isoWATFLOOD

Stable water isotope simulation in the WATFLOOD hydrologic model

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Contents

1 Introduction: What is isoWATFLOOD

isoWATFLOOD is a stable water isotope model which runs with the WATFLOOD hydrologic model (Kouwen, 2014). The isoWATFLOOD model, like the WATFLOOD model on which it depends, is a partially-physically based, distributed computer model. The isotope model simulates δ^{18}O, and optionally δ^2H, in the hydrologic storages and fluxes defined by continuous hydrologic simulation within a watershed model in WATFLOOD. Watersheds have ranged in size from 500 km^2 to >1,000,000 km^2, and have been run with hourly (and sub-hourly for routing), daily or monthly time-steps.

1.1 Purpose

Stable water isotopes are naturally occurring tracers in the water cycle, which can provide additional information on flow generation processes to improve our understanding and simulation of streamflow in a watershed. Uses for simulated stable water isotope data include:

- Additional data for parameter calibration

- Verification of internal hydrologic storage simulations

- Streamflow separation into source components

- Identification of physically-unrepresentative parameter sets

- Reducing equifinality and simulation uncertainty

- Characterization of the impact of climatic conditions on the hydrologic cycle in a basin, particularly in regards to evaporation

1.2 Version history

The original isoWATFLOOD model was developed by Dr. Tricia Stadnyk for the simulation of δ^{18}O (see Stadnyk-Falcone (2008)). The model was expanded to additionally simulate δ^2H, and further improved

by Tegan Holmes (see Holmes (2016)). Additional improvements have been made by Dr. Nicholas Kouwen and Carly Delavau.

- Version 1.0 (2008) Simulation of oxygen-18 in all WATFLOOD storages

- Version 1.1 Isotope pumping added

- Version 1.2 (2013) isotope.par file added for isotope initialization and forcing

- Version 1.3 (June 2015) Gridded isotope precipitation data read-in added

- Version 2.0 (July 2015) Optional simulation of deuterium in all WATFLOOD storages

- Version 2.1 (September 2015) Snowpack isotope evolution, relative humidity data added as an optional input, isotopes in diverted and nudged flows and functionality with sub-hourly routing

- Version 2.2 (November 2015) Transpiration added as an explicit flux, with user defined parameters, observed isotope input added and switch from iterated to direct solutions for all mass balance calculations

- Version 2.3 (August 2016) ISOsurface, ISOinter and ISOground merged into ISOland, connected wetland ET split added to ET parameter file, and evaporative fractionation included for rivers

2 How to run isoWATFLOOD

Running isoWATFLOOD is quite simple, provided you can already use WATFLOOD. This section covers

how to switch on the isotope simulation, the isotope simulation options and input files, and the output

from the simulation.

2.1 Requirements

In order to run isoWATFLOOD, you need:

1) A WATFLOOD splx.exe with the isoWATFLOOD module

2) A complete and functional WATFLOOD basin, with temperature data

3) An isotope initialization file (see Section 2.1.1) in the basin folder

Once you have these three things, go to the event file (event\event.evt) and in the flag section switch

the fractionation flag to 'y':

```
:frcflg                    y
```

Add the frcflg if it isn't there already (the tracer flag (trcflg) does not need to be turned on to run the

isotope tracer, but it can be set to y if you want the virtual tracer result in addition to the isotope tracer

simulation). Run WATFLOOD as usual, and if "RUNNING ISOTOPE FRACTIONATION" appears at the end of the

header then isoWATFLOOD is running too.

The additional simulation isotopes substantially increases the simulation run-time. Running a single

isotope simulation will approximately double the run-time. The options chosen for the simulation (see

Section 2.2) will alter the simulation run-time.

2.1.1 The isotope initialization file

The isotope initialization file is the only additional file required to run isoWATFLOOD (it needs all sorts of data and parameters but those are also required by WATFLOOD and are therefore specified in the normal WATFLOOD PAR file). The initialization file initializes the isotope compositions of various hydrologic storages (data for which should be obtained from long-term isotope monitoring data), but also contains the basic isotope precipitation data. An example of `basin\isotope.init`:

```
1                                       !2H flag
3                                       !number of years for isotopes
1                                       !output land class
delta1          -10.50                  !bkgd for water
delta2          -15.85                  !bkgd for soil water
delta3          -15.85                  !bkgd for groundwater
delta4          -25.00                  !bkgd for snow
isoyear           2002     2003     2004        !year for isotope values
deltar          -19.10   -19.10   -20.10        !delta value for rain
deltas          -29.35   -29.35   -25.03        !delta value for snow
rfoffset          0.00     0.00     1.00        !depletion for refreezing
smoffset          0.00     0.00     5.00        !enrichment for snow melt
```

This is a text file input, so copy the spacing to avoid data input errors. Going through the lines in order:

- The 2H flag: this will turn on the dual-isotope simulation if set to 2 (see Section 2.2.1)

- This number determines how may columns of input data the program looks for, from isoyear on

- This number determines the land class which gets used in isotope output (see Section 2.3.1)

- Initial oxygen-18 composition for surface water (surface, stream, lake and wetland) in δ‰

- Initial oxygen-18 composition for soil water (upper zone/interflow) in δ‰

- Initial oxygen-18 composition for groundwater (groundwater/baseflow) in δ‰

- Initial oxygen-18 composition for snow (existing snowpack) in δ‰

- The years for the input data. You need to have all the years of the isotope simulation listed. The years must match those in the event files. Having extra years won't cause problems, they just won't get used.

- The oxygen-18 δ‰ value for rain for the year

- The oxygen-18 δ‰ value for snow for the year

- The snowpack depletion for refreezing for oxygen-18 in ‰, for the year. If you don't know what this is, leave it as 0.0

- The snowpack enrichment for melting for oxygen-18 in ‰, for the year. If you don't know what this is, leave it as 0.0

The initialization values are only significant for the beginning of the isotope simulation. The length of time the storage unit is affected by these values depends on its residence time. Generally, these values stop affecting the simulation after the first freshet. The precipitation data must be included, but the values may not be used if better precipitation is provided (Section 2.2.2).

2.2   Options

The isoWATFLOOD model has simulation options beyond the most basic model. These also require more data. This section covers the other things that the isotope simulation can do.

2.2.1   Dual-isotope simulation

The dual-isotope (deuterium and oxygen-18) simulation is switched on using the isotope.init file. In the first line, set the value to '2' to flag the deuterium simulation on. You will also need to provide all the information for deuterium that you did for oxygen-18, so isotope.init gets longer:

```
2                              !2H flag
3                              !number of years for isotopes
1                              !output land class
delta1        -10.50           !bkgd for water
```

```
delta2          -15.85                           !bkgd for soil water
delta3          -15.85                           !bkgd for groundwater
delta4          -25.00                           !bkgd for snow
isoyear          2002     2003     2004          !year for isotope values
deltar          -19.10   -19.10   -20.10         !delta value for rain
deltas          -29.35   -29.35   -25.03         !delta value for snow
rfoffset          0.00     0.00     1.00         !depletion for refreezing
smoffset          0.00     0.00     5.00         !enrichment for snow melt
delta2H1         -90.0                       !bkgd for water
delta2H2        -119.8                       !bkgd for soil water
delta2H3        -119.8                       !bkgd for groundwater
delta2H4        -193.0                       !bkgd for snow
deltar2H        -152.0   -152.0   -152.0         !delta value for rain
deltas2H        -228.0   -228.0   -188.0         !delta value for snow
rfoffset2H        5.00     5.00     6.00         !depletion for refreezing
smoffset2H        8.00     8.00     9.00         !enrichment for snow melt
1                                            ! framework flag
```

This is a text file input, so copy the spacing to avoid data input errors. Going through the new lines (after

smoffset) in order:

- Initial deuterium composition for surface water (surface, stream, lake and wetland) in δ‰

- Initial deuterium composition for soil water (upper zone/interflow) in δ‰

- Initial deuterium composition for groundwater (groundwater/baseflow) in δ‰

- Initial deuterium composition for snow (existing snowpack) in δ‰

- The deuterium δ‰ value for rain for the year

- The deuterium δ‰ value for snow for the year

- The snowpack depletion for refreezing for deuterium in ‰, for the year. If you don't know what

  this is, leave it as 0.0

- The snowpack enrichment for melting for deuterium in ‰, for the year. If you don't know what

  this is, leave it as 0.0

- The framework flag, which determines what kind of isotope framework you get. 1- an average

  framework for the whole basin 2- a framework for each gauge 3- user determined framework

areas. More information on the differences in Section 2.3.3. Option three requires another input file.

As with oxygen-18, the deuterium initialization is only temporarily significant to the simulation output.

If you do want to use the third option for producing frameworks, you need to add another input file, to combine sub-basins. An example of `basin\isobasin_combine.txt`:

```
1               1
2               2
3               3
4               3
5               1
```

This is a text file input, so copy the spacing to avoid data input errors. Each sub-basin (there are 5 in this example) is included in a framework, but multiple sub-basin can be included in the same framework (there will be three frameworks in this example).

2.2.2   Gridded forcing for isotopes in precipitation

Developed by Carly Delavau and Nick Kouwen

Gridded forcing for isotopes in precipitation can be used in place of the annual average values specified in the isotope.init file. Gridded forcing data allows for the isotopic composition input to vary over the basin area, and over a shorter time period than annually. This is particularly helpful in very large basins, and for producing time-series results in smaller basins. The method for producing gridded isotope forcing data developed by Carly Delavau is covered in Appendix A.

To read in gridded isotope input data for oxygen-18, list the file name and location in the event files in the gridded file section:

```
:griddeddrain              isoP\20090101_drn_m.r2c
```

If the file listed in the event file for gridded δ rain can be found, the data in it will be used in place of the annual values from isotope.init for oxygen-18 in all precipitation (both rain and snow). To read in gridded isotope input data for deuterium, if running a dual-isotope simulation, list the file name and location in the event files in the gridded file section:

```
:griddeddsnow                    isoP\20090101_drn_m2H.r2c
```

If the file listed in the event file for gridded δ snow can be found, the data in it will be used in place of the annual values from isotope.init for deuterium in all precipitation (both rain and snow) (the nonsensical naming came from re-purposing old code for gridded deuterium inputs).

2.2.3   Observed isotopic composition of streamflow

Developed by Nick Kouwen and Tegan Holmes

Simulated isotopes in streamflow can be compared to observed values within the isoWATFLOOD program with isotope observation input files. With isotope observation input files, the RMSE is calculated for each observation site, and this error can be used in the DDS process, with error flag 100. There will also be more output data (see Section 2.3.2). The input files are in the .ts5 format. Each observation site adds a column to the input file data. The input files are annual, with one row per day. Data is in δ‰. If there is no observed isotopic composition available for the day, -99999.9 should be entered instead. The inputs must be located in a folder called isoObs, and must be named either iso_18O_YYYY.ts5 for oxygen-18 or iso_2H_YYYY.ts5 for deuterium. An example of the beginning of an isotope observation input file, `'isoObs\iso_2H_2010.ts5'` follows:

```
##############################################################

:FileType   ts5    ASCII EnSim 1
#      Canadian    Hydraulics    Centre/National    Research    Council    (c)
       1998-2007
#      DataType    Type  5    Time   Series
#
:Application        isoWATFLOOD
:Version    3.1.33
:WrittenBy  TH
:CreationDate      28/07/2016
#
#-------------------------------------------------------------------------

#
:AttributeName     1_2H
:AttributeUnits    1
:AttributeName     2_2H
:AttributeUnits    1
:AttributeName     3_2H
:AttributeUnits    1
:BeginLine  3
:Point      -97.354    55.996
:Point      -98.492    55.8
:Point      -98   55.6
:EndLine
#      25    Odei River
#      9     Sapochi River
#      24    Taylor River
:EndHeader
2010-01-01  -99999.9    -99999.9    -99999.9
2010-01-02  -99999.9    -99999.9    -99999.9
2010-01-03  -99999.9    -115.193388 -99999.9
2010-01-04  -99999.9    -99999.9    -99999.9
```

2.2.4 Observed relative humidity data

Calculating evaporative fractionation in isoWATFLOOD requires values for the relative humidity (see

Section 3.1.1). Relative humidity is estimated by the program as:

```
relh(n)=(10/1000.)/(((1e-06*tempv(n)**4.-3e-05*tempv(n)**3.
+0.0036*tempv(n)**2.+0.0182*tempv(n)+0.6607)*1000.)/101325.*0.625)
```

Where tempv(n) is the air temperature in the grid cell. However, relative humidity is not solely

dependent on air temperature so this estimate is not particularly accurate, beyond capturing general

seasonal trends. There is therefore an option to read-in observed relative humidity data, and use

observed humidity rather than the estimate. Like temperature and precipitation data, relative humidity

is read into the program as distributed data, with 1 value per grid cell. To read in relative humidity data, list the file name and location in the event files in the gridded file section:

```
:griddedhumidity              humid\20090101_hum.r2c
```

The .r2c file format for relative humidity is identical to that for temperature. The simplest way to generate the humidity .r2c files is to use the air temperature distributer for WATFLOOD (see the WATFLOOD manual (Kouwen, 2014)). Enter humidity rather than air temperature point observations, and rename the resulting files to avoid further confusion.

Using observed rather than estimated relative humidity will slow the simulation down, but will improve the isotope simulation, particularly at finer temporal scales. Using observed humidity data is therefore recommended when simulating to compare to an observed isotope data time-series.

2.2.5   Evaporation-Transpiration split parameters

While evaporation and transpiration can be lumped together as evapotranspiration for hydrologic modeling, the two processes are significantly different for isotope simulations as evaporation fractionates isotopes and transpiration does not. Therefore isoWATFLOOD splits the evapotranspiration loss calculated by WATFLOOD into evaporation and transpiration. However, this split requires parameters, an 'a' and 'b' value for each land class which might have both evaporation and transpiration (see Section 3.1.2 for how this works, and what the parameters actually do). These parameters can be selected by the user if an ET.par file is added to the basin folder, with an example of the contents shown below, for three land classes:

```
ii 1 a        0.4
ii 1 b        6.0
ii 2 a        0.2
ii 2 b        8.0
ii 3 a        0.3
ii 3 b        2.0
```

This is a text input, so the spacing should be copied to avoid input errors. If there is no `basin\ET.par` then all 'a' values will be set to 0.3 and all 'b' values to 4.0. Adding an ET.par file is optional, but recommended, as the E/T split will influence the final isotope simulation result and different land cover do have different splits between E and T (for example, more E in wetlands than forest).

