Model agnostic isotope tracer simulator

Model compatibility limitations

- Works with 'flux-state' hydrologic models: water volume or mass is simulated in storages (state) and moves between modeled storages (fluxes)
- Water must be fully tracked in the simulation: conservation of simulated mass in the model domain
- All storages must share simulation time intervals (all storages have the same start and end times for simulation time step)
- Connections between modeled storages must be one directional (no bi-directional connections)
    - 'Upstream' to 'downstream' storage order cannot change during the simulation
- Simulating isotope tracers requires state and flux values to be passed to the MA simulator
    - All storage state and flux values must be output for the external simulator

Currently only precipitation is allowable as an external water input to the model domain (intended to change in later versions).

Standardized data requirements

The model agnostic isotope tracer simulator requires hydrologic and atmospheric data to be organized in a standardized format. There are three 'large' and three 'small' inputs needed for a successful isotope tracer simulation. The major inputs are:

1. <u>Storage matrix</u>

- One row per modeled storage (e.g., water mass in sub-basin 3, soil layer 2)
- Two columns: mass in storage at end of time interval, associated atmosphere #
- 3rd dimension is time: one data 'sheet' per time interval
- Storages **MUST** be in an 'upstream' to 'downstream' order
    - Order of storages in the storage matrix is the order of calculation
    - Concentration of first row calculated first, 2nd next, ect.
    - E.g., headwater sub-basins must be listed prior to outlet sub-basins and surface storage must be listed before lower soil layers
    - Depending on model structure there may be only one valid order or multiple valid storage calculation orders
- The order of the list of storages must be identical for all simulation time intervals

2. <u>Atmosphere matrix</u>

- Each row is an 'atmosphere', with the row number matching that listed in the storage matrix
- Three columns: air temperature (°C), relative humidity (%), δ value of isotopes in precipitation (‰)
- Must be at least one atmosphere to simulate precipitation and evaporative fractionation
- 3rd dimension is time: one data 'sheet' per time interval

3. <u>Flux matrix</u>

- One row per individual simulated flux (e.g., evapotranspiration from sub-basin 3, soil layer 2)
- 4 columns: flux rate, source #, destination #, evaporative fraction

    - Flux rate must match units of other inputs (mass from storage matrix, time from time vectors, e.g., if storage is tracked in kg and time in days, fluxes must be in kg/day)
    - Source # is the row # of the flux source storage (from storage matrix) if internal, 0 if the flux is precipitation
    - Destination # is the row # of the destination storage (from storage matrix) for the flux if internal, 0 if the flux leaves the model domain
    - Evaporative fraction: fraction of the flux which is evaporation (0 if not evaporative, 1 if flux is exclusively evaporation, equal to E/ET for evapotranspiration)
- 3rd dimension is time: one data 'sheet' per time interval
- No known restrictions on number or order (flux list may change between simulation time intervals, fluxes with all values equal to zero are permissible)

The remaining inputs are:

1. Storage initialization matrix
    - Rows match those in the storage matrix
    - 2 columns: mass in storage at simulation time=0, delta value of isotopes in storage at simulation time=0
2. Time 1
    - Vector of simulation interval start times (units agree with flux rate units)
    - E.g., 0, 2, 3, 4, 6…
    - Not required to start at zero or have equal intervals
3. Time 2
    - Vector of simulation interval end times (units agree with flux rate units)
    - E.g., 2, 3, 4, 6, 8…
    - Time 2 - Time 1 determines simulation time step lengths

Output

Currently, simulated isotope delta values are output for all storages in the storage matrix in an output data matrix (rows are storages in storage matrix order, columns are time intervals).

For storages which are dry for the entirety of a simulation interval (no storage, inflow or outflow) the simulated mass concentration is 0, producing -1000‰ as output.