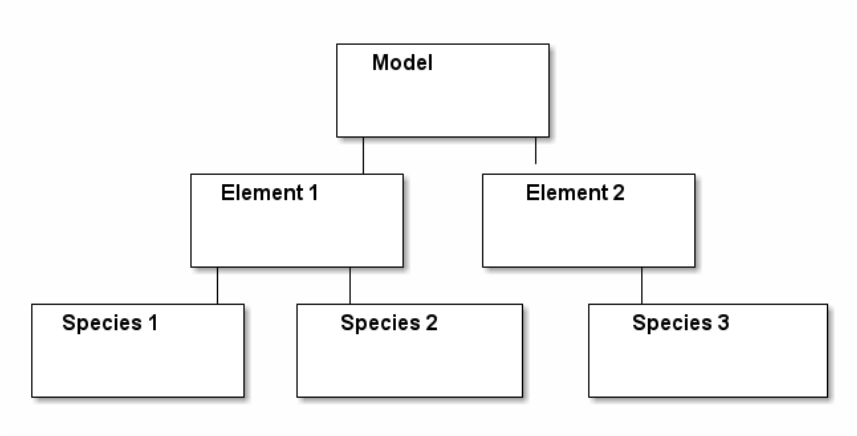
1 Overview

Please note that the current code is under rapid development, and that this quick-start guide is not in sync. While the principle has not changed, the syntax shown below will not work without producing errors. An updated guide will be published once the API is stable.

ESBMTK provides a couple of classes which are used to define a model. The classes are arranged in a hierarchical manner, starting with the model class. The model class (or object), set's global parameters like the model name, the time step etc. Next comes one or more element objects which define basic element properties. Each element can have one or more species. Note that these classes specify units, however at present, there is incomplete support for unit conversions. So it is up to the author to ensure proper unit conversions. It is therefore best, to use the same units throughout.

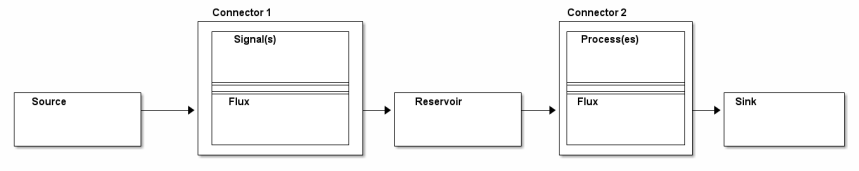


At present, these classes only specify the isotopic reference ratios, and plot labels.

Next comes the source and sink class, which simply specify the name and species, followed by reservoir object which specifies things like reservoir name, reservoir size, reservoir species etc. Each reservoir can only have one element. This is counter intuitive since we would think of the ocean as single reservoir with many elements. However, the model only attempts to track the transfer of mass between reservoirs, for a given element. For multi element models, you need to setup reservoirs and connections for each element.

Sources, sinks, and reservoirs are connected through fluxes, and fluxes are either forced by signals, or affected by processes. Most processes can be derived implicitly from the way we connect reservoirs (see below), however signal must be specified explicitly. It is thus best to define these first (see the worked example below).

The connection between a source and a sink (or two reservoirs) is handled by the connection class. This class will create the necessary fluxes, and where possible add processes. Fluxes and processes are also implemented as objects.