2.2.6   Isotope forcing for diversions and nudged flow stations

Diversions and nudged flow stations are separate WATFLOOD features, but they are lumped together in this section since the isotope forcing files are the same.

Diversions: These add water to grid cells at the edge of a basin. If you have a diversion in your basin, and don't give isoWATFLOOD any forcing data for it, the program will run the simulation, but you will get very poor isotope simulation results downstream of the diversion, as there will be a large volume of isotopes missing. So if you have diversions, add a folder called isoForcing and make annual input files for each diversion. Name them YYYY_divDIV#.txt (i.e. 2010_div2.txt for the second diversion in 2010). If you are running deuterium, also add YYYY_divDIV#_2H.txt (i.e. 2010_div2_2H.txt).

Nudging: Nudging adjusts the outflow of a grid cell to match the observed flow from a flow gauge in the cell. If you don't give isoWATFLOOD any forcing data for a nudged station, the adjusted flow is given the isotopic concentration of the unadjusted flow. This is fine for minor corrections. However, if nudging is being used as diversion in the interior of a basin area (e.g., the Churchill River Diversion at Notigi in the middle of the lower Nelson River basin) the simulated isotope concentration will not be representative of the actual flow. If this is the case, add forcing data files, and isoWATFLOOD will use those instead of the calculated concentration. Put the files in a folder called isoForcing and make annual input files, named YYYY_nudGAUGE#.txt (i.e. 2010_nud17.txt for nudging forcing at the 17th gauge in 2010). Also, the gauge number is assumed to be 2 digits, so if you want to use forcing for the 6th gauge the file would

have to be named 2010_nud 6.txt. If you are running deuterium, also add YYYY_nudGAUGE#_2H.txt (i.e.

2010_nud17_2H.txt).

Other than the names, the nudging and diversion input files are the same. The file must be a text file 366

lines long with 1 real number per line and no header. Each line corresponds to one day. The input data

should be in δ‰. If you aren't in a leap year, you can just put a 0 in the last line. An example of the last 4

lines for an oxygen-18 input file in 2010 (not a leap year):

```
-10.6520000000000
-10.6520000000000
-10.6520000000000
0.
```

You don't need that many decimal places, but it doesn't matter if they are there. Do make sure there is a

decimal point.

The isotope value you assigned to the diverted or nudged flow should be estimated from observations

of the diverted or nudged flow (long term average data), or the nearest downstream station in the

watershed (preferably upstream of a confluence). Either use a step-wise function or interpolate

between data points to get a value for every day.

2.3   Output

The isoWATFLOOD model calculates lots of things, and therefore can produce lots of output too. This

section covers what is actually produced as standard output in the results folder from the compiled

version of the code. Custom outputs are possible based on collaboration with model developers.

2.3.1 Standard output files

Running isoWATFLOOD with only oxygen-18 produces:

- dCG.csv- Craig-Gordon (1965) model results, including the isotopic composition of the vapour phase, δE. Output for each cell containing a flow gauge (as defined in the WATFLOOD streamflow file). Columns are: time, <gauge>(relative humidity, δ_E, δ^*). Delta values are for oxygen-18 based on evaporation from the water class.

- dGW.csv- isotopic composition of groundwater results, or δGW. Output for each cell containing a flow gauge (as defined in the WATFLOOD streamflow file). Columns are: time, <gauge>(δ_{GW}). Delta values are for oxygen-18 in the lower zone storage compartment in the grid cell.

- dIF.csv- isotopic composition of interflow results, or δIF. Output for each cell containing a flow gauge (as defined in the WATFLOOD streamflow file). Columns are: time, <gauge>(δ_{IF}). Delta values are for oxygen-18 in an upper zone compartment in the grid cell. The upper zone compartment output is determined by the land class entered in the third line of the isotope.init file (each land class has a separate UZ compartment).

- dLK.csv- isotopic composition of lake water results, or δLK. Output for each lake/reservoir in the basin (as defined in the WATFLOOD basin file, as "reaches"). Columns are: time, <reservoir>(δ_{LK}). Delta values are for oxygen-18 of the water in a defined WATFLOOD lake.

- dRAIN_raw.csv- Isotopes in rain input. Output for each cell containing a flow gauge (as defined in the WATFLOOD streamflow file). Columns are: time, <gauge>(δ_R). Delta values are for oxygen-18 in rainfall. This is input data being returned for verification purposes, not simulation results.

- dSNOW_raw.csv- Isotopes in snow input. Output for each cell containing a flow gauge (as defined in the WATFLOOD streamflow file). Columns are: time, <gauge>(δ_S). Delta values are for

oxygen-18 in snowfall. This is input data being returned for verification purposes, not simulation results.

- dSNW.csv- isotopic composition of the snowpack results, or δSNW. Output for each cell containing a flow gauge (as defined in the WATFLOOD streamflow file). Columns are: time, <gauge>(δ_{SNW}). Delta values are for oxygen-18 in a snowpack in the grid cell. The snowpack output is determined by the land class entered in the third line of the isotope.init file (each land class has a separate snowpack).

- dSTR.csv- isotopic composition of streamflow results, or δSTR. Output for each cell containing a flow gauge (as defined in the WATFLOOD streamflow file). Columns are: time, <gauge>(δ_{STR}). Delta values are for oxygen-18 in the water class within a grid containing a streamflow gauge, and represent the routed flow isotopic composition.

- dSW.csv- isotopic composition of surface water results, or δSW. Output for each cell containing a flow gauge (as defined in the WATFLOOD streamflow file). Columns are: time, <gauge>(δ_{SW}). Delta values are for oxygen-18 in a surface water compartment in the grid cell. The surface water compartment output is determined by the land class entered in the third line of the isotope.init file (each land class has a separate UZ compartment). There is often no surface water, in which case -1000 is the null value output.

- dWET.csv- isotopic composition of connected wetland (fen) results, or δWET. Output for each cell containing a flow gauge (as defined in the WATFLOOD streamflow file). Columns are: time, <gauge>(δ_{WET}). Delta values are for oxygen-18 in the connected wetland class storage, and represent the wetland routed flow isotopic composition.

These files are not produced if DDS is turned on in the par file.

2.3.2 Comparison to observed data

When there is observed streamflow data to compare with (see Section 2.2.3), the simulated and observed isotope values are output:

- iso_info.txt- This file contains the full time-series for simulated and observed streamflow isotopic compositions at isotope observation sites, listed comparisons of simulated and observed data for all days with observed data, and RMSE values for every isotope observation site.

- iso_18O_conc.csv- Streamflow results at isotope observation sites for oxygen-18 water composition. Includes outputs for each isotope observation site in the .ts5 file. Columns are: day, <site>(δ_{OBS}, δ_{SIM}). Simulated values come from the water land class in the grid cell containing an observation site.

- iso_2H_conc.csv- Streamflow results at isotope observation sites for deuterium water composition. Includes outputs for each isotope observation site in the .ts5 file. Columns are: day, <site>(δ_{OBS}, δ_{SIM}). Simulated values come from the water land class in the grid cell. Only produced if running a dual-isotope simulation.

These files are produced even if DDS is turned on in the par file. This data is from isotope observation sites, not streamflow gauges. Isotope observation sites are independent of flow gauges and are defined in the isoObs .ts5 files.

2.3.3 Dual-isotope output

When the dual-isotope simulation is turned on, most of the standard output files have additional data, and two new files are output. The dSW, dIF, dGW, dSNW, dWET, dSTR, dRAIN_raw and dSNOW_raw files include both oxygen-18 and deuterium simulation output, in the form: time, <gauge>(δ^{18O}, δ^{2H}). The dCG and dLK output files do not change. The two new output files are:

- dexcess.csv- The *d*-excess value for the isotope in streamflow simulation. The *d*-excess value is computed as δ^{2H}-8*δ^{18O}. Output is for each cell containing a flow gauge (as defined in the WATFLOOD streamflow file). Columns are: time, <gauge>(*d*-excess). Values are calculated using the stream channel isotope compositions (δ_{STR}).

- frame.csv- the simulated isotope framework end points. The output here depends on what was entered in the last line of the isotope.init file.

    1= One set of end points, with δ values averaged over the entire basin area

    2= A set of end points for every gauge in the basin (defined by the number of streamflow gauges), with δ values averaged over the area associated with the gauge. This associated area is the area upstream of the gauge, less the area of any upstream gauges (e.g. if there were 2 gauges along the channel, with gauge 2 downstream of 1, the area for gauge 1 would be the drainage area of gauge 1, and the area for gauge 2 would be the drainage area of gauge 2 minus the drainage area of gauge 1).

    3=User determined number of end point sets (see Section 2.2.1 for the input file), where the areas associated with gauges can be grouped together, with the δ values averaged over the grouped areas. Helpful if you want to group together a series of gauges along a stream channel, or main stem to get a framework for a particular sub-basin.

Each framework point set consists of three sets of line end points and two additional points. The first two columns (x (oxygen-18) values in the first, y (deuterium) in the second) are for the global meteoric water line (GMWL) which always has the same equation: δ^{2H}=8* δ^{18O}+10. Next are two columns for the local meteoric water line (LMWL), based on a precipitation flux weighted average of the input precipitation composition, averaged over the framework area. The last line set is the local evaporation line (LEL), calculated from evaporation flux weighted

average values of δ_E and $\delta*$, averaged over the framework area. The evaporation flux weighted

average values, averaged over the framework area, for δ_A and $\delta*$ are the two points output, in

the final four columns of the framework point set. Averaged values (for δ_E, δ_A and $\delta*$) are

calculated as:

$$\delta_{avg} = \sum_{n=a}^{b}\sum_{t=1}^{T} E_{t,n}\delta_{t,n} \bigg/ \sum_{n=a}^{b}\sum_{t=1}^{T} E_{t,n}$$

(2.1)

Where T is the total simulation length (in hours), a and b are the initial and final grid cells in the

framework area, $\delta_{t,n}$ is the delta value at time t in grid cell n, and $E_{t,n}$ is the evaporation volume

loss from open water over time t in grid cell n.

The d-excess file is not produced if DDS is turned on in the par file, and the framework file is not

produced properly.

3 The stable water isotope model in isoWATFLOOD

The isoWATFLOOD model simulates isotope mass balances for all of the hydrologic storages in the WATFLOOD model. The stable water isotope volume in every grouped response unit, in every grid cell, is calculated based on the fluxes in and out of the storage unit. Figure 3.1 shows the storage units and fluxes for a single grid cell with five grouped response units, including a connected wetland.
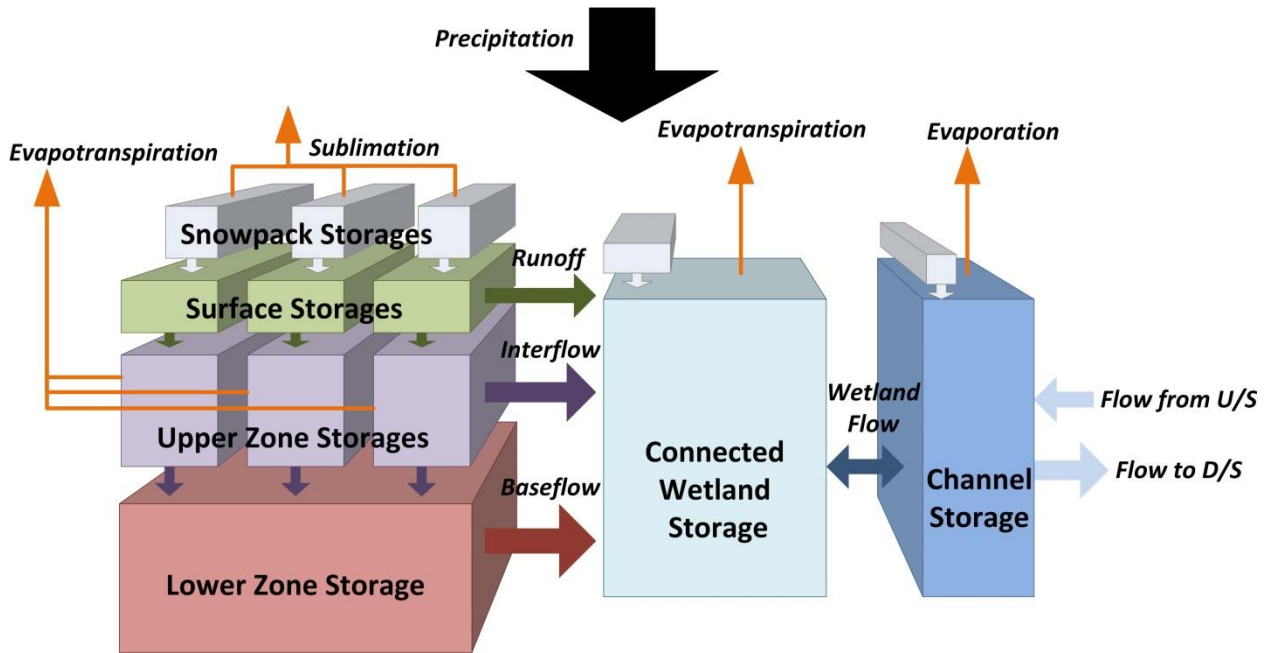
Figure 3.1 Grouped response units within a WATFLOOD grid cell

The stable water isotope volume in each storage compartment is computed each time interval based on the stored volume at the beginning of the time interval, and the inflow and outflow over the time interval. Volumes within WATFLOOD and isoWATFLOOD are measured in cubic meters, while isotopic concentrations are unitless (m^3/m^3), but are later converted into delta values for output relative to Vienna Standard Mean Ocean Water (VSMOW). The δ value is defined as:

$$\delta‰=(R/R_{std}-1) \times 10^3 \tag{3.1}$$

Where R is the relative abundance of D/H or $^{18}O/^{16}O$, and R_{std} comes from the world standard (Vienna Standard Mean Ocean Water, VSMOW2, or previously VSMOW) (Gat, 1996). Isotopes are transferred between compartments based on the isotopic concentration within the storage and the water flux calculated by WATFLOOD. Evaporated water has a different concentration of isotope species than the source water, as stable water isotopes fractionate.

This chapter will describe the models used to simulate stable water isotopes in each type of hydrologic storage, and in evaporated water. Much of the content comes from Holmes (2016).

