PITLAKQ Documentation

Release 1.6.0

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CHAPTER 1

Installing PITLAKQ

1.1 A Python Program

PITLAKQ is written in Python and FORTRAN. It includes CE-QUAL-W2, a public domain code for hydrodynamics and water quality of lakes and reservoirs version 2.0. The latter is implemented in FORTRAN. Therefore, you need to install Python. You don't need to know how to program in Python in order to use PITLAKQ. However, it can be very useful to have some basic Python knowledge. There is no need to understand FORTRAN because the FORTRAN source code is complied into Python extension.

1.2 Installing of Miniconda or Anaconda

PITLAKQ relies on many external packages. Therefore, you need to install either Miniconda or Anaconda. Anaconda is a Python distribution with about 200 Python packages. It is a download of about 400 to 500 MB and will take about 2 GB on your hard drive. Miniconda is much much smaller and is therefore the preferred option. Both allow the comfortable installation of further packages as well as creating of so called environments. We will take advantage of both features.

PITLAKQ works on Microsoft Windows, Mac OS X, and Linux. It is packaged as a conda package.

Please download Miniconda. Please choose the right version for your operating system and take Python 3.9 (or higher, if available.) Install, following the instructions on the download web site. Please install only for you, with your user rights, **not** for all, which would require administrator rights. You can check if the installation was successful by opening a new terminal window. On Windows this can be achieved by typing `Anaconda Prompt` while hovering with the cursor over the Windows start button (lower left on a standard install) and clicking on the entry `Anaconda Prompt`. On Mac OS X and Linux a normal terminal window should work.

Now type:

```
python
```

You should see a response and >>> with a blinking curses.

Type:

```
>>> exit()
```

to terminate this Python session. You can also identify the installed Python version with:

```
python --version
```

1.3 Installing PITLAKQ

In a terminal window type:

```
conda config --add channels conda-forge
conda config --add channels msys2
conda config --add channels hydrocomputing
```

Currently, PITLAKQ is available for Python 3.9. If you have an installed Python with the same version (see above for finding out the current Python version), you may skipp the following steps that create a new environment. However, creating a new environment can be useful even if you already have the right Python version, because it allows to separate the Python installation for PITLAKQ from potential other Python applications. There are many more interesting details about conda environments.

1.3.1 Creating a *conda* environment

Type:

```
conda create -n pitlakq39 python=3.9
```

Answer "Yes" to the question(s) and type enter.

Next, type:

```
activate pitlakq39
```

On Linux or Mac this needs to be:

```
source activate pitlakq39
```

Note: There might be `pitlakq` packages for different Python versions. To find out, type:

```
conda search pitlakq
```

You should see an answer like this:

```
pitlakq   1.6    py39_0  hydrocomputing/win-64
```

This means version 1.6 of `pitlakq` is available for Python 3.9. If it would say `py36_x`, you should create an environment for Python 3.6. For example:

```
conda create -n pitlakq36 python=3.6
```

and activate accordingly:

```
activate pitlakq36
```

You can choose a different name but you need to be consistent. Here we use `pitlakq39`.

The prompt should change to `(pitlakq39)`.

1.3.2 Installing PITLAKQ

Type:

```
conda install pitlakq
```

Answer "Yes" to the question(s) and type enter.

This will take a while. After this is finished, you can check if `pitlakq` is properly installed by typing:

```
pitlakq
```

You should see something like this:

```
usage: run_pitlakq.py [-h] [-v] {init,run,create,introspect} ...

positional arguments:
  {init,run,create,introspect}
    init                initialize PITLAKQ and create `.pitlakq`
    run                 start the calculation of a model
    create              creates a new project folder with empty sub folders
    introspect          find out internals of PITLAKQ or your projects

optional arguments:
  -h, --help            show this help message and exit
  -v, --version         show version info and exit
```

1.4 Initializing PITLAKQ

PITLAKQ needs to know about two directories:

1. A path for the models
2. A temporary path to copy internal files during model execution

The easiest way to do let PITLAKQ know is to run:

```
pitlakq init
```

This will create a file named `.pitlakq` in your home directory. It will contain content like this:

```
model_path:
    C:\Users\<user_name>\pitlakq_work\models

ram_path:
    C:\Users\<user_name>\pitlakq_work\RAM

resources_path:
    <install_dir>\pitlakq\resources

template_path:
    <install_dir>\pitlakq\templates
```

Where `<user_name>` is your user name and `<install_dir>` is the directory `pitlakq` is installed in. You can change these paths, forcing PITLAKQ to look into a different directory for models (`model_path`) of using a different directory for temporary files (`ram_path`). This is an advanced technique and not needed for normal use.

You can place `.pitlakq` somewhere else. Just choose a directory and set the environmental variable `PITLAKQHOME` pointing this path.

1.5 Check if it runs

You can find out what projects are available with:

```
pitlakq introspect --projects
```

If the are no projects, you get an according message:

```
Projects:
Currently no projects.
```

Copy one or more projects, i.e. directories, from the provided tutorial projects into this path.

Now

```
pitlakq introspect --projects
```

should show you the projects you can run:

```
Projects:
     pitlakq_tut
     pitlakq_tut_gwh
     pitlakq_tut_loadin
     pitlakq_tut_qual
```

Choose a name from this list and run the model with:

```
pitlakq run pitlakq_tut
```

This should produce a lot of screen output. The model might run several minutes or longer. You can always stop a model run with the key combination <Ctrl><C>.

CHAPTER 2

PITLAKQ Tutorial

2.1 Preliminaries

This tutorial assumes that you have installed PITLAKQ properly and can run it from the command line as explained in the section *A Python Program*.

2.2 Running Python Scripts

Some of the task are done via Python scripts. There are two options:

1. Run the script saved in a file from the command-line via `python my_script.py`
2. Run from inside a Jupyter notebook.

For the second option type:

```
jupyter lab
```

A browser window will open. Click on the drop-down menu `New` and select `Python 3`. This will open a new notebook. Enter the Python commands into a cell and type `<Shift><Enter>`.

2.3 Create a new project

The first thing we need to do is to create new, still empty, project. Create a new project named `my_project` by typing:

```
pitlakq create my_project
```

Now you should have a directory inside your `models` directory with a layout that looks like this:

```
pitlakq_tut
|
+---balance
+---input
|   +---main
```

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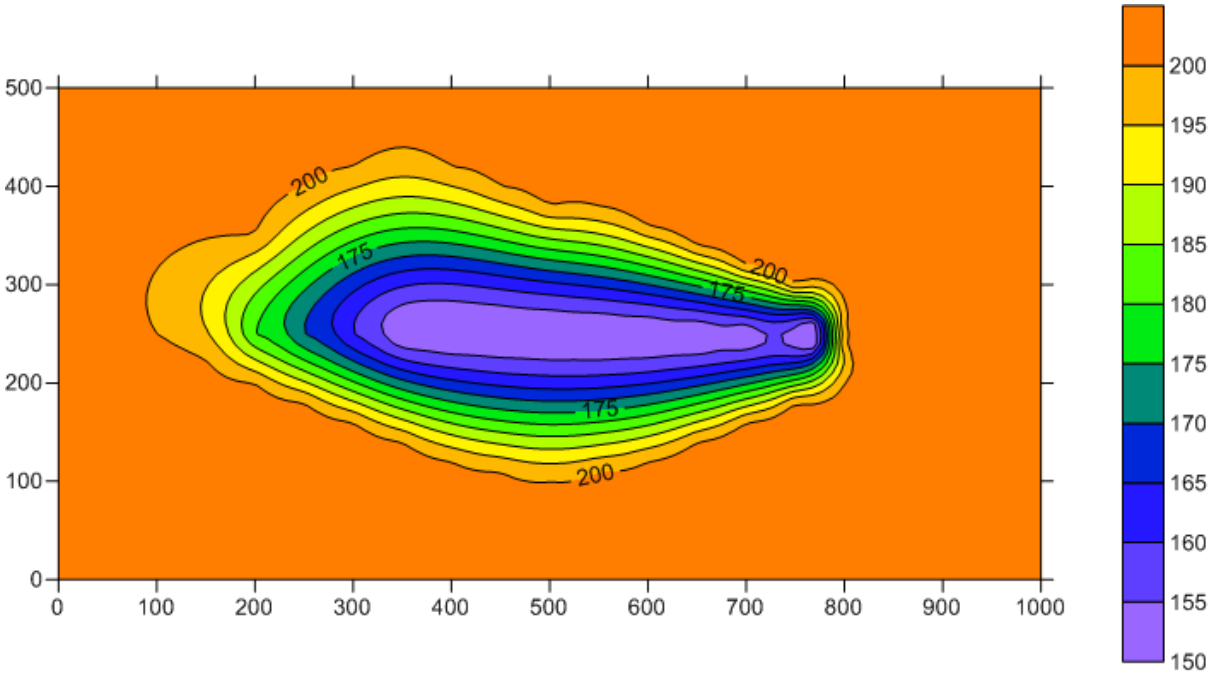
```
|   +---w2
+---output
|   +---sediment
|   +---w2
+---postprocessing
+---preprocessing
    +---input
    +---output
    +---tmp
```

2.4 Preprocess the bathymetry data

The bathymetry of the lake needs to be discretized. CE-QUAL-W2 and therefore PITLAKQ is two-dimensional along x and z. The y-direction is parametrized as cell width. Let's assume we have a lake that looks like the following picture.



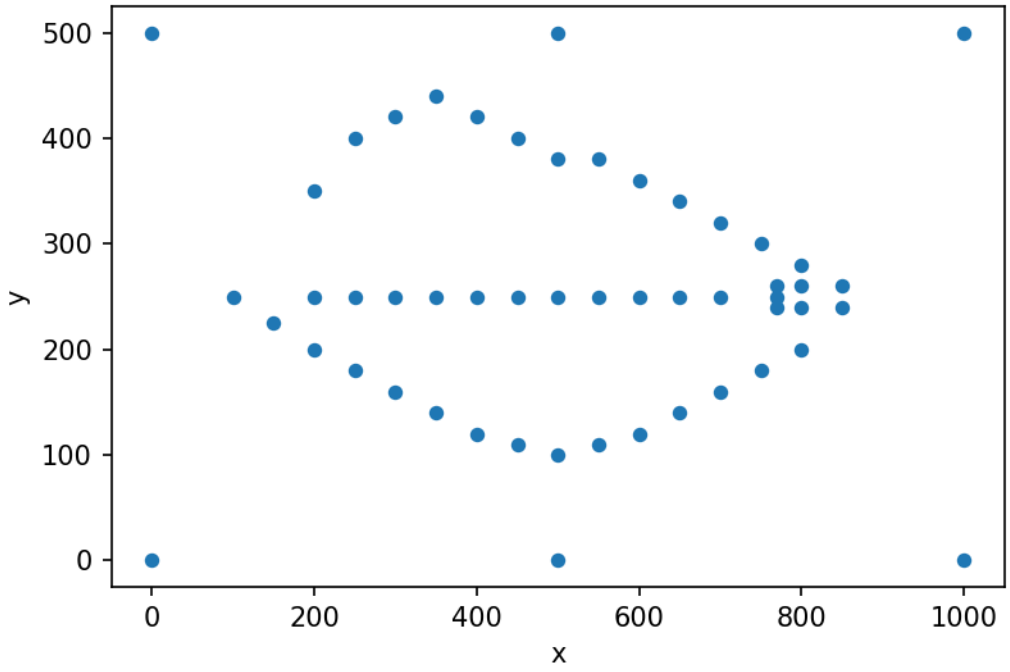
We save the gridded data that where used to generate this contour plot in a a SURFER 6 text file named `bath_asci.grd` (this default name can be changed with configuration options if needed). The file content look like this:

```
DSAA
100 51
0 1000
0 500
150.03254732465 214.3417454463
202.0000000052914 202.5142874143128 203.0243218381507
```

Currently, PITLAKQ only supports this file format. Adding more formats is possible.

If there are many points with lake bottom elevation data, linear interpolation may be accurate enough. PITLAKQ provides a pre-processing tool for creating a SURFER 6 text file with linear interpolation.

