostly through dissolved atmospheric CO2 enrichment of the fluid
- Dissolution of the minerals depends on the specific surface area --> area of the mineral which might be in contact with the fluid
- Flow following preferential paths : concentration of the advective alteration and dissolution until a breakthrough --> changing in the flow regime, concentration of the most part of the fluid flow in one main path
- 2 governing numbers in karst formation :
  - Péclet number : Describes the rate of influence between advection and diffusion processes in the model (depends on the fluid rate and the coefficient of diffusivity)
  - Damköhler number : Describes the rate of influence between reaction and flow of the reactives in the model
  - (a third indicative number, the Reynolds number, used in the calculation of the Péclet number, describes the linear or turbulent nature of the flow)



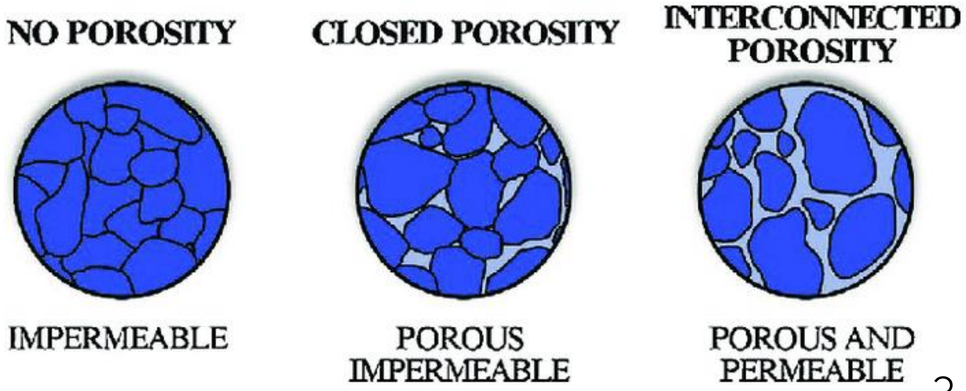
Tóth J., 1962



Mádlné Szőnyi J. et al., 2022



Radhi Wattan et al., 2022



Evangelista et al., 2019

Ghost-rock process

I – Chemical alteration of the matrix

-Slow alteration of the matrix by a weak acidic fluid infiltrating in apertures such as fracturations

-High Damköhler number

-Low advection

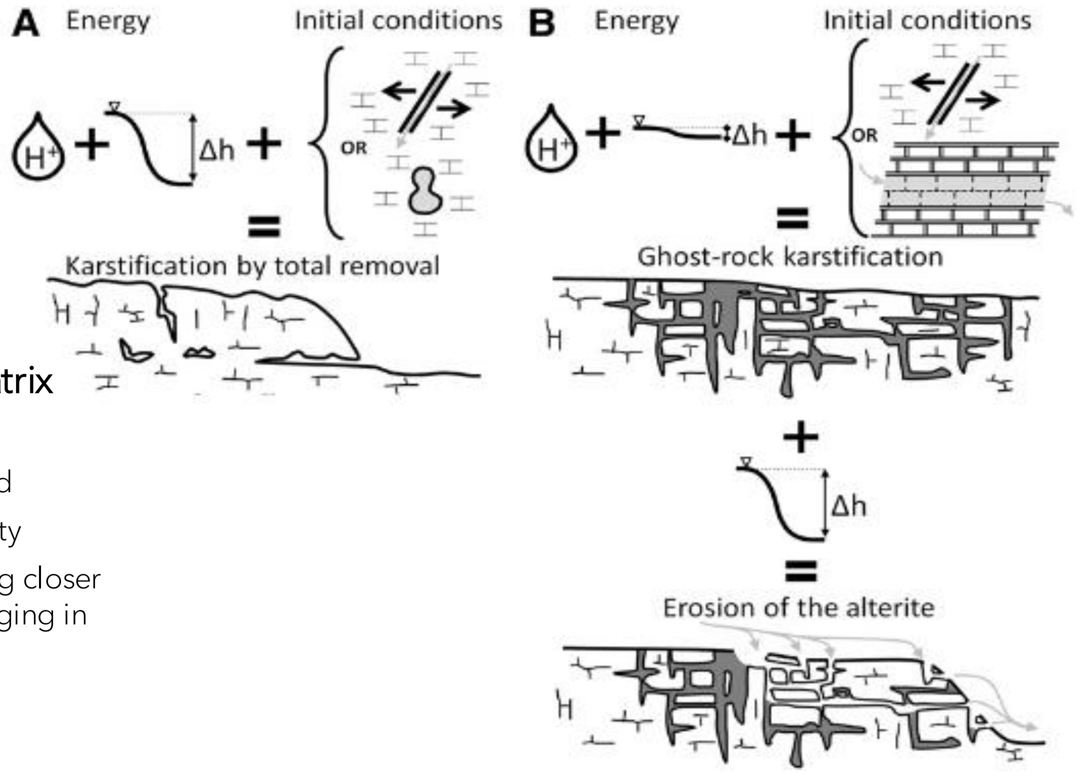
-Dissolution affected by heterogeneities and tortuosity of the apertures

II - Emptying the altered matrix

-Carried by advection of the fluid

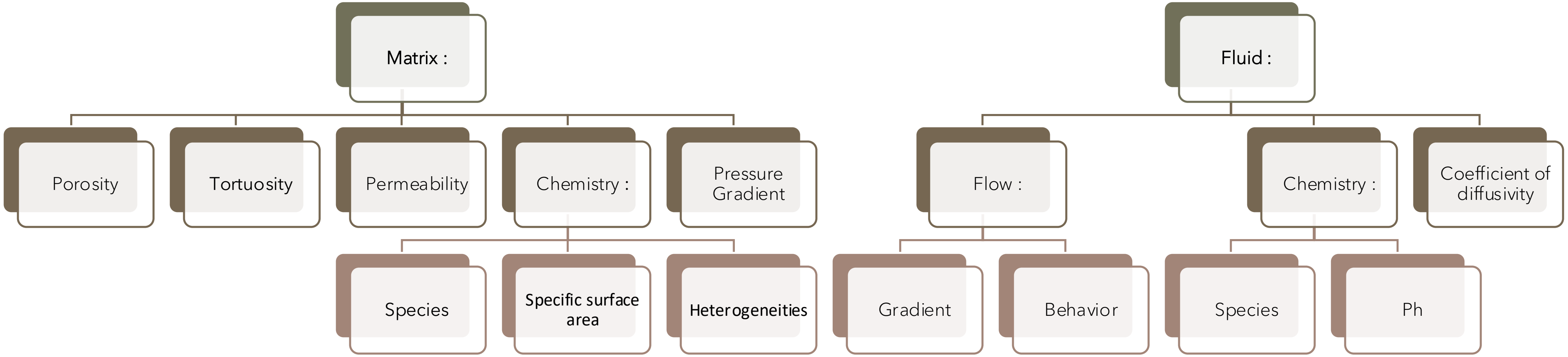
-Collapsing by the effect of gravity

-Deep structures, emptied while getting closer to the surface, and affected by a changing in the hydraulic gradient



Dubois C. et al., 2014

Key elements governing karst formation



Matrix :

- Porosity
- Tortuosity
- Permeability
- Chemistry :
  - Species
  - Specific surface area
  - Heterogeneities
- Pressure Gradient

Fluid :

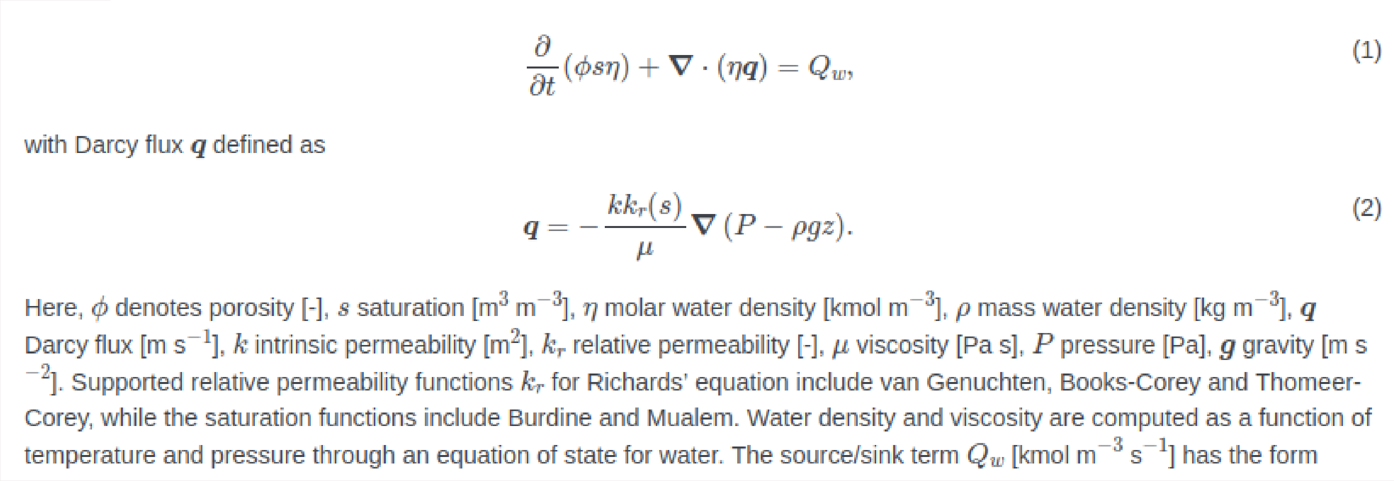
- Flow :
  - Gradient
  - Behavior
- Chemistry :
  - Species
  - Ph
- Coefficient of diffusivity

Purpose of the simulation

- Karsts : major water management possibilities : source of ¼ of water consumption worldwide, and major domestic water source in Mediterranean region (Ford D. et al.) --> need of more understanding of this phenomenon which can highly impact human water consumption
- Main objective of the simulation : numerical simulation of ghost-rock karstification process in a fractured matrix
- Simulations inspired by laboratory experiments carried-out by Linda LUQUOT in 2016 (Interaction between a fractured marl caprock and CO2 -rich sulfate solution under supercritical CO2 conditions) --> reproduction of this experiment on PFLOTRAN software

Simulation

- Flow equation : Richards model (saturated matrix)
- Transport equation : GIRT (Global Implicite Reactive Transport) : requires high computational capacities --> OSRT (Operator-Split Reactive Transport) might be an alternative
- Solver : Linear (Newton ?)