3.1 Evaporation

The different physical properties of stable water isotopes mean that isotopes do not evaporate at the same rate, which alters the isotope concentration of water undergoing evaporation: lighter isotopes are preferentially removed, and the remaining water enriches in the rarer, heavier isotopes. The change in concentration due to evaporative fractionation is significant enough to warrant its inclusion in the isotope simulation.

3.1.1 Evaporative fractionation

To model fractionation due to evaporation the concentration of stable water isotopes in the evaporated water vapor, C_E^{iso}, is needed; this concentration is dependent on both atmospheric conditions and the concentration of the evaporating water body. There are two significant components to fractionation: equilibrium and kinetic separation (Gibson, et al., 2008). Equilibrium isotopic fractionation is temperature dependent, with the equilibrium isotopic separation between liquid and water, ε^*, calculated as (Gibson, et al., 2008):

$$\varepsilon^* = \alpha^* - 1 \tag{3.2}$$

The equilibrium fractionation factor for the liquid to vapor transition, α^*, is calculated using the empirically derived equations from Horita and Wesolowski (1994):

$$\alpha^*_{18O} = e^{(-7.685+6.7123*(10^3/\text{T})-1.6664*(10^6/\text{T}^2)+0.35041*(10^9/T^3))/1000}$$ (3.3)

$$\alpha^*_{2H} = e^{(1158.8*(T^3/10^9)-1620.1*(\text{T}^2/10^6)+794.84*(\text{T}/10^3)-161.04+2.9992*(10^9/T^3))/1000}$$ (3.4)

Where α is in decimal format, and T is air temperature in degrees kelvin. The kinetic separation of isotope species is dependent on both surface properties and relative humidity, with kinetic isotopic separation, ε_k, defined as (Gat, 1996):

$$\varepsilon_k = C_D n\theta(1-h)$$ (3.5)

Where C_D is 28.55‰ for ^{18}O and 25.115‰ for D, h is the relative humidity, n is a turbulence parameter, and θ is a transport resistance factor reduced from unity for large open water bodies (Gibson, et al., 2008). In isoWATFLOOD, n is equal to 2/3 for wetlands, 1/2 for lakes, 1 for soil water, and 0 for river channels (the water is assumed to be too turbulent for kinetic fractionation). The θ parameter is equal to 1, except for lakes, which are assumed to have some additional resistance, with θ equal to 0.88.

The isotopic composition of the evaporated water vapor, δ_E, was first modeled by Craig & Gordon (1965) for oceanic waters. A simplified version of the Craig-Gordon equation describing the composition of the water vapor as a function of the composition of the evaporating water body, δ_L, is used in the simulation (Gonfiantini, 1986):

$$\delta_E = \frac{\dfrac{(\delta_L - \varepsilon^*)}{\alpha^*} - h\delta_a - \varepsilon_k}{1 - h + \varepsilon_k}$$ (3.6)

Where δ_a is the isotopic composition of the ambient atmospheric moisture; h, ε and δ are in decimal notation. The evaporating water composition, δ_L, is dependent on the composition of the water source undergoing evaporation, which can be different for each storage compartment in the model, and is

assumed to be the last computed (previous time step) isotopic composition of any given evaporating

compartment. The isotopes in atmospheric moisture are often assumed to be in equilibrium with those

in precipitation, although if evaporated water constitutes a significant fraction of the vapor, this

assumption may not be valid (Gibson, et al., 2008). With the assumed relationship between the isotopic

composition of atmospheric moisture and the isotopic composition of precipitation, δ_P, which depends

on there being no recirculated moisture, δ_a can be calculated as (Gibson, et al., 2016):

$$\delta_A = \frac{\delta_P - \varepsilon^*}{1 + \varepsilon^*} \tag{3.7}$$

with ε^* and δ in decimal notation.

Enrichment is limited by atmospheric conditions, such that a desiccating water body has a limiting

isotopic composition, δ^*, reached as the water volume approaches zero (Gibson, et al., 2016):

$$\delta^* = \frac{h\delta_a + \varepsilon_k + \varepsilon^*/\alpha^*}{h - \varepsilon_k - \varepsilon^*/\alpha^*} \tag{3.8}$$

The simulation uses the composition from the previous time interval in calculating δ_E for any storage

undergoing evaporative fractionation, including soil storages, connected wetlands, rivers and lakes. The

concentration of stable water isotopes in the evaporated water vapor, C_E^{iso}, is calculated simply as the

concentration form of δ_E (which is in δ form). The simulated evaporative fractionation assumes that the

evaporation source is well mixed, and that the source water composition and all atmospheric conditions

remain constant through the simulation time interval (i.e., one hour, or potentially less for wetlands and

lakes).

3.1.2 Evaporation and transpiration partition

Evaporative fractionation is assumed to apply only to the evaporation portion of evapotranspiration.

Therefore, the evapotranspiration flux calculated by WATFLOOD must be partitioned into evaporation

and transpiration. The split between evaporation and transpiration depends on the water held in the upper zone of the soil, quantified by the upper zone storage indicator, *UZSI* in WATFLOOD which is a function of the soil moisture. Evapotranspiration in WATFLOOD ranges from the potential rate when the soil is saturated, to zero when water content reaches the permanent wilting point, *PWP.* The upper zone indicator is computed as (Neff, 1996):

$$UZSI = \left(\frac{UZS - PWP}{SAT - PWP}\right)^{1/2}$$

(3.9)

Where *UZSI* is the upper zone storage and *SAT* is the saturated soil storage.

As the soil dries, the transpiration fraction of evapotranspiration increases and the evaporation fraction decreases. The proportion of evaporation, *E*, to evapotranspiration, *ET*, is estimated using a power law function (Stadnyk-Falcone, 2008):

$$\frac{E}{ET} = a \cdot UZSI^b$$

(3.10)

Where *a* is the maximum evaporation to evapotranspiration fraction for the land class (typically between 0.3 and 0.5), and *b* is the rate at which the evaporative component of evapotranspiration increases with soil water content. Increasing *b* or decreasing *a* reduces the amount of evaporation in different ways, as shown in Figure 3.2.
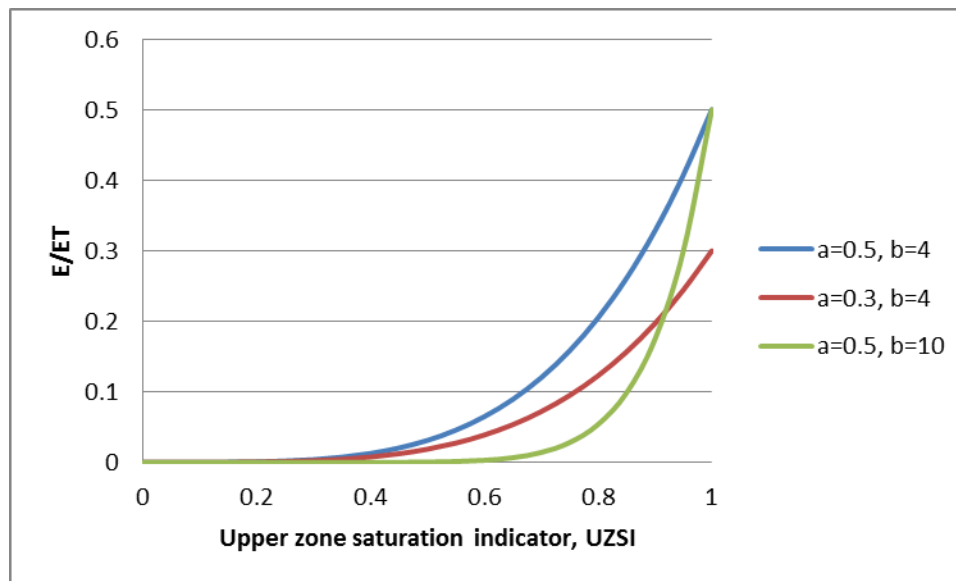
Figure 3.2 Effect of parameters on E/ET partition

Evapotranspiration in connected wetlands is not partitioned in this way, as they do not have an upper

zone, or *UZSI*. Instead, the *a* value is used as a constant value for E/ET.

3.2 Snow

All land classes have a snowpack storage, which collects frozen precipitation and releases it later as

snow melt. Whether precipitation is snow or rain is defined in WATFLOOD based on the air temperature

when it is falling. Snowfall covers the entire area of a grid and the volume of the snowpack increases

with subsequent snowfalls. Sublimation removes water from a grids snowpack. Snowmelt is modeled

using the air temperature. When the air temperature exceeds the specified melting temperature for a

given land class (*base* in WATFLOOD), frozen water melts and the snowpack area can decrease. The

snowpack contains both liquid and frozen water during the ripening phase, with liquid water coming

either from snowmelt or rain on snow. When the amount of liquid water in the snowpack exceeds the

storage capacity, melt water flows into the surface storage, or into the channel or connected wetland

for those two classes. The mass balance for the snowpack is illustrated in Figure 3.3.
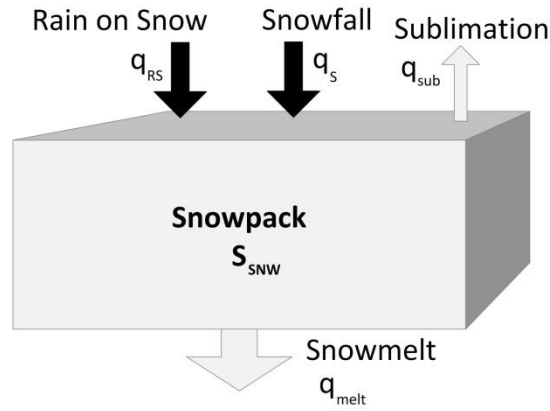
Figure 3.3 Snowpack mass balance

The isotope volume added to the snowpack, I_{SNW}^{iso}, is a function of the precipitation over the time interval:

$$I_{SNW}^{iso} = \left(C_{RS}^{iso} q_{RS} + C_S^{iso} q_S\right)\Delta t \qquad (3.11)$$

Where C_S^{iso} and C_{RS}^{iso} are the isotopic concentrations of snow and rain and q_S and q_{RS} are the inflows from snow and rain on the snowpack. The water volume removed from the snowpack, Q_{SNW}, includes snowmelt, q_{melt}, and sublimation, q_{sub}:

$$Q_{SNW} = (q_{melt} + q_{sub})\Delta t \qquad (3.12)$$

The volume of water stored in the snowpack at the end of the time interval, $S_{SNW,2}$, is known because WATFLOOD`s calculations for the time interval are completed prior to the isotope module run. The volume of isotopes in the snowpack at the end of the time interval, $S_{SNW,2}^{iso}$, can therefore be directly computed as:

$$S_{SNW,2}^{iso} = \frac{S_{SNW,1}^{iso} + I_{SNW}^{iso}}{1 + Q_{SNW}/S_{SNW,2}} \qquad (3.13)$$

Where $S_{SNW,1}^{iso}$ is the volume of isotopes in the snowpack at the beginning of the time interval. The concentration of isotopes in the snowpack, C_{SNW}^{iso}, is calculated using the storage volumes at the end of the time interval:

$$C_{SNW}^{iso} = \frac{S_{SNW,2}^{iso}}{S_{SNW,2}}$$

(3.14)

The concentration of the snowpack is also the concentration of the snowmelt and sublimation fluxes removed from the snowpack based on the assumption that fractionation from melt and sublimation is negligible. The snowpack composition is constant through the pack depth, and through the time interval, based on an assumption of instant and complete mixing of the snowpack through its depth. While this is not physically possible, as the pack is solid water and does not readily mix, the implication of this assumption is that melt and sublimation occur evenly through the entire snowpack depth.

3.3 Land

Land classes (except for the connected wetland and water classes) have surface and upper soil storages. All upper soil storages are connected to the lower soil storage for the grid cell.

3.3.1 Surface

The surface storage represents water ponded on the surface in small depressions. The surface storage is divided into snow-covered and bare areas, with the snow-covered area defined by the area of the snowpack. Melt water from the snowpack and rainfall on the bare area are added to the surface storage, along with glacier melt if it is present in the grid cell. The rainfall reaching the surface storage may be reduced by interception capacity (defined by WATFLOOD parameters). Infiltration from the surface to the upper zone of soil is calculated based on the soil properties and the depth of ponded water. If the volume of water in the surface storage exceeds the allowable depression storage for the

land class, the excess becomes direct runoff. Surface storage is highly transient, so evaporation is

assumed to be negligible. Figure 3.4 shows a surface storage with all possible fluxes.
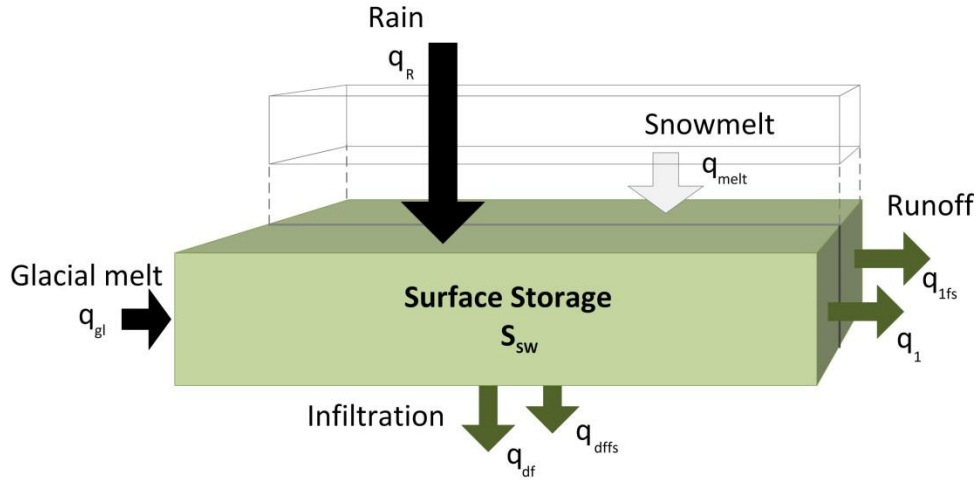
Figure 3.4 Surface storage mass balance

The isotope volume added to the surface compartment, I_{SW}^{iso}, includes rain on bare ground, q_R,

snowmelt, q_{melt}, and glacial melt, q_{gl}:

$$I_{SW}^{iso} = \left(C_R^{iso} q_R + C_{SNW}^{iso} q_{melt} + C_{gl}^{iso} q_{gl} \right) \Delta t \qquad (3.15)$$

Where C_R^{iso} is the isotope concentration of rain, C_{SNW}^{iso} is the isotope concentration of snowmelt and

C_{gl}^{iso} is the isotope concentration of glacial melt. The volume of water removed from surface storage,

Q_{SW}, includes infiltration from bare and frozen soil, q_1 and q_{1fs}, and lateral runoff into the channel or

wetlands from bare and frozen soil, q_{df} and q_{dffs} :

$$Q_{SW} = \left(q_1 + q_{1fs} + q_{df} + q_{dffs} \right) \Delta t \qquad (3.16)$$

The volume of water in the surface compartment at the end of the time interval, $S_{SW,2}$, is known from

the calculations completed in WATFLOOD before the isotope module is run. Two separate cases exist for

the surface isotope mass balance, depending on the water volume retained in the surface compartment.

