## 1 Equilibrating two reservoirs

Two reservoirs which are connected via forward and backward fluxes will equilibrate their concentrations (and thus their isotope ratios). The equilibrium depends on the actual concentration plus any optional equilibrium constants.

We can model this situation by creating two explicit fluxes between two reservoirs, which mimics the actual nature of exchange fluxes. However, we can also express the flux balance between both fluxes, and only compute the difference. The latter approach is more succinct. ESBMTK implements this case with the flux\_balance connection type, takes three parameters

- left is a list which can contain constants and/or reservoirs. The list must contain at least one valid element. All elements in this list will be multiplied with each other. E.g. if we have a list with one constant and one reservoir, the reservoir concentration will be multiplied with the constant. If we have two reservoirs, the respective reservoir concentrations will be multiplied with each other.
- right similar to left The final flux rate will be computed as the difference between left and right
- k\_value a constant which will be multiplied with the difference between left=and =right

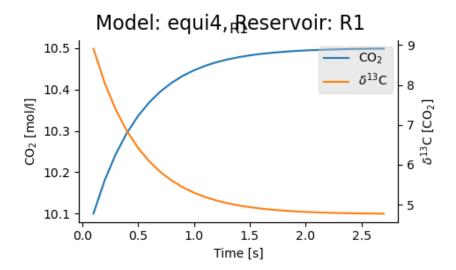
Here a simple example.

```
from esbmtk import Model, Reservoir, Signal
   from esbmtk import Connect, Source, Sink
   volume = "1 liter"
5
   # create model
6
   Model(
7
       name="equi4", # model name
8
        stop="3 s",
                       # end time of model
9
       timestep="0.1 s",
10
                                     # time step
        element=["Carbon"], # initialize carbon species
11
       mass_unit="mol",
12
       volume_unit="1",
13
```

```
14 )
15
  Reservoir(
16
       name="R1",
                   # Name of reservoir
17
       species=CO2,
                              # Species handle
18
19
       delta=10,
                               # initial delta
       concentration=f"10 mol/l", # concentration
20
       volume=volume, # reservoir size (m^3)
21
22 )
23
24 Reservoir(
       name="R2",
25
                   # Name of reservoir
       species=CO2,
                       # Species handle
26
       delta=0,
                              # initial delta
27
       concentration=f"11 mol/l", # concentration
28
       volume=volume, # reservoir size (m^3)
29
  )
30
31
  Connect(
32
       source=R1, # target of flux
33
       sink=R2, # source of flux
       rate="1 mol/s",
                              # flux rate
35
       ctype="flux_balance",
36
       k_value=1,
37
       left=[R1],
38
       right=[R2],
39
                              # isotope fractionation
40
       #alpha=0,
       plot="no",
41
  )
42
43
44
45 # Run the model
46 equi4.run()
48 # plot the results
49 equi4.plot_data()
```

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Execution took 0.0010554550000003715 seconds



<Figure size 500x300 with 2 Axes>