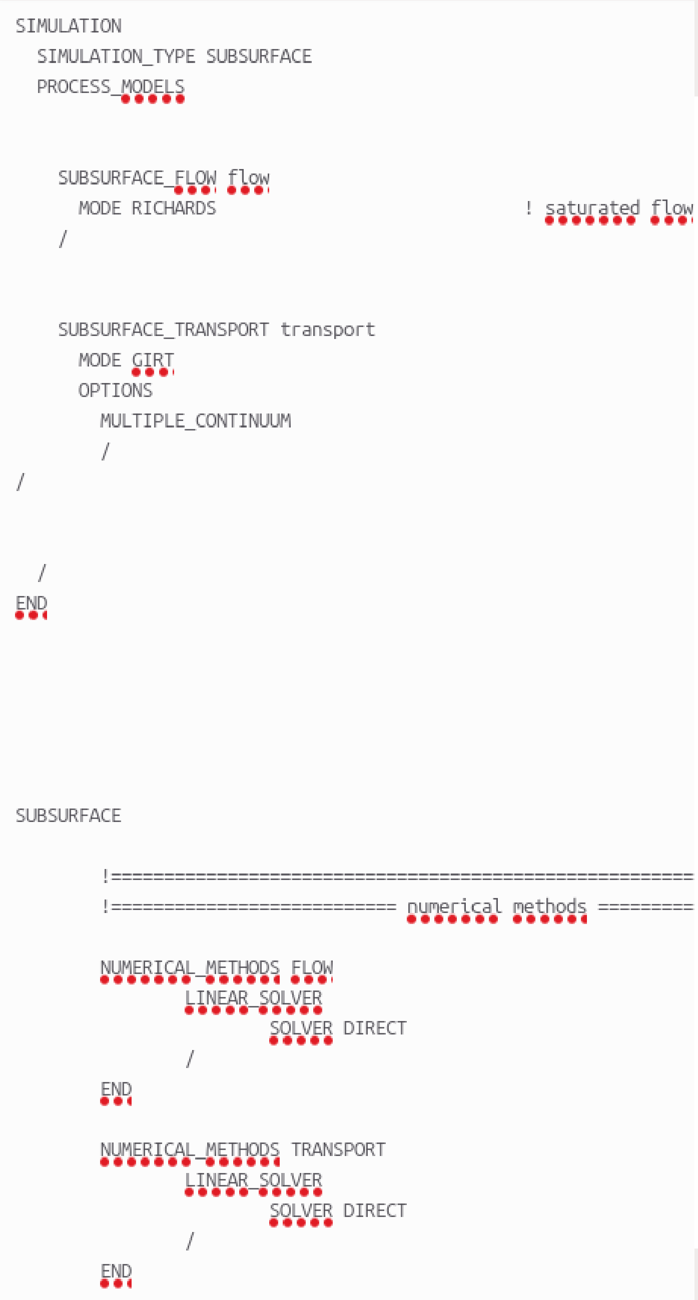


$$\frac{\partial}{\partial t}(\phi s \eta) + \boldsymbol{\nabla} \cdot (\eta \boldsymbol{q}) = Q_w, \tag{1}$$

with Darcy flux $\boldsymbol{q}$ defined as

$$\boldsymbol{q} = -\frac{k k_r(s)}{\mu} \boldsymbol{\nabla}(P - \rho g z). \tag{2}$$

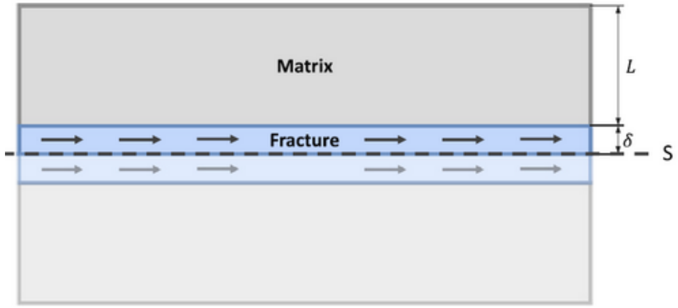
Here, ϕ denotes porosity [-], s saturation [m^3 m^{-3}], η molar water density [kmol m^{-3}], ρ mass water density [kg m^{-3}], $\boldsymbol{q}$ Darcy flux [m s^{-1}], k intrinsic permeability [m^2], k_r relative permeability [-], μ viscosity [Pa s], P pressure [Pa], $\boldsymbol{g}$ gravity [m s^{-2}]. Supported relative permeability functions k_r for Richards' equation include van Genuchten, Books-Corey and Thomeer-Corey, while the saturation functions include Burdine and Mualem. Water density and viscosity are computed as a function of temperature and pressure through an equation of state for water. The source/sink term Q_w [kmol m^{-3} s^{-1}] has the form



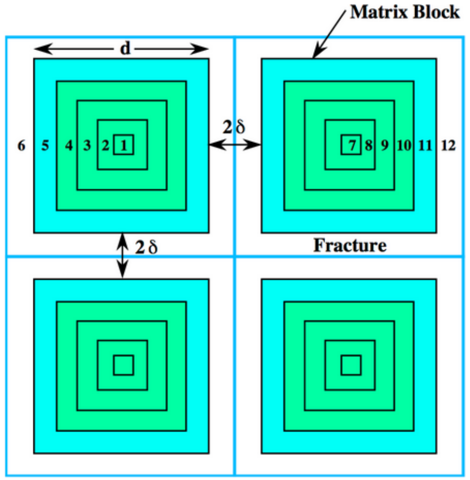
```
SIMULATION
  SIMULATION_TYPE SUBSURFACE
  PROCESS_MODELS


    SUBSURFACE_FLOW flow
      MODE RICHARDS                             ! saturated flow
    /


    SUBSURFACE_TRANSPORT transport
      MODE GIRT
      OPTIONS
        MULTIPLE_CONTINUUM
        /
/


  /
END









SUBSURFACE


        !=======================================================
        !=========================== numerical methods =========


        NUMERICAL_METHODS FLOW
                LINEAR_SOLVER
                        SOLVER DIRECT
                /
        END

        NUMERICAL_METHODS TRANSPORT
                LINEAR_SOLVER
                        SOLVER DIRECT
                /
        END
```

System Environment

- Fractured matrix
- High porosity (0.15) and permeability (1e-12)
- Secondary continuum : only diffusion considered



