Documentation: data input

Compute lambdas	Read lambdas
"_discr_temp.dat"	"_WMA_discr.dat"
"_discr_esp.dat"	"_WMA_lambdas.dat"
"_tpt_props.dat"	
"_BCs.dat"	
"_flux_inflow.dat" *	
"_sist_quim.dat"	
"_quim_loc.dat"	
"_tar_wat.dat"	
"_out_options.dat"	
"_chem_opts.dat"	

* Only if the flux is non uniform.

- **"_WMA_discr.dat":** This file contains the time discretisation for the WMA.
  - **Class:** 1D transient reactive transport
  - **Line 1**: Name of the problem
  - **Line 2**: Section separation
  - **Line 3**: Section name
  - **Line 4**: *Num_time* (integer)
    - Number of time steps
  - **Line 5**: *Delta_t* (real)
    - Time step
    - Note: If discretization is not uniform, you must write the array of time steps on the same line
  - **Line 6**: *int_method* (integer)
    - Time integration method:
      1. Euler explicit
      2. Euler fully implicit
      3. Crank-Nicolson
  - **Line 7**: end of section

```
'TITLE OF THE PROBLEM: Gypsum in equilibrium'
'-------------------------------------------------------------------------------------------------------------'
'TIME'
10              ! number of time steps
1d1             ! time step ( we assume uniform time discretisation )   Δt
1               ! time integration method for chemical reactions
'*'
'-------------------------------------------------------------------------------------------------------------'
'end'
```

- **"_WMA_lambdas.dat"**: This file contains the mixing ratios and their associated target waters to apply the WMA.
    - **Class:** Transient 1D transport
    - **Line 1**: Name of the problem
    - **Line 2**: Section separation
    - Section name: 'MIXING RATIOS'
    - **Lines 1-nº mixing waters:** *num_mix_ratios* (integer), *mixing_ratios* (real vector)
        - *num_mix_ratios*: number of mixing ratios in each target
        - *mixing_ratios*: mixing ratios in each target (contains sink/sources and boundary terms)
    - **Line nº mixing waters+1**: end of mixing ratios pseudomatrix
    - **Line nº mixing waters+2**: end of section
    - section separation
    - Section name: 'MIXING WATERS'
    - **Lines 1-nº mixing waters**: *ind_tar_wat* (integer), *mix_wat_indices* (integer vector)
        - *ind_tar_wat*: index of target water
        - *mix_wat_indices*: indices of target waters associated to each mixing ratio
    - **Line nº mixing waters+1**: end of section
    - end of file

'TITLE OF THE PROBLEM: Gypsum in equilibrium'

'----------'

'MIXING RATIOS' ! in each line: number of mixing ratios, mixing ratios at each target (including sink/sources and boundary terms)

1 1.00000E+00

3 9.20000E-01 4.20000E-02 3.80000E-02

3 9.20000E-01 4.20000E-02 3.80000E-02

3 9.20000E-01 4.20000E-02 3.80000E-02

3 9.20000E-01 4.20000E-02 3.80000E-02

3 9.20000E-01 4.20000E-02 3.80000E-02

3 9.20000E-01 4.20000E-02 3.80000E-02

3 9.20000E-01 4.20000E-02 3.80000E-02

3 9.20000E-01 4.20000E-02 3.80000E-02

3 9.20000E-01 4.20000E-02 3.80000E-02

1 1.00000E+00

0 ! indicates the end of the mixing ratios pseudomatrix

'*'

$$\lambda_{ij}$$

'----------'

'MIXING WATERS' ! target water index, water indices in 'MIXING RATIOS'

1	1		
2	2	1	3
3	3	2	4
4	4	3	5
5	5	4	6
6	6	5	7
7	7	6	8
8	8	7	9
9	9	8	10
10	10	9	11
11	11		

$$\mathbf{c}_i^{k+1} = \sum_{j \in I_i} \lambda_{ij} \mathbf{c}_j^k$$

$$I_1, I_2, I_3, \ldots$$

'----------'

'end'

