Manual For Darcy Impes Leaching

Before using the mobile immobile model and leaching chemical model

- please TURN ON the porosity on the pressure mesh (/material_phase::Phase2/scalar_field::Porosity_pmesh) and liquid viscosity on the pressure mesh (/material_phase::Phase2/scalar_field::Viscosity_pmesh)
- please TURN ON the field for average ore diameter (/porous_media/scalar_field::Rock_diameter)

❖ **Mobile-Immobile model:**

(1). TURN ON: < /material_phase::Phase2/MobileImmobileModel >

(a). The immobile saturation and mass transfer coefficient between mobile and immobile phase could either be a prescribed field or calculated by an internal algorithm proposed by Lima (2006).

(b). tensor_field(Dispersivity_MIM):

- To include the dynamic dispersivity according to the dynamic liquid velocity, turn on this field and turn off the dispersivity of all of the scalar fields under this phase, the dispersivitiy is assumed to be same for all the scalar fields.
- Otherwise, turn off 'Dispersivity_MIM' and include the dispersivity individually under each scaler field.
- There are two internal algorithms for the dynamic dispersivity, one is proposed by Lima (2006). Another one is fitted by the curve presented by Ilankoon (2012)

(2). Under EACH prognostic scalar field of liquid phase,

(a). TURN ON the mass of this field in the stagnant region:
< /material_phase::Phase2/scalar_field/prognostic/scalar_field::Immobile >

i. scalar_field(Average_mass): the average bulk concentration of this field
ii. scalar_field(Mobile_ratio) and scalar_field(Immobile_ratio): is the weighting ratio of the mobile and immobile mass to the total mass

(b). IF there is the leaching chemical source term of this field, also TURN ON:
< /material_phase::Phase2/scalar_field/prognostic/LeachingChemicalSourceTerm/Mobile_Immobile_Model > for chemical species OR < /material_phase::Phase2/scalar_field::Temperature/prognostic/leaching_temperature_sources/Mobile_Immobile_Model > for liquid temperature

i. scalar_field(Mobile_chemical_src): the chemical source term for mobile field (mass/m^3 mobile Liquid/s)
ii. scalar_field(immobile_chemical_src): the chemical source term for immobile field (mass/m^3 immobile Liquid /s)

❖ **Leaching chemical model**:

(1). Mineral dissolution

(a). reaction(CuFeS2_oxidation_aqueous_ferric_sulfate) and reaction(FeS2_oxidation_aqueous_ferric_sulfate): chalcopyrite and pyrite dissolution

- scalar_field(dCuFeS2_dt) and scalar_field(dFeS2_dt) is the mass conversion rate with the unite of (mol/m^3 heap/s)
- scalar_field(extraction_rate) is the conversion rate of the mineral with the unit (s^-1)
- scalar_field(current_extraction) is the current conversion of the mineral (-)
- scalar_field(molar_concentration) is the total molar mass of the mineral per volume

of heap (mol/m^3 heap), this is the initial mass available inside the heap before leaching.

- experiment data: the data from the semi-empirical lookup curve, $\frac{d\varepsilon}{dt}\frac{1}{\eta_t \kappa} = f(\varepsilon)$
  i. number_of_data_points: the total number of the point to interpolate the semi-empirical curve
  ii. extraction: the x axis of the semi-empirical curve, ε. Write down the corresponding value of each the data point
  iii. empirical_extraction_rate_over_k: the y axis of the semi-empirical curve, $\frac{d\varepsilon}{dt}\frac{1}{\eta_t \kappa}$. Write down the corresponding values of the each data point.

- rate_constant_Arrhenius: it is the reaction rate constant calculated by the Arrhenius equation. In semi-empirical model, it is the κ in the equation, which is from literature.
  i. scalar_field(prefactor): it is the prefacter k inside the Arrhenius equation, in semi-empirical model it is negelected (set as 1.0) since the pre-factor is neglected when calibrating the semi-empirical curve, the error of from the pre-factor can be cancelled as long as the same value of the pre-factor is used in the simulation with the one used in the calibration.
  ii. activation_energy: it is the activation energy of the corresponding reactions in the Arrhenius equation.
  iii. gas_constant: 8.314 J/(K mol)