Slab

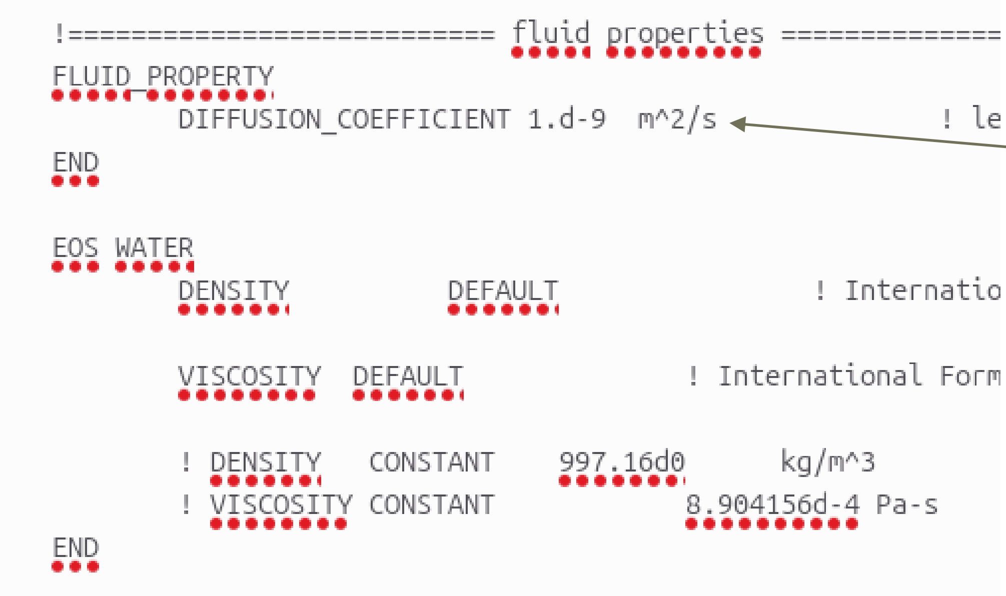


Nested cubes

Lichtner P.C. et al., 2020, modified

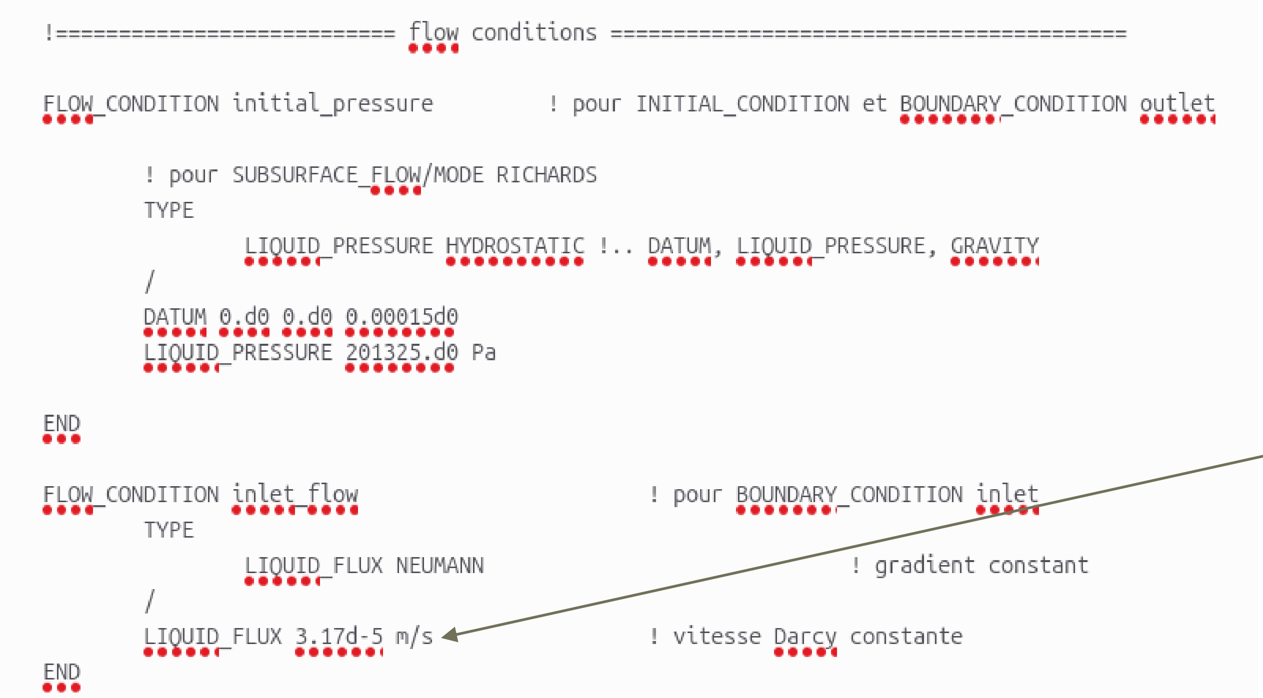
```
!=========================== porous properties =======================================

CHARACTERISTIC_CURVES saturated ! For MODE RICHARDS. Relative permeability and saturation functi

        DEFAULT         ! Sets up dummy saturation and permeability functions for saturated sing
END

MATERIAL_PROPERTY porous
        ID 1

        ! transient if CHEMISTRY/UPDATE_POROSITY
        POROSITY 0.15000003d0           ! inhibé par CHEMISTRY/CALCULATE_INITIAL_POROSITY

        ! transient if CHEMISTRY/UPDATE_PERMEABILITY
        PERMEABILITY
                ISOTROPIC
                PERM_ISO 1.d-12 m^2
        /
        PERMEABILITY_CRITICAL_POROSITY 0.0      ! theory guide : phi_c
        PERMEABILITY_POWER 0.66667                                      ! theory guide : n=a doc
        PERMEABILITY_MIN_SCALE_FACTOR 0.0               ! theory guide : fmin

        ! transient if CHEMISTRY/UPDATE_TORTUOSITY
        TORTUOSITY 1.0
        TORTUOSITY_POWER 1.0                                                            ! theory

        LONGITUDINAL_DISPERSIVITY 0.0
        TRANSVERSE_DISPERSIVITY_H 0.0
        TRANSVERSE_DISPERSIVITY_V 0.0

        CHARACTERISTIC_CURVES saturated ! For MODE RICHARDS. Relative permeability and saturatio
        SECONDARY_CONTINUUM
                TYPE SLAB
                LENGTH 0.01
                NUM_CELLS 5
                POROSITY 0.25d0
                LIQUID_DIFFUSION_COEFFICIENT 5.1d-10
                EPSILON 0.00909
        /
END
```

```
MATERIAL_PROPERTY mat
        ID 1

        ! transient if CHEMISTRY/UPDATE_POROSITY
        POROSITY 0.15000003d0           ! inhibé par CHEMISTRY/CALCULATE_INITIAL_POROSITY

        ! transient if CHEMISTRY/UPDATE_PERMEABILITY
        PERMEABILITY
                ISOTROPIC
                PERM_ISO 1d-12  m^2                                                             ! initial value for transient
        /
        PERMEABILITY_CRITICAL_POROSITY 0.0      ! theory guide : phi_c
        PERMEABILITY_POWER 0.66667                                      ! theory guide : n=a doc 2015
        PERMEABILITY_MIN_SCALE_FACTOR 0.0               ! theory guide : fmin

        ! transient if CHEMISTRY/UPDATE_TORTUOSITY
        TORTUOSITY 1.0
        TORTUOSITY_POWER 1.0                                                            ! theory guide : b

        LONGITUDINAL_DISPERSIVITY 0.0
        TRANSVERSE_DISPERSIVITY_H 0.0
        TRANSVERSE_DISPERSIVITY_V 0.0

        CHARACTERISTIC_CURVES saturated ! For MODE RICHARDS. Relative permeability and saturation functions and associated parameters.
END

MATERIAL_PROPERTY fracture
        ID 2

        ! transient if CHEMISTRY/UPDATE_POROSITY
        POROSITY 1d0            ! inhibé par CHEMISTRY/CALCULATE_INITIAL_POROSITY

        ! transient if CHEMISTRY/UPDATE_PERMEABILITY
        PERMEABILITY
                ISOTROPIC
                PERM_ISO 8.333d-10      m^2                                                             ! initial value for transient
        /
        PERMEABILITY_CRITICAL_POROSITY 0.0      ! theory guide : phi_c
        PERMEABILITY_POWER 0.66667                                      ! theory guide : n=a doc 2015
        PERMEABILITY_MIN_SCALE_FACTOR 0.0               ! theory guide : fmin

        ! transient if CHEMISTRY/UPDATE_TORTUOSITY
        TORTUOSITY 1.0
        TORTUOSITY_POWER 1.0                                                            ! theory guide : b

        LONGITUDINAL_DISPERSIVITY 0.0
        TRANSVERSE_DISPERSIVITY_H 0.0
        TRANSVERSE_DISPERSIVITY_V 0.0
        CHARACTERISTIC_CURVES saturated ! For MODE RICHARDS. Relative permeability and saturation functions and associated parameters.
END
```



```
!=========================== fluid properties ==============
FLUID_PROPERTY
        DIFFUSION_COEFFICIENT 1.d-9  m^2/s              ! le
END


EOS WATER
        DENSITY          DEFAULT                ! Internatio

        VISCOSITY  DEFAULT              ! International Form

        ! DENSITY   CONSTANT    997.16d0      kg/m^3
        ! VISCOSITY CONSTANT            8.904156d-4 Pa-s
END
```

/!\ : Diffusion coefficient identical for all species in the simulation



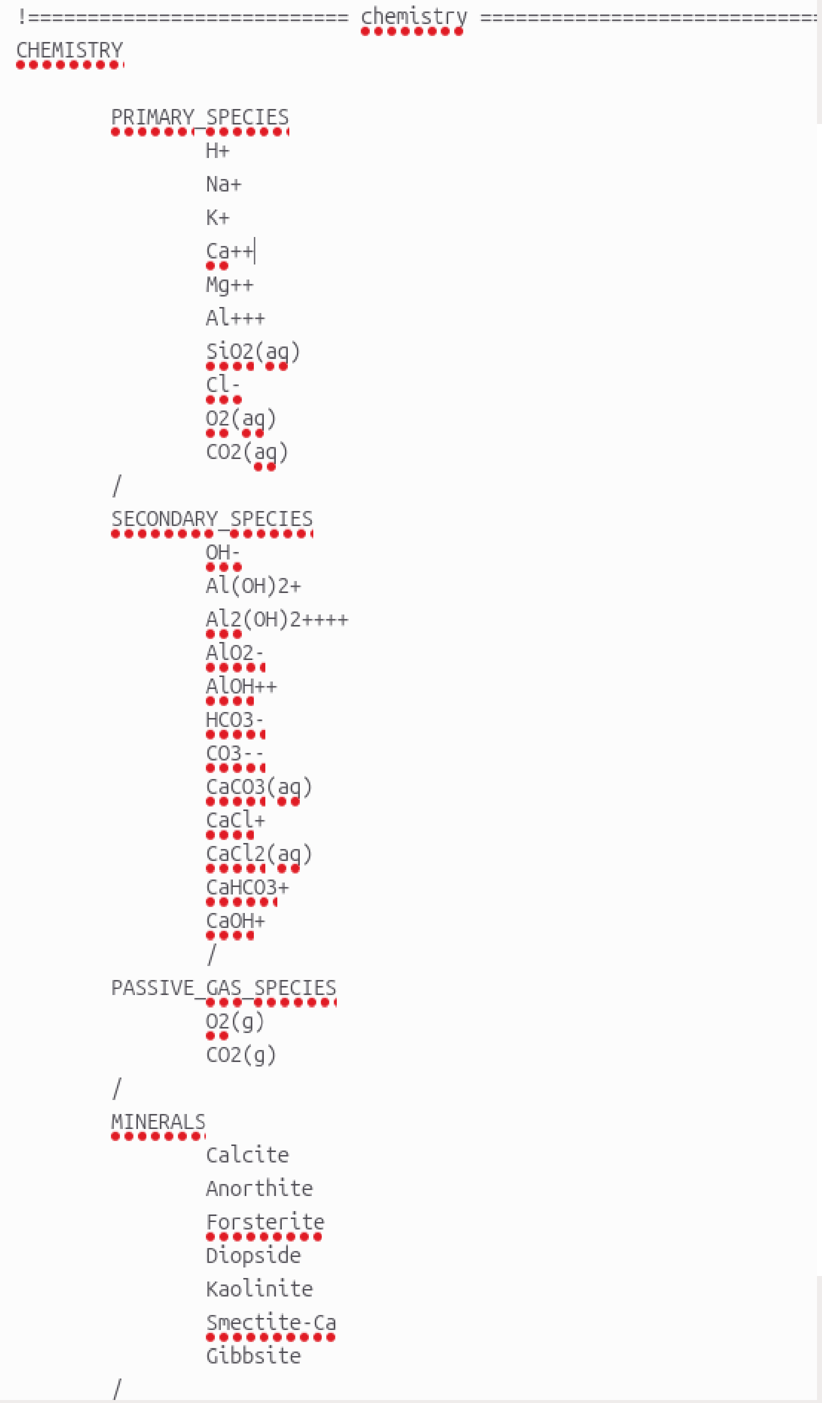
```
!=========================== flow conditions =========================================

FLOW_CONDITION initial_pressure         ! pour INITIAL_CONDITION et BOUNDARY_CONDITION outlet

        ! pour SUBSURFACE_FLOW/MODE RICHARDS
        TYPE
                LIQUID_PRESSURE HYDROSTATIC !.. DATUM, LIQUID_PRESSURE, GRAVITY
        /
        DATUM 0.d0 0.d0 0.00015d0
        LIQUID_PRESSURE 201325.d0 Pa

END

FLOW_CONDITION inlet_flow                       ! pour BOUNDARY_CONDITION inlet
        TYPE
                LIQUID_FLUX NEUMANN                             ! gradient constant
        /
        LIQUID_FLUX 3.17d-5 m/s                 ! vitesse Darcy constante
END
```