- **"_sist_quim.dat":** This file contains the information related to the chemical system (species, reactions, etc)
    - **Class:** Chemical system
    - **Line 1**: Name of the problem
    - **Line 2**: Section separation
    - **Line 3**: Section name
        - If Section name = 'PRIMARY AQUEOUS SPECIES' or 'AQUEOUS COMPLEXES':
            0. **Line 3a**: *sp_name* (string)
                - Name of species in database **"master25_modif.dat"**
            1. **Line 3b**: end of section
        - If Section name = 'MINERALS' or 'GASES':
            0. **Line 3a**: *sp_name* (string), *flag_eq* (logical), *flag_cst_act* (logical)
                - *sp_name:* Name of species in database **"master25_modif.dat"**
                - *flag_eq*: TRUE if equilibrium reaction, FALSE otherwise
                - *flag_cst_act*: TRUE if species has constant activity, FALSE otherwise
            1. **Line 3b**: end of section
        - If Section name = 'REDOX REACTIONS':
            0. **Line 3a**: *react_name* (string), *flag_eq* (logical)
                - *react_name:* Name of redox reaction in database **"reacciones_monod_JW.dat"**
                - *flag_eq*: TRUE if equilibrium reaction, FALSE otherwise
            1. **Line 3b**: end of section
        - If Section name = 'SURFACE COMPLEXES':
            0. **Line 3a**: *sp_name* (string)
                - *sp_name:* Name of species in database **"master25_modif.dat"**
            1. **Line 3b**: end of section
    - **Line 4**: end of section
    - **Line 5**: end of file

```
'TITLE OF THE PROBLEM: Gypsum in equilibrium'

'-----------------------------------------------------------------------------------------------------------------------------------------------------------'

'PRIMARY AQUEOUS SPECIES'

'h2o(p)'                                                    ! name of primary aqueous species

'ca+2'

'so4-2'

'*'

'MINERALS'

'gypsum' .true. .true.                                      ! name of mineral, flag equilibrium, flag constant activity

'*' .true. .true.

'GASES'

'co2(g)'  .true. .true.                                     ! name of gas, flag equilibrium, flag constant activity

'o2(g)'  .true. .true.                                  ! name of gas, flag equilibrium, flag constant activity

'*'  .true. .true.

'-----------------------------------------------------------------------------------------------------------------------------------------------------------'

'end'
```

- **"_quim_loc.dat"**: This file contains the **local** chemical information (water types, mineral zones, gas zones)
    - **Class:** Chemistry
    - **Line 1**: Name of the problem
    - **Line 2**: Section separation
    - Section name: 'INITIAL AND BOUNDARY WATER TYPES'
    - **Line 1**: *act_coeffs_model* (integer)
        0. Ideal
        1. Debye-Hückel
        2. Debye-Hückel extended
        3. Davies
        4. Truesdell-Jones
    - **Line 2**: *num_wat_types* (integer)
        0. Number of water types (include initial, recharge, boundary etc)
    - **Line 3**: *ind_wat_type* (integer), *temp* (real)
        - *ind_wat_type*: index of water type
        - *temp*: temperature of solution
    - **Line 3a**: *name* (string)
        - Name of water type
    - **Line 3b**: water type data begins
        - *Icon*: initial condition type
            1. prescribed primary concentration
            2. prescribed total concentration
            3. prescribed activity
            4. primary species is in equilibrium with a phase
        - *Guess*: Initial guess for primary species concentration
        - *Ctot*: (all concentrations are expressed in molalities)
            0. *Icon=1*: primary species concentration
            1. *Icon=2*: total concentration of primary species
            2. *Icon=3*: activity of primary species
            3. *Icon=4*: activity of phase that is in equilibrium with this primary species
        - *Constrain*: if *icon=4*, it is the phase in equilibrium with the primary species
    - **Line 3c:** *prim_sp_name* (string), *icon* (integer), *guess* (real), *ctot* (real), *constrain* (string)
    - **Line 3d**: end of water type data
    - **Line 4**: end of section

```
'TITLE OF THE PROBLEM: Gypsum in equilibrium'
'-------------------------------------------------------------------------------------------------------------------------------------------------------------'
'INITIAL AND BOUNDARY WATER TYPES'
0                                                    ! activity coefficients model
2                                                    ! number of water types
1    25.0                                            ! index water type, temperature (C)
'boundary'                                           ! name of water type
'     icon      guess      ctot       constrain'
'h2o(p)'    3          1d0     1d0              ''
'ca+2'     1       1d-3     1d-3             ''
'so4-2'    4          1d-5          1d0          'gypsum'
'*'     0       0.0        0.0         ' '
2    25.0                                            ! index water type, temperature (C)
'initial'                                            ! name of water type
'     icon      guess      ctot       constrain'
'h2o(p)'    3          1d0     1d0              ''
'ca+2'     1       1d-5     1d-5             ''
'so4-2'    4          1d-5          1d0          'gypsum'
'*'     0       0.0        0.0         ' '
'-------------------------------------------------------------------------------------------------------------------------------------------------------------'
```