These are the data points that were used to create the above contour map:



You can create this plot with this code:

```
from pitlakq.preprocessing.create_bathgrid import show_points

show_points(project_name='pitlakq_tut', bath_data_file_name='bath_data.txt')
```

The file named `bath_data.txt` with the data looks like this:

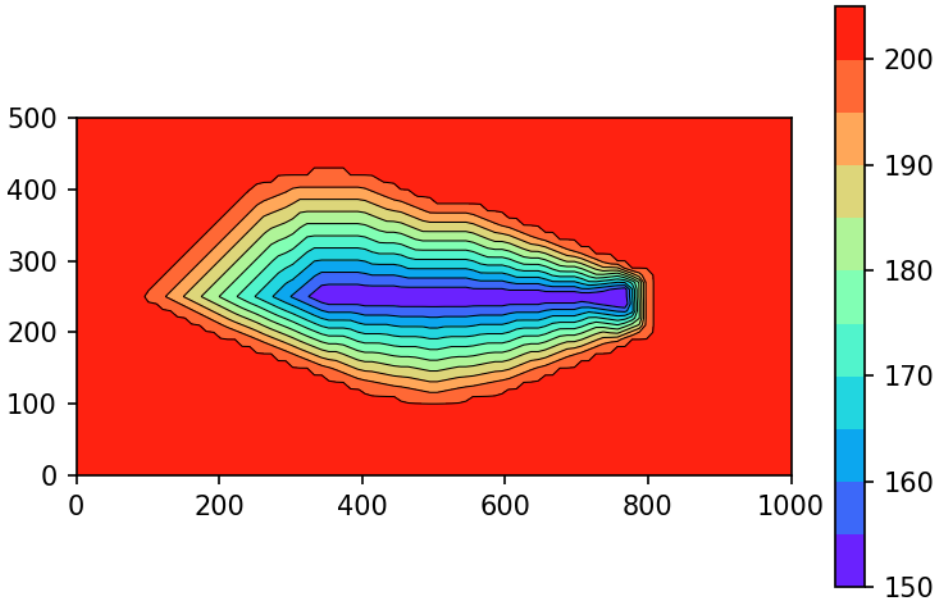
```
x y z
100 250 200
150 225 200
200 200 200
250 180 200
300 160 200
350 140 200
400 120 200
450 110 200
500 100 200
```

This Python program creates the SURFER file for the project `pitlakq_tut`, using 100 grid locations in x and 51 grid locations in y direction:

```
from pitlakq.preprocessing import create_bathgrid

create_bathgrid.main('pitlakq_tut', 'bath_data.txt', num_x=100, num_y=51)
```

The resulting grid file allows to generate this contour plot:



You can create this plot with this code:

```
from pitlakq.preprocessing.create_bathgrid import show_contours

show_contours(project_name='pitlakq_tut',
              bath_data_file_name='bath_data.txt',
              num_x=100, num_y=51, show_plot=True)
```

This looks similar to the SURFER-generated contour plot. An analyses shows that the surface area differs by about 6% and the lake volume by about 9%. The differences will be smaller for denser data points.

This tool can also be used to apply a different griding algorithm or program:

1. Save the griding result in x-y-z format such as in the file `bath_data.txt` with high resolution, i.e. many data points.
2. Apply the tool as described above with many interpolation points in x and y direction.

Alternatively, you can save the griding results directly in the SURFAER text format.

Now, we specify how our lake grid is going to look like. PITLAKQ currently supports either East-West or North-South directed grid layouts. This due to the (here not covered coupling to regularly gridded groundwater models. We place a file called `reservoir.txt` inside our directory `preprocessing/input`. This is the file content:

```
Columns         RW
1          100
2          200
3          300
4          400
5          500
6          600
7          700
8          800
9          900
Layers ZU
1 150
```

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```
2 151
3 152
4 153
5 154
6 155
7 156
8 157
9 158
10 159
11 160
12 161
13 162
14 163
15 164
16 165
17 166
18 167
19 168
20 169
21 170
22 171
23 172
24 173
25 174
26 175
27 176
28 177
29 178
30 179
31 180
32 181
33 182
34 183
35 184
36 185
37 186
38 187
39 188
40 189
41 190
42 191
43 192
44 193
45 194
46 195
47 196
48 197
49 198
50 199
51 200
```

We have 9 columns running from East to West with a distance of 100 each. We could vary the distance for each column (or segment). We also choose a equi-distant discretization in the vertical with 1 m per layer for 50 layers.

We supply more information in the file `preprocessing.yaml`:

```
bathymetry:
    initial_water_surface:
        value: 185
    max_water_surface:
        value: 200
```

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```
    orientations:
        value: [1.57]
```

This file is in the YAML format. The entry `orientations` here says that our first (sub)lake (we only have one sub-lake, which takes up the total lake) is in East-West direction.

Now we start our preprocessing program in a similar fashion as setting up a new project. Create file called `do_preprocessing.py` with this content:

```
from pitlakq.preprocessing import preprocess

preprocess.main('pitlakq_tut')
```

Replace the name `pitlakq_tut` with your project name. e.g. `my_project`.

Run it: `python do_preprocessing.py`. If everything goes well you will have a file named `bath.nc` in the `output` directory under `preprocessing`. This file `bath.nc` will be used as input for our model run. It is in netCDF format.

The file `bath.nc` can be converted into a human readable format with `ncdump bath.nc`:

```
netcdf bath {
dimensions:
        segment_lenght = 10 ;
        layer_height = 52 ;
variables:
        double segment_lenght(segment_lenght) ;
        double starting_water_level(segment_lenght) ;
        double segment_orientation(segment_lenght) ;
        double layer_height(layer_height) ;
        double cell_width(layer_height, segment_lenght) ;
data:

 segment_lenght = 100, 100, 100, 100, 100, 100, 100, 100, 100, 100 ;

 starting_water_level = 200, 200, 200, 200, 200, 200, 200, 200, 200, 200 ;

 segment_orientation = 9.99, 1.57, 1.57, 1.57, 1.57, 1.57, 1.57, 1.57, 1.57,
    9.99 ;

 layer_height = 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
    1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
    1, 1, 1, 1, 1, 1, 1, 1 ;

 cell_width =
  0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
  0, 75.6157364131951, 145.089953029845, 222.101772341138, 279.100893272702,
    279.22978559541, 222.26566587868, 141.54165990374, 27.8009873136653, 0,
  0, 64.9264248803291, 139.74267671092, 215.582246846721, 274.371310775368,
    274.382373960408, 216.115799371682, 134.929618517385, 23.2367196470327, 0,
...
```

We can visualize our lake grid. Create a file called `do_show_bath.py` with this content:

```
from pitlakq.postprocessing import show_bath

show_bath.main("output/bath.nc", bottom=150)
```

Run it: `python do_show_bath.py`. You should see a picture like this:

Copy the file `bath.nc` into the directory `/tut/pitlakq_tut/input/w2/`.

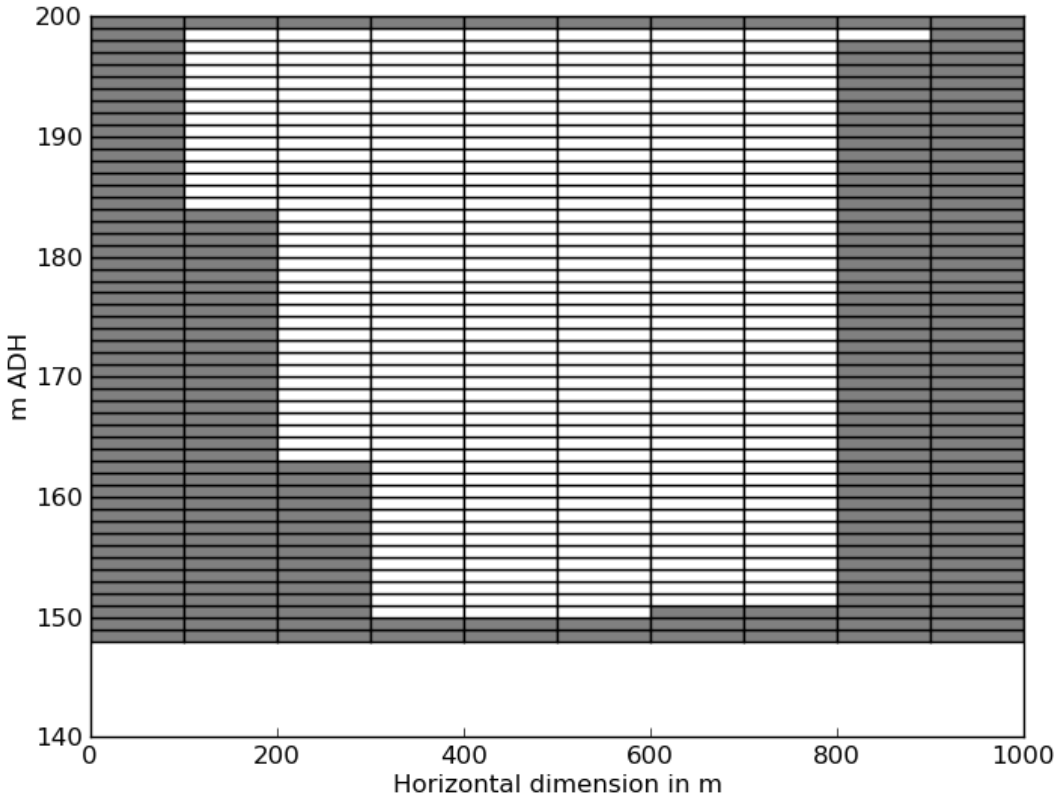

Fig. 1: Lake Bathymetry

2.5 Create the main input file

Now we need to create input files. PITLAKQ has many hundreds of input variables. Fortunately, for many applications sensible default will values can be used. In the `template` directory (see your `.pitlakq` for its location). You will find many templates of input files that contain default values. The following input files contain only a minimal, site-specific data set. Most of the input is taken from the defaults. Since we do only a very simple model (hydrodynamics only, no inflow, no precipitation no evaporation) to show the general principal how PITLAKQ works, this is approach is useful. For real-world applications the amount of (different) input data is typically much larger. We look at the many options that are involved when water quality calculations that couple chemical and biological process or treatment, erosion or sediment interactions come into play in later tutorials.

The input files are either in YAML or CSV (text in columns) format. Both formats are easily readable by humans and computers. The YAML files use the so called `!File` directive, which allows to include YAML into other YAML by referencing them rather than copying their content. This means the same file can be used from several other YAML files. Furthermore, the input can be spread over as many or a as few input files as desired. This gives great flexibility how to arrange the model best for each specific task.

This is a minimal PITLAKQ input file with information about the whole model. For an overview of all available options see the file `pitlakq.yaml` in the directory `<install_dir>/pitlakq/templates` (See *Initializing PITLAKQ* for details about where this path is located.):

```
general:
    start:
        value: 01.01.1998
    gw_start:
        value: 01.01.1998
    lake_time_step:
        value: .1
    number_of_gw_time_steps:
        value: 120
    dump_input:
        value: False
lake:
    max_water_surface:
        value: 200.0
    deepest_segment:
        value: 8
```

It is located in the directory where all your PITLAKQ projects are: `<my_project_name>/input/main/pitlakq.yaml`. Change `<my_project_name>` to the name of your project. This file has two groups `general` and `lake`. There are several more groups. But since we can use the default values from `<install_dir>\pitlakq\templates` we don't need to repeat them here. All values must be indented by four space, not tabs. Best is to turn the option in your editor to display non-printing characters. For example, with Notepad++ the menu `View | Show Symbol | Show White Space and TAB` allows you to make them visible. We always edit the attribute `value` there can be more attributes like `unit` but we don't use them here.

The value for `start` is `01.01.1998`. Note: Currently, dates always have to be in `DD.MM.YYYY`-format. Other formats would be possible but are not implemented yet. There is a second date for the start called `gw_start`. This is doe to historical reasons. Please use `gw_start` plus `number_of_gw_time_steps` to specify actual model run. A `gw_time_step` is by default one calendar month long. So `120` month will be exactly 10 years. Leap years are considered. The option `dump_input` make PITLAKQ to stop after reading all inputs to give you the possibility to dump the input, which is combination of the defaults and the user settings into one big YAML file. While this can take several seconds, it can be interesting to see these data.

The group `lake` allows you to give more information about the lake model. Here we only provide `max_water_surface` and `deepest_segment`. The later could be induced from the bathymetry data in `bath.nc` but for various reasons it can be supplied here.