Injected flux as inflow

Chemistry of the system

Injection of a CO2-enriched water in a carbonate rock

- Weak acid --> high concentration but slow reaction
- 2 main processes of particles kinetics : diffusion and advection --> controlled by the Peclet number, requiring the diffusion coefficient (set as identical for every chemical species)
- Definition of primary species and secondary species to be precipitated
- Very low flow rate to be settled --> uniform dissolution ; if too high --> risk of wormhole structure, then breakthrough and end of the phantomisation

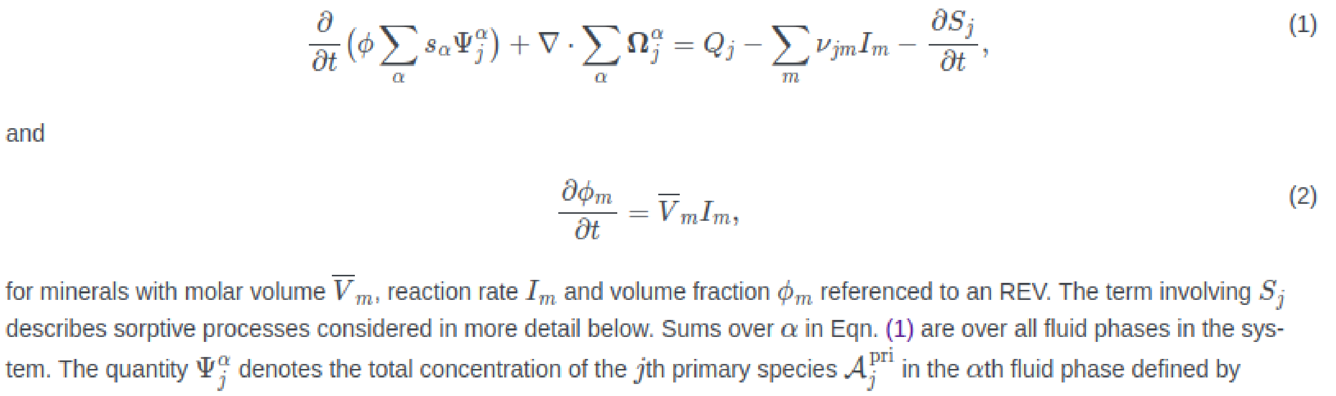


```
!========================= chemistry ===========================
CHEMISTRY

        PRIMARY_SPECIES
                H+
                Na+
                K+
                Ca++
                Mg++
                Al+++
                SiO2(aq)
                Cl-
                O2(aq)
                CO2(aq)
        /
        SECONDARY_SPECIES
                OH-
                Al(OH)2+
                Al2(OH)2++++
                AlO2-
                AlOH++
                HCO3-
                CO3--
                CaCO3(aq)
                CaCl+
                CaCl2(aq)
                CaHCO3+
                CaOH+
                /
        PASSIVE_GAS_SPECIES
                O2(g)
                CO2(g)
        /
        MINERALS
                Calcite
                Anorthite
                Forsterite
                Diopside
                Kaolinite
                Smectite-Ca
                Gibbsite
        /
```

Chemical mass conservation equations

ALPHA = 1 --> EQUATION SIMPLIFIED

QJ --> SOURCE/SINK = 0



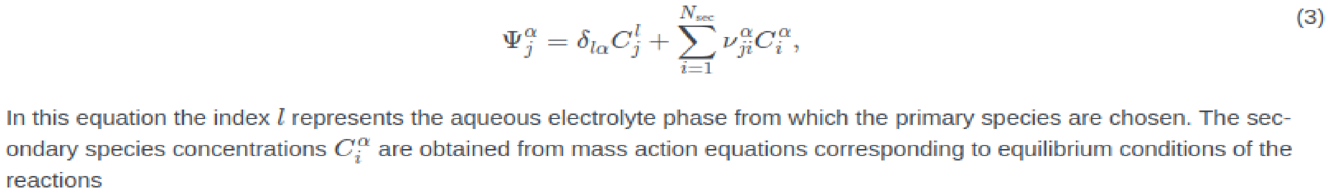
$$\frac{\partial}{\partial t}\Big(\phi\sum_\alpha s_\alpha \Psi_j^\alpha\Big) + \nabla\cdot\sum_\alpha \boldsymbol{\Omega}_j^\alpha = Q_j - \sum_m \nu_{jm} I_m - \frac{\partial S_j}{\partial t}, \tag{1}$$

and

$$\frac{\partial \phi_m}{\partial t} = \overline{V}_m I_m, \tag{2}$$

for minerals with molar volume $\overline{V}_m$, reaction rate I_m and volume fraction ϕ_m referenced to an REV. The term involving S_j describes sorptive processes considered in more detail below. Sums over α in Eqn. (1) are over all fluid phases in the system. The quantity Ψ_j^α denotes the total concentration of the jth primary species $\mathcal{A}_j^{\text{pri}}$ in the αth fluid phase defined by

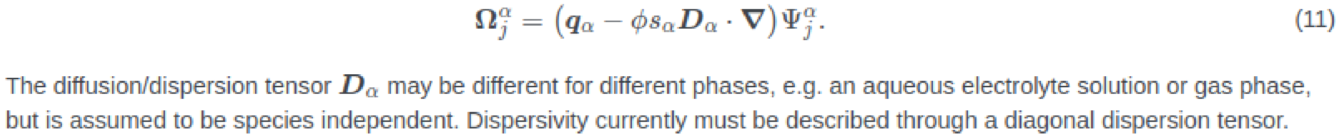
Lichtner P.C. et al., 2020



$$\Psi_j^\alpha = \delta_{l\alpha} C_j^l + \sum_{i=1}^{N_{\text{sec}}} \nu_{ji}^\alpha C_i^\alpha, \tag{3}$$

In this equation the index l represents the aqueous electrolyte phase from which the primary species are chosen. The secondary species concentrations C_i^α are obtained from mass action equations corresponding to equilibrium conditions of the reactions

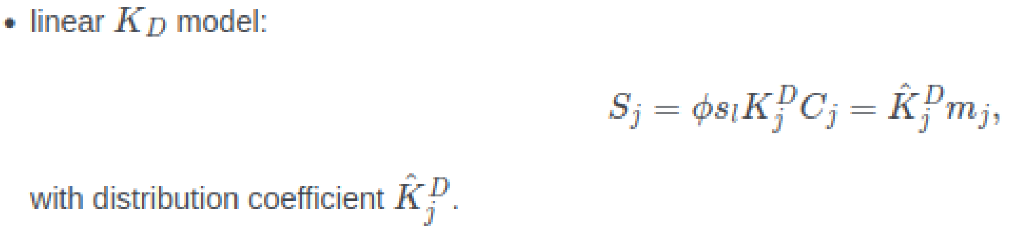
Lichtner P.C. et al., 2020



$$\boldsymbol{\Omega}_j^\alpha = \big(\boldsymbol{q}_\alpha - \phi s_\alpha \boldsymbol{D}_\alpha \cdot \boldsymbol{\nabla}\big)\Psi_j^\alpha. \tag{11}$$

The diffusion/dispersion tensor $\boldsymbol{D}_\alpha$ may be different for different phases, e.g. an aqueous electrolyte solution or gas phase, but is assumed to be species independent. Dispersivity currently must be described through a diagonal dispersion tensor.