- **"_quim_loc.dat":**
  - Section name: 'INITIAL MINERAL ZONES'
  - **Line 1**: *num_min_zones* (integer)
    - Number of mineral zones
  - **Line 2a**: *ind_min_zone* (integer), *temp* (real)
    - *ind_min_zone*: index of mineral zone
    - *temp*: temperature of mineral zone
  - **Line 2b**: *name* (string)
    - Name of initial mineral zone
  - **Line 2c**: mineral zone data begins
  - **Line 2d**: *min _name* (string), *vol_frac* (real), *react_surf* (real)
    - *min_name*: name of mineral in mineral zone (must be in the chemical system)
    - *vol_frac.:* initial volumetric fraction of mineral
    - *react_surf*: specific surface of mineral (surface of mineral per unit volume of medium)
  - **Line 2e**: end of block
  - **Line 3**: end of section

```
'INITIAL MINERAL ZONES'

1                                                    ! number of mineral zones

1        25.0                                        ! index of mineral zone, temp (C)

'gypsum'                                             ! name of mineral zone

'mineral       vol.frac.   area'

'gypsum'        0.50       0.1d+3

'*'            0.00        0.00

'-------------------------------------------------------------------------------------------------------------------------------------------------------'
```

- **"_quim_loc.dat":**
  - Section name: 'INITIAL AND BOUNDARY GAS ZONES'
  - **Line 1**: *num_gas_zones* (integer)
    - Number of gas zones
  - **Line 2a**: *ind_gas_zone* (integer), *temp* (real), *vol* (real)
    - *ind_gas_zone*: index of gas zone
    - *temp*: temperature of gas zone
    - *vol*: total volume of gas
  - **Line 2b**: gas zone data begins
  - **Line 2c**: *name* (string)
    - Name of gas zone
  - **Line 2d**: *gas _name* (string), *part_press* (real)
    - *gas_name*: name of gas in gas zone (must be in the chemical system)
    - *part_press:* initial partial pressure (equivalent to activity) of gas
  - **Line 2e**: end of block
  - **Line 3**: end of section
  - **Line 4**: end of file

```
'INITIAL AND BOUNDARY GAS ZONES'
1                                                    ! number of gas zones
1       25      1d9                                  ! index gas zone, temp (ºC), volume
'atmosphere'                                         ! name of gas zone
'gas                    partial pressure'            ! pressure (in atm)
'co2(g)'                    3.5d-4
'o2(g)'                     2d-1
'*'                         0.00
'-------------------------------------------------------------------------------------------------------------------------------------------'
'end'
```

- **"_tar_wat.dat":** This file contains the **association** between target waters, target solids and/or target gases, and it also indicates if the target waters belong to the domain or not.
    - **Class: Chemistry**
    - **Line 1**: Name of the problem
    - **Line 2**: Section separation
    - Section name: 'TARGET WATERS'
    - **Line 1**: *num_tar_wat* (integer)
        - Number of target waters
    - **Line 2**: *num_ext_wat* (integer)
        - Number of external target waters
    - **Lines 3 - *num_tar_wat*+2**: *ind_tar_wat* (integer), *iwtype* (integer), *ind_min_zone* (integer), *ind_gas_zone(*integer), *flag_wat_type*(logical)*
        - *ind_tar_wat*: Index target water
        - *iwtype*: Index water type in section 'INITIAL AND BOUNDARY WATER TYPES'
        - *ind_min_zone*: Index mineral zone in section 'INITIAL MINERAL ZONES'
        - *ind_gas_zone*: Index gas zone in section 'INITIAL AND BOUNDARY GAS ZONES'
        - *flag_wat_type:* Flag to indicate target water type. **Optional** variable.
            - 0: Boundary
            - 1: Domain
            - 2: Recharge
    - end of section

* Only if there are external and/or boundary waters

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'TITLE OF THE PROBLEM: Gypsum in equilibrium'

'-----------------------------------------------------------------------------------------------------------------------------------------------------------'

'TARGET WATERS'

11                                          ! number of target waters

0                                           ! number of recharge target waters

2                                           ! number of boundary target waters

1       1       1       0       0       ! target water index, water type index, mineral zone index, gas zone index, flag water type

2       2       1       0       1

3       2       1       0       1

4       2       1       0       1

5       2       1       0       1

6       2       1       0       1

7       2       1       0       1

8       2       1       0       1

9       2       1       0       1

10      2       1       0       1

11      2       1       0       0

'-----------------------------------------------------------------------------------------------------------------------------------------------------------'