2.6 Create a W2 input file

The file <my_project_name>/input/w2/w2.yaml has more entries:

```
general:
    titel:
        value: A simple PITLAKQ test model
bounds:
    number_of_segments:
        value: 10
    number_of_layers:
        value: 52
    number_of_constituents_segments:
        value: 10
    number_of_constituents_layers:
        value: 52
times:
    start:
        value: 01.01.1998
    end:
        value: 31.01.2009
---
!File
    name: bath.nc
    format: netcdf
    group_name: bathymetry
---
bathymetry:
    starting_water_level:
        value: 195.0
---
branch_geometry:
    branch_name:
        value:
            - test lake                              # no w2 variable
    branch_upstream_segments:
        value:
            - 2
    branch_downstream_segments:
        value:
            - 8


waterbody_coordinates:
    latitude:
        value: -33.21 # degrees
    longitude:
        value: 116.093  # degrees
    bottom_elevation:
        value: 150.0

tributaries:
    number_of_tributaries:
        value: 1
    tributary_names:
        value:
            - mytribname
    tributary_segment:
        value:
            - 5

ice_cover:
```

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```
    allow_ice_calculations:
        value: False

initial_conditions:
    initial_temperature:
        value: 10 # isothermal
    temperature:
        value: 10.0
    ice_thickness:
        value: 0.0

initial_concentrations:
    tracer:
        value: 10.0

---
!File
    name: meteorology.txt
    format: columns_whitespace
    group_name: meteorology


---
!File
    name: precipitation.txt
    format: columns_whitespace
    group_name: precipitation


---
!File
    name: precipitation_temperature.txt
    format: columns_whitespace
    group_name: precipitation_temperature


---
!File
    name: precipitation_concentration.txt
    format: columns_whitespace
    group_name: precipitation_concentration
```

Most of the information in this file are handed down to CE-QUAL-W2. In fact, the file `<install_dir>/pitlakq/templates/w2.yaml` has an attribute `w2_code_name` for most of the entries. This corresponds to variable name in CE-QUAL-W2. Therefore, more information about each of this entries can be found in the CE-QUAL-W2 manual or in FORTRAN source code.

We provide a model title and detailed information about the model bounds. Here we just repeat the 10 by 52 setup from our `bath.nc`. These dimensions will be used to check if other input values we will specify later are of the correct shape.

Then we start a new stream with `---` and include the file `bath.nc` with help of the directive `!File`- This file is in netCDF format and we would like it to be in the group `bathymetry`. The specification of this group allows to override parts of the data in `bath.nc`. We do this by providing an different value for the starting water label and set `starting_water_level` in the group `bathymetry` to 195.0 (meters). No need to go into the netCDF file and change data there.

The group `branch_geometry` provides information for each branch. We only have one branch in this case. Multi-branch setups are possible but more complicated and only recommend for complex cases such as complex geometries or large difference in lake water levels. The `branch_upstream_segments` is typically `2` for the first branch. The value for `branch_downstream_segments` is `8` instead of `9`, which would be the last active segment. Looking at the lake cells (*Lake Bathymetry*), we can see that the last segment in only one meter deep.

This means setting `branch_upstream_segments` to `9` works only if the water level is at 200 m. Below this segment is dry and CE-QUAL-W2 terminates with an error message.

The `waterbody_coordinates` are in degrees of latitude and longitude, where the southern hemisphere gets negative values for latitude. Even though, we don't have any tributary inflow yet, wen need (for input reasons in CE-QUAL-W2) provide on tributary, which we do in group `tributaries`. As we will see, we just put a value of zero for inflow to turn it off. We don't want to calculate the ice cover and therefore set `allow_ice_calculations` in the group `ice_cover` to `False`.

We use very simple initial conditions. Setting `initial_temperature` to positive value uses this value for isothermal conditions throughout the entire lake. Using a `-1` or `-2`, we can specify a one-dimensional or two-dimensional temperature distribution in `temperature`. That is also the reason we need to repeat this `temperature`. Similarly, even though we turned ice calculations of, we need to set `ice_thickness` because the default value has different dimensions. Similarly, we set the `initial_concentrations` of a specie `tracer` to `10.00` even though, we don't calculate species yet.

Now we include more files using the directive `!File`. Let's have a look at these files.

The meteorology file provides input data for:

- air temperature,
- dew point temperature,
- wind speed,
- wind direction and
- cloud cover

The time resolution can be as fine as desired up to one minute. Finer resolution would be possible but the input format does not support it yet.

```
date            time  air_temperature  dewpoint_temperature  wind_speed  wind_
↪direction  cloud_cover
01.03.1997     00:00            14.4                  6.80       3.06           2.
↪27           0
01.03.1997     01:00            13.9                  7.00       3.06           2.
↪09           0
01.03.1997     02:00            13.4                  7.00       2.50           2.
↪09           0
01.03.1997     03:00            12.8                  7.10       1.39           2.
↪09           0
01.03.1997     04:00            12.8                  7.10       1.39           2.
↪27           0
01.03.1997     05:00            13.1                  7.40       2.50           2.
↪09           0
01.03.1997     06:00            13.0                  7.50       1.39           2.
↪27           0
01.03.1997     07:00            13.9                  7.90       2.22           2.
↪09           0
01.03.1997     08:00            15.3                  8.10       3.06           1.
↪92           0
```

The precipitation file is simpler. It only has the entry for precipitation in m/s:

```
date            time  precipitation
01.03.1997     00:00      0.000e+00
01.03.1997     01:00      0.000e+00
01.03.1997     02:00      0.000e+00
01.03.1997     03:00      0.000e+00
01.03.1997     04:00      0.000e+00
01.03.1997     05:00      0.000e+00
01.03.1997     06:00      0.000e+00
01.03.1997     07:00      0.000e+00
01.03.1997     08:00      0.000e+00
```

Likewise, the precipitation temperature:

```
date        time       precipitation_temperature
01.01.2001  00:00         15.5
02.01.2001  00:00         15.5
01.02.2001  12:00:00.0    15.5
02.02.2001  12:00:00.0    15.5
31.12.2020  00:00:00.0    15.5
31.12.2100  00:00:00.0    15.5
```

and the concentration:

```
date        time      tracer
01.01.1993  00:00:00.0          0.0
01.01.2020  00:00:00.0          0.0
```

For each entry in `tributary_names`, we need to specify:

- <mytribname>_inflow.txt
- <mytribname>_temperature.txt
- <mytribname>_concentration.txt

Replace `<mytribname>` with name(s) you used.

We don't have any inflow:

```
date            time  tributary_inflow
01.01.1997     00:00      0.0
01.01.2011     00:00      0.0
```

Therefore, data in the temperate file:

```
date        time       tributary_temperature
01.01.1997  00:00         15.0
01.01.2011  00:00         15.0
```

and the concentration file:

```
date    time    tracer
01.03.1997      00:00:00.0      0.0
01.01.2020      00:00:00.0      0.0
```

are ignore.

The specification of not-used values can be a bit misleading. PITLAKQ follows CE-QUAL-W2 as close as possible to allow the of the CE-QUAL-W2's manual as much as possible.

2.7 Looking at results

Run your model with `pitlakq run <project_name>`. The calculation should be finished after a few minutes. Now we can visualize the temperature at one point over time. Create a file called `do_show_temp.py` with this content:

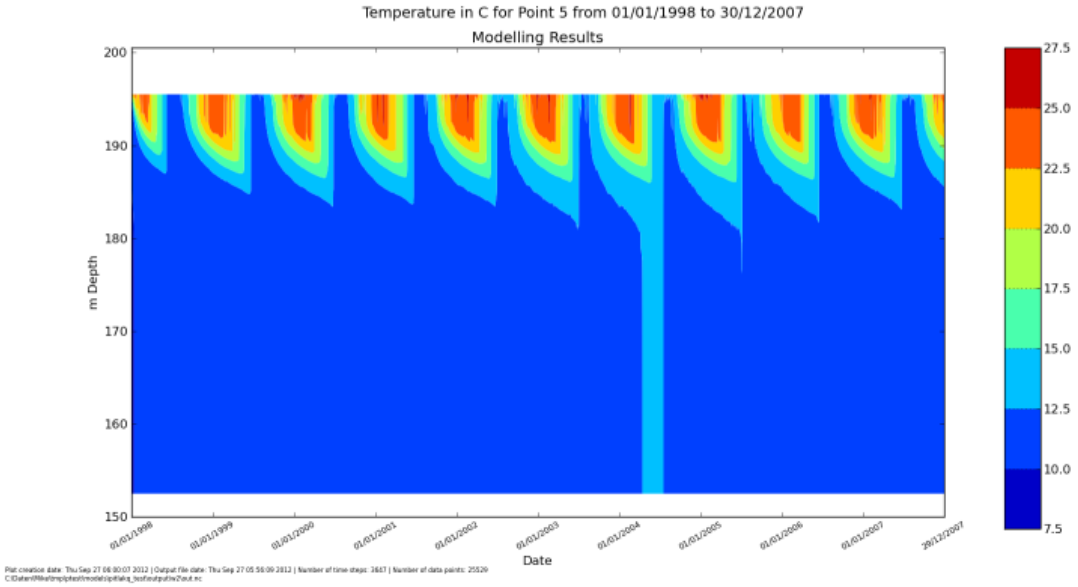
```
from pitlakq.postprocessing import depth_time_contour

species=[{"name": "t2", "levels": "auto"}]
depth_time_contour.main("../output/w2/out.nc", species=species, location=5)
```

This assumes the file is located in the `postprocessing` directory of your project. Now run it:

```
python do_show_temp.py
```

You should see a picture like this:



2.8 Turning on precipitation

You can see that the water level does not change over the whole runtime of the model. This is due to fact that there no sources or sinks to our lake. Let's add some precipitation. Add this to your `w2.yaml` file:

```
calculations:
    precipitation_included:
        value: True
```

Now re-run your model and look at the water level that is printed to the screen. It should drop with each time step. We can visualize the lake water level with this script:

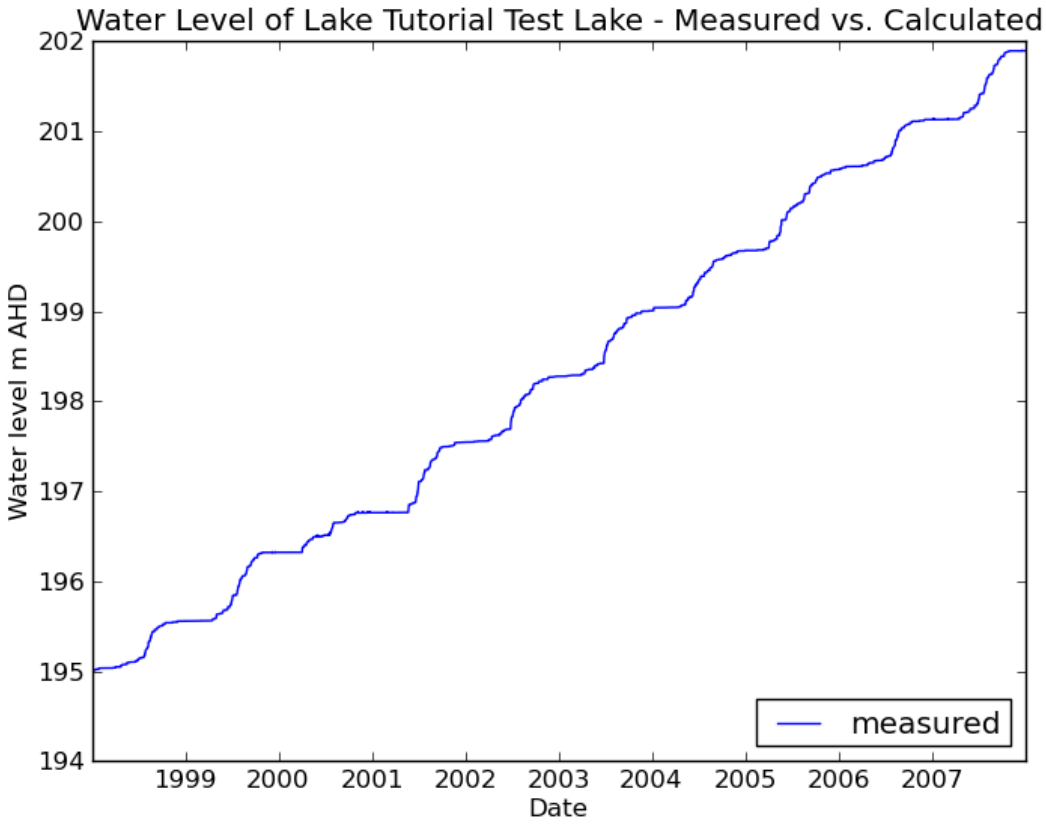
```
from pitlakq.postprocessing import waterlevel


waterlevel.main("../output/w2/out.nc", lake_name="Tutorial Test Lake",
                loc="lower right")
```

This assumes the file is located in the `postprocessing` directory of your project. Now run it:

```
python do_show_wl.py
```

You should see a picture like this:



2.9 Adding evaporation

Now we also turn on evaporation:

```
calculations:
    evaporation_included_in_water_budget:
        value: True
```

Now re-run your model and look at the water level that printed to the screen. It should drop with each time step. Now we also us measured water level data to compare to our calculations:

```
date            level
01.01.1998       195.0
01.01.2000       193.0
01.01.2003       191.0
01.01.2007       190.0
```

We modify our script a bit:

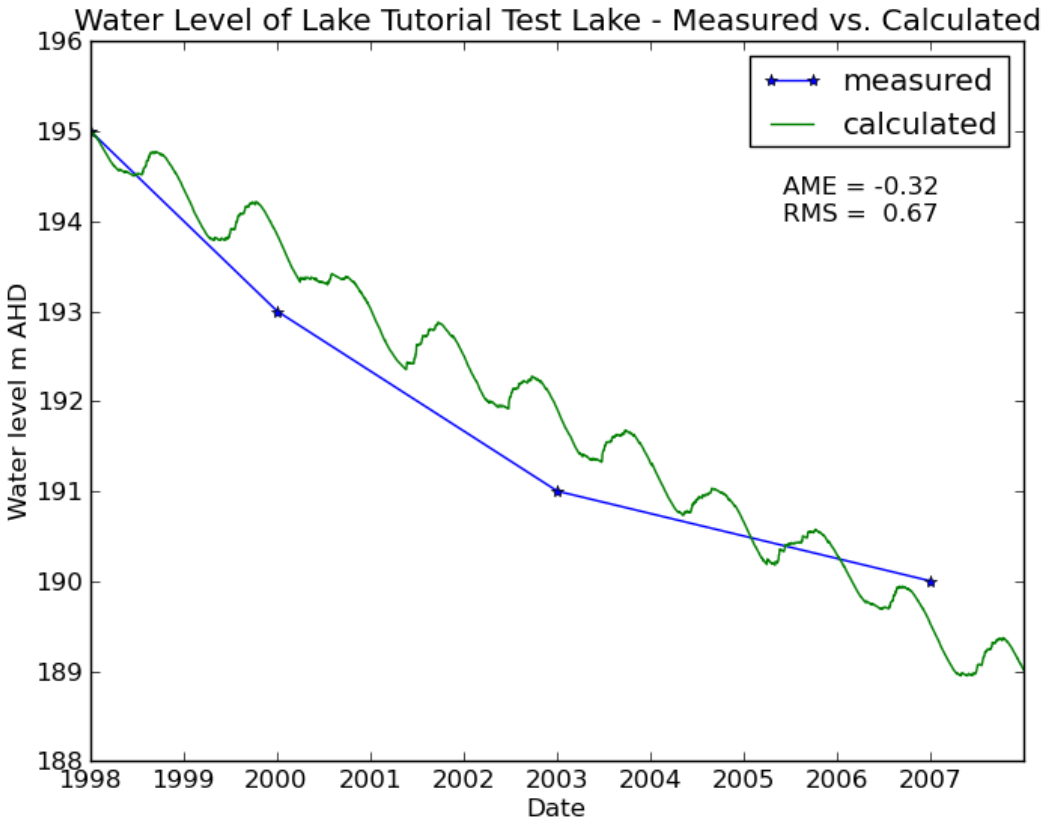
```
from pitlakq.postprocessing import waterlevel


waterlevel.main("../output/w2/out.nc", lake_name="Tutorial Test Lake",
                measured_values_path="measured_wl.txt")
```

and run it:

```
python do_show_wl_measured.py
```

You should see a picture like this:



2.10 Adding inflow

`mytribname_inflow.txt`

We add some inflow:

```
date            time  tributary_inflow
01.01.1997     00:00       0.005
01.01.2011     00:00       0.0
```

Re-run the model and see how the water level in the lake changes.

2.11 Charge balancing

The initial lake composition and all inflows need to be charge balanced. This is important because the pH value is calculated via the charge. PITLAKQ offers tools to make charge balancing of inflows easier, especially if many inflow time steps need to be charged.

We supply measured concentrations for all inflows in an CSV `sample_concentration.csv` file:

```
Cequal;date;time;ph;dissolved_oxygen;ammonium;nitrate_nitrite;phosphorus;tracer;
↪sulfate;chlorid;calcium;magnesium;sodium;potassium;iron_II;iron_III;manganese_II;
↪manganese_III;aluminium;inorganic_carbon;ks43;factor
phreeqc;;;pH;O(0);Amm;N(+5);P;skip;Sulfat;Cl;Ca;Mg;Na;K;Fe(+2);Fe(+3);Mn(+2);
↪Mn(+3);Al;C;ks43;factor
```

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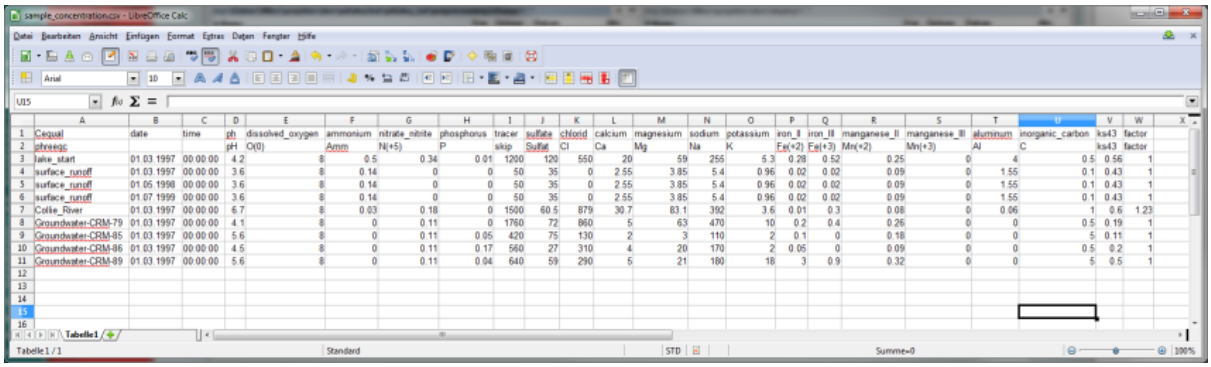
```
lake_start;01.03.1997;00:00:00;4.2;8;0.5;0.34;0.01;1200;120;550;20;59;255;5.3;0.28;
↪0.52;0.25;0;4;0.5;0.56;1
surface_runoff;01.03.1997;00:00:00;3.6;8;0.14;0;0;50;35;0;2.55;3.85;5.4;0.96;0.02;
↪0.02;0.09;0;1.55;0.1;0.43;1
surface_runoff;01.05.1998;00:00:00;3.6;8;0.14;0;0;50;35;0;2.55;3.85;5.4;0.96;0.02;
↪0.02;0.09;0;1.55;0.1;0.43;1
surface_runoff;01.07.1999;00:00:00;3.6;8;0.14;0;0;50;35;0;2.55;3.85;5.4;0.96;0.02;
↪0.02;0.09;0;1.55;0.1;0.43;1
Collie_River;01.03.1997;00:00:00;6.7;8;0.03;0.18;0;1500;60.5;879;30.7;83.1;392;3.6;
↪0.01;0.3;0.08;0;0.06;1;0.6;1.23
Groundwater-CRM-79;01.03.1997;00:00:00;4.1;8;0;0.11;0;1760;72;860;5;63;470;10;0.2;
↪0.4;0.26;0;0;0.5;0.19;1
Groundwater-CRM-85;01.03.1997;00:00:00;5.6;8;0;0.11;0.05;420;75;130;2;3;110;2;0.1;
↪0;0.18;0;0;5;0.11;1
Groundwater-CRM-86;01.03.1997;00:00:00;4.5;8;0;0.11;0.17;560;27;310;4;20;170;2;0.
↪05;0;0.09;0;0;0.5;0.2;1
Groundwater-CRM-89;01.03.1997;00:00:00;5.6;8;0;0.11;0.04;640;59;290;5;21;180;18;3;
↪0.9;0.32;0;0;5;0.5;1
```

Opened in a spreadsheet program, it looks like this:



Now we create a script to start our charge balancing run:

```
import datetime
import os

from pitlakq.preprocessing import charge_tributaries

# Get current working directory.
base = os.getcwd()
# Build absolute path.
in_file_name = os.path.join(base, 'sample_concentration.csv')
# Start charging.
charge_tributaries.main(project_name='pitlakq_tut',
                        in_file_name=in_file_name,
                        out_dir=base,
                        charging_species='Cl',
                        last_date=datetime.datetime(2012, 1, 5))
```

and execute it:

```
python do_trib_charge.py
```

This will generate the files:

- `Collie_River.txt`
- `Groundwater-CRM-79.txt`
- `Groundwater-CRM-85.txt`

- Groundwater-CRM-86.txt
- Groundwater-CRM-89.txt
- lake_start.txt
- sample_concentration_.txt
- surface_runoff.txt

that contain this kind of information:

```
      date       time                          ph          dissolved_oxygen          ␣
↪         ammonium          nitrate_nitrite ...
01.03.1997  00:00:00                  6.70000                   8.00000          ␣
↪         0.03000                   0.18000  ...
05.01.2012  00:00:00                  6.70000                   8.00000          ␣
↪         0.03000                   0.18000  ...
```

Tributaries that are in contact with atmosphere my exhibit some deviations in terms of carbon concentration. If the acid capacity is known, it can be used as additional information. We run the script `do_check_trib_charge.py`:

```
import os
from pitlakq.preprocessing import check_kb_balance

# Get current working directory.
base = os.getcwd()
# Build absolute path.
in_file_name = os.path.join(base, "Collie_River.txt")
# Specify project name.
project_name  = "pitlakq_tut"
target_ph = 4.3
# Start charging.
check_kb_balance.main(project_name,in_file_name, target_ph)
```

```
python do_check_trib_charge.py
```

It titrates the water toward a pH of 4.3 and compares the used amount acid with of the measured value for this titration. It will output something like this:

```
           date  calc  meas ratio
     01.03.1997  0.60  0.60  1.00
     05.01.2012  0.60  0.60  1.00
min 0.0018992835095
max 0.0018992835095
average 0.0018992835095
abs average 0.0018992835095
run time 0.0929999351501
```

If the ratio is different from 1.0 you may adjust the value for `factor` in `sample_concentration.csv` for the Collie River water, re-run `do_trib_charge.py` and `do_check_trib_charge.py`. Repeat until the the ratio approaches 1.0. This excises has to be supported by fundamental chemical understanding of the underlying process.

2.12 Water quality calculations

To do water quality calculations, we need to add more entries to our `pitlakq.yaml`:

```
general:
    start:
        value: 01.01.1998
```

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```
    gw_start:
        value: 01.01.1998
    lake_time_step:
        value: .1
    number_of_gw_time_steps:
        value: 120
    dump_input:
        value: False
lake:
    lake_calculations:
        value: True
    max_water_surface:
        value: 200.0
    deepest_segment:
        value: 8
    kinetics:
        value: True

phreeqc:
    lake_active_const_names:
        value:
            - na
            - cl
            - dox
            - no3
            - nh4
            - po4
            - ca
            - so4
            - mg
            - mn
            - ka
            - al
            - tic
            - fe3
            - mn3
            - fe
    rates:
        value:
            - fe
            - fe3
            - mn
            - mn3
            - so4

    mineral_rates:
        value:
            - feoh3
    lake_active_minerals_names:
        value:
            - feoh3
            - aloh3
            - po4precip
    charge:
        value: Cl #Ca
    parallel_phreeqc:
        value: False
    c_as_c:
        value: True
    monthly_phreeqc:
        value: False
```

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```
    phreeqc_step:
        value: 1
    fe_po4_ratio:
        value: 10
couplings:
    phreeqc_coupling_lake:
        value: True
```

We set the options `lake_calculations` and `kinetic` in the group `lake` to `True`. We want to couple with PHREEQC. Therefore, we set `phreeqc_coupling_lake` in the group `couplings` to `True`. In addition, we add the group `phreeqc`, in which we specify the active constituents as list of names under `lake_active_const_names`. We like to have some of constituents to be calculated with rate equations rather than an equilibrium approach. We list these names under `rates`.

The mapping of different names is defined in `resources/const_names.txt` This is an expert from this file with the constituents we calculate:

key	name	w2ssp	w2ssgw	phreeqc_name	molar_weight	rate_name
fe	iron_II	fessp	fessgw	Fe(+2)	55.847	Fe_di
fe3	iron_III	fe3ssp	fe3ssgw	Fe(+3)	55.847	Fe_tri
so4	sulfate	so4ssp	so4ssgw	Sulfat	96.064	Sulfat
mn	manganese_II	mnssp	mnssgw	Mn(+2)	54.938	Mn_di
mn3	manganese_III	mn3ssp	mn3ssgw	Mn(+3)	54.938	Mn_tri

Important here are the columns `key`, `phreeqc_name` and `rate_name`. The rates themselves are defined in `resources/phreeqc_w2.dat`

Analogous we allow the minerals given in `lake_active_minerals_names` to form. We specify with `mineral_rates` what minerals are formed from rate constituent. The relevant part from `resources/mineral_names.txt` looks like this:

key	name	w2ssp	w2ssgw	phreeqc_name	molar_weight	rate_name
feoh3	iron_hydroxide	feoh3ssp	noGW	Fe(OH)3(a)	106.871	Fe(OH)3(a)r

We need to start with a charge balanced water. Therefore we choose one constituent to be used for charging. We choose `Cl` for `charge` because we don't need to evaluate chloride.

PITLAKQ supports parallel processing of PHREEQC calculations. This an advanced feature and we turn `parallel_phreeqc` off. All our carbon concentrations are given in terms of `C`, therefore we set `c_as_c` to true. This will run all PHREEQC calculation with the option `as C`. We want daily PHREEQC time steps. Actually they are the default.

Iron precipitation co-precipitates phosphorus. We specify the ratio for this process with `fe_po4_ratio` a typical value is `10`.

We also modify our `w2.yaml` file:

```
general:
    titel:
        value: A simple PITLAKQ test model
bounds:
    number_of_segments:
        value: 10
    number_of_layers:
        value: 52
    number_of_constituents_segments:
        value: 10
    number_of_constituents_layers:
        value: 52
    number_of_tributaries:
        value: 2
times:
```

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```
    start:
        value: 01.01.1998
    end:
        value: 31.01.2009
---
!File
    name: bath.nc
    format: netcdf
    group_name: bathymetry
---
bathymetry:
    starting_water_level:
        value: 195.0
---
branch_geometry:
    branch_name:
        value:
            - test lake                          # no w2 variable
    branch_upstream_segments:
        value:
            - 2
    branch_downstream_segments:
        value:
            - 8


waterbody_coordinates:
    latitude:
        value: -33.21 # degrees
    longitude:
        value: 116.093  # degrees
    bottom_elevation:
        value: 150.0

calculations:
    precipitation_included:
        value: True
    evaporation_included_in_water_budget:
        value: True

tributaries:
    number_of_tributaries:
        value: 2
    tributary_names:
        value:
            - mytribname
            - groundwater
    tributary_segment:
        value:
            - 5
            - 6
    #placement_key:
    #    distributed: 0
    #    density: 1
    #    specify: 2
    #    default: 1
    tributary_inflow_placement:
        value:
            - 1 # density
            - 1 # density
    tributary_inflow_top_elevation:
```

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```
        value:
            - 180
            - 180
    tributary_inflow_bottom_elevation:
        value:
            - 155
            - 155

ice_cover:
    allow_ice_calculations:
        value: False

initial_conditions:
    initial_temperature:
        value: 10 # isothermal
    temperature:
        value: 10
    ice_thickness:
        value: 0.0

---
!File
    name: w2const.yaml
    format: yaml
---

initial_concentrations:
    tracer:
        value: 1.0
        unit: mg/l
    labile_dom: #((TOC-algae)*0.75)*0.3
        value: 0.1 #0.63
        unit: mg/l
    refractory_dom: #((TOC-algae)*0.75)*0.7
        value: 0.1 #1.47
        unit: mg/l
    algae:
        value: 0.05
        unit: mg/l
    labile_pom: #((TOC-algae)*0.25)*0.3 detritus
        value: 0.1 #0.21
        unit: mg/l
    phosphorus: #o-PO4
        value: 0.06
        unit: mg/l
    ammonium:
        value: 0.01
        unit: mg/l
    nitrate_nitrite:
        value: 0.001
        unit: mg/l
        # als NO3-N (=Nitrat/4.42)
    dissolved_oxygen:
        value: 9.0
        unit: mg/l
    sediment:
        value: 0.0 #4.0 TOC im Sediment
        unit: mg/l
    inorganic_carbon: # tic
        value: 0.15 # 22.5
        unit: mg/l
```

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```
    ph:
        value: 5.0
        unit: mg/l
    carbon_dioxide: # aus ph und DIC
        value: 0.0 #0.37
        unit: mg/l
    iron_II:
        value: 0.01
        unit: mg/l
    aluminium:
        value: 0.1
        unit: mg/l
    sulfate:
        value: 30
        unit: mg/l
    calcium:
        value: 7
        unit: mg/l
    magnesium:
        value: 14
        unit: mg/l
    sodium:
        value: 14
        unit: mg/l
    potassium:
        value: 1.5
        unit: mg/l
    manganese_II:
        value: 0.05
        unit: mg/l
    chlorid:
        value: 56
        unit: mg/l
    iron_III:
        value: 0.05
        unit: mg/l
    manganese_III:
        value: 0.01
        unit: mg/l
    iron_hydroxide:
        value: 0.01
        unit: mg/l
    aluminium_hydroxide:
        value: 0.01
        unit: mg/l


---
!File
    name: meteorology.txt
    format: columns_whitespace
    group_name: meteorology


---
!File
    name: precipitation.txt
    format: columns_whitespace
    group_name: precipitation
```

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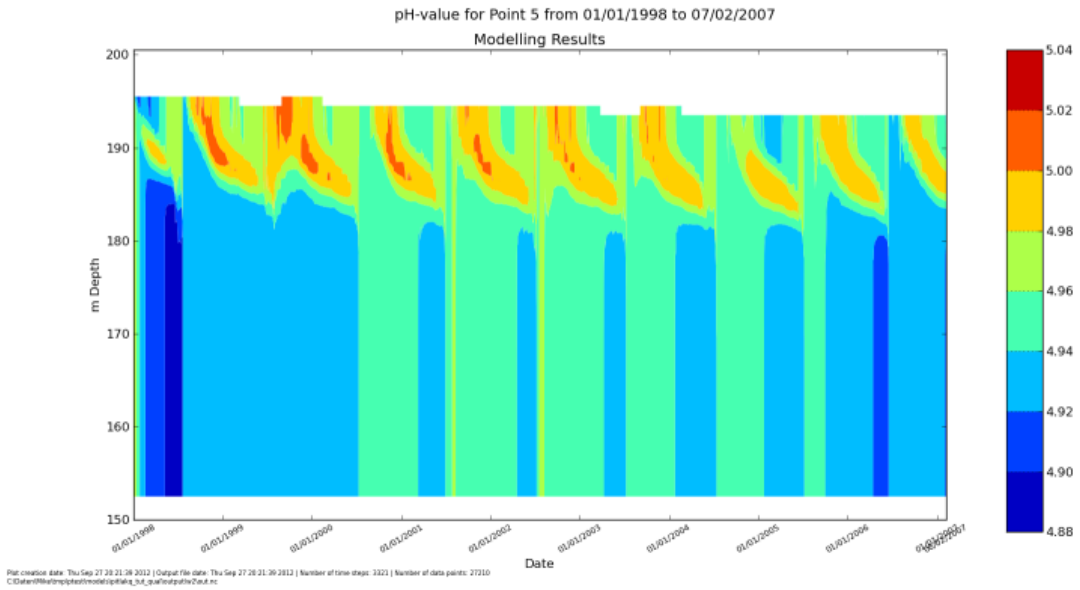
```
---
!File
    name: precipitation_temperature.txt
    format: columns_whitespace
    group_name: precipitation_temperature


---
!File
    name: precipitation_concentration.txt
    format: columns_whitespace
    group_name: precipitation_concentration
```

We add another tributary and specify initial concentrations. Add a second tributary requires to add some more information how we would like tributary inflows to placed. We choose by density. Due to logic of the input, we go have to specify top and bottom elevations, even though they are not used. This could be improved in PITLAKQ but would require to modify the input system.

After we start our run with `pitlakq -p pitlakq_tut_qual` and let it run for a while. In the mean create this script:

```
from pitlakq.postprocessing import depth_time_contour

species=[{"name": "ph", "levels": "auto"}]
depth_time_contour.main("../output/w2/out.nc", species=species, location=5)
```

Running it `pythont do_show_ph.py` (remember the calculations should have run for few minutes), you should see a figure like this:

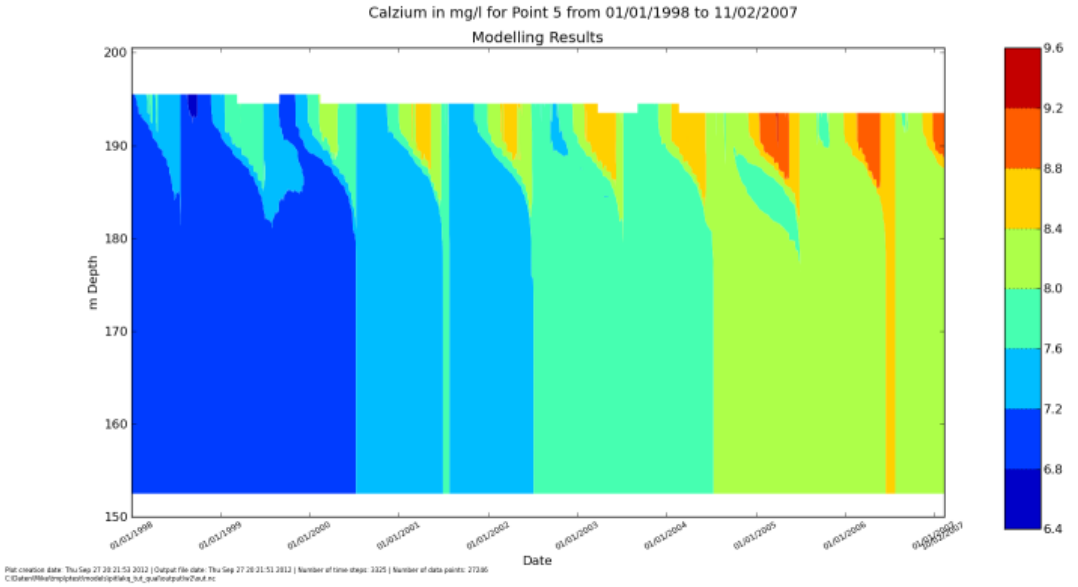


Depending on how long you model run the figure might look considerably different.

This script:

```
from pitlakq.postprocessing import depth_time_contour

species=[{"name": "ca", "levels": "auto"}]
depth_time_contour.main("../output/w2/out.nc", species=species, location=5)
```

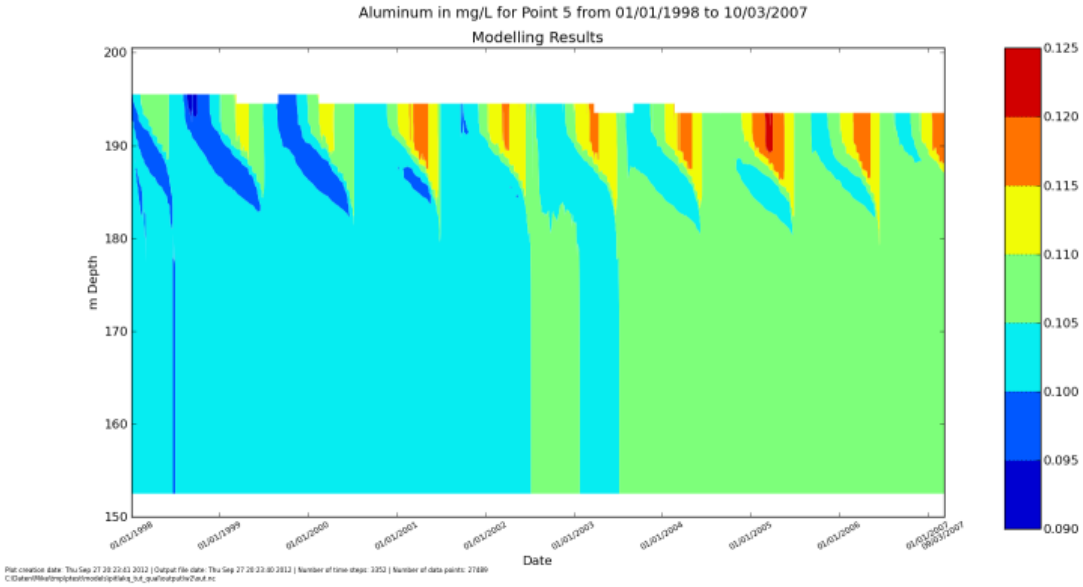
after run `pythont do_show_ca.py` displays this figure