If the water volume is greater than zero, the isotope volume in the surface compartment at the end of the time interval, $S_{SW,2}^{iso}$, is calculated using the isotope volume in the surface compartment at the beginning of the time interval, $S_{SW,1}^{iso}$:

$$S_{SW,2}^{iso} = \frac{S_{SW,1}^{iso} + I_{SW}^{iso}}{1 + Q_{SW}/S_{SW,2}} \tag{3.17}$$

The concentration of the outflow from surface storage, C_{SW}^{iso}, is then:

$$C_{SW}^{iso} = \frac{S_{SW,2}^{iso}}{S_{SW,2}} \tag{3.18}$$

In the case where there is no water volume remaining at the end of the time interval (i.e., outflow exceeds storage), $S_{SW,2}$ will be equal to zero and the isotope volume will be:

$$S_{SW,2}^{iso} = 0 \tag{3.19}$$

However, the outflow from the surface compartment may still be positive, either from the infiltration of old storage, new inflows, or some combination of the two. The concentration of the outflow from surface storage is then:

$$C_{SW}^{iso} = \frac{S_{SW,1}^{iso} + I_{SW}^{iso}}{S_{SW,1} + I_{SW}} \tag{3.20}$$

Where $S_{SW,1}$ is the water volume in the surface compartment at the beginning of the time interval, and I_{SW} is the volume of water added over the time interval:

$$I_{SW} = (q_R + q_{melt} + q_{gl})\Delta t \tag{3.21}$$

The surface water isotope model assumes instant and complete mixing of the surface water and constant isotopic composition within the hourly time interval. These assumptions are reasonable, as the surface water storage volume is small and very shallow and likely turbulent, such that any new inputs

(which would be of constant composition across the GRU area) would be mixed throughout the surface water depth immediately.

3.3.2 Upper zone

The upper zone soil storage resides immediately below the land surface compartment, and may be either saturated or unsaturated. As with the surface storage, the upper zone is divided into snow-covered and bare areas, with the snow-covered area defined by the snowpack area. Water is added to the upper zone via infiltration from the surface storage for the land class. Evapotranspiration is removed from the upper zone, with losses being a function of the amount of water stored in the upper zone (i.e., more storage resulting in higher evapotranspiration rates). If sufficient water is stored in the upper zone, vertical drainage to the lower zone storage and lateral interflow will both remove water from the upper zone, controlled by WATFLOOD parameters. An upper zone storage compartment with all possible fluxes is shown in Figure 3.5.
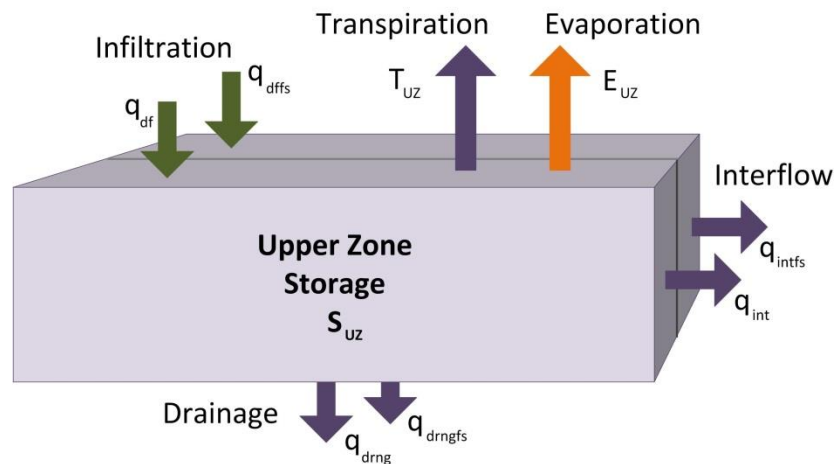
Figure 3.5 Upper zone soil storage mass balance

The isotope volume entering the upper zone, I_{UZ}^{iso}, includes both infiltration from bare soil, q_{df}, and from frozen soil, q_{dffs}:

$$I_{UZ}^{iso} = C_{SW}^{iso}(q_{df} + q_{dffs})\Delta t \qquad (3.22)$$

The isotopic concentration of the inflow, C_{SW}^{iso}, is the concentration of the surface storage. The volume of

water moved from the upper zone to other compartments, Q_{UZ}, is the sum of vertical drainage and

lateral interflow:

$$Q_{UZ} = (q_{int} + q_{intfs} + q_{drng} + q_{drngfs})\Delta t \qquad (3.23)$$

Where q_{int} and q_{intfs} are interflow from bare and frozen soil, and q_{drng} and q_{drngfs} are drainage from

bare and frozen soil. The volume of water both transpired, T_{UZ}, and evaporated, E_{UZ}, from the upper

zone over the time interval are also removed (see 3.1.2 for split between evaporation and

transpiration). Transpiration is assumed to be non-fractionating in isoWATFLOOD, with transpired water

having the same isotopic concentration as the upper zone storage. Evaporated water is given the

isotopic concentration $C_{UZ,E}^{iso}$, (see 3.1.1 for evaporative fractionation calculations). The volume of

isotopes in the upper zone at the end of the time interval, $S_{UZ,2}^{iso}$, can be calculated directly, since all

other variables; including $S_{UZ,1}^{iso}$, the volume of isotopes in the upper zone at the beginning of the time

interval and $S_{UZ,2}$, the water volume in the upper zone at the end of the time interval; are known:

$$S_{UZ,2}^{iso} = \frac{S_{UZ,1}^{iso} + I_{UZ}^{iso} - C_{UZ,E}^{iso}E_{UZ}}{1 + (Q_{UZ} + T_{UZ})/S_{UZ,2}} \qquad (3.24)$$

The isotopic concentration of the drainage and interflow depends on the concentration of the upper

zone storage:

$$C_{UZ}^{iso} = \frac{S_{UZ,2}^{iso}}{S_{UZ,2}} \qquad (3.25)$$

The upper zone isotope model also assumes instant and complete mixing through the upper zone depth

in a given time step (i.e., 1 hour), such that the source water for the evaporated water isotope

composition is fully mixed. This assumption is not entirely realistic when new water is added to the

storage in a given time step since the rate of movement through the soil will be less than needed for complete mixing. The isotopic composition of the upper zone storage and fluxes are assumed to be constant through the one hour simulation time interval, and meteorological conditions affecting evaporative fractionation are also assumed to be constant through this period. Given the resolution of most commonly available climate data inputs, this assumption is realistic. The isotopic composition of the lower zone storage is assumed to have no effect on the upper zone composition.

It is also assumed that there will always be water in the upper zone (at least, based on WATFLOOD, the PWP depth). In rare cases, when there is low upper zone retention and high interflow coefficients, this may be violated, resulting in no simulated values from then on.

3.3.3 Lower zone

The lower soil zone represents the saturated depth unaffected by surface conditions, such that land cover (vegetation) or snow cover do not separate the lower zone into distinct storages. All upper soil zone storages in a grid cell drain into the same lower zone storage. This lower zone storage has a single outflow, the baseflow, which increases as the volume stored in the lower zone increases. Deep groundwater flows either into or out of a grid are not currently included in the WATFLOOD or isoWATFLOOD models. A lower zone storage compartment is illustrated in Figure 3.6.
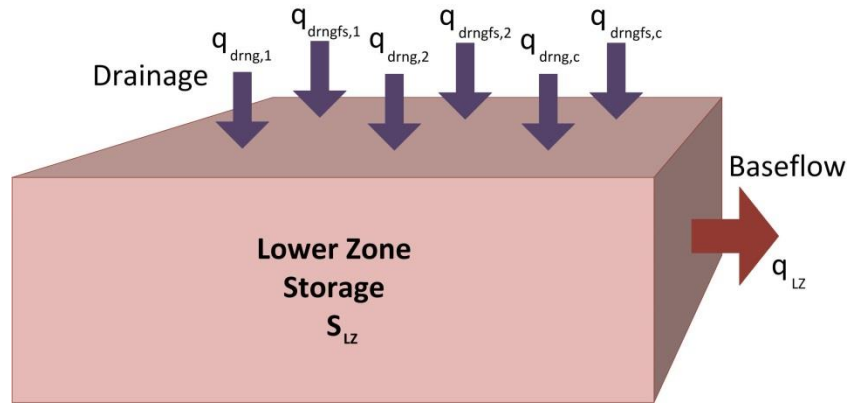
Figure 3.6 Lower soil zone storage mass balance

All drainages originating in upper zone storages, including bare soil drainage, q_{drng}, and frozen soil drainage, q_{drngfs}, are included in the isotope volume added to the lower zone, I_{LZ}^{iso}:

$$I_{LZ}^{iso} = \sum_{i=1}^{c} C_{UZ,i}^{iso}(q_{drng,i} + q_{drngfs,i})\Delta t$$

(3.26)

Where c is the number of land classes with upper zone storages and C_{UZ}^{iso} is the isotopic concentration of the upper zone. The only outflow from the lower zone is the baseflow, q_{lz}, so the volume of water removed from the lower zone storage, Q_{LZ}, is:

$$Q_{LZ} = q_{lz}\Delta t$$

(3.27)

The volume of isotopes in the lower zone at the beginning of the time interval, $S_{LZ,1}^{iso}$, and the volume of water in the lower zone at the end of the time interval, $S_{LZ,2}$, are known from WATFLOOD, so the volume of isotopes in the lower zone storage can be calculated directly:

$$S_{LZ,2}^{iso} = \frac{S_{LZ,1}^{iso} + I_{LZ}^{iso}}{1 + Q_{LZ}/S_{LZ,2}}$$

(3.28)

The baseflow concentration, C_{LZ}^{iso}, depends on the lower zone storage at the end of the time interval:

$$C_{LZ}^{iso} = \frac{S_{LZ,2}^{iso}}{S_{LZ,2}}$$

<div align="right">(3.29)</div>

The lower zone storage is assumed to be instantly and completely mixed regardless of the storage volume, and the isotopic composition of the lower zone storage and outflow are assumed to be unvarying through the one hour simulation time interval. The instant and completing mixing assumption for the lower zone will be less accurate in the timestep where new inflows are added to the stored volume, as the groundwater volume can be very large.

3.4   Connected wetland

The WATFLOOD model has optional connected wetlands to represent wetlands (fens, or riparian zones) directly connected to the river or stream. There is the potential for water to flow from the wetland to the stream, and for water to flow from the stream into the wetland (depending on the hydraulic gradient) (Kouwen, 2014). Water coming from the land is added to the connected wetland inflow, as the wetland is assumed to occur as a buffer along the edges of the channel. Connected wetlands have their own snow pack and the melt water is added directly to the wetland storage. Rain falling over the wetland is also added directly to the storage. Both evaporation and transpiration remove water from the wetland. A connected wetland storage compartment with all possible fluxes is shown in Figure 3.7, with the number of runoff and interflow fluxes dependent on the number of GRU in the grid cell.
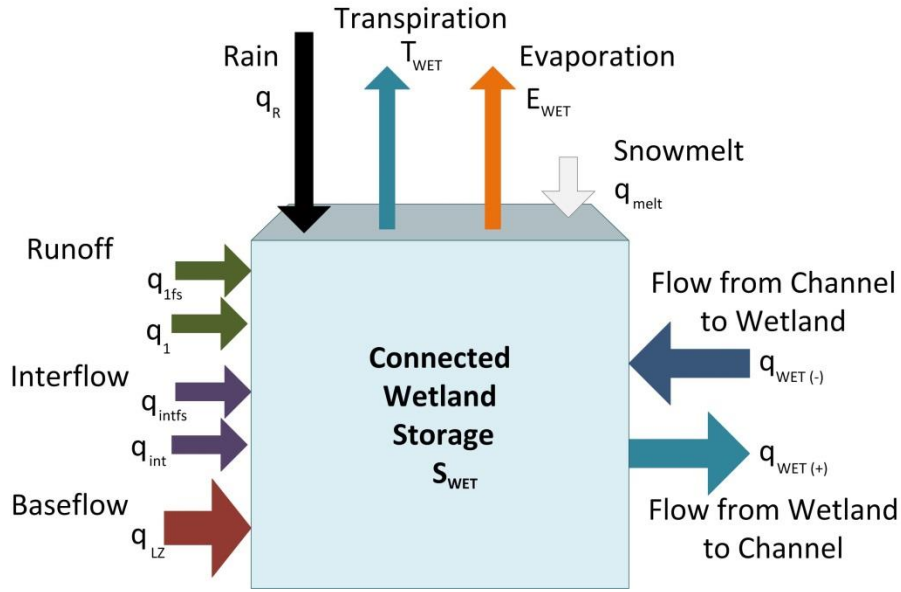
Figure 3.7 Connected wetland mass balance

The first step for calculation the isotopic composition of the connected wetland is to find the isotopic concentration of the wetland without evaporative enrichment. The inflow and outflow from the wetland depends on the direction of flow between the wetland and the channel. If the flow, q_{WET}, is positive, water is moving from the wetland to the channel. The volume of isotopes added to the wetland storage over the current time interval, $I_{WET,2}^{iso}$, includes isotopes from direct rainfall, q_R, snowmelt from the wetland snowpack, q_{melt}, interflow from bare and frozen soil, q_{int} and q_{intfs}, direct runoff from bare and frozen soil, q_1 and q_{1fs}, and baseflow, q_{lz}:

$$I_{WET,2}^{iso} = \left(C_R^{iso}q_R + C_{SNW}^{iso}q_{melt}\right)\Delta t + \sum_{i=1}^{c}\left(C_{UZ,i}^{iso}\left(q_{int,i} + q_{intfs,i}\right) + C_{SW,i}^{iso}\left(q_{1,i} + q_{1fs,i}\right)\right)\Delta t$$

$$+ C_{LZ}^{iso}q_{lz}\Delta t - C_{WET,1}^{iso}(E_{WET} + T_{WET})\Delta t$$

(3.30)

Where c is the number of terrestrial land classes, C_R^{iso} is the isotopic concentration of rainfall, C_{SNW}^{iso} is the isotopic concentration of snowmelt, C_{UZ}^{iso} is the isotopic concentration of the upper zone, C_{SW}^{iso} is the isotopic concentration of surface water, and C_{LZ}^{iso} is the isotopic concentration of the lower zone.