'end'
```

- **"_out_options.dat":** This file contains the **variables** whose values will be **written** during the simulation.
    - **Type:** Chem_out_options
    - **Line 1**: Name of the problem
    - **Line 2**: Section separation
    - Section 'TIME STEPS':
        - **Line 1**: *nits* (integer)
            - Nº intermediate time steps
            - If *nits* = 0: only initial and final waters are considered for output
            - If *nits* = -1: all intermediate time steps considered
        - **Line 2**: *inter_time_steps* (integer array)
            - Intermediate time steps
            - If *nits* < 1: skip line
            - Else: must have dimension = *nits*
    - Section 'TARGET WATERS':
        - **Line 1**: *notw* (integer)
            - Nº output target waters
            - If *notw* = 0: all target waters considered
        - **Line 2**: *tar_wat* (integer array)
            - target waters
            - If *notw* = 0: skip line
            - Else: must have dimension = *notw*
    - Section 'VARIABLES':
        - **Line 1**: *var* (string)
            - name of variable that will be included in output file
            - if *var*='all': all of them will be written
            - if *var*='conc': concentrations
            - if *var*='act': activities
            - if *var*='react_rate': reaction rates
            - if *var*='vol_frac': volumetric fractions of minerals
    - Section 'AQUEOUS SPECIES':
        - **Line 1**: *aq_sp_name* (string)
            - Name of aqueous species that will be included in output file
            - If *aq_sp_name*='all': all aqueous species included
    - Section 'MINERALS':
        - **Line 1**: *min_name* (string)
            - Name of minerals that will be included in output file
            - If *min_name*='all': all minerals included
    - Section 'REACTIONS':
        - **Line 1**: *react_name* (string)
            - Name of reaction that will be included in output file
            - If *react_name*='all': all reactions included

```
'TITLE OF THE PROBLEM: Gypsum in equilibrium'
'-------------------------------------------------------------------------------------------------------------------------------------------'
'TIME STEPS'
2                              ! number of intermediate output time steps
1 5                            ! intermediate time steps for output file
'-------------------------------------------------------------------------------------------------------------------------------------------'
'TARGET WATERS'
6                              ! number of output target waters
1 3 5 7 9 11                   ! target waters for output file
'-------------------------------------------------------------------------------------------------------------------------------------------'
'VARIABLES'                    ! names of variables that will be written in output file
'conc'
'react_rate'
'vol_frac'
'*'
'-------------------------------------------------------------------------------------------------------------------------------------------'
'AQUEOUS SPECIES'              ! names of aqueous species that will be considered in output file
'all'
'*'
'-------------------------------------------------------------------------------------------------------------------------------------------'
'MINERALS'                     ! names of minerals that will be considered in output file
'all'
'*'
'-------------------------------------------------------------------------------------------------------------------------------------------'
'REACTIONS'                    ! names of reactions that will be considered in output file
'gypsum'
'*'
'-------------------------------------------------------------------------------------------------------------------------------------------'
'end'
```

- **"_chem_opts.dat"**: This file contains the different **options** to **solve** reactive mixing with the **WMA**.
    - **Class**: **Chemistry**
    - **Line 1**: Name of the problem
    - **Line 2**: Section separation
    - **Line 3**: Section name
    - **Line 4**: *opt* (integer)
        - Chemical input data option
    - **Line 5**: *opt* (integer)
        - Jacobian option
    - **Line 6**: *flag* (logical)
        - Lumping flag
    - **Line 7**: *opt* (integer)
        - Consistent WMA option
    - **Line 8**: *opt* (integer)
        - Estimation of downstream waters kinetic reaction amounts option
    - **Line 9**: *opt* (integer)
        - Time weighting kinetic reaction rates option
    - **Line 10**: end of section

```
'TITLE OF THE PROBLEM: Gypsum in equilibrium'
'-------------------------------------------------------------------------------------------------------------------------------------------'
'CHEMICAL OPTIONS'
1                       ! Chemical input data option (1: CHEPROO-based, 2: PHREEQC, 3: PFLOTRAN)
1                       ! Option to compute Jacobians (0: incremental coefficients, 1: analytically)
.true.                  ! Lumping flag
2                       ! Consistent WMA option (1: explicit, 2: upstream to downstream)
1                       ! Estimation of downstream waters rk (4 options, see documentation for details)
2                       ! Time weighting rk option (1: concentrations, 2: reaction rates)
'-------------------------------------------------------------------------------------------------------------------------------------------'
'end'
```