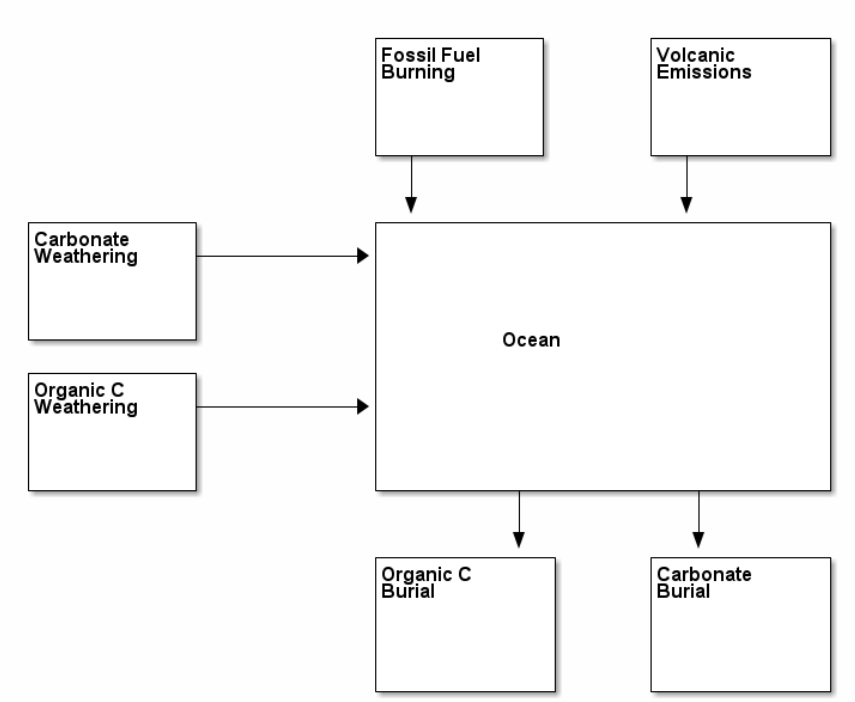


Each connector object can have more than one signal or process (or a mixture of signals and processes). Each reservoir can have more than one connector object.

1.1 A worked example

In the following example we will set up a simple carbon cycle model. The data forcing the anthropogenic carbon flux will be read from a csv file. Interaction with external data is handled through the external data object which allows to integrate external data into the model framework. It can then be used to generate a signal, or it can be associated with a reservoir so that the data is plotted with the reservoir data.

The model consists of four sources, two sinks, and one reservoir



1.2 Setting up the model

We need to load all required libraries and all classes we want to use. Interaction with the model classes is done through keyword/value pairs. Use `help()` to inquire about the supported keyword value pairs.

ESBMTK is unit aware. The units are used to map all input data to internal units. The type of internal units needs to specified when creating the model object. The time unit is derived from the timestep variable. I.e., if the timestep is given in seconds, all other time related input will be mapped to seconds. Similarly you have to define the base mass unit. Typically, this will be moles, but other units like grams etc can also be used. At present ESBMTK cannot convert between different types of mass units (e.g., kg to moles). The usual prefixes like kilo, mega, milli etc are recognized. Volume units like `l` or `m**3` are recognized as well. ESBMTK also defines the sverdrup ("Sv")

Once the input units are mapped to base units specified by the model object, all data will be reported in the base units. The only exception is the

`object.plot()` method which will transform the data back into the original unit. In other words, if your timestep is in years, but you specify your endtime in kyrs, the time axis will be plotted in kyrs. Similarly for all other data, with the exception of the isotope delta values.

```
from esbmtk import Model, Element, Species, Reservoir
from esbmtk import Signal, Connect, Source, Sink, Flux
from esbmtk import ExternalData

# create model
Model(
    name="C_Cycle",      # model name
    stop="200 yrs",      # end time of model
    timestep=" 1 yr",    # time unit
    mass_unit = "mol",   # mass unit
    volume_unit = "l",   # volume unit
    m_type = "both",      # calculate mass and isotopes
)
```

Note that per default, ESBMTK will ignore isotope calculations. You need to set `m_type = 'both'` to enable isotope calculations.

1.3 Declare elements and species

We register the elements(s) with the model by providing the model name. Note that this is not a string, but the model handle which is derived from the model name in the model definition above. We use the element handle in a similar way to register the species with an element.

```
# Element properties
Element(
    name="C",                   # Element Name
    model=C_Cycle,              # Model handle
    mass_unit="mmol",           # base mass unit
    li_label="C^{12$S",         # Name of light isotope
    hi_label="C^{13}$S",        # Name of heavy isotope
    d_label="$\delta^{13}$C",       # Name of isotope delta
    d_scale="VPDB",             # Isotope scale. End of plot labels
    r=0.0112372,  # VPDB C13/C12 ratio https://www-pub.iaea.org/MTCD/publications/PDF/te_825_
)
```

```
12
13 # add species
14 Species(name="CO2", element=C)  # Name & element handle
15 Species(name="DIC", element=C)
16 Species(name="OM", element=C)
17 Species(name="CaCO3", element=C)
```

You can do this explicitly as in the example above, or use the builtin definition by providing the element keyword in the model definition. This keyword takes and element name, and causes the model to initialize an `Element` object and a variety of `Species` objects. At present ESBMT contains definitions for "Carbon" and "Sulfur" which will create the element objects `C` and `S` respectively. You can query which species are known to an element by calling the `list_species` method, e.g., `C.list_species()`

You can initialize more than one element by providing a list as argument (i.e., `["Sulfur", "Carbon"]`). In other words, you can replace the above code block by adding `=element = "Carbon"` to the model parameters.