Evaporation, E_{WET}, and transpiration, T_{WET}, from the wetland are removed from the inflow; both are assumed to have the isotope concentration of the wetland storage at the beginning of the time interval, $C_{WET,1}^{iso}$ in the initial mass balance. Because evapotranspiration is removed from the inflow, the volume of water removed from the wetland storage over the current time interval, $Q_{WET,2}$, depends only on the flow into the channel:

$$Q_{WET,2} = q_{WET}\Delta t \tag{3.31}$$

WATFLOOD calculates the storage in connected wetlands using the inflow and outflow from the current and the previous time interval. The isotope storage calculation must match the method used for water, but because the water mass balance has already been calculated for the time interval, the storage of isotopes in the wetland at the end of the time interval, $S_{WET,2}^{iso}$, can be calculated directly, without iteration:

$$S_{WET,2}^{iso} = \frac{S_{WET,1}^{iso} + \left(I_{WET,1}^{iso} + I_{WET,2}^{iso} - Q_{WET,1}^{iso}\right)/2}{1 + Q_{WET,2}/2S_{WET,2}} \tag{3.32}$$

where $S_{WET,1}^{iso}$ is the storage of isotopes in the wetland at the beginning of the time interval, $I_{WET,1}^{iso}$ is the volume of isotopes added to the wetland in the previous time interval, $Q_{WET,1}^{iso}$ is the volume of isotopes removed from the wetland in the previous time interval, and $S_{WET,2}$ is the storage of water in the wetland at the end of the time interval.

If the flow, q_{WET}, is negative, water is moving from the channel into the wetland. In this case, the volume added to the wetland also includes the wetland flow, which is subtracted since it is negative:

$$
\begin{aligned}
I_{WET,2}^{iso} = \left(C_R^{iso} q_R + C_{SNW}^{iso} q_{melt}\right)\Delta t + \sum_{i=1}^{c} \left(C_{UZ,i}^{iso}\left(q_{int,i} + q_{intfs,i}\right) + C_{SW,i}^{iso}\left(q_{1,i} + q_{1fs,i}\right)\right)\Delta t \\
+ C_{LZ}^{iso} q_{lz}\Delta t - C_{WET,1}^{iso}(E_{WET} + T_{WET})\Delta t - C_{STR,1}^{iso} q_{WET}\Delta t
\end{aligned}
\tag{3.33}
$$

The flow from the channel is assumed to have the same concentration as the streamflow in the previous time interval, $C_{STR,1}^{iso}$. Both evapotranspiration and the wetland-channel flow are included in $I_{WET,2}^{iso}$, therefore:

$$Q_{WET,2} = 0 \qquad (3.34)$$

The equation for $S_{WET,2}^{iso}$ is then simplified to:

$$S_{WET,2}^{iso} = S_{WET,1}^{iso} + \left(I_{WET,1}^{iso} + I_{WET,2}^{iso} - Q_{WET,1}^{iso}\right)/2 \qquad (3.35)$$

For either case the current isotopic concentration of the connected wetland storage, $C_{WET,2}^{iso}$, is:

$$C_{WET,2}^{iso} = \frac{S_{WET,2}^{iso}}{S_{WET,2}} \qquad (3.36)$$

The second step, which is only needed if there is evaporation occurring over the time interval, is to calculate the enrichment of the wetland due to evaporation. The isotopic concentration in delta format of an evaporating water body is calculated using the isotopic concentration of the connected wetland in delta format, $\delta_{WET,2}$:

$$\delta_{WET,E} = \delta_S - \left(\delta_S - \delta_{WET,2}\right)\left(\frac{S_{WET,2}}{S_{WET,1}}\right)^{-\left(1+m\frac{E}{I}\right)/\left(1-\frac{E}{I}-\frac{Q}{I}\right)} \qquad (3.37)$$

Where E is the volume of water evaporated over the time interval, I is the volume of water added to the wetland over the time interval from land outflows, precipitation, snowmelt and flow from the channel and Q is the volume of water removed from the wetland either into the stream channel or through transpiration. $S_{WET,2}$ is the volume of water at the end of the time interval, and $S_{WET,1}$ is the water volume at the beginning of the time interval. The value m is:

$$m = \frac{h - \varepsilon^*/\alpha^* - \varepsilon_k}{1 - h - \varepsilon_k} \qquad (3.38)$$

Where h is the fractional relative humidity, and ε^*, α^* and ε_k are calculated as described in Section

3.1.1. δ_S is the steady state isotopic concentration of the evaporating water body:

$$\delta_S = \frac{\delta_I + m\frac{E}{I}\delta^*}{1 + m\frac{E}{I}}$$

(3.39)

Where δ_I is the isotopic concentration of I in delta format, and δ^* is calculated as described in Section

3.1.1.

The enriched isotopic concentration is then used to update the isotope volume in storage, and the

isotope concentration of the storage:

$$S_{WET,2}^{iso} = C_{WET,E}^{iso}S_{WET,2}$$

(3.40)

$$C_{WET,2}^{iso} = C_{WET,E}^{iso}$$

(3.41)

Regardless of whether the wetland was enriched, the isotope outflow volume $Q_{WET,2}^{iso}$ is calculated for

the mass balance calculation in the subsequent time interval:

$$Q_{WET,2}^{iso} = C_{WET,2}^{iso}Q_{WET,2}$$

(3.42)

The connected wetland isotope model assumes that all inflows, whether precipitation or groundwater,

are instantly and completely mixed into the wetland storage. Meteorological conditions affecting

evaporative fractionation and the isotopic composition of the wetland outflow are assumed to be

constant over the simulation time interval, which may be hourly or sub-hourly depending on the routing

time interval.

3.5 Channel

The WATFLOOD hydrologic model routes flow through channels with a defined drainage network (with

drainage order determined by the elevation). Each grid contains one section of the total channel

storage, which can receive water from multiple upstream grids. Rain and snowmelt over the channel

area are added to the grid channel storage, as is the flow generated in the grid land area if connected

wetlands are not present, and evaporation is removed. If connected wetlands are included, flow from

the wetland to the channel is added to the storage, or removed if the flow reverses directions. The

outflow from the channel storage to the downstream receiving grid is calculated using hydrologic

storage routing, based on the continuity equation, and using the Manning equation to relate flow and

discharge. A channel storage compartment with fluxes is illustrated in Figure 3.8; there may be multiple

flows from upstream grids, depending on the drainage network.
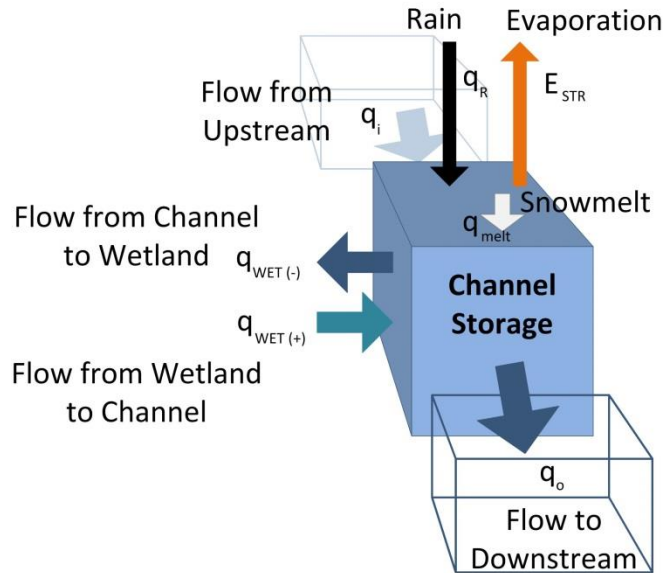
Figure 3.8 Channel mass balance

The flow of isotopes matches that of water, with the change in storage dependent on the inflow and

outflow at the beginning and end of the time interval. There are three possible cases for the calculation

of the incoming volume of isotopes for the current time interval, $I_{STR,2}^{iso}$. In the most common case, $I_{STR,2}^{iso}$

includes all isotopes coming from upstream grids, $Q_{STR,2,U/S}^{iso}$, and inflows from the connected wetland,

rainfall and snowmelt, with evaporation removed:

$$I_{STR,2}^{iso} = \sum Q_{STR,2,U/S}^{iso} + \left(C_{WET,2}^{iso} q_{WET} + C_R^{iso} q_R + C_{SNW}^{iso} q_{melt} - C_{STR,E}^{iso} E_{STR} \right) \Delta t \qquad (3.43)$$

Where $C_{WET,2}^{iso}$ is the isotopic concentration of the wetland at the end of the time interval (from

ISOwetland.f or ISO2Hwetland.f), q_{WET} is the flow between the channel and wetland, C_R^{iso} is the isotopic

concentration of rainfall, q_R is the rainfall over the channel, C_{SNW}^{iso} is the isotopic concentration of

snowmelt, q_{melt} is the snowmelt from the channel snowpack, $C_{STR,E}^{iso}$ is the isotopic concentration of the

evaporating moisture (see Section 3.1.1) and E_{STR} is the volume of water evaporated from the channel

over the time interval. The flow from the connected wetland can also be negative, such that channel

water is transferred to the connected wetland, with the wetland flow having the concentration of the

channel at the beginning of the time interval:

$$I_{STR,2}^{iso} = \sum Q_{STR,2,U/S}^{iso} + \left(C_{STR,1}^{iso} q_{WET} + C_R^{iso} q_R + C_{SNW}^{iso} q_{melt} - C_{STR,E}^{iso} E_{STR} \right) \Delta t \qquad (3.44)$$

Where $C_{STR,1}^{iso}$ is the isotopic concentration of the channel at the beginning of the time interval. Finally, if

connected wetlands are not used in the WATFLOOD model, water from the land area is added to the

channel directly:

$$I_{STR,2}^{iso} = \sum Q_{STR,2,U/S}^{iso} + \sum_{i=1}^{c} \left(C_{UZ,i}^{iso}(q_{int,i} + q_{intfs,i}) + C_{SW,i}^{iso}(q_{1,i} + q_{1fs,i}) \right) \Delta t + C_{LZ}^{iso} q_{lz} \Delta t$$
$$+ \left(C_R^{iso} q_R + C_{SNW}^{iso} q_{melt} - C_{STR,E}^{iso} E_{STR} \right) \Delta t \qquad (3.45)$$

Where c is the number of terrestrial land classes, q_{int} and q_{intfs} are interflow from bare and frozen soil,

C_{UZ}^{iso} is the isotopic concentration of the upper zone, C_{SW}^{iso} is the isotopic concentration of surface water,

q_1 and q_{1fs} are direct runoff from bare and frozen soil, C_{LZ}^{iso} is the isotopic concentration of the lower

zone and q_{lz} is baseflow. Only the outflow to the downstream grid, q_o, is included in the outflow

volume in the current time interval, $Q_{STR,2}$:

$$Q_{STR,2} = q_o \Delta t \qquad (3.46)$$

The isotope storage in the channel at the end of the time interval, $S_{STR,2}^{iso}$, is calculated from the isotope storage at the beginning of the time interval, $S_{STR,1}^{iso}$; the isotope volume added in the current and previous time intervals, $I_{STR,1}^{iso}$ and $I_{STR,2}^{iso}$; the isotope volume removed in the previous time interval, $Q_{STR,1}^{iso}$; and the water stored in the channel at the end of the time interval, $S_{STR,2}$:

$$S_{STR,2}^{iso} = \frac{S_{STR,1}^{iso} + \left(I_{STR,1}^{iso} + I_{STR,2}^{iso} - Q_{STR,1}^{iso}\right)/2}{1 + Q_{STR,2}/2S_{STR,2}} \tag{3.47}$$

The concentration of isotopes in the channel storage and outflow is:

$$C_{STR,2}^{iso} = \frac{S_{STR,2}^{iso}}{S_{STR,2}} \tag{3.48}$$

The volume of isotopes removed in the current time interval is also calculated for the mass balance in the subsequent interval:

$$Q_{STR,2}^{iso} = C_{STR,2}^{iso} Q_{STR,2} \tag{3.49}$$

All channel storage in a grid cell is assumed to be instantly and completely mixed, and the outflow composition is assumed to be constant for the simulation time interval, which may be hourly or sub-hourly depending on the routing time interval.