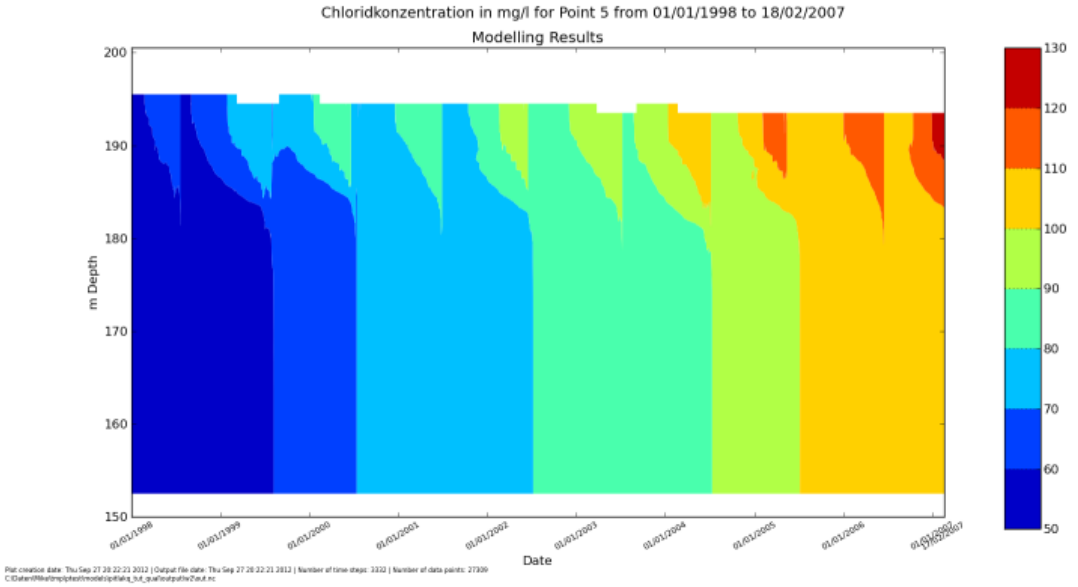


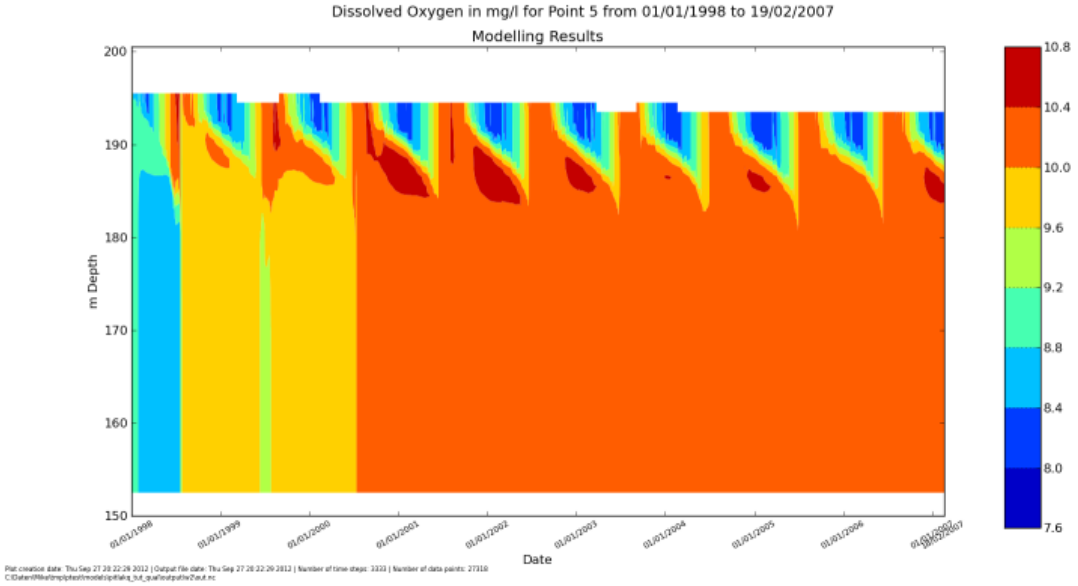
We can pout several constituents in one script:

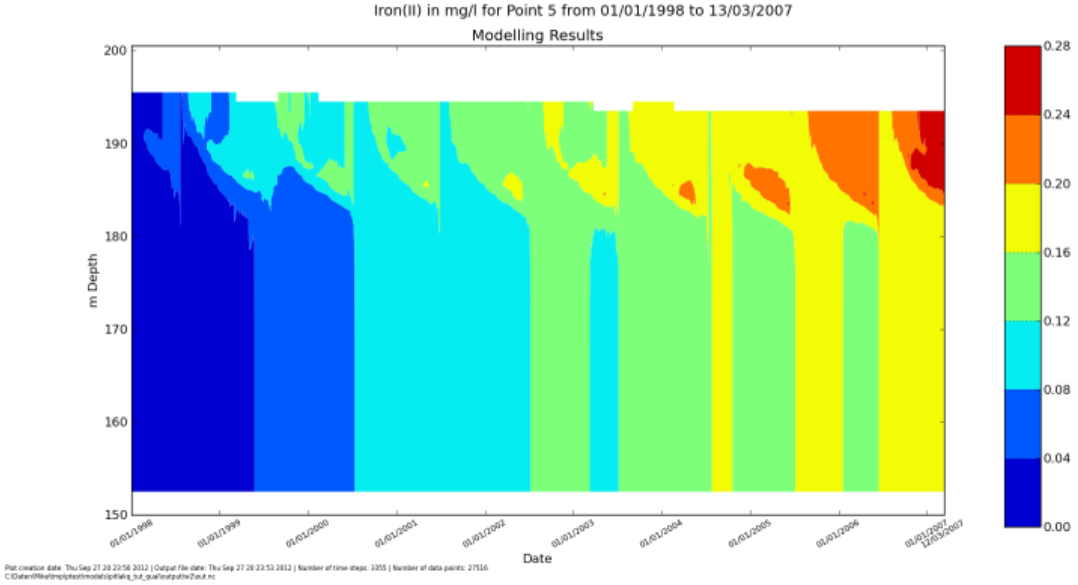
```
from pitlakq.postprocessing import depth_time_contour

for name in ["na", "cl", "dox", "po4", "ca", "so4", "mg",
             "al", "fe3", "fe"]:
    species=[{"name": name, "levels": "auto"}]
    depth_time_contour.main("../output/w2/out.nc", species=species, location=5)
```

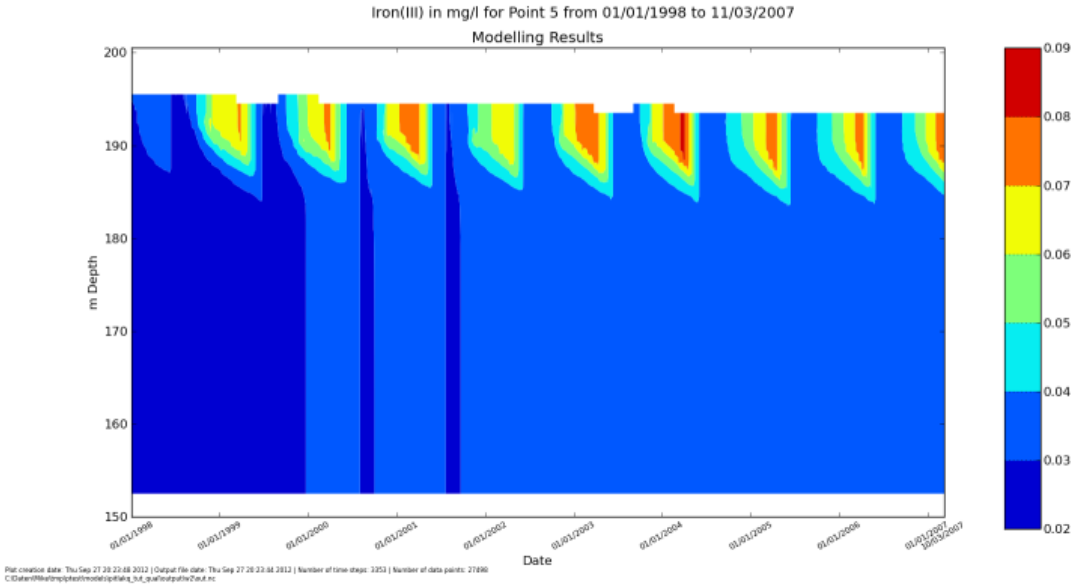
After running it with `python do_show_many.py` you should see the windows popping up with these figures. After you close one, the next will up.

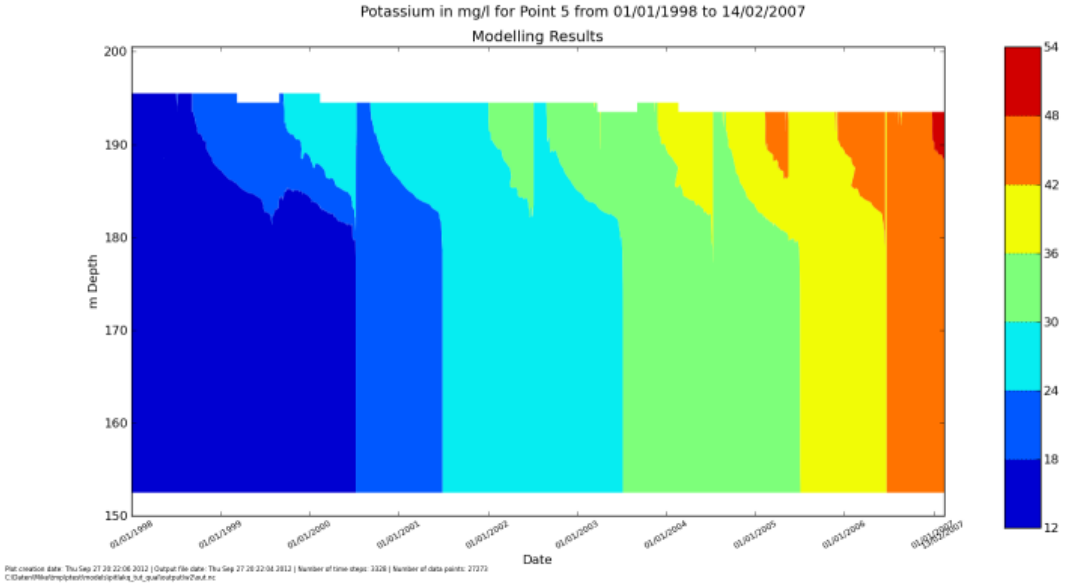


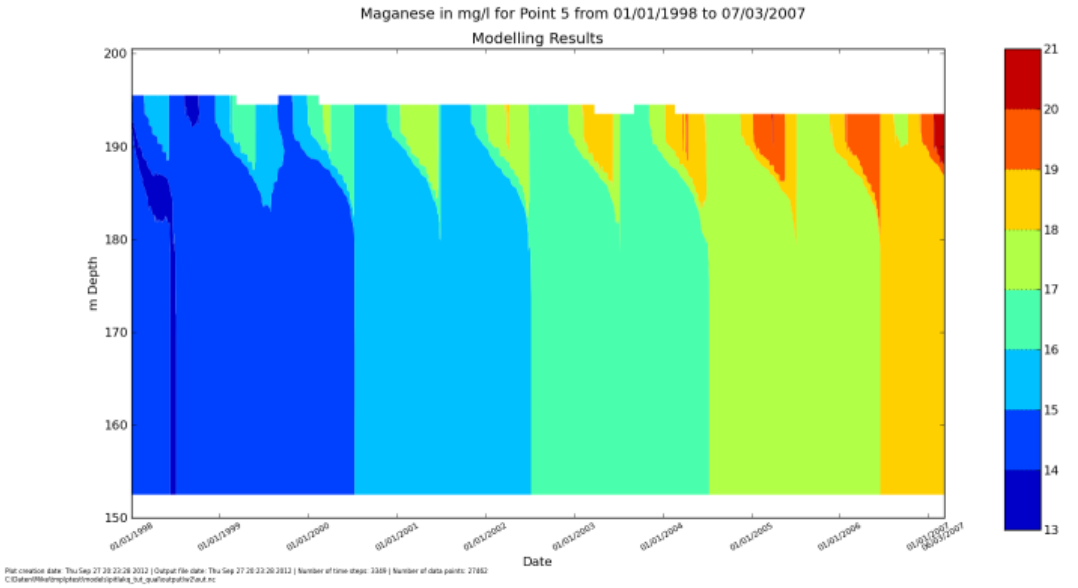

Chloridkonzentration in mg/l for Point 5 from 01/01/1998 to 18/02/2007
Modelling Results
m Depth
Date
200
190
180
170
160
150
130
120
110
100
90
80
70
60
50