1.4 Using external data to initialize a signal

We can use an external csv file to create a signal. The first column contains the time coordinates, the second the flux rate, and the third the delta value of the flux. The first row must contain a header, and the header must contain a variable name followed by a unit:

Age [kyr]	Volcanic Flux [mol/s]	δ^{13}C [permille]
0	20	0
1	30	2

Note that the unit must be specified inside square brackets. All values will be mapped into the model units and interpolated to fit the model time resolution.

Signals can also by created by specifying a signal type. At present the class understands, square, and pyramidal signal forms, as well as repetition. Signal can be added to each other (i.e., you can specify a signal which effects the flux, and then add another signal which effects the isotope ratio).

```
1 Signal(name = "ACR",              # Signal name
2        species = CO2,             # Species
```

```
        filename = "test-data.csv" # filename
)
```

Once a signal instance has been created, it can be passed to a connector object in order to associate it with a flux (see the first connection below as an example).

1.5 Sources, Sinks and Reservoirs

The fundamental model object is the reservoir. Reservoirs are connected to each other by one or more fluxes. Fluxes are created implicitly by connecting two reservoirs.

Connecting a reservoir with a Source or Sink also creates a flux, but unlike reservoirs, sources and sinks do not have any associated data. They are merely there to allow the creation of a flux.

```
Source(name="Fossil_Fuel_Burning", species=CO2)
Source(name="Carbonate_Weathering", species=CO2)
Source(name="Organic_Weathering", species=CO2)
Source(name="Volcanic", species=CO2)
Sink(name="Carbonate_burial", species=CaCO3)
Sink(name="OM_burial", species=OM)

Reservoir(
    name="Ocean",                # Name of reservoir
    species=DIC,                 # Species handle
    delta=2,                     # initial delta
    concentration="2.62 mmol/l", # cocentration
    volume="1.332E18 m**3",      # reservoir size (m^3)
)
```

1.6 Connecting sources, reservoirs and sinks

Now that all model elements are specified, we can connect everything. The first statement below, connects the source `Fossil_Fuel_Burning` with the reservoir `Ocean`. This will create a flux with the name `Fossil_Fuel_-Burning_to_Ocean`. The rate and delta keywords indicate that this flux will be zero. However, we provide `pl = [ACR]` which is the carbon flux data which we imported via the signal object above. This data will be added to

the `Fossil_Fuel_Burning_to_Ocean` flux (since the process is additive, the initial flux has to be zero!)

The type of flux depends on how we specify the connection. In the previous example we provided a signal, so the flux will change with time according to the signal data. If you look at the connection between `Carbonate_Weathering` and `Ocean` below, we specify a given rate and delta value. So this flux will not change over time. If you look at the connection between `Ocean` and `OM_burial` the connection specifies a constant flux but with an `alpha = -26.3`. This indicates that this flux involves a fixed isotope offset relative to the upstream reservoir, i.e., the isotope ratio of this flux will change dynamically in response to the isotope ratio of the reservoir, but with a constant offset. See below for a full list of connection options.

Fluxes can be circular, care must however be taken in which sequence they are defined, since the solver computes each flux and reservoir in the order they are initialized (see the Examples directory for a more complete example).

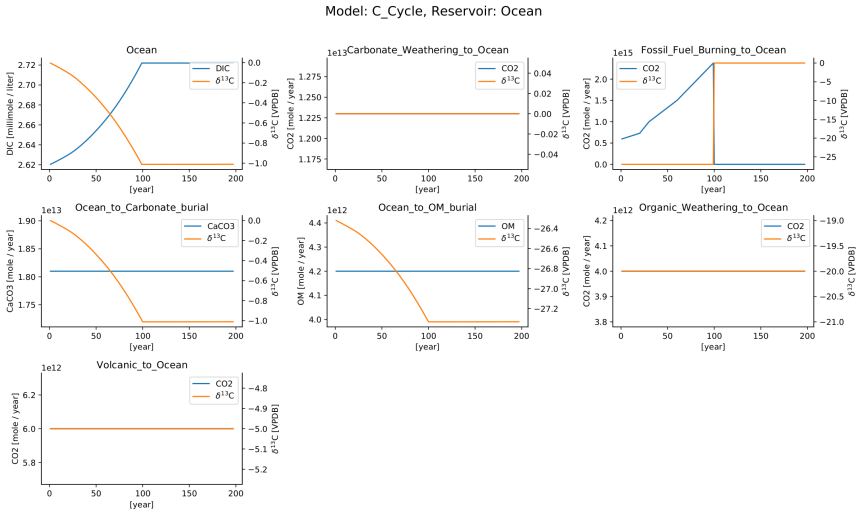
```
# connect source to reservoir
Connect(
    source=Fossil_Fuel_Burning,  # source of flux
    sink=Ocean,                  # target of flux
    rate="0 mol/yr",             # weathering flux in
    delta=0,                     # set a default flux
    pl=[ACR],                    # process list, here the anthropogenic carbon release
)

Connect(
    source=Carbonate_Weathering,  # source of flux
    sink=Ocean,                   # target of flux
    rate="12.3E12 mol/yr",        # weathering flux in
    delta=0,                      # isotope ratio
)

Connect(
    source=Organic_Weathering,  # source of flux
    sink=Ocean,                 # target of flux
    rate="4.0E12 mol/yr",       # flux rate
    delta=-20,                  # isotope ratio
)

Connect(
```

```
    source=Volcanic,       # source of flux
    sink=Ocean,            # target of flux
    rate="6.0E12 mol/yr", # flux rate
    delta=-5,              # isotope ratio
)

Connect(
    source=Ocean,          # source of flux
    sink=OM_burial,        # target of flux
    rate="4.2E12 mol/yr",  # burial rate
    alpha=-26.32,          # fractionation factor
)

Connect(
    source=Ocean,          # source of flux
    sink=Carbonate_burial, # target of flux
    rate="18.1E12 mol/yr", # burial rate
    alpha=0,               # set the isotope fractionation
)
```

