Documentation: data input

- **Transient 1D reactive transport class**:
  - **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'
```

- **Transient 1D transport class**:
  - **Line 1**: Name of the problem
  - **Line 2**: Section separation
  - **Line 3**: Section name
  - **Line 4**: *Flag_porosity* (logical), *porosity* (real scalar or vector)
    - *Flag_porosity*=true*:* porosity is homogenous
    - *Flag_porosity*=false: porosity is heterogeneous (in this case you must write the porosities in the same line)
  - **Line 5**: end of section
  - **Line 6**: Section separation
  - **Line 7**: Section name
  - **Line 8**: *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 9**: end of mixing ratios pseudomatrix
  - **Line 10**: end of section
  - **Line 11**: section separation
  - **Line 12**: name of section
  - **Line 13**: *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 14**: end of section
  - **Line 15**: end of file

'TITLE OF THE PROBLEM: Gypsum in equilibrium'

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

'TRANSPORT PROPERTIES'

.true. 5d-1 ! in this line: flag for homogeneous property, porosity ϕ

'*'

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

'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

λ_{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'

- **Chemical system class:**
  - **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.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'                                   ! name of primary aqueous species
'ca+2'
'so4-2'
'*'
'AQUEOUS COMPLEXES'
'*'                                     ! name of aqueous complex
'MINERALS'
'gypsum' .true. .true.                  ! name of mineral, flag equilibrium, flag constant activity
'*' .true. .true.
'GASES'
'*'  .true. .true.                      ! name of gas, flag equilibrium, flag constant activity
'SURFACE COMPLEXES'
'*'                                     ! name of surface complex
'-----------------------------------------------------------------------------------------------------------------------------------------------------------------------'
'end'
```

- **Aqueous chemistry class**:
  - **Line 1**: Name of the problem
  - **Line 2**: Section separation
  - **Line 3**: Section name: 'INITIAL AND BOUNDARY WATER TYPES'
  - **Line 4**: *act_coeffs_model* (integer)
    0. Ideal
    1. Debye-Hückel
    2. Debye-Hückel extended
    3. Davies
    4. Truesdell-Jones
  - **Line 5**: *num_wat_types* (integer)
    0. Number of water types (include initial, recharge, boundary etc)
  - **Line 6**: *ind_wat_type* (integer), *temp* (real)
    - *ind_wat_type*: index of water type
    - *temp*: temperature of solution
  - **Line 6a**: *name* (string)
    - **Name of water type**
  - **Line 6b**: 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*:
      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 6c:** *prim_sp_name* (string), *icon* (integer), *guess* (real), *ctot* (real), *constrain* (string)
  - **Line 6d**: end of water type data
  - **Line 7**: 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, temp (C)
'boundary'                                           ! name of water type
'     icon      guess      ctot       constrain'
'h2o'       1          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, temp (C)
'initial'                                            ! name of water type
'     icon      guess      ctot       constrain'
'h2o'       1          1d0     1d0              ''
'ca+2'     1       1d-5     1d-5             ''
'so4-2'   4           1d-5          1d0          'gypsum'
'*'     0       0.0        0.0         ' '
'-------------------------------------------------------------------------------------------------------------------------------------------------------------------'
```

- **Solid chemistry class**:
  - **Line 1**: Section name: 'INITIAL MINERAL ZONES'
  - **Line 2**: *num_min_zones* (integer)
    - Number of mineral zones
  - **Line 3a**: *ind_min_zone* (integer), *temp* (real)
    - *ind_min_zone*: index of mineral zone
    - *temp*: temperature of mineral zone
  - **Line 3b**: mineral zone data begins
  - **Line 3c**: *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 area
  - **Line 3d**: end of block
  - **Line 4**: end of section

```
'INITIAL MINERAL ZONES'

1                                                    ! number of mineral zones

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

'mineral      vol.frac.   area(m2/m3rock)'

'gypsum'      0.50      0.1d+3

'*'           0.00      0.00

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

- **Gas chemistry class**:
  - **Line 1**: Section name: 'INITIAL GAS ZONES'
  - **Line 2**: *num_gas_zones* (integer)
    - Number of gas zones
  - **Line 3a**: *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 3b**: gas zone data begins
  - **Line 3c**: *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 3d**: end of block
  - **Line 4**: end of section
  - **Line 5**: end of file

```
'INITIAL GAS ZONES'

1                                                    ! number of initial gas zones

1          25          1d0                           ! index gas type, temp (ºC), volume

'gas                          partial pressure'      ! pressure in atm

'co2(g)'                          3.5d-4

'o2(g)'                           2d-1

'n2(g)'                           7.99965d-1

'*'                               0.00

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

'end'
```

- **Chemistry class**:
  - **Line 3**: Section name: 'TARGET WATERS'
  - **Line 4**: *num_tar_wat* (integer)
    - Number of target waters
  - **Line 5**: Subsection name: 'external waters'
  - **Line 5a**: *num_ext_wat* (integer)
    - Number of external target waters
  - **Line 5b**: *ind_tar_wat* (integer), *iwtype* (integer)
    - *ind_tar_wat*: Index target water
    - *iwtype*: Index water type
  - **Line 6**: Subsection name: 'domain waters'
  - **Line 6a**: *ind_tar_wat* (integer), *iwtype* (integer), *ind_sol_zone* (integer), *ind_gas_zone* (integer)
    - *ind_tar_wat*: Index target water
    - *iwtype*: Index water type
    - *ind_sol_zone*: Index solid zone
    - *ind_gas_zone*: Index gas zone
  - **Line 7**: end of section

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

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

'TARGET WATERS'

11                                      ! number of target waters

'external waters'

1                                       ! number of external target waters (recharge, boundary, etc)

1       1                               ! target water index, water type index

'domain waters'

2       2       1       0               ! target water index, water type index, solid zone index, gas zone index

3       2       1       0

4       2       1       0

5       2       1       0

6       2       1       0

7       2       1       0

8       2       1       0

9       2       1       0

10      2       1       0

11      2       1       0

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

'end'
```

- **Chem_out_options type**:
  - 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 targets
1 3 5 7 9 11               ! targets 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'
```