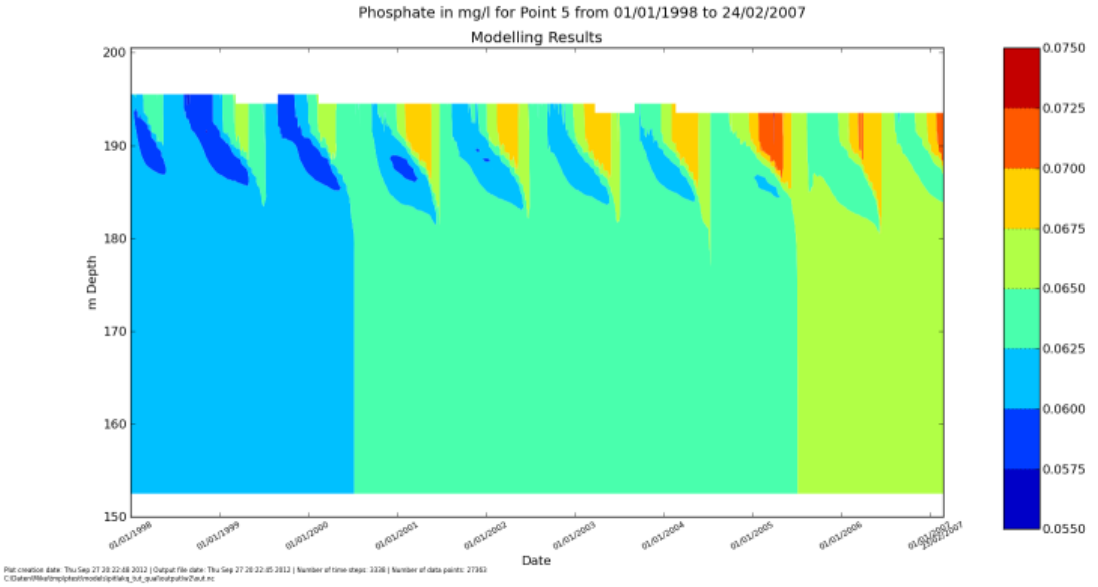

Dissolved Oxygen in mg/l for Point 5 from 01/01/1998 to 19/02/2007
Modelling Results
m Depth
Date
200
190
180
170
160
150
10.8
10.4
10.0
9.6
9.2
8.8
8.4
8.0
7.6

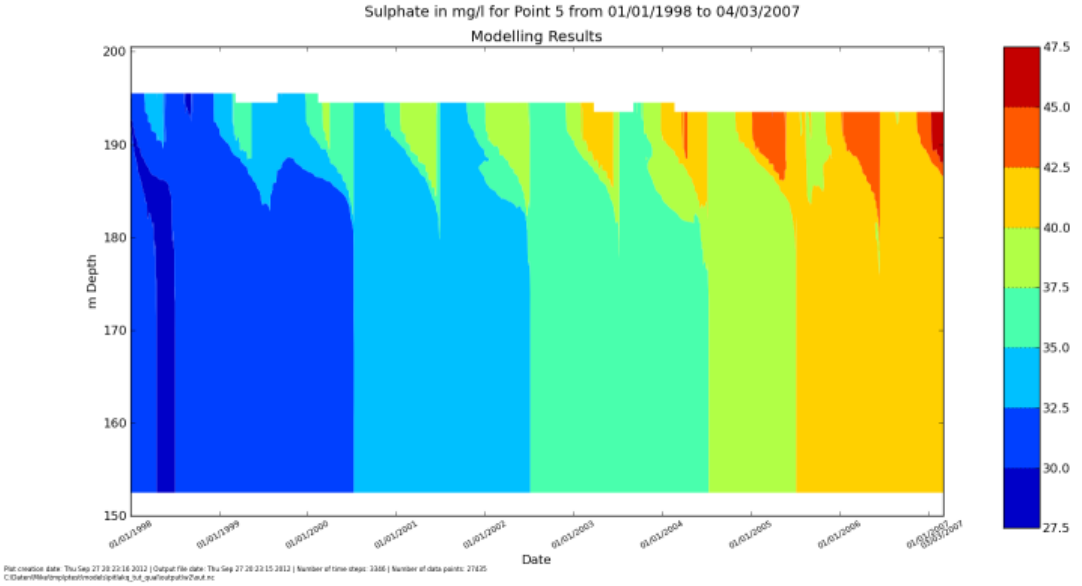

Iron(II) in mg/l for Point 5 from 01/01/1998 to 13/03/2007
Modelling Results
m Depth
Date
200
190
180
170
160
150
0.28
0.24
0.20
0.16
0.12
0.08
0.04
0.00


Iron(III) in mg/l for Point 5 from 01/01/1998 to 11/03/2007
Modelling Results
m Depth
Date
200
190
180
170
160
150
01/01/1998
01/01/1999
01/01/2000
01/01/2001
01/01/2002
01/01/2003
01/01/2004
01/01/2005
01/01/2006
01/01/2007
10/03/2007
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02


Potassium in mg/l for Point 5 from 01/01/1998 to 14/02/2007
Modelling Results
m Depth
Date
200
190
180
170
160
150
01/01/1998
01/01/1999
01/01/2000
01/01/2001
01/01/2002
01/01/2003
01/01/2004
01/01/2005
01/01/2006
01/01/2007
14/02/2007
54
48
42
36
30
24
18
12


Maganese in mg/l for Point 5 from 01/01/1998 to 07/03/2007
Modelling Results
m Depth
Date
200
190
180
170
160
150
01/01/1998
01/01/1999
01/01/2000
01/01/2001
01/01/2002
01/01/2003
01/01/2004
01/01/2005
01/01/2006
01/01/2007
08/03/2007
21
20
19
18
17
16
15
14
13





2.13 Making groundwater inflow a function of lake water level

So far we have specified the groundwater inflow as a tributary inflow. For this we needed to provide the inflow for each desired time step. An alternative solution is to specify groundwater inflows as a function of lake water level.

First, we create a new project with `pitlakq create pitlakq_tut_gwh`. We just copy the `input` folder from our former project `pitlakq_tut_qual`. Introducing a new feature, it is always a good idea to turn of water quality calculations for the first steps. This makes setting up our new inflow simpler and test runs considerately faster.

To do this we just turn off the PHREEQC coupling. In `pitlakq.yaml` we set this option for this to `False`:

```
couplings:
    phreeqc_coupling_lake:
        value: False
```

Furthermore, for know we also turn of kinetic calculations in W2 setting the corresponding option in `pitlakq.yaml` to `False`:

```
lake:
    ...
    kinetics:
        value: False
```

Now we also turn off our groundwater inflow tributary. In `w2.yaml` we set the number of tributaries to one.

```
bounds:
  ...
  number_of_tributaries:
      value: 1
```

And also change the tributary section to one tributary:

```
tributaries:
    number_of_tributaries:
        value: 1
    tributary_names:
        value:
            - mytribname
    tributary_segment:
        value:
            - 5
    tributary_inflow_placement:
        value:
            - 1 # density
    tributary_inflow_top_elevation:
        value:
            - 180
    tributary_inflow_bottom_elevation:
        value:
            - 155
```

Now we do a test run to see if the model still works:

`pitlakq run pitlakq_tut_gwh`

We turn on the option `gwh` in `pitlakq.yaml`:

```
gw:
    gwh:
        value: True
```

The only thing missing now is the actual input. We create a template input file with this script:

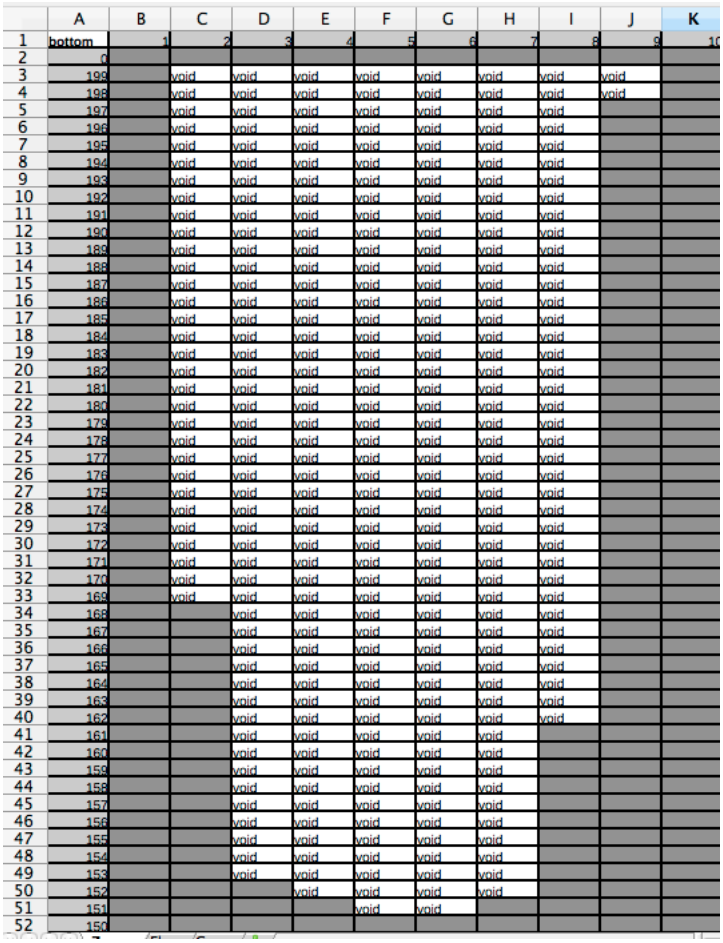
```
from pitlakq.preprocessing import create_xlsx_input

create_xlsx_input.main("pitlakq_tut_gwh")
```

Running it:

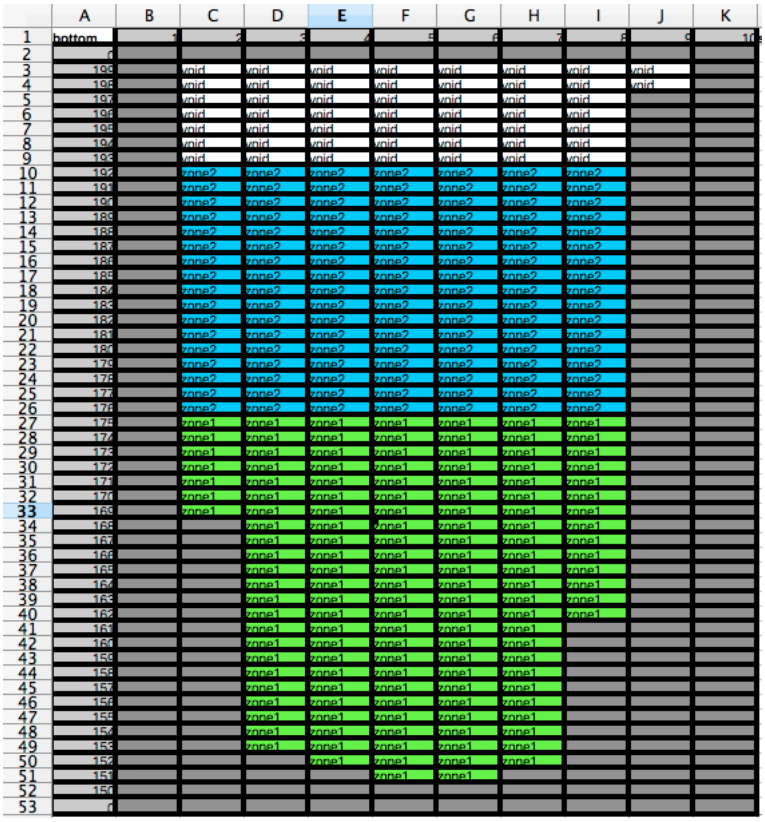
`python do_gwh_xlsx.py`

creates a file `gwh_template.xlsx` in `input/gwh`. Rename this file to `gwh.xlsx`. This renaming is a safety measure to avoid accidental re-creation of the file and loosing the entered in input.

This file has three tabs. The first one represents the zones:



Only the white cells with the `void` inside are editable



We added two zones. The color are optional and don't mean anything to PITLAKQ. But the name is important. There is no limit on the number of zones as long as there are at least two cells in two adjacent layers in one zone. The inflows will be distributed over these cells according to there current water filled volume.

Inflows will activate only if the water level specified in the column `Level` on the tab `Flow` will be reached by the lake water level. A soon as the next level is reached, its inflow will be active and not the one below anymore. This way inflows can vary in many ways. Inflows can be negative which results in groundwater outflow.

Zone name	Level	Flow
zone1	155	0.02
zone1	160	0.01
zone1	170	0.05
zone1	180	0.001
zone2	180	0.002
zone2	185	0.001
zone2	190	-0.0

Each zone has one concentration specified in the tab `Conc`. We just use the concentration from our groundwater tributary. This table shows the first entries. Add all that from the original groundwater tributary file.

Zone name	dissolved_oxygen	ammonium	nitrate_nitrite
zone1	8	0	0.11
zone2	8	0	0.11

Now run the model. Modify levels and flow values to see the effect on the water level.

Finally, we can turn the water quality calculations back on.

2.14 Adding New Species to the Database

PITLAKQ currently comes with 56 pre-defined solute species and 7 minerals. It is also possible to add user-defined species. There are several steps to incorporate own species in PITLAKQ. These species will be transported in CE-QUAL-W2 as tracers. All water quality processes will take place in PHREEQC. Furthermore, minerals that are allowed to form and precipitate can also be added. As with other minerals, they can be allowed to fully precipitate as soon as they are over-saturated or can be allowed to settle with potential dissolution on their way to the bottom if conditions change.