1.7 Running the model

The model is executed via the `run()` method. The results can be displayed withe the `plot_data()` method which will generate an overview graph for each reservoir. Export of the results to a csv file is done via the `save_data()` method which will create csv file for each reservoir.

```
# Run the model
C_Cycle.run()

# plot the results
C_Cycle.plot_data()
# save the results
C_Cycle.save_data()
```



2 Controlling the flux type

Connecting two reservoirs creates a flux. In order to keep the connection definition concise, basic flux properties are derived implicitly from the way the connection is specified:

- If both `rate` and `delta` are given, the flux is treated as a fixed flux with a given isotope ratio. This is usually the case for most source objects (they can still be affected by a signal, see above), but makes little sense for reservoirs and sinks.
- If both the `rate` and `alpha` are given, the flux rate is fixed (subject to any signals), but the isotopic ratio of the output flux depends on the isotopic ratio of the upstream reservoir plus and isotopic offset specified by `alpha`. This is typically the case for fluxes which include an isotopic fractionation (i.e., pyrite burial). This combination is not particularly useful for source objects.
- If the connection specifies only `delta` the flux is treated as a variable flux which is computed in such a way that the reservoir maintains steady state with respect to it's mass.
- If the connection specifies only `rate` the flux is treated as a fixed flux which is computed in such a way that the reservoir maintains steady state with respect to it's isotope ratio.

2.1 Advanced flux properties

Often is desirable to modify a flux is response to something else. A typical example would be some sort of signal to force an input flux. This can be done by first creating a signal, and then by adding this signal to the list of processes registered with this connection:

```
Signal(name = "ACR",    # name of signal
       species = CO2,   # species
       filename = "emissions.csv",
       scale  = 0.3,
)

Connect(
    source=Fossil_Fuel_Burning,  # source of flux
    sink=Shallow_Ocean,          # target of flux
    rate="0 mol/year",           # baseline flux
    delta=0,                     # baseline delta
    pl=[ACR],                    # add signal to process list
)
```

The above method will work for all process types, often used processes can also be specified directly during connection creation by providing the ctype keyword as in this example

```
Connect(
    source=Deep_Ocean,          # source of flux
    sink=Carbonate_burial,      # target of flux
    rate="18.1E12 mol/year",    # flux rate
    ctype="scale_with_concentration_normalized", #type
    ref_reservoir = Deep_Ocean, #
    k_value = 1e3,              # scaling value
    ref_value = "2.6 mmol/l",   # target concentration
    alpha=0,                    # isotope fractionation
)
```

Note that in most cases, the below scaling functions will relate to the upstream reservoir. As such, `ref_reservoir` defaults to the upstream reservoir, and the `ref_reservoir` keyword can be omittted.

2.1.1 Currently recognized ctype values

In most cases, the below scaling functions will relate to the upstream reservoir. As such, `ref_reservoir` defaults to the upstream reservoir.