- bulk_fluid_conditions: the dependence of the bulk concentrations in the Arrhenius equation, write down
  i. phase: the material phase of that field (i.e. if it is in the liquid phase then write 2)
  ii. order: the order of the reaction in that field according to the Arrhenius equation (for example, the reaction rate of chalcopyrite dissolution is $\kappa_{CuFeS_2} = 4\pi r^2 k e^{-Ea/RT}[H^+]^{0.8}[Fe^{3+}]^{0.42}$, write down 0.42 for the order of bulk_concentration(Fe3) and 0.8 for the bulk_concentration(H))

(b). reaction(S0_dissolution): elemental sulphur dissolution, $\kappa_{gangue} = \upsilon_{gangue} C_{H^+}$
- scalar(S0): the molar concentration of S0, (mole/m^3 heap)
- scalar_field(dS0_dt): change rate of the S0 concentration, (mole/m^3 heap/s)
- Dissolution_Algorithm(Non-bio_leaching): only the non-bioleaching algorithm is available, which linearly depends on the S0 formation from chalcopyrite dissolution,
  i. percentage_of_dissolve: which indicate the percentage of the S0 formed from chalcppyrite dissolution are dissolved, υ_{gangue} .

- o2_name: which is the scalar field name of the liquid oxygen in liquid phase.
- H_name: which is the scalar field name of H+ in liquid phase.

(c). reaction(Gangue_mineral_acid_dissolution): $\kappa_{S_0} = 2\upsilon_{S_0}\kappa_{CuFeS_2}$ for $\upsilon_{S_0} \in [0, 1]$
- scalar_field(dG_dt): change rate of the gangue mineral concentration, (mole/m^3 heap/s)
- rate_constant: the gangue mineral dissolution is assumed to be under linear rate, please specify the rate constant of dissolution, υ_{S_0}, (s^-1)
- H_name: which is the scalar field name of H+ in liquid phase.

(2). Solution phase reactions

(a). reaction(Ferrous_Oxidation)

- scalar_field(dFe2_dt): the oxidation rate of Fe2, (mole/m^3 heap/s)
- Dissolution_Algorithm(Non-bio_leaching): the reaction rate is calculated by empirical Arrhenius equation
  i. rate_constant_Arrhenius: it is the reaction rate constant calculated by the Arrhenius equation
  ii. scalar_field(prefactor): it is the prefacter k inside the Arrhenius equation
  iii. activation_energy: it is the activation energy of the corresponding reactions in the Arrhenius equation.
  iv. gas_constant: 8.314 J/(K mol)

- bulk_fluid_conditions: the dependence of the bulk concentrations in the Arrhenius equation, write down
  i. name: the corresponding scalar field name of the reactant that is in the Arrhenius equation (could be a name that is different from the name in the Arrhenius equation but it should be the same name given to the prognostic scalar field.)
  ii. phase: he material phase of that field (i.e. if it is in the liquid phase then write 2)
  iii. order: the reaction order of that reactant.

✓ Dissolution_Algorithm(bio_leaching): this is the bio-leaching algorithm for ferrous oxidation and it will be explained in a separate part below.

(b). reaction(Jarosite_Precipitation): the algorithm is based on Leahy and Schwarz (2009),
$\kappa_{jarosite} = \upsilon_{jarosite}\,[Fe^{3+}]$
if $\log_{10}(0.056[Fe^{3+}]) > -1.43pH + 0.87$

- scalar_field(dM_dt): precipitation rate of Fe3+ by jarosite (mole/ m^3 heap/s)
- scalar_field(molar_concentration): the current molar concentration of jarosite, (mol/ m^3 liquid solution)
- H_name: The scalar filed name for H+ in Phase 2 used to calculate pH
- Fe3_name: The scalar filed name for Fe3 in Phase 2 used to calculate jarosite precipitation
- rate_constant: The jarosite precipitation rate constant, which is a linear constant , $\upsilon_{jarosite}$

(c). reaction(Oxygen_dissolution): the equilibrium algorithm based on Tromans (1998)

- scalar_field(dOg_dt): the change rate of gas oxygen (mole/ m^3 of heap/s)
- scalar_field(molar_concentration): the current molar concentration of jarosite (mol/ m^3 liquid solution)
- og_name: The scalar filed name for gas phase oxygen in Phase 1
- o2_name: The scalar filed name for liquid phase oxygen in Phase 2

(3) heat transfer model

(a). single_phases_heat_transfer: only calculate the heat change of the liquid phase
(b). two_phases_heat_transfer: the heat generations by solution phase reactions are added to liquid phase temperature, while the heat generations by mineral dissolutions are added to rock temperature.