3.6 Lake or reservoir

Natural lakes and regulated reservoirs can be included in the model by designating grid cells (in WATFLOOD) as contributing to the same lake or reservoir. In these grid cells, the water land class is lake area, rather than channel area as it is in standard grid cells. Lakes can be made up of a single or multiple grid cells, the water area in each cell being part of the same lake storage compartment. Any flow generated in the land area of a reservoir cell is added directly to the lake, along with flow from all upstream grid cells. Connected wetlands are not present in reservoir grid cells; all wetlands are treated as normal land classes with upper zone storages. As with channel storage, rainfall and snowmelt over

the water area are added directly to the lake, and evaporation is removed. There is a single discharge to the downstream receiving grid cell, with the flow rate typically determined from a user-specified storage-discharge relationship (Kouwen, 2014). A lake storage compartment with fluxes is illustrated in Figure 3.9; the number of runoff, interflow and base flow influxes depends on the number of GRU present in reservoir grid cells and the total number of grid cells included in the reservoir.
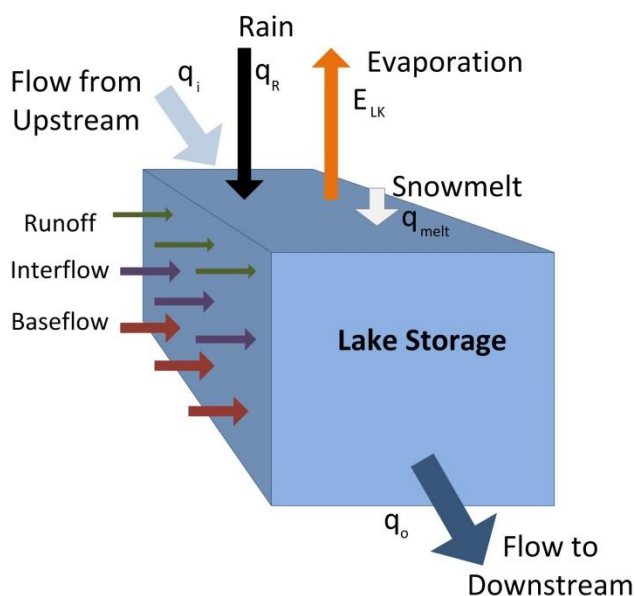
Figure 3.9 Reservoir mass balance

Evaporative fractionation is modeled using the equations for the time-dependent model lakes presented in Gibson (2002). Firstly, the isotopic concentration of the lake prior to evaporative enrichment is calculated from the mass balance in the lake. The isotope volume added into the lake in the current time interval, $I_{LK,2}^{iso}$; including upstream flows, $Q_{STR,2,U/S}^{iso}$; and flows generated from land in the lake grids, snowmelt, and rainfall:

$$I_{LK,2}^{iso} = \sum Q_{STR,2,U/S}^{iso} \tag{3.50}$$

$$+ \sum_{r=1}^{n} \left(\sum_{i=1}^{c} \left(C_{UZ,i,r}^{iso}(q_{int,i,r} + q_{intfs,i,r}) + C_{SW,i,r}^{iso}(q_{1,i,r} + q_{1fs,i,r}) \right) \Delta t \right.$$

$$\left. + C_{LZ,r}^{iso} q_{lz,r} \Delta t \right) + \left(C_R^{iso} q_R + C_{SNW}^{iso} q_{melt} - C_{LK,1}^{iso} E_{LK} \right) \Delta t$$

Where c is the number of non-water land classes, n is the number of grids in the lake, q_{int} and q_{intfs} are

interflow from bare and frozen soil, C_{UZ}^{iso} is the isotopic concentration of the upper zone, C_{SW}^{iso} is the

isotopic concentration of surface water, q_1 and q_{1fs} are direct runoff from bare and frozen soil, C_{LZ}^{iso} is

the isotopic concentration of the lower zone, q_{lz} is baseflow, C_R^{iso} is the isotopic concentration of

rainfall, q_R is the rainfall over the lake, C_{SNW}^{iso} is the isotopic concentration of snowmelt and q_{melt} is the

snowmelt from the lake snowpack. Evaporation over the time interval, E_{LK}, is assigned the

concentration of the lake at the beginning of the time interval, $C_{LK,1}^{iso}$, in the initial mass balance. Only

the outflow from the lake to the downstream receiving grid, q_o, is included in $Q_{LK,2}$, the volume of

water removed from the lake storage over the current time interval:

$$Q_{LK,2} = q_o \Delta t \tag{3.51}$$

The isotope storage in the lake at the end of the time interval, $S_{LK,2}^{iso}$ is first calculated from the isotope

storage at the beginning of the time interval, $S_{LK,1}^{iso}$, the isotope volume added in the current and

previous time interval, $I_{LK,1}^{iso}$ and $I_{LK,2}^{iso}$, the isotope volume removed in the previous time interval, $Q_{LK,1}^{iso}$,

and the water stored in the lake at the end of the time interval, $S_{LK,2}$:

$$S_{LK,2}^{iso} = \frac{S_{LK,1}^{iso} + \left(I_{LK,1}^{iso} + I_{LK,2}^{iso} - Q_{LK,1}^{iso} \right)/2}{1 + Q_{LK,2}/2S_{LK,2}} \tag{3.52}$$

The isotope concentration of the lake without evaporative enrichment is then calculated as:

$$C_{LK,2}^{iso} = \frac{S_{LK,2}^{iso}}{S_{LK,2}} \tag{3.53}$$

If any evaporation occurs over the time interval, a new enriched isotope concentration in delta notation,

$\delta_{LK,E}$, is calculated using the equations from Gibson (2002):

$$\delta_{LK,E} = \delta_S - \left(\delta_S - \delta_{LK,2}\right)e^{-\left(1+m\frac{E}{I}\right)\frac{It}{V}} \tag{3.54}$$

Where *E* is the volume of water evaporated over the time interval, *I* is the volume of water added to the

lake over the time interval from land outflows, precipitation, snowmelt and flow from upstream and *V* is

the volume of water in the lake at the beginning of the time interval. This equation assumes that the

lake volume is constant over the simulation time interval. $\delta_{LK,2}$ is the isotope concentration of the lake

without evaporative enrichment in delta notation. The value *m* is defined by Welhan and Fritz (1977)

(see equation 3.37). The enriched isotopic concentration is then used to update the isotope volume in

storage, and the isotope concentration of the storage:

$$S_{LK,2}^{iso} = C_{LK,E}^{iso}S_{LK,2} \tag{3.55}$$

$$C_{LK,2}^{iso} = C_{LK,E}^{iso} \tag{3.56}$$

Regardless of whether the lake was enriched, the isotope volume removed in the current time interval,

$Q_{LK,2}^{iso}$ is calculated for the mass balance calculation in the subsequent time interval:

$$Q_{LK,2}^{iso} = C_{LK,E}^{iso}Q_{LK,2} \tag{3.57}$$

The lake isotope simulation assumes instant and complete mixing of the lake, and constant isotopic

compositions for the lake storage and outflow over the simulation time interval, which may be hourly or

sub-hourly depending on the routing time interval. The meteorological conditions affecting evaporative

fractionation are assumed to be constant over the simulation time interval, and evaporation is assumed

to have no effect on the isotopic composition of atmospheric moisture.

4 The isoWATFLOOD code

This section provides a brief overview of the isoWATFLOOD code, and its connection to the WATFLOOD code.
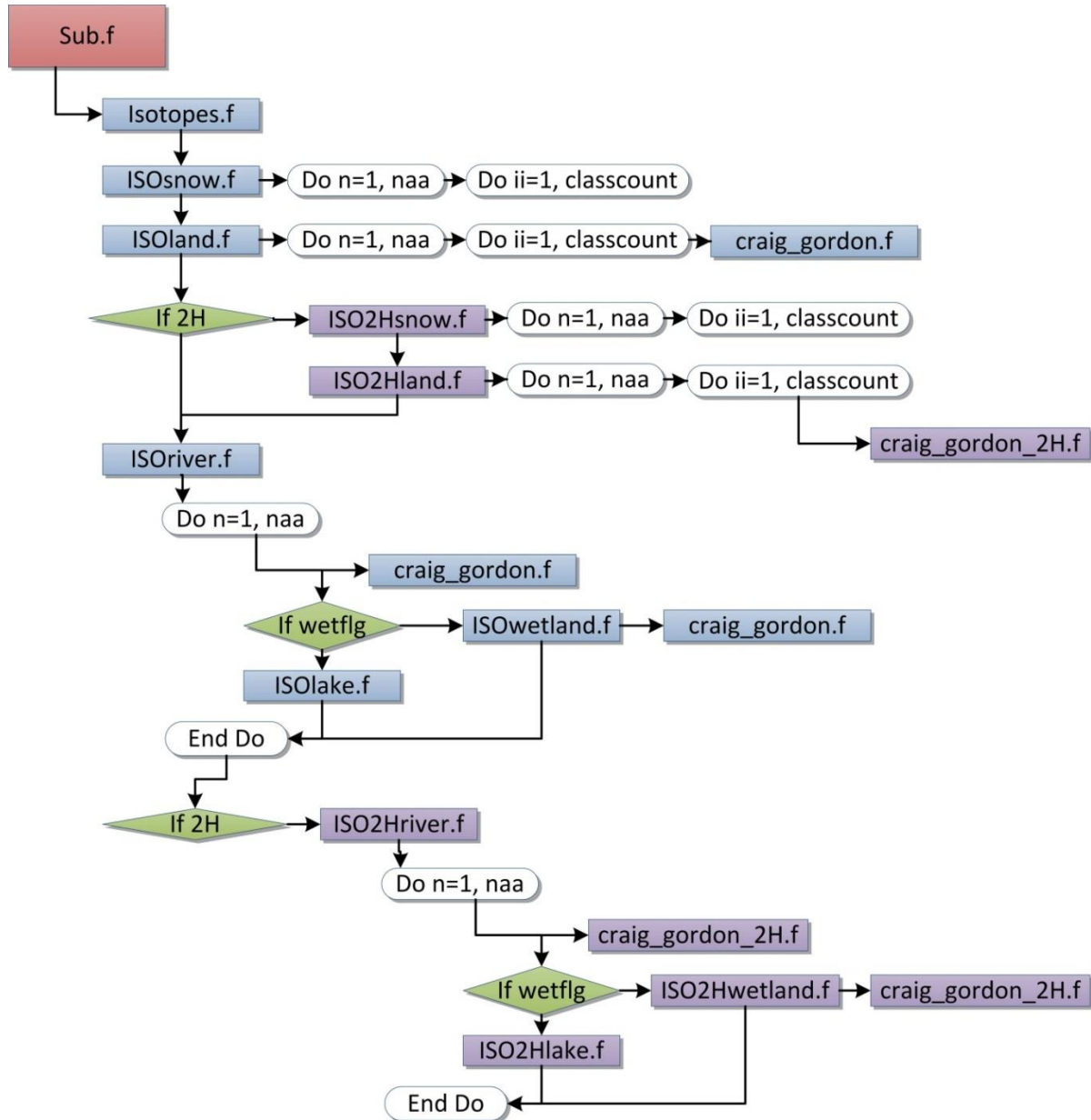
4.1 Stable water isotope simulation

Figure 4.1 Code structure for the isoWATFLOOD module

Figure 4.1 shows the structure of the isotope simulation code, with all isotope subroutines. The isotope module controlled by isotopes.f, which calls the primary isotope subroutines. The isotope subroutines are:

- ISOsnow.f: Calculates snowpack O^{18} isotope mass balances for all land classes in all grid cells and is called hourly.

- ISOland.f: Calculates surface water and upper zone O^{18} isotope mass balances for all land classes that have surface and upper zone compartments in all grid cells, and lower zone O^{18} isotope mass balances for all grid cells. It is also called hourly.

- ISOriver.f: Calculates stream channel O^{18} isotope mass balances in all grid cells. If connected wetlands are present, ISOwetland is called before calculating channel O^{18} isotope mass balance. If a grid cell is a lake cell, ISOlake is called instead of calculating channel O^{18} isotope mass balance. This routine is called hourly or sub-hourly, using the routing time step.

- ISOwetland.f: Calculates connected wetland O^{18} isotope mass balance for grid cells with connected wetland, and is called on the routing time step.

- ISOlake.f: Calculates the lake O^{18} isotope mass balance, and is called on the routing time-step.

- craig_gordon.f: Calculates the O^{18} isotopic composition of evaporated moisture. Called whenever there is evaporation (for the upper zone in ISOland, the stream or lake in ISOriver and the wetland in ISOwetland) to update the isotopic concentration of evaporating moisture from that storage.

- ISO2Hsnow.f: Calculates snowpack H^2 isotope mass balances for all land classes in all grid cells, and is called hourly. Only run if the dual-isotope simulation is turned on.

- ISO2Hland.f: Calculates surface water and upper zone H^2 isotope mass balances for all land classes that have surface and upper zone compartments in all grid cells, and lower zone H^2

isotope mass balances for all grid cells. It is also called hourly and only run if the dual-isotope simulation is turned on.

- ISO2Hriver.f: Calculates stream channel H^2 isotope mass balances in all grid cells. If connected wetlands are present, ISO2Hwetland is called before calculating channel H^2 isotope mass balance. If a grid cell is a lake cell, ISO2Hlake is called instead of calculating channel H^2 isotope mass balance. The routine is called hourly or sub-hourly, using the routing time step and is only run if the dual-isotope simulation is turned on.

- ISO2Hwetland.f: Calculates connected wetland H^2 isotope mass balance for grid cells with connected wetlands and is called on the routing time step. It is only run if the dual-isotope simulation is turned on.

- ISO2Hlake.f: Calculates the lake H^2 isotope mass balance on the routing time-step; only run if the dual-isotope simulation is turned on.

- craig_gordon_2H.f: Calculates the H^2 isotopic composition of evaporated moisture, and is called whenever there is evaporation (for the upper zone in ISO2Hland, the stream or lake in ISO2Hriver and the wetland in ISO2Hwetland).

Water and oxygen-18 volumes are calculated in the standard ISO subroutines, but only deuterium volumes are calculated in the ISO2H routines. The second isotope simulation therefore requires running the first.

4.2 Tie-ins to WATFLOOD

While the majority of isotope simulation code is located in the isoWATFLOOD code, the model does require some additional code in WATFLOOD subroutines, in order to track all required inputs and produce some output files.

- Areacg.f- Contains the declarations for the isoWATFLOOD variables.

- aet.f- Flags for evaporation, and splits evapotranspiration into transpiration and evaporation.

- lst.f- Error calculation and output for observed isotopic composition of streamflow.

- route.f- Change in treatment of evaporation variable storage when channel drying up.

- runof6.f- Stores additional variables for use in isoWATFLOOD.

- spl9.f- Allocation of some isoWATFLOOD related variables, and framework file output.

- sub.f- Calls isotopes.f, calculates relative humidity if there is no data files, and reads in initialization file, gridded isotopic precipitation data, gridded relative humidity, ET parameters, and framework basin combinations.

5 References

Gat, J., 1996. Oxygen and hydrogen isotopes in the hydrologic cycle. *Annual Review Earth Planet Science,* Volume 24, pp. 225-262.

Gibson, J., Birks, S. & Edwards, T., 2008. Global prediction of dA and d2H-d18O evaporation slopes for lakes and soil water accounting for seasonality. *Global Biogeochemical Cycles,* Volume 22, p. GB2031.

Gibson, J., Birks, S. & Yi, Y., 2016. Stable isotope mass balance of lakes: a contemporary perspective. *Quarternary Science Reviews,* Volume 131, pp. 316-328.