Lichtner P.C. et al., 2020

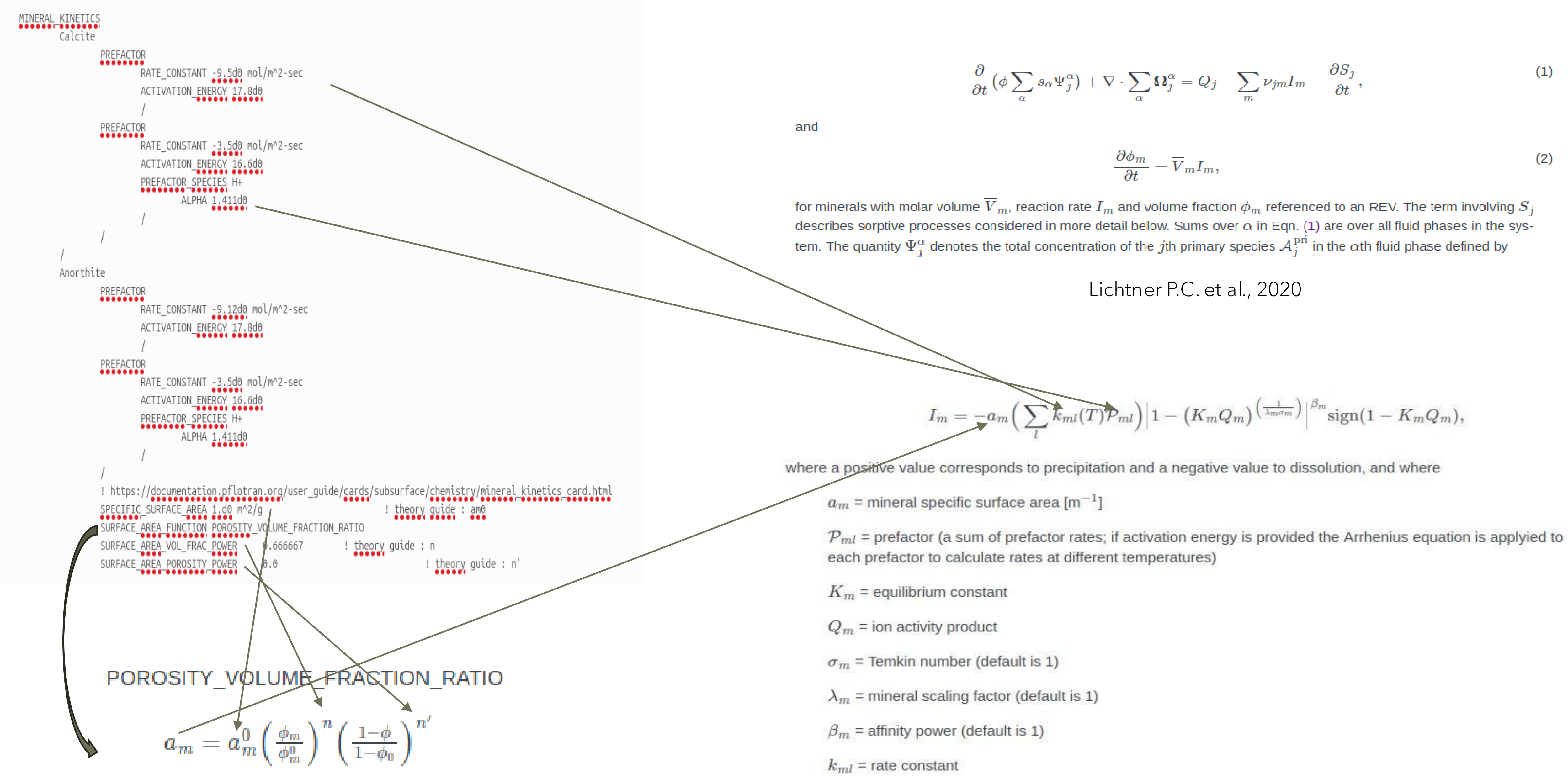


- linear K_D model:

$$S_j = \phi s_l K_j^D C_j = \hat{K}_j^D m_j,$$

with distribution coefficient $\hat{K}_j^D$.

Lichtner P.C. et al., 2020



```
MINERAL_KINETICS
        Calcite
                PREFACTOR
                        RATE_CONSTANT -9.5d0 mol/m^2-sec
                        ACTIVATION_ENERGY 17.8d0
                        /
                PREFACTOR
                        RATE_CONSTANT -3.5d0 mol/m^2-sec
                        ACTIVATION_ENERGY 16.6d0
                        PREFACTOR_SPECIES H+
                                ALPHA 1.411d0
                        /
                /
        /
        Anorthite
                PREFACTOR
                        RATE_CONSTANT -9.12d0 mol/m^2-sec
                        ACTIVATION_ENERGY 17.8d0
                        /
                PREFACTOR
                        RATE_CONSTANT -3.5d0 mol/m^2-sec
                        ACTIVATION_ENERGY 16.6d0
                        PREFACTOR_SPECIES H+
                                ALPHA 1.411d0
                        /
                /
                ! https://documentation.pflotran.org/user_guide/cards/subsurface/chemistry/mineral_kinetics_card.html
                SPECIFIC_SURFACE_AREA 1.d0 m^2/g                          ! theory guide : am0
                SURFACE_AREA_FUNCTION POROSITY_VOLUME_FRACTION_RATIO
                SURFACE_AREA_VOL_FRAC_POWER     0.666667         ! theory guide : n
                SURFACE_AREA_POROSITY_POWER     0.0                          ! theory guide : n'
```

$$\frac{\partial}{\partial t}\left(\phi\sum_\alpha s_\alpha\Psi_j^\alpha\right)+\nabla\cdot\sum_\alpha\boldsymbol{\Omega}_j^\alpha=Q_j-\sum_m\nu_{jm}I_m-\frac{\partial S_j}{\partial t}, \tag{1}$$

and

$$\frac{\partial\phi_m}{\partial t}=\overline{V}_m I_m, \tag{2}$$

for minerals with molar volume $\overline{V}_m$, reaction rate I_m and volume fraction ϕ_m referenced to an REV. The term involving S_j describes sorptive processes considered in more detail below. Sums over α in Eqn. (1) are over all fluid phases in the system. The quantity Ψ_j^α denotes the total concentration of the jth primary species $\mathcal{A}_j^{\rm pri}$ in the αth fluid phase defined by

Lichtner P.C. et al., 2020

$$I_m=-a_m\left(\sum_l k_{ml}(T)\mathcal{P}_{ml}\right)\left|1-\left(K_mQ_m\right)^{\left(\frac{1}{\lambda_m\sigma_m}\right)}\right|^{\beta_m}\mathrm{sign}(1-K_mQ_m),$$

where a positive value corresponds to precipitation and a negative value to dissolution, and where

a_m = mineral specific surface area [m^{-1}]

$\mathcal{P}_{ml}$ = prefactor (a sum of prefactor rates; if activation energy is provided the Arrhenius equation is applyied to each prefactor to calculate rates at different temperatures)

K_m = equilibrium constant

Q_m = ion activity product

σ_m = Temkin number (default is 1)

λ_m = mineral scaling factor (default is 1)

β_m = affinity power (default is 1)