- scalar_field(Rock_Temperature): the rock temperature which is calculated by a conduction equation with the source terms from dissolution reactions and liquid-solid heat transfers. (unite: k)
- scalar_field(Rock_density): in kg/m^3
- scalar_field(Rock_Cp): heat capasity of the rock, kJ/kg/k

- heat transfer sources: the source terms of the rock temperature
  i. scalar_field(solid_liquid_heat_transfer_rock_phase), it is the heat transfer from the rock to liquid. $[-\Delta H = h_t a_t (T_r - T_l)]$, unite: (k/s)
     - scalar_field(K_eff_sl): effective heat transfer coefficient between solid and liquid, (kw/k/m^3), $h_t a_t$. Ether using a prescribed value OR diagnostic field by using an internal algorithm.
  ii. scalar_field(mineral_dissolution_heat_sources): unite is (k/s)*(m^3_rock/m^3_heap)
     - please SELECT the mineral dissolutions which can generate heat to the rock, and specify the enthalpy (KJ/mol) of each reaction

✓ If using the heat transfer model, please TURN ON the liquid temperature under phase 2, < /material_phase::Phase2/scalar_field::Temperature>
AND
TURN ON
</material_phase::Phase2/scalar_field::Temperature/prognostic/leaching_temperature_sources>

- scalar_field(Liquid_Cp): liquid heat capasity, kJ/Kg/K
- heat_transfer_sources:
  i. scalar_field(solid_liquid_heat_transfer_rock_phase), it is the heat transfer from the rock to liquid. k/s
  ii. scalar_field(solution_phase_heat_sources): unite is (k/s)*(m^3_liquid/m^3_heap)
     - please SELECT the solution phase reactions which can generate heat to the rock, and specify the enthalpy (KJ/mol) of each reaction

(4). **Liquid_solid_wetting_efficiency**: please TURN ON it IF using heat transfer model and semi-empirical model.

- scalar_field(Wetting_efficiency): it is the non-dimentional parameter. It is calculated by the algorithm from Al-Dahhan and Dudukovic (1995).

When using leaching chemical model, under EACH prognostic field of the solutes (including Og in phase 1):

(1). TURN ON < /material_phase::Phase2/scalar_field/prognostic/LeachingChemicalSourceTerm >

- According to the equations of chemical reactions, SELECT the corresponding solution phase or/and mineral dissolution reactions which can change the value of this scalar field. Write down the stoichiometric factor of this field in the reaction equation (positive if on the left hand side, negative if on the right hand side).

❖ **Bioleaching model for ferrous oxidation**:

(1). Under Phase 2, TURN ON the fields phi_l (now it supports 3 different phi_l, it could be extended to include more phi, and it is not necessary to turn on all of the phi), phi_l is φ_i in the bioleaching model.

(2). TURN ON < /Leaching_chemical_model/SolutionPhaseReactions/reaction::Ferrous_Oxidation/Dissolution_Algorithm::bio_leaching >

(a). TURN ON the corresponding scalar_field(phi_l) under the bio_leaching algorithm, (e.g, phi_l2 under the phase 2, then turn on phi_l2 under the bio_leaching model)

(b). TURN ON the corresponding scalar_field(miu) under the bio_leaching algorithm, (e.g,

phi_l2 under the phase 2, then turn on miu2 under the bio_leaching model) , miu is μ in the model.

i. k1: rate constant of attachment
ii. k2: rate constant of detachment
iii. k_death: death rate constant
iv. phi_max: Ψ_{max}
v. miu_max: μ_{max}
vi. T_shift: $T_{shift,i} = T_{optimal,i} - T_{optimal,1}$

(c). Y: yield coefficient
(d). kmo: Monod parameter for oxygen
(e). kmfe2: Monod parameter for ferrous ions
(f). ferrous_name: the name of the scalar field of Fe2 in liquid phase
(g). oxygen_name: the name of the scalar field liquid phase oxygen