Gonfiantini, R., 1986. Environmental isotopes in lake studies. In: P. Fritz & J. Fontes, eds. *Handbook of environmental isotope geochemistry, the terrestrial environment.* New York: Elsevier, pp. 113-168.

Holmes, T., 2016. *Assessing the value of stable water isotopes in hydrologic modeling: a dual-isotope approach,* University of Manitoba: M.Sc Thesis.

Kouwen, N., 2014. *WATFLOOD/WATROUTE Hydrological Model Routing & Flood Forecasting System,* User's Manual, University of Waterloo, Waterloo, ON. www.watflood.ca.

Neff, T. A. M., 1996. *Mesoscale water balance of the boreal forest using operational evapotranspiration approaches in a distributed hydrologic model,* Waterloo: M.A.Sc Thesis, University of Waterloo.

Stadnyk-Falcone, T. A., 2008. *Mesoscale Hydrological Model Validation and Verification using Stable Water Isotopes: The isoWATFLOOD Model,* Waterloo: Ph.D. Thesis, University of Waterloo.

Stadnyk, T. A., Delavau, C., Kouwen, N. & Edwards, T. W. D., 2013. Towards hydrological model calibration and validation: simulation of stable water isotopes using the isoWATFLOOD model. *Hydrological Processes,* Volume 27, pp. 3791-3810.

Appendix A- IsoP

Written by Carly Delavau

Background Information and Folder Structure

Building off the existing WATFLOOD folder structure (shown below in **Error! Reference source not found.**, adapted from Kouwen, 2014), the *isoP* code and required files are housed under the main SPL directory in a folder titled *isoP_Code*. Within the same directory level is the main watershed folder (e.g. lnrb, simpson_ef, etc).

Moving down one level into the watershed folder, *isoP* requires a folder structure as detailed on the left
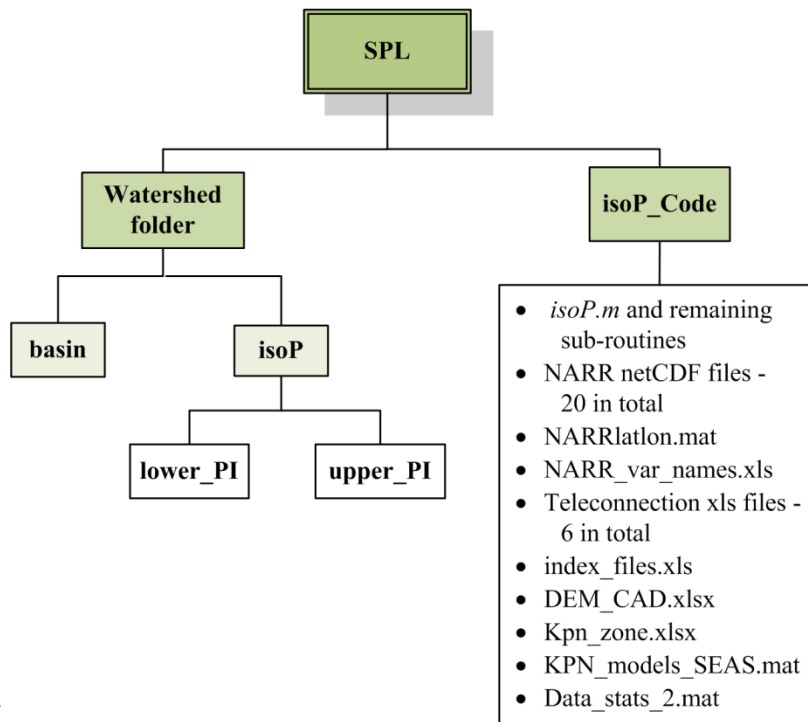
portion of

Figure *A-*. This includes an *SPL\watershed\basin* folder with the *_shd.r2c* file, and a *SPL\watershed\isoP* folder. For watersheds that have been previously setup, the *basin* folder and *_shd.r2c* file will already exist and only the *isoP* folder and sub-folders must be created.

If the user plans on simulating upper and lower prediction intervals, they are required to include two empty folders within the *SPL\watershed\isoP* folder: the folders must be named *upper_PI* and *lower_PI*. As the *isoP* program runs, it will eventually fill the *isoP* folder (and *upper_PI* and *lower_PI* folders, if applicable) with monthly y*yyymmdd_drn.r2c* files. R2C stands for 2D rectangular cell format. All gridded

WATFLOOD inputs are in this particular format (Kouwen, 2014); therefore for both simplicity and consistency, the *yyyymmdd_drn.r2c* files are produced in this format as well.
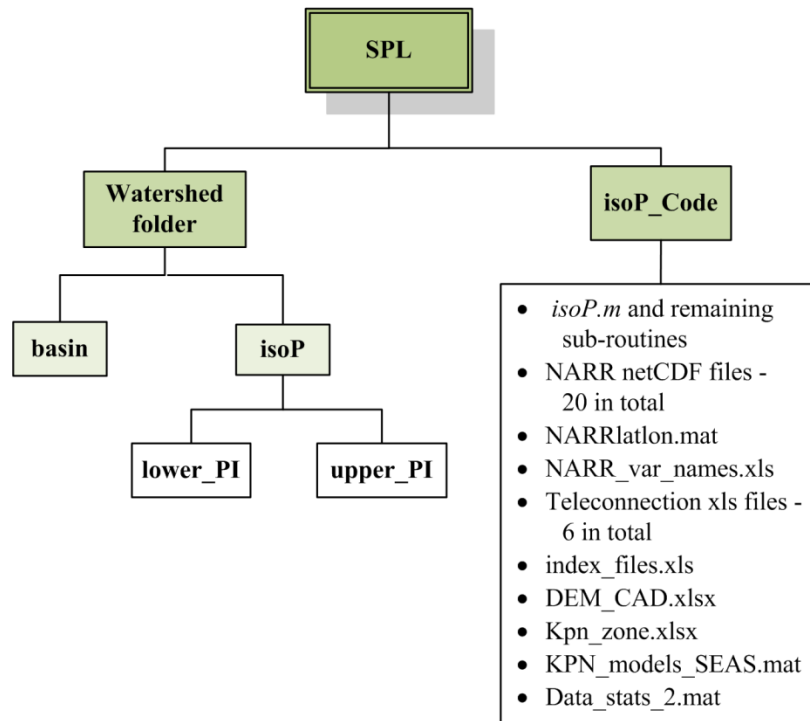

Figure A-1: Folder structure required by the isoP program, and the files housed in the isoP_Code folder on local drive:\SPL\isoP_Code.

Within the *SPL\isoP_Code* folder are a series of files that are read in and used by *isoP.m*. The first, and most important, are nine m-files that include the *isoP.m* code and remaining sub-routines. These are described in detail below.

The next set of files relate to NARR climate data. Twenty netCDF files (one for each climate variable) are included in this directory. It should be noted that these netCDF files will need to be updated from time to time as new data is incorporated by NOAA (National Oceanic and Atmospheric Administration). Additional information on this is provided below. The remaining two NARR files (*NARRlatlon.mat* and *NARR_var_names.xls*) are used to determine which NARR variables to read in, and what location to read the data in for.

The teleconnection excel files (AMO, AO, NAO, PDO, PNA, SOI) store monthly teleconnection indices from January 1950 until December 2014. This data will also need updating for post-2014 simulation. All

of the indices, with the exception of the PDO index, can be found on the NOAA website. PDO is available through the University of Washington's Joint Institute for the Study of Atmosphere and Ocean (JISAO) website (JISAO, 2016). *Index_files.xls* stores the list of teleconnection indices to read into the *isoP.m* program. Currently, this list contains all six of the aforementioned indices.

DEM_CAD.xls is a file of latitude and longitude coordinates with an estimate of the elevation at each xy grid. Elevations are obtained from the GTOPP30 digital elevation model (DEM) at a resolution of 30 arc seconds (approximately 1km). This mapping product is from a collaborative effort lead by the United States Geological Survey (USGS) and is available on their website (USGS, 1997). *Kpn_zone.xls* is a similar type of coordinate file and contains the Köppen-Geiger zone number at each point of a 17 arc-second grid, derived from a publically available global ACSII file of Köppen-Geiger climate classifications (Institute for Veterinary Public Health, 2011).

As previously described, empirical $\delta^{18}O_{ppt}$ models are developed for five of the 10 Köppen zones that exist in Canada (35, 42, 43, 47 and 62; Figure a), which account for almost 95% of Canada's contributing drainage area. It should be noted that outside of the Köppen zones outlined above, $\delta^{18}O_{ppt}$ cannot be simulated using the isoP modelling approach due to a lack of $\delta^{18}O_{ppt}$ data within these climate regions to develop empirical prediction models. If more data become available and/or the need exists, $\delta^{18}O_{ppt}$ prediction models may be developed in the additional unmodelled regions outlined on Figure b (Köppen zones 26, 32, 41, 46, 61) Conversely, one of the existing models could be applied outside of the zone of development; however this is not recommended as the models have not been tested or applied outside of their respective zones. Regions of Canada currently without a KPN model include some transboundary watersheds (Skagit and Milk Rivers), the downstream portions of the Bow and Red Deer Rivers, a section of the South Saskatchewan River near the Alberta/Saskatchewan border, the northern portion of Vancouver Island, and regions of Ellesmere and Axel Heiberg Islands in the Arctic Archipelago (Figure b).
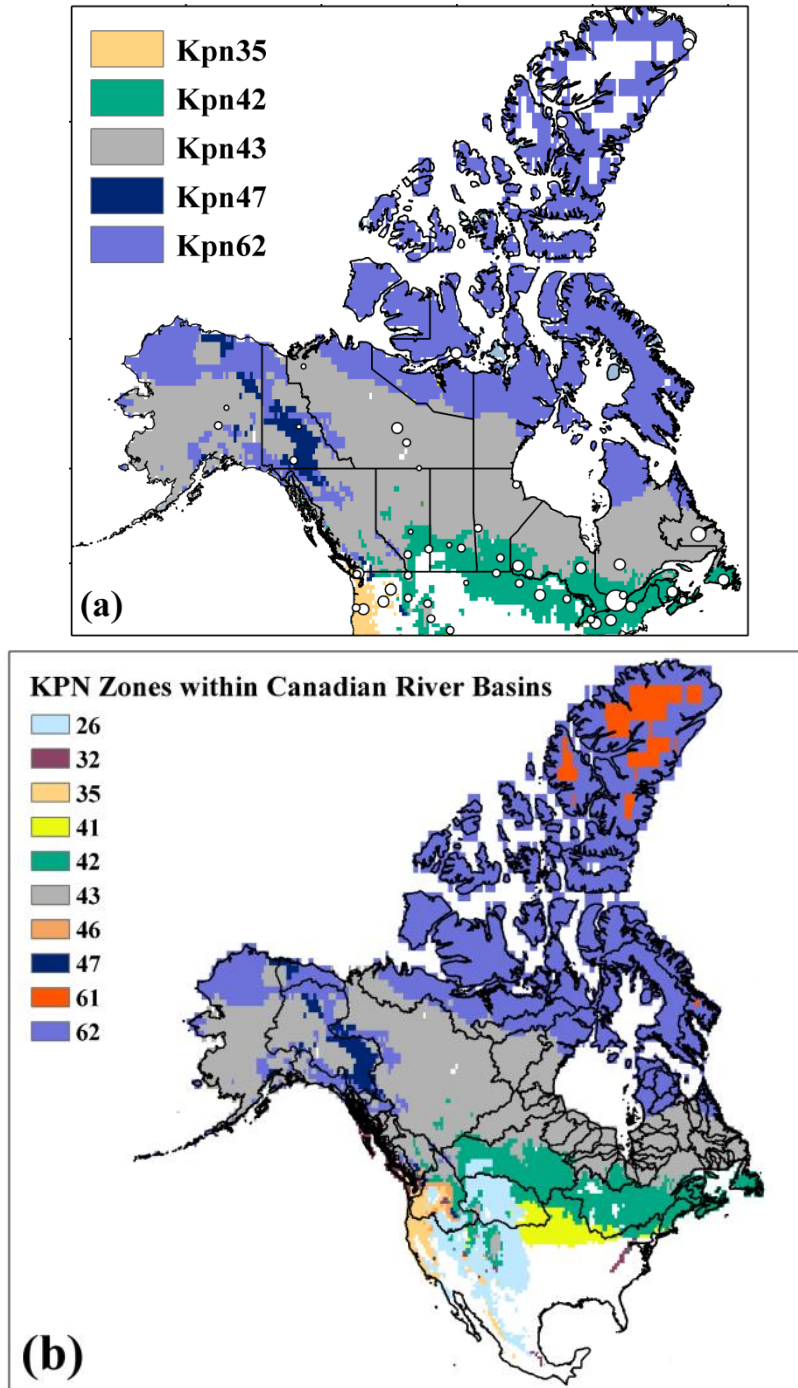
Figure A-2: (a) The five Köppen Zones for which $\delta^{18}O_{ppt}$ prediction models are developed, and (b) the ten Köppen Zones located within Canadian river basins.

Finally, *KPN_models_SEAS.mat* is a Matlab workspace storing the 12 empirical models for the Köppen Zone regionalization (as outlined in Delavau *et al.*, 2015). The models are stored in a LinearModel format

(Mathworks, 2016a) and the details of the models can be viewed (but not changed) in Matlab if required.

The *isoP* Program

The *isoP* program is a series of eight Matlab scripts (m-files) that are called from the main program module, *isoP.m* (Figure). The code was developed in version R2013a, however has been tested and successfully executed in version R2014b.