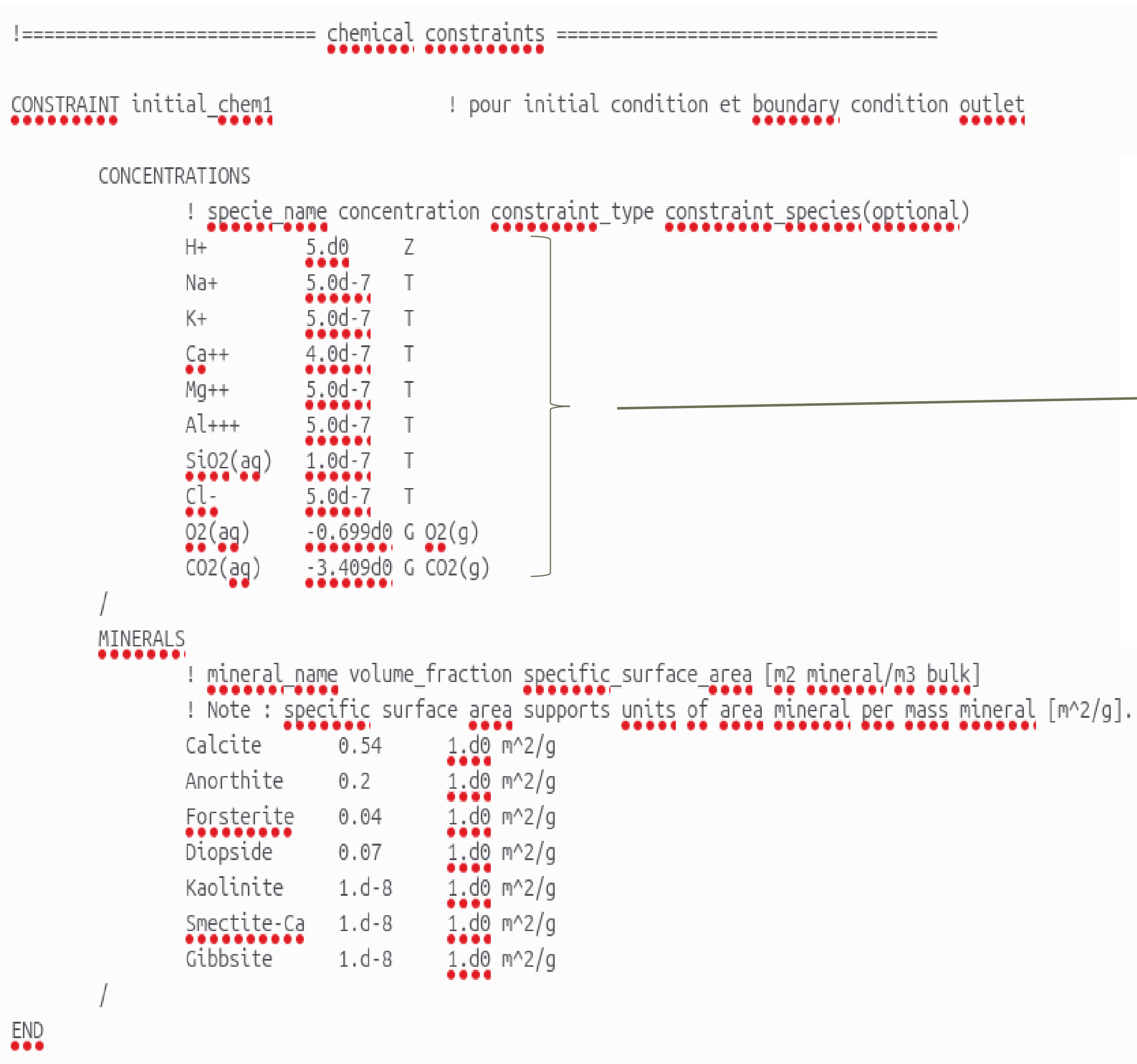
k_{ml} = rate constant

POROSITY_VOLUME_FRACTION_RATIO

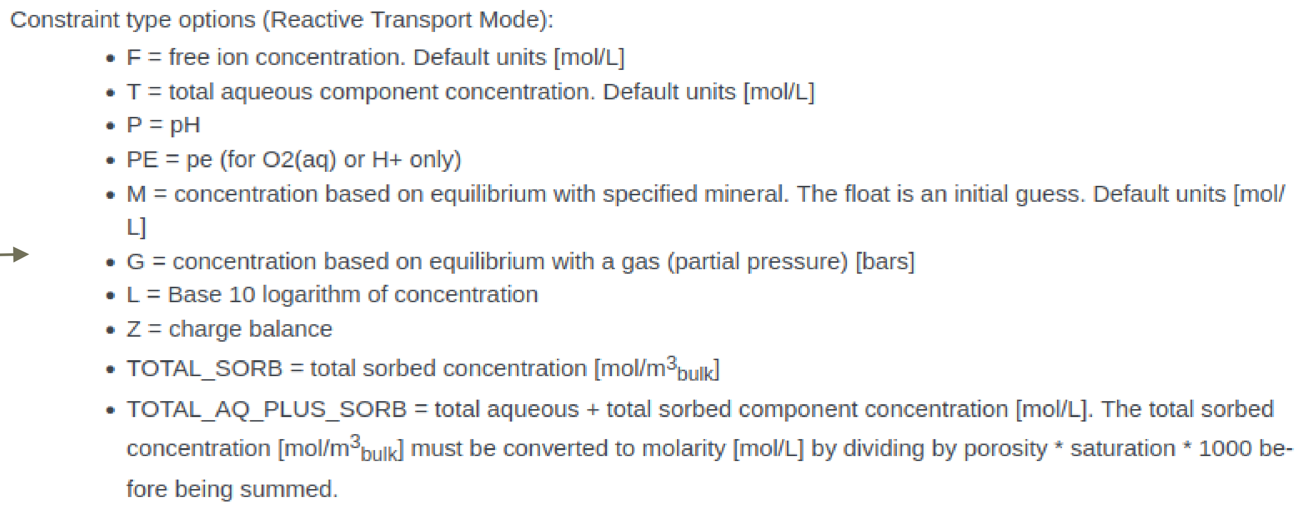
$$a_m=a_m^0\left(\frac{\phi_m}{\phi_m^0}\right)^n\left(\frac{1-\phi}{1-\phi_0}\right)^{n'}$$

Lichtner P.C. et al., 2020

Lichtner P.C. et al., 2020



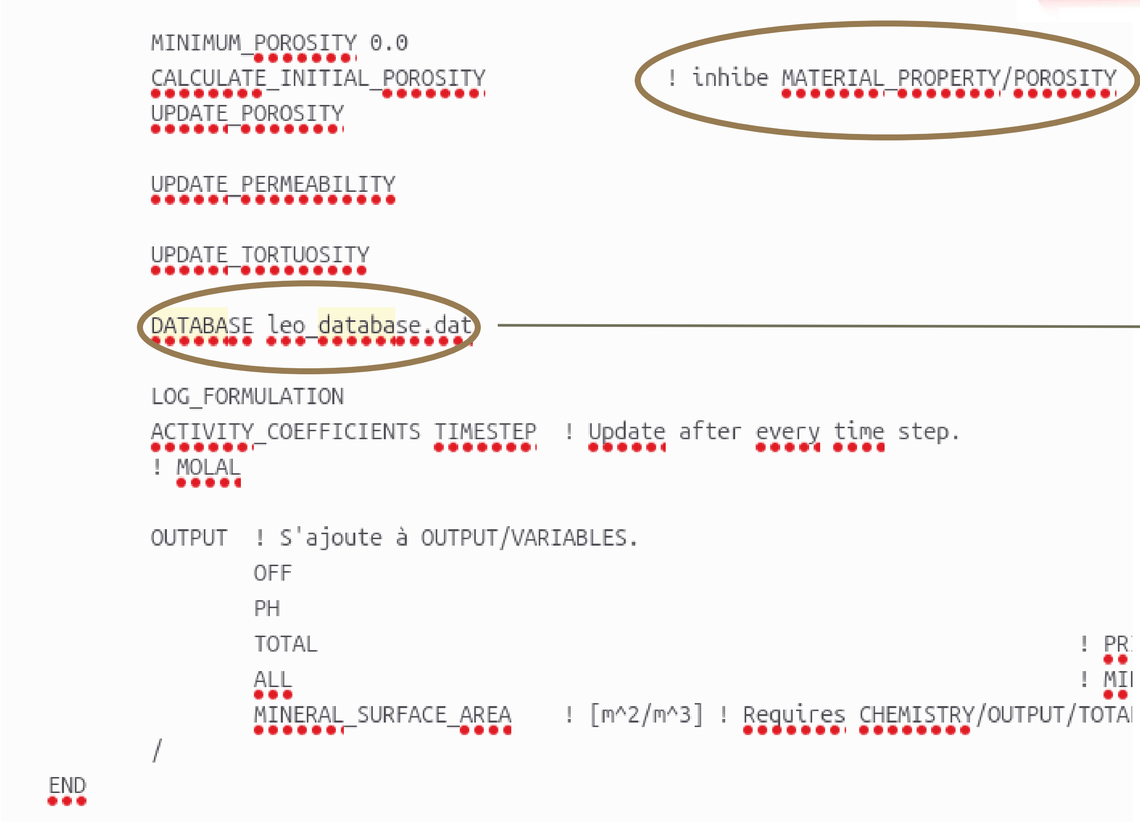
```
!========================== chemical constraints ==================================

CONSTRAINT initial_chem1                ! pour initial condition et boundary condition outlet

       CONCENTRATIONS
              ! specie_name concentration constraint_type constraint_species(optional)
              H+         5.d0     Z
              Na+        5.0d-7   T
              K+         5.0d-7   T
              Ca++       4.0d-7   T
              Mg++       5.0d-7   T
              Al+++      5.0d-7   T
              SiO2(aq)   1.0d-7   T
              Cl-        5.0d-7   T
              O2(aq)     -0.699d0 G O2(g)
              CO2(aq)    -3.409d0 G CO2(g)
       /
       MINERALS
              ! mineral_name volume_fraction specific_surface_area [m2 mineral/m3 bulk]
              ! Note : specific surface area supports units of area mineral per mass mineral [m^2/g].
              Calcite      0.54     1.d0 m^2/g
              Anorthite    0.2      1.d0 m^2/g
              Forsterite   0.04     1.d0 m^2/g
              Diopside     0.07     1.d0 m^2/g
              Kaolinite    1.d-8    1.d0 m^2/g
              Smectite-Ca  1.d-8    1.d0 m^2/g
              Gibbsite     1.d-8    1.d0 m^2/g
       /
END
```



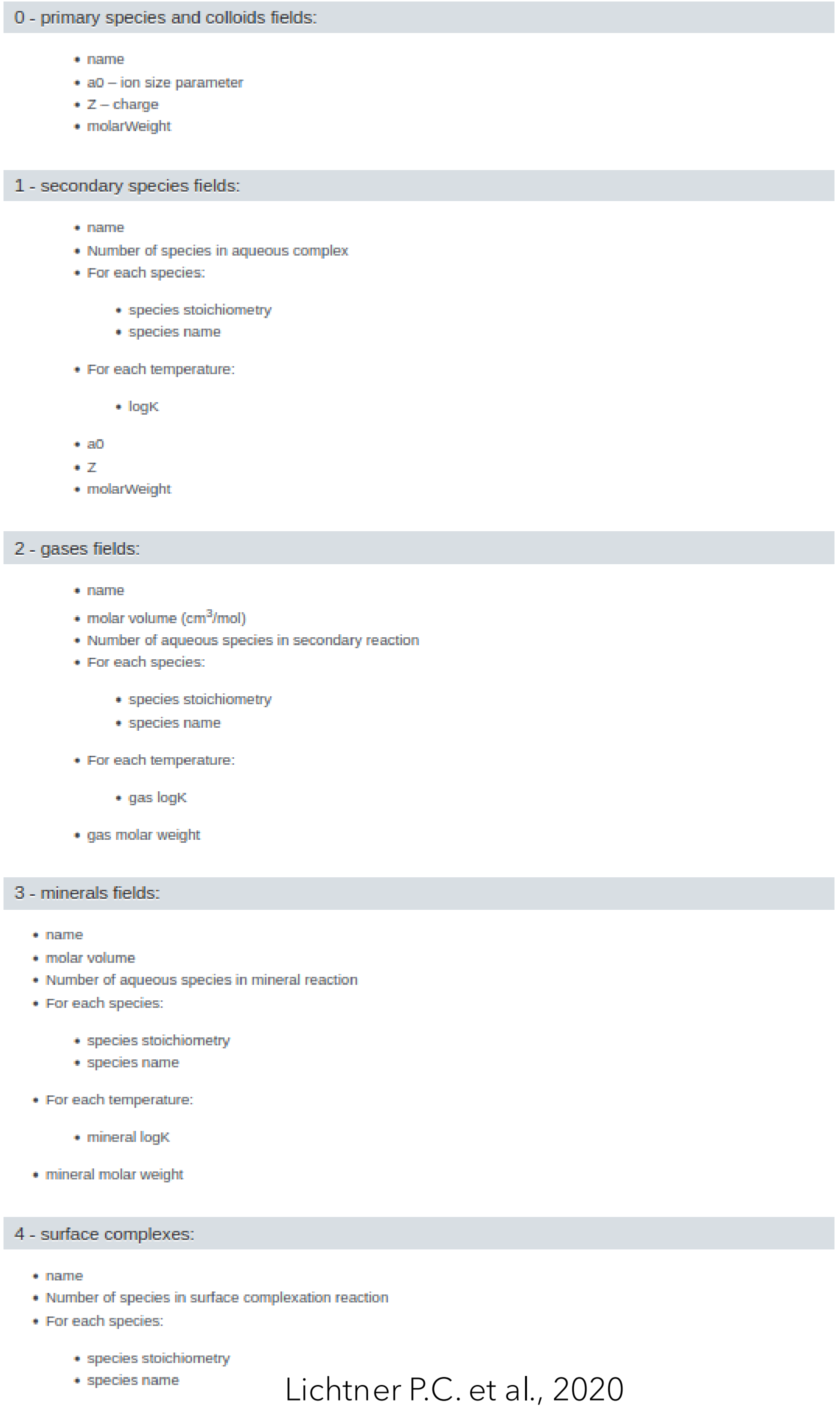
Constraint type options (Reactive Transport Mode):

- F = free ion concentration. Default units [mol/L]
- T = total aqueous component concentration. Default units [mol/L]
- P = pH
- PE = pe (for O2(aq) or H+ only)
- M = concentration based on equilibrium with specified mineral. The float is an initial guess. Default units [mol/L]
- G = concentration based on equilibrium with a gas (partial pressure) [bars]
- L = Base 10 logarithm of concentration
- Z = charge balance
- TOTAL_SORB = total sorbed concentration [mol/m$^3_{bulk}$]
- TOTAL_AQ_PLUS_SORB = total aqueous + total sorbed component concentration [mol/L]. The total sorbed concentration [mol/m$^3_{bulk}$] must be converted to molarity [mol/L] by dividing by porosity * saturation * 1000 before being summed.