- `scale_with_mass` scale a flux relative to the mass in a given reservoir. Required parameters are `ref_reservoir` which must be a reservoir handle, and `k_value` which must be a constant. Note that this will scale the flux based on the initial flux rate you specify.
- `scale_with_concentration` scale a flux relative to the concentration in a given reservoir. Required parameters are `ref_reservoir` which must be a reservoir handle, and `k_value` which must be a constant. Note that this will scale the flux based on the initial flux rate you specify.
- `scale_with_mass_normalized` scale a flux relative to the mass in a given reservoir. Required parameters are `ref_reservoir` which must be a reservoir handle, and `k_value` which must be a constant. Additionally, `ref_value` must be specified. This will scale the flux in such a way that it maintains the mass specified by `ref_value`. The scaling factor `k_value` defines how fast the system returns to equilibrium

  $F = (M(t)/ref_{value} -1) * k_{value}$
- `scale_with_concentration_normalized` same as above, but this time the scaling is relative to concentration

  $F = (c(t)/ref_{value} -1) * k_{value}$
- `monod_type_limit` Fluxes can be scaled with a Michalis-Menten type scaling function

  F = F * a * F0 x C/(b+C)
- `flux_balance` This can be used to express equilibration fluxes between two reservoirs (see the equilibration example in the example directory). This 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`

2.2 Introspection

The object names can be used to query almost all object parameters. I addition to the usual commands (e.g., `print`, `help`, `dir`), the `model`, `reservoir` and `connection` classes provide a `describe()` method. This method can be used e.g., to query the name and type of the connections, fluxes and processes which are associated with a reservoir.

The code will echo the names of the connector objects on to the console as `Source_2_Sink_Connector`. The corresponding flux name is `Source_2_Sink_Flux` and any associated Processes will be named `Source_2_Sink_Pname` where `Source` and `Sink` refer too the corresponding upstream and downstream reservoirs/sources/sinks.

Lastly, it is possible to update connection properties after the connection has been specified. Individual values can be updated by simple assignment, e.g., `Connection.alpha = 34`. If you need to update more than one value, you can use update method

```
Connection.update(
    ctype='flux_balance',
    left=[R1, K],
    right=[R2, R3],
)
```

This is particularly useful in connection with reservoir groups

2.3 External Data

You can associate external datasets to a reservoir (or flux) in order to compare model results against measured data. See the `one-box-ocean` example in the examples directory.

2.4 Working with Units

ESBMTK supports unit parsing in it's arguments, i.e., "1 ky" is understood to be equivalent to 1000 yrs. It also supports some units which are useful in Oceanography (i.e., the Sverdrup). The unit parsing is handled by the `pint` library, please see `https://github.com/hgrecco/pint` for details.

Sometimes is useful to leverage unit parsing in your code which establishes the boundary conditions for the model. An immediate example is the definition of the time units. Default alias for year is `a`, which works well in a geological context. However, for models which deal with historic times, "yrs" my be more appropriate. You can redefine the year unit definition in the following way

```
from esbmtk import ureg

ureg.define("year = 365.25 * day = yrs = julian_year")
```

where the first alias after the definition (i.e.,"yrs") is the one which will be used by ESBMTK for plotting.

Similarly, we can create some shorthands to simplify calculations

```
from esbmtk import ureg

meter = ureg.meter
mol = ureg.mol
mmol = ureg.mmol
Mol = ureg.Mol
mMol = ureg.mMol
Sv = ureg.Sv
years = ureg.years
seconds = ureg.seconds
liter = ureg.liter
```

and then do some dimensionality correct calculations similar to this one

```
volume = 1.38E21 * liter  # Total ocean volume in m**3
area = 361E12 * meter**2  # m^2 # Total ocean area
average_depth = volume/area # average depth, about 4000m
print(f"average_depth = {average_depth:.2e~P}")
```

2.5 Saving and reading model state

Some models require a spin up period to reach steady state. The `save_state()` method allows to the save the model state, and use it as the initial conditions for a new model run.

Notes: The model definition must remain the same. Similarly, if you change a boundary condition in the model definition between two runs, it will be overwritten by the `read_state()` method. It is however possible to add signals to the new run, in order to change the steady state.

2.6 Adding data after the fact

Data which is computed after the model finishes, can be integrated into the summary plots via the DataField class. The data will be plotted in the same window as the reservoir it has been associated with.

```
Example:
             DataField(name = "Name"
                       associated_with = reservoir_handle
                       y1_data = np.Ndarray
                       y1_label = Y-Axis label
                       y1_legend = Data legend
                       y2_data = np.Ndarray    # optional
                       y2_label = Y-Axis label # optional
                       y2_legend = Data legend # optional
```

```
Note that Datafield data is not mapped to model units. Care must be taken
that the data units match the model units.
```