Figure provides a summary of the structure of the *isoP* code, and the inputs and outputs passed from one sub-routine to the next. The following section provides an overview of each of the eight sub-routines, as well as the main executing module, *isoP.m*.
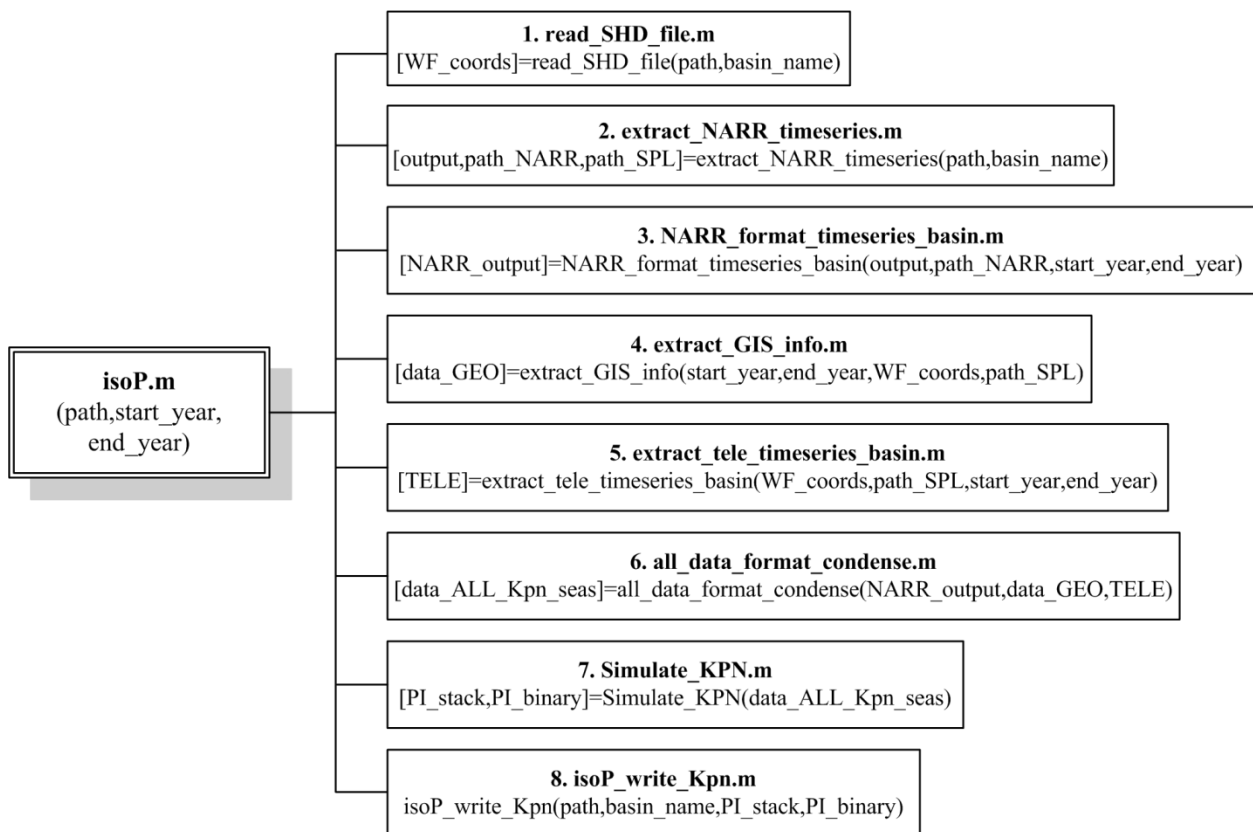

Figure A-3: IsoP program code structure.

isoP.m

isoP.m is the main module for the creation of gridded δ^{18}O$_{ppt}$ simulations. All other sub-routines are called from this main module in the order listed on Figure , beginning with reading in the *_shd.r2c* file, and completing with writing out the *yyyymmdd_drn.r2c* files for input into isoWATFLOOD.

To execute the isoP program, the user must first open Matlab and browse to the *SPL\isoP_Code* folder. Once in this folder, from the command window the user calls the isoP program, and is required to provide the path of the main watershed directory in the form of a text string (e.g. *'G:\spl\lnrb'*) and the start year and end year of the simulation they would like to carry out at that time, for example:

```
isoP('G\SPL\lnrb',2009,2012)
```

From this point forward, the program will provide updates as it progresses through each sub-routine, and the user will be prompted for input at least on one occasion, potentially twice (as will be described later within this documentation). As previously mentioned, at the end of program execution, gridded $\delta^{18}O_{ppt}$ files will be placed within the *SPL\watershed\isoP* folder.

The remainder of this document describes the function of each sub-routine, as well as any pertinent information required by the user of isoP.

read_SHD_file.m

This program reads in the *_shd.r2c* file and extracts the geographic information required to locate the basin, such as the x and y origins, and the number and size of the grids. This information is used to construct a grid of lat/long points at which the required data will be extracted at, and time series $\delta^{18}O_{ppt}$ will be simulated for. The points represent the "WATFLOOD grid", and are located at the centre of each grid point within the WATFLOOD model of interest (Figure).

IMPORTANT NOTE: the program will output this list of coordinates under *SPL\watershed\isoP\watershed_coords.xls.* If you re-run *isoP.m* without first deleting the existing *watershed_coords.xls* file, the program will vertically concatenate another set of coordinates below the coordinates form the first execution of the program. **Make sure if you are re-running *isoP.m* that you have first deleted this file.**
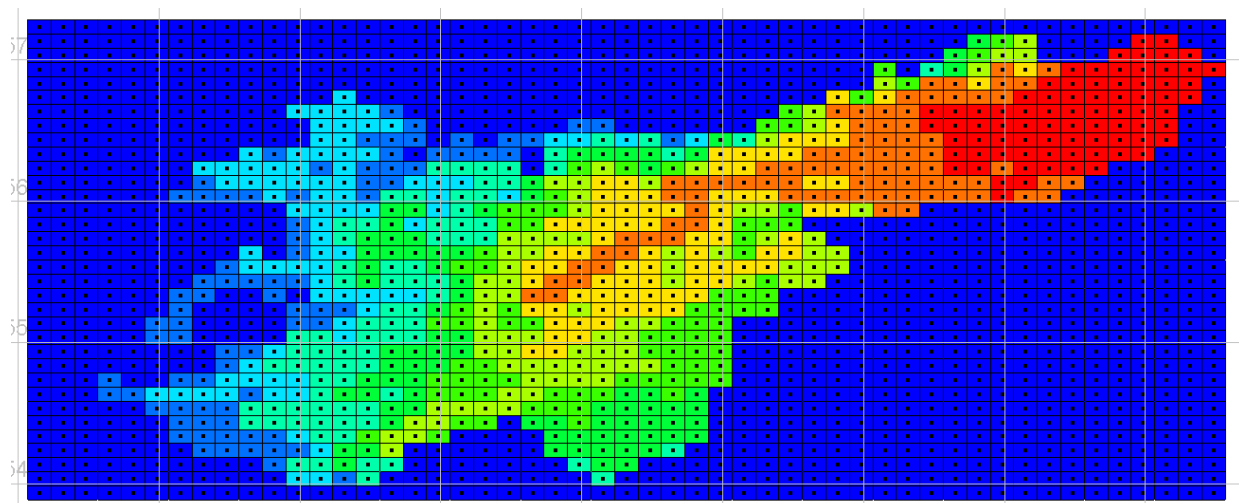
Figure A-4: The WATFLOOD grid for the Lower Nelson River watershed.

This is the first sub-routine that may prompt the user for feedback. If the watershed coordinate system is in Cartesian or UTM, then the user will be prompted to select what UTM zone the basin in located within. If the coordinate system is specified as lat/long, then there will be no user feedback required. The *isoP* program uses these coordinates as the locations to extract geographic and climate data, and to carry out all further computations, eventually simulating a time series of monthly $\delta^{18}O_{ppt}$ at each grid point. Upon completion of *read_SHD_file.m*, the program passes the WATFLOOD grid onto *extract_NARR_timeseries.m*.

Extract_NARR_timeseries.m

Extract_NARR_timeseries.m reads in the list of NARR climate variable names (*NARR_var_names.xls*) from the *SPL\isoP_Code* directory and using the coordinate grid established in *read_SHD_file.m*, it extracts all 20 NARR variables at the specified grid locations for the entirety of the time series within the netCDF (.nc extension) files (1979 – 2014). NARR data are provided in netCDF format, which is a multi-dimensional format where data are stored in layers made of up several dimensions (in this case, x, y and time). A complete directory and access to all NARR climate output can be found at:

http://www.esrl.noaa.gov/psd/data/gridded/data.narr.monolevel.html

For this particular application, monthly means are required. NARR data does not exist for pre-1979. If you need to update the netCDF files for more recent years, visit the website and download the most recent version of the files. Replace the previous files with the most up to date files. A list of the required

climate variables along with some important netCDF file information for each variable is provided in the *isoP\Documentation* folder. Once the netCDF files are updated (if required), place them in the *isoP_Code* folder. The program has been written dynamically so that it can adapt to accommodate updated data and changing time frames. Once *extract_NARR_timeseries.m* has completed extracting the climate time series at each of the WATFLOOD grids, it passes that output, along with two folder paths to *NARR_format_timeseries_basin.m*.

NARR_format_timeseries_basin.m

NARR_format_timeseries_basin.m formats the NARR climate variables into metric units, and for some variables, calculates monthly totals from monthly averages. The NARR output is then passed to *all_data_format_condense.m*.

extract_GIS_info.m

extract_GIS_info.m uses a nearest neighbour method (Mathworks, 2016b) to find the DEM grid point (from the previously described *DEM_CAD.xls*) that is closest to each WATFLOOD grid point. Once located, the program extracts the elevation from that grid and assigns it to the corresponding WATFLOOD grid. *extract_GIS_info.m* uses this same procedure to extract the Köppen Zone identifier (35, 42, 43, 47, or 62, as stipulated within the *Kpn_zone.xls* file) at each grid point as well. This identifier tells the program which zone(s) the watershed is in, and which seasonal regression models to utilize at each grid point. This program then passes the geographic output to *all_data_format_condense.m.*

extract_tele_timeseries_basin.m

extract_tele_timeseries_basin.m reads in the six teleconnection index time series as stipulated in the *index_files.xls* document (*AMO.xls*, *AO.xls*, *NAO.xls*, *PDO.xls*, *PNA.xls*, *SOI.xls*). These indices are not spatially variable, and therefore are the same at each WATFLOOD grid point. Currently, these indices have been updated until December 2014. Similarly to NARR, this data requires updating if post 2014 $\delta^{18}O_{ppt}$ simulations are required. As previously mentioned, this data can be found on the NOAA and JISAO sites.

_All_data_format_condense.m_

All_data_format_condense.m essentially brings the three major data sources together (NARR, geographic, and teleconnection), standardizes and condenses them into a single cell, which stores a matrix of data for each grid point. This sub-routine reads in *Data_stats_2.mat*, which is a workspace with the averages and standard deviations for all predictor variables used in model development. isoP uses this information to standardize the data before $\delta^{18}O_{ppt}$ simulation commences. This is required as the Koppen zone models are developed based on standardized data (for stability purposes), and use of these models requires data to be standardized, and is then converted back to normal reporting convention after $\delta^{18}O_{ppt}$ simulation.

_Simulate_KPN.m_

Simulate_KPN.m uses these data output by the previous sub-routine, alongside the *KPN_models_SEAS.mat* workspace to simulate a monthly time series of $\delta^{18}O_{ppt}$ at each WATFLOOD grid for the specified time frame. As each grid point is now associated with a Köppen zone number, this sub-routine utilizes that number to determine which regression model to employ. This sub-routine also prompts the user for feedback regarding if they would like to simulate $\delta^{18}O_{ppt}$ prediction intervals (i.e., account for input data uncertainty) utilizing the bootstrapping methodology outlined in Delavau *et al*. (2015).

The program asks the user the following:

```
Would you like to account for 18Oppt input uncertainty by calculating prediction intervals?
NOTE: this is a very time consuming, computationally heavy process. Y/N';
```

The user must respond with a Y to incorporate uncertainty, or an N to bypass. **As a warning**, it should be mentioned that bootstrapping prediction intervals adds significant time to your simulation- this is especially true for larger basins and longer time periods. If you require uncertainty bounds, it is best to let these simulations run overnight.

_isoP_write_Kpn.m_

isoP_write_Kpn.m reads in simulated $\delta^{18}O_{ppt}$ (and prediction intervals, if specified by the user required), and utilizing the standard WATFLOOD header, creates monthly *yyymmdd_drn.r2c* files for the specified

time period. Upon completion of the program, the main files are exported into the *SPL\watershed\isoP* folder. An example of the program output is included below. If upper and lower prediction intervals are simulated, these files will be output to the *SPL\watershed\upper_PI* and *SPL\watershed\lower_PI* folders, respectively. The naming convention of the files will still follow the aforementioned format (*yyyymmdd_drn.r2c*), as this is the file name isoWATFLOOD searches for when reading time series $\delta^{18}O_{ppt}$ forcing. However, within the WATFLOOD header of each file, the upper and lower prediction interval $\delta^{18}O_{ppt}$ simulations are named *18Oppt_KPN_90percentile* and *18Oppt_KPN_10percentile*, respectively.

References

Delavau, C., K. P. Chun, T. Stadnyk, S. J. Birks, and J. M. Welker (2015), North American precipitation isotope (d18O) zones revealed in time series modeling across Canada and northern United States, Water Resour. Res., 51, doi:10.1002/2014WR015687.

ECHMWF, (2016), ERA-40, Daily, Retrieved 07/11, 2016, from: http://apps.ecmwf.int/datasets/data/era40-daily/levtype=sfc/

Institute for Veterinary Public Health, (2011), World Map of the Köppen-Geiger climate classification updated, Retrieved 07/11, 2016, from: http://koeppen-geiger.vu-wien.ac.at/present.htm

JASAO, (2016), PDO index, Retrieved 07/11, 2016, from: http://jisao.washington.edu/pdo/PDO.latest.

Kouwen, N., (2014), WATFLOOD/WATROUTE Hydrological Model Routing and Flood Forecasting System. User's Manual, University of Waterloo, Waterloo, ON. www.watflood.ca.

Mathworks, (2016a), LinearModel class, Retrieved 07/11, 2016, from: http://www.mathworks.com/help/stats/linearmodel-class.html.

Mathworks, (2016b), NearestNeighbor, Retrieved 07/11, 2016, from: http://www.mathworks.com/help/matlab/ref/triangulation.nearestneighbor.html

NOAA, (2016a), Teleconnections - Spatially and temporally large-scale anomalies that influence the variability of the atmospheric circulation, Retrieved 07/11, 2016, from: http://www.ncdc.noaa.gov/teleconnections/

NOAA, (2016b), NCEP North American Regional Reanalysis: NARR, Retrieved 07/11, 2016, from: http://www.esrl.noaa.gov/psd/data/gridded/data.narr.monolevel.html.

USGS, (1997), Global 30 Arc-Second Elevation (GTOPO30) - Computational and Information Systems Laboratory Research Data Archive, Retrieved 07/11, 2016, from: https://lta.cr.usgs.gov/GTOPO30.)