Lichtner P.C. et al., 2020



```
    MINIMUM_POROSITY 0.0
    CALCULATE_INITIAL_POROSITY          ! inhibe MATERIAL_PROPERTY/POROSITY
    UPDATE_POROSITY

    UPDATE_PERMEABILITY

    UPDATE_TORTUOSITY

    DATABASE leo_database.dat

    LOG_FORMULATION
    ACTIVITY_COEFFICIENTS TIMESTEP  ! Update after every time step.
    ! MOLAL

    OUTPUT  ! S'ajoute à OUTPUT/VARIABLES.
            OFF
            PH
            TOTAL                                                          ! PR
            ALL                                                            ! MI
            MINERAL_SURFACE_AREA    ! [m^2/m^3] ! Requires CHEMISTRY/OUTPUT/TOTA
    /
END
```



0 - primary species and colloids fields:

- name
- a0 – ion size parameter
- Z – charge
- molarWeight

1 - secondary species fields:

- name
- Number of species in aqueous complex
- For each species:
  - species stoichiometry
  - species name
- For each temperature:
  - logK
- a0
- Z
- molarWeight

2 - gases fields:

- name
- molar volume (cm^3/mol)
- Number of aqueous species in secondary reaction
- For each species:
  - species stoichiometry
  - species name
- For each temperature:
  - gas logK
- gas molar weight

3 - minerals fields:

- name
- molar volume
- Number of aqueous species in mineral reaction
- For each species:
  - species stoichiometry
  - species name
- For each temperature:
  - mineral logK
- mineral molar weight

4 - surface complexes:

- name
- Number of species in surface complexation reaction
- For each species:
  - species stoichiometry
  - species name

Lichtner P.C. et al., 2020

Boundary conditions

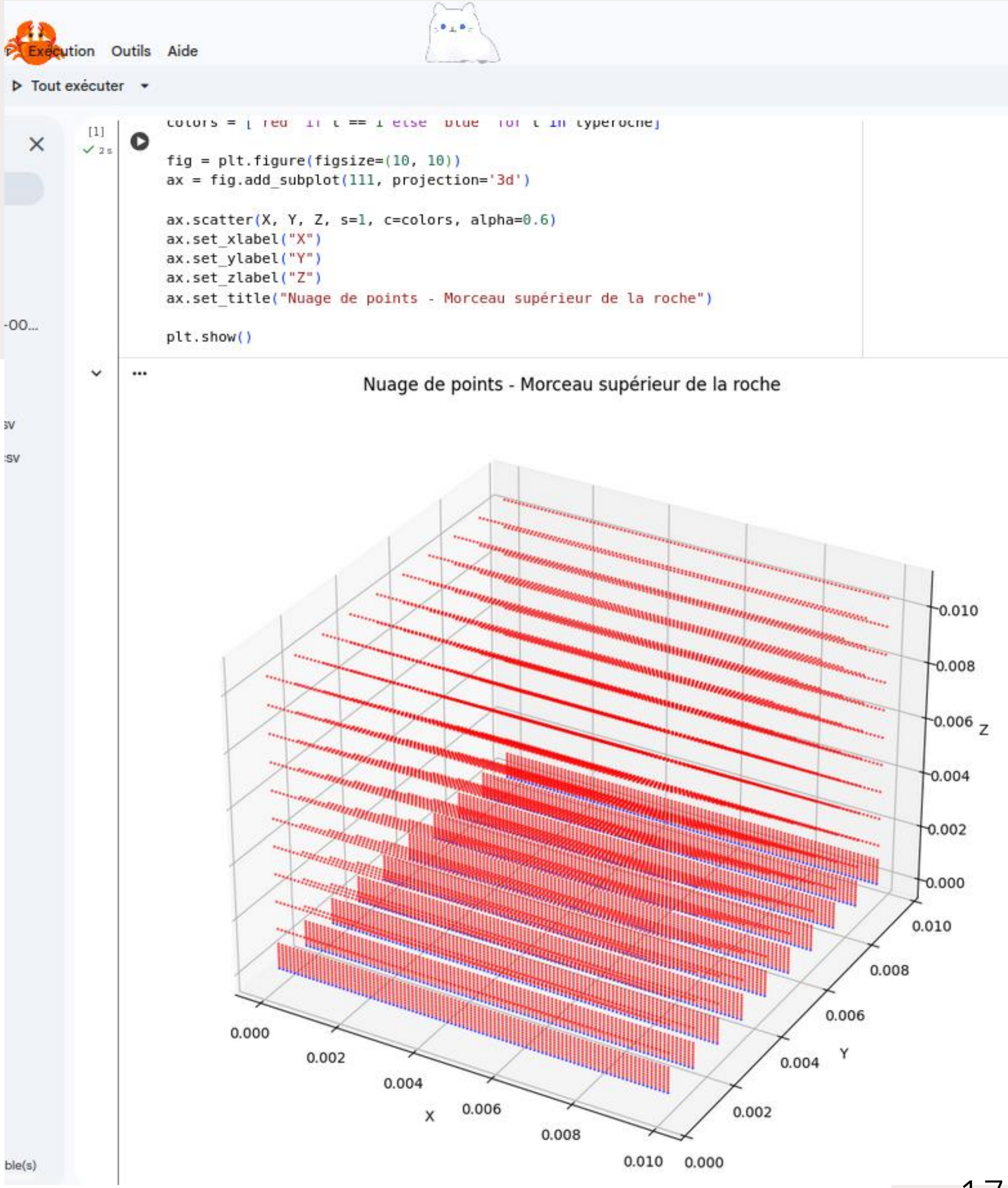
- One inlet on the left border of the model : Flux of 3.17e-5 m/s
- One outlet at the right border of the model
- Other faces of the model : no specification --> defined as no flow

Type Dirichlet : Only advection considered --> no diffusion at the boundary conditions

```
!========================== transport conditions ==================================

TRANSPORT_CONDITION initial_chem1        ! pour INITIAL_CONDITION et BOUNDARY_CONDITION out
        TYPE ZERO_GRADIENT                       ! inflow  : third-type or Robin boundary c

        CONSTRAINT_LIST
                0.d0 initial_chem1       ! appliqué à partir de t=0
        /
END


TRANSPORT_CONDITION outlet_chem          ! pour BOUNDARY_CONDITION inlet
        TYPE DIRICHLET_ZERO_GRADIENT     ! inflow  : constant concentration

        CONSTRAINT_LIST
                0.d0 inlet_chem1         ! appliqué à partir de t=0
        /
END

TRANSPORT_CONDITION inlet_chem           ! pour BOUNDARY_CONDITION inlet
        TYPE DIRICHLET_ZERO_GRADIENT     ! inflow  : constant concentration

        CONSTRAINT_LIST
                0.d0 inlet_chem ! appliqué à partir de t=0
        /
END


!==================================================================================
!========================== initial and boundary conditions =======================

INITIAL_CONDITION
        FLOW_CONDITION      initial_pressure
        TRANSPORT_CONDITION initial_chem1
        REGION porous
END


BOUNDARY_CONDITION outlet
        FLOW_CONDITION      initial_pressure
        TRANSPORT_CONDITION outlet_chem
        REGION outlet
END

BOUNDARY_CONDITION inlet
        FLOW_CONDITION      initial_pressure
        TRANSPORT_CONDITION inlet_chem
        REGION inlet
END
```

Grid view of the model

- 1cm/1cm/1,1cm (X/Y/Z)
- On X axis :
    - 100 cells : 0.0001m resolution
- On Y axis :
    - 1 cell : 0.01m resolution (2D simulation)
- On Z axis :
    - 10 cells : 0.0001m resolution
    - 10 cells 0.001m resolution

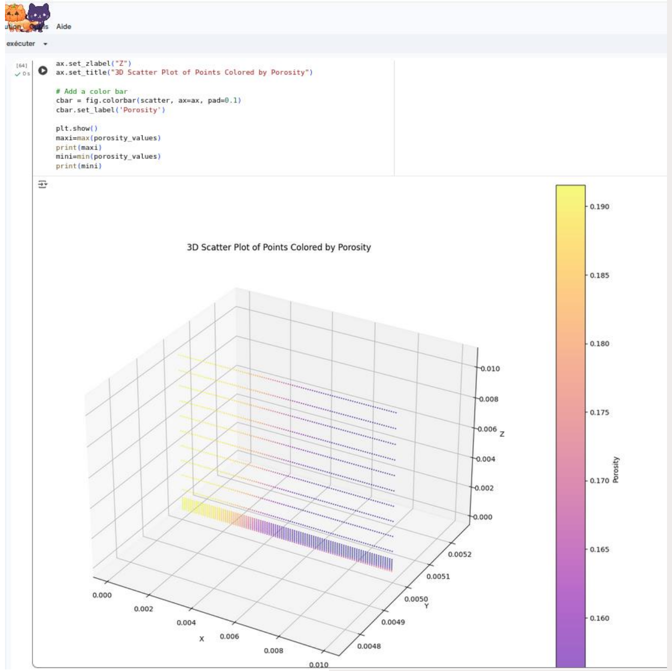


```
colors = ['red' if t == 1 else 'blue' for t in typeroche]

fig = plt.figure(figsize=(10, 10))
ax = fig.add_subplot(111, projection='3d')

ax.scatter(X, Y, Z, s=1, c=colors, alpha=0.6)
ax.set_xlabel("X")
ax.set_ylabel("Y")
ax.set_zlabel("Z")
ax.set_title("Nuage de points - Morceau supérieur de la roche")

plt.show()
```

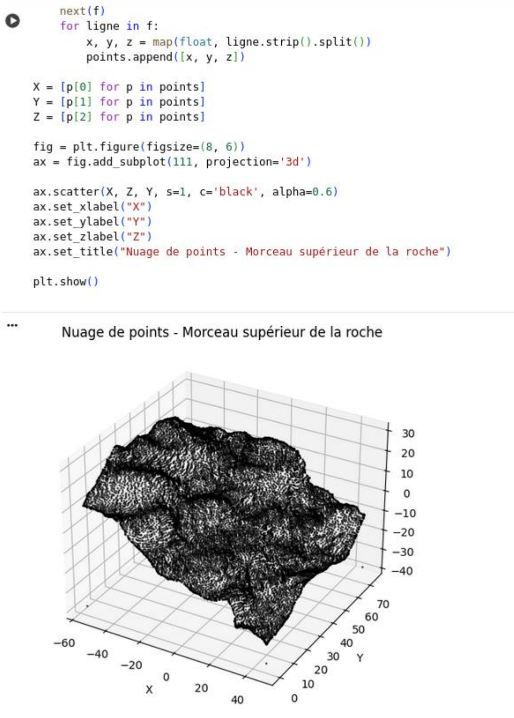
Nuage de points - Morceau supérieur de la roche

What was done so far

- Bibliography/Familiarisation with the topic
    - Karsts
    - Ghost rock
    - Geochemistry
- Introduction to PFLOTRAN
    - Test simulations with different grids/materials
    - Test simulations with a fracture in the model
- Modeling of a cloud points on python of the surface of a natural fracturation mesh



```
ax.set_zlabel("Z")
ax.set_title("3D Scatter Plot of Points Colored by Porosity")

# Add a color bar
cbar = fig.colorbar(scatter, ax=ax, pad=0.1)
cbar.set_label('Porosity')

plt.show()
maxi=max(porosity_values)
print(maxi)
mini=min(porosity_values)
print(mini)
```



```
    next(f)
    for ligne in f:
        x, y, z = map(float, ligne.strip().split())
        points.append([x, y, z])

X = [p[0] for p in points]
Y = [p[1] for p in points]
Z = [p[2] for p in points]

fig = plt.figure(figsize=(8, 6))
ax = fig.add_subplot(111, projection='3d')

ax.scatter(X, Z, Y, s=1, c='black', alpha=0.6)
ax.set_xlabel("X")
ax.set_ylabel("Y")
ax.set_zlabel("Z")
ax.set_title("Nuage de points - Morceau supérieur de la roche")

plt.show()
```

Next step

- Run a simulation reproducing the experiment of Linda :
  - New mineralogy
  - New fluid compositions and flow rates
  - New size of model
  - New matrix properties
  - New elements

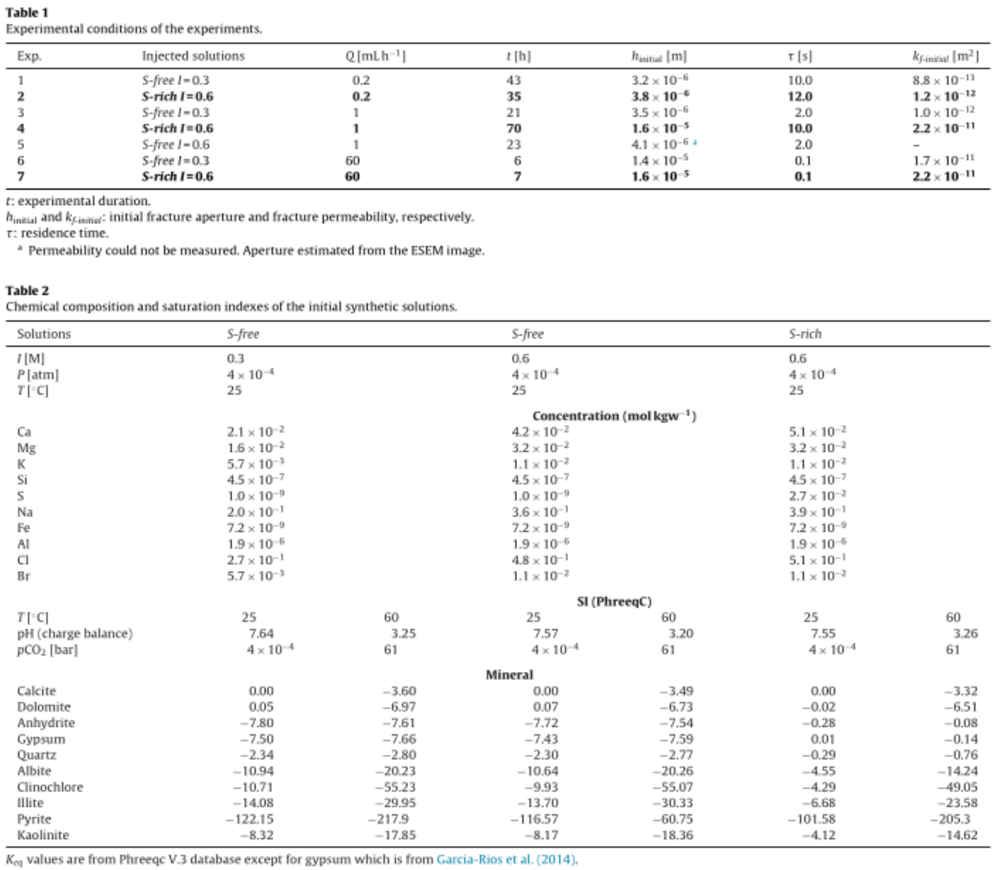


Table 1
Experimental conditions of the experiments.

Exp.	Injected solutions	Q [mL h^{-1}]	*t* [h]	$h_{initial}$ [m]	τ [s]	$k_{f\text{-}initial}$ [m^2]
1	*S-free* I = 0.3	0.2	43	3.2×10^{-6}	10.0	8.8×10^{-13}
2	***S-rich* I = 0.6**	**0.2**	**35**	3.8×10^{-6}	**12.0**	1.2×10^{-12}
3	*S-free* I = 0.3	1	21	3.5×10^{-6}	2.0	1.0×10^{-12}
4	***S-rich* I = 0.6**	**1**	**70**	1.6×10^{-5}	**10.0**	2.2×10^{-11}
5	*S-free* I = 0.6	1	23	4.1×10^{-6} [a]	2.0	–
6	*S-free* I = 0.3	60	6	1.4×10^{-5}	0.1	1.7×10^{-11}
7	***S-rich* I = 0.6**	**60**	**7**	1.6×10^{-5}	**0.1**	2.2×10^{-11}

t: experimental duration.
$h_{initial}$ and $k_{f\text{-}initial}$: initial fracture aperture and fracture permeability, respectively.
τ: residence time.
[a] Permeability could not be measured. Aperture estimated from the ESEM image.

Table 2
Chemical composition and saturation indexes of the initial synthetic solutions.

Solutions	*S-free*		*S-free*		*S-rich*	
I [M]	0.3		0.6		0.6	
P [atm]	4×10^{-4}		4×10^{-4}		4×10^{-4}	
T [°C]	25		25		25	
			Concentration (mol kgw^{-1})			
Ca	2.1×10^{-2}		4.2×10^{-2}		5.1×10^{-2}	
Mg	1.6×10^{-2}		3.2×10^{-2}		3.2×10^{-2}	
K	5.7×10^{-3}		1.1×10^{-2}		1.1×10^{-2}	
Si	4.5×10^{-7}		4.5×10^{-7}		4.5×10^{-7}	
S	1.0×10^{-9}		1.0×10^{-9}		2.7×10^{-2}	
Na	2.0×10^{-1}		3.6×10^{-1}		3.9×10^{-1}	
Fe	7.2×10^{-9}		7.2×10^{-9}		7.2×10^{-9}	
Al	1.9×10^{-6}		1.9×10^{-6}		1.9×10^{-6}	
Cl	2.7×10^{-1}		4.8×10^{-1}		5.1×10^{-1}	
Br	5.7×10^{-3}		1.1×10^{-2}		1.1×10^{-2}	
				SI (PhreeqC)		
T [°C]	25	60	25	60	25	60
pH (charge balance)	7.64	3.25	7.57	3.20	7.55	3.26
pCO_2 [bar]	4×10^{-4}	61	4×10^{-4}	61	4×10^{-4}	61
			Mineral			
Calcite	0.00	−3.60	0.00	−3.49	0.00	−3.32
Dolomite	0.05	−6.97	0.07	−6.73	−0.02	−6.51
Anhydrite	−7.80	−7.61	−7.72	−7.54	−0.28	−0.08
Gypsum	−7.50	−7.66	−7.43	−7.59	0.01	−0.14
Quartz	−2.34	−2.80	−2.30	−2.77	−0.29	−0.76
Albite	−10.94	−20.23	−10.64	−20.26	−4.55	−14.24
Clinochlore	−10.71	−55.23	−9.93	−55.07	−4.29	−49.05
Illite	−14.08	−29.95	−13.70	−30.33	−6.68	−23.58
Pyrite	−122.15	−217.9	−116.57	−60.75	−101.58	−205.3
Kaolinite	−8.32	−17.85	−8.17	−18.36	−4.12	−14.62

K_{eq} values are from Phreeqc V.3 database except for gypsum which is from Garcia-Rios et al. (2014).

Upcoming steps

- Continue to accumulate knowledge about karstic and Ghost rock mechanisms, as well as geochemistry and PFLOTRAN software
- Simulate in 2D, then in 3D the model with a fracture
- From this model :
  - Add heterogeneities to the model
  - Simulate different natures of matrix
  - Combine different fractures