The next steps will modify files in the installation directory. To avoid overwriting these files with defaults when updating `pitlakq`, it is recommend to copy the directories `<install_dir>/pitlakq/templates` and `<install_dir>/pitlakq/resources` into different locations. These new locations need to be listed in your `` `.pitlakq `` file. (See *Initializing PITLAKQ* for details.)

There are four steps involved in adding a new specie:

1. Add a new line in the file `resources/const_names.txt` for solute or in the file `resources/mineral_names.txt` for mineral species.
2. Add a corresponding entry in the file `templates/w2.yaml`.
3. Add a corresponding entry in the file `templates/activeconst.txt`.
4. Optional: Update the PHREEQC database if it **does not contain** the new specie and the corresponding reactions yet.

These steps may get a bit more stream-lined in the future. Due to the fact that PITLAKQ was not designed from ground up for adding new species by the user, consolidating the information from steps 1. to 3. in one place would mean a major re-arrangement of the code base. Let's go over the steps in detail.

2.14.1 Add a line to the files `resources/const_names.txt` or `resources/mineral_names.txt`

The file `resources/const_names.txt` has this structure:

```
key    name           w2ssp  w2ssgw  phreeqc_name  molar_weight  rate_name

alkal  alkalinity     void   void    void          void          void
mn     manganese_II   mnssp  mnssgw  Mn(+2)        54.938        Mn_di
na     sodium         nassp  nassgw  Na            22.9898       void
```

There are more lines in this file. The three lines above are chosen to exemplify how different options look like.

The file `resources/mineral_names.txt` has this structure:

```
key     name            w2ssp     w2ssgw  phreeqc_name  molar_weight  rate_name

feoh3   iron_hydroxide  feoh3ssp  void    Fe(OH)3       106.871       Fe(OH)3(a)r
caco3   calcite         auto      void    Calcite       100.071       void
```

There are more lines in this file. The two lines above are chosen to exemplify how different options look like.

The columns have these meanings:

key Internal key used for CE-QUAL-W2 and other purposes. It must be unique. It is likely that one-letter names or very short names are already taken. PITLAKQ will warn you when this is the case. In this case, please choose another name. It is recommended to use a name that is as close as possible to the chemical symbol. Technically, any name consisting of English lowercase letters, digits and the underscore (_) can be used. However, digits cannot appear at the beginning of a name.

name A descriptive name for the specie. The name must be unique among the names in this column. The same name rules as for `key` apply.

w2ssp Name used for exchange with PHREEQC. This is typically `<name>ssp`. A specific name is only used for pre-defined species. As a user you can only choose between the option `auto` or `void`. The entry `auto` should be used for all species for which you want PHREEQC to use in its reactions. The actual name will be generated internally. Using `void` in this column prevents the specie to be used for PHREEQC calculations. This is useful for species that don't make sense in PHREEQC. For example, `alkalinity` in the example above is not used. It is the original alkalinity calculated in CE-QUAL-W2. It is contained only for technical reasons and serves no actual purpose for modeling. Due to the way the source code of CE-QUAL-W2 is structured, it would require a major re-write to turn off alkalinity with other means. Using `void` can be useful for other species such as tracers. This way you can add an unlimited number of tracers.

w2ssgw Name used for exchange with groundwater. This is typically `<name>ssgw`. A specific name is only used for pre-defined species. As a user you can only choose between the option `auto` or `void`. The entry `auto` should be used for all species for which the groundwater should act as source and sink. The actual name will be generated internally. Using `void` in this column prevents any exchange with the groundwater for this specie. This is useful for minerals that can be transported in the lake but typically not in the groundwater due to velocities that are orders of magnitude smaller.

phreeqc_name This is the name of the specie used in PHREEQC. It must appear in the database in `SOLUTION_MASTER_SPECIES` for solutes or in `PHASES` for minerals. See the PHREEQC manual for more details.

molar_weight The molar weight of the specie. This must be the same value as used in the PHREEQC database. So far there are no know use cases where this value differs from the one in PHREEQC. It you know of one, please tell the model developers.

rate_name This is an alternative name for the specie used in PHREEQC's rate reactions. You must name the specie matching the corresponding entry under `KINETICS` in the PHREEQC database.

A typical entry in `resources/const_names.txt` would look like this:

```
key name       w2ssp    w2ssgw  phreeqc_name     molar_weight     rate_name

.... other lines here ....

van vanadium   auto     auto    V                50.9415          void
```

Since `v` is already used in CE-QUAL-W2 (PITLAKQ will warn you about it), we choose `van` for `key`. The entry for `name` is just the lower case version of the chemical name. The entry for `w2ssp` must be `auto` because we want our species to react in PHREEQC. Likewise, the entry for `w2ssgw` is also `auto` because we would like the exchange with groundwater to be possible. It can be enabled and disabled for each model but must be `auto`, otherwise it cannot be enabled at all. The PHREEQC name is just the normal chemical name and you must use the same name as in the PHREEQC database. The molar weight is copied from the PHREEQC database. We don't want to use kinetic rate reactions, therefore `rate_name` is `void`.

Adding a new line at the end of the file `resources/mineral_names.txt` should look like this:

```
key      name             w2ssp      w2ssgw   phreeqc_name   molar_weight   rate_name

.... other lines here ....

caco3    calcite          auto       void     Calcite        100.071        void
```

The meanings are the same as above. We choose a unique name for the `key`. In our case the lowercase version of the chemical formula. The `name` is the lowercased PHREEQC name. We want reactions in PHREEQC, hence `auto` for `w2ssp`. Minerals typically are not transported in the groundwater, therefore `void` in `w2ssgw`. The molar weight is again the value PHREEQC uses. We also do not want rate reactions and set `rate_name` to `void`.

2.14.2 Add an entry in `templates/w2.yaml`

We need to tell CE-QUAL-W2 about the new specie. We need to add an entry inside the group `initial_concentrations`. Going with our example for vanadium it would look like this:

```
initial_concentrations:
    # many more entries here
    vanadium:
        default: 0.0
        w2_code_name: van
        dimension:
            - number_of_layers
            - number_of_segments
```

Unless you want a default initial concentration different from zero, add `default: 0.0`. The entry for `w2_code_name` must be the same as in the column `key` in `resources/const_names.txt` or `resources/mineral_names.txt`. Always use the same entries for `dimension`.

2.14.3 Add an entry in `templates/activeconst.txt`

The file `templates/activeconst.txt` looks like this:

```
constituent_name active_constituents initial_concentration inflow_active_
↪constituents tributary_active_constituents precipitation_active_constituents
.... other lines here ....
iron_II          0                    0                     0                    ⌐
↪   0                              0
.... other lines here ....
silver           0                    0                     0                    ⌐
↪   0                              0
.... other lines here ....
```

Per default all species should be inactive. Using this file copied to your model input, you can activate any specie you need for any if the columns.

Adding a new specie is simple. Just use the name you entered in the column `name` in `resources/const_names.txt` or `resources/mineral_names.txt` and copy all the zeros from the line above:

```
constituent_name active_constituents initial_concentration inflow_active_
↪constituents tributary_active_constituents precipitation_active_constituents
.... other lines here ....
vanadium           0                    0                     0                  ␣
↪      0                              0
```

2.14.4 Update the PHREEQC database

You may need to update your PHREEQC database to reflect your changes. You don't need to do anything, if the database already contains all species you added including all the reactions that are needed for your site.

You can also specify a different database. Just add this to your `pitlakq.yaml`:

```
phreeqc:
    # more lines here
    phreeqc_database_name:
        value: my_database.dat ## default is phreeqc_w2.dat
```

You need to copy the database file `my_database.dat` into the directory `resources` of you PITLAKQ install. Refer to `.pitlakq` where this is on your computer.

2.15 Pit Wall Loading

2.15.1 Needed information

The water quality of a pit lake can be significantly influenced by material from the pit wall entering the lake. PITLAKQ offers a way to simulate these loadings. There are several prerequisites that need to be satisfied for the modeling approach to work:

1. You need to specify loading rates expressed in mass per area per time from the pit walls for all species that you would like to model. Such loading rates are typically measured in laboratory experiments. The rates need to be assigned to pit wall zones. There is no limit on the number of zones. There can be as few as one zone, covering all pit walls, or as many as dozens, hundreds, or thousands of zones if such detailed information is available.
2. You need to specify surface areas of the pit wall for each zone for different lake water levels. There is no limit on the number of lake water levels with different surface areas you can specify. However, there must be at least two levels. This surface areas will be used to calculate the effective loadings for each zone for the current water level.
3. You also need to specify planar areas in the fashion as surface areas. These planar areas will be used to calculate the run off from the pit walls using the precipitation specified in the model input for the CE-QUAL-W2 part of PITLAKQ.

2.15.2 The procedure

PITLAKQ is calculating the following:

1. For each loading time step, typically one day but it can be set by the user, the model determines the surface area of each zone. Each area is multiplied by the given loading rate for this zone and the elapsed time (one day for our example case). These masses are accumulated to be added to the lake as soon as there is runoff.

2. The precipitation for the time period is calculated. If there is no precipitation, nothing happens. If there is precipitation, it will be multiplied with the planar area of each zone to yield the water volume supplied by each zone.
3. The water volume is added to a specified region of the lake. This region is determined by a user-defined number of layers counted from the lake surface and active lake segments per zone. In addition, the lake receives the accumulated masses from step 1. and an amount of heat provided by a given temperature multiplied by the volumes. After adding the masses to the lake, the accumulated masses are set to zero. This means the accumulation can begin anew with the next time step.

For example, if there is a 10-day period without precipitation, the model would accumulate masses for all species for all zones according to the specified loading rates and current surface areas for all zones. After 10 days the calculated precipitation volumes for each zone would carry these masses into the lake. For wet climates with frequent precipitation this results in a steady loading from the pit walls. On the other hand, for dry climates with infrequent precipitation this simulates longer periods without any loading followed by short peaks of loading.

2.15.3 Model input

The input for the loading is contained in the file `loading.xlsx` in the directory `input/loading`. The tab "Area" holds a table of surface areas and planar areas in m^2 for each desired water table as well as start and end segment of the lake in between which the load should be applied. For one zone this table could look like this:

water_level	zone1_planar	zone1_surface	zone1_start_segment	zone1_end_segment
152	0	0	4	5
155	73278.2	97704.3	4	5
153	69492.0	92656.0	6	8
154	67777.0	90370.4	6	8
155	67048.0	89398.1	6	8

Typically there are more lines in a table, covering the whole expected range of water table changes. Using a value of zero for areas effectively turns them off for this water table. This allows to represent inactive areas for certain areas. A table for three zones would have this header:

Header	
water_level	
zone1_planar	
zone2_planar	
zone3_planar	
zone1_surface	
zone2_surface	
zone3_surface	
zone1_start_segment	
zone1_end_segment	
zone2_start_segment	
zone2_end_segment	
zone3_start_segment	
zone3_end_segment	

The numbers for the areas need to be supplied by the user. Currently, there is no extra tool for preprocessing that would generate the area information from bathymetry information. Using GIS software, generation of the area information should be straight forward.

The table under the tab "Conc" holds the loading data in $g/m^2/s$. Each zone name that was used in the table under tab "Area" must appear in the column `zone`. All species that are to be active for loading have to given in the columns of the table as headings:

zone	cobalt	silver	zinc	tracer	calcium
zone1	1.00E-011	1.00E-010	1.00E-010	1.00E-010	1.00E-010
zone2	5.00E-011	1.00E-010	4.00E-010	1.00E-010	1.00E-010
zone3	0	1.00E-010	1.00E-011	1.00E-010	1.00E-010

In addition, all species in this table must be turned on using a `1` for `active_constituents` in the file `input/w2/activeconst.txt` in your **model input**. Please **do not** turn them on as default in `resources\activeconst.txt` as this would affect all other models, which is typically undesirable.

CHAPTER 3

Command-line Options

PITLAKQ provides command-line options.

Just typing *pitlakq* or *pitlakq -h* at the command line will bring up this output:

```
usage: pitlakq [-h] [-v] {init,run,create,introspect} ...

positional arguments:
  {init,run,create,introspect}
    init                initialize PITLAKQ and create `.pitlakq`
    run                 start the calculation of a model
    create              creates a new project folder with empty sub folders
    introspect          find out internals of PITLAKQ or your projects

optional arguments:
  -h, --help            show this help message and exit
  -v, --version         show version info and exit
```

The program is organized in subcommands such as `init` or `run`. For example, `run` takes the name of the project to be run as obligatory argument:

```
pitlakq run -h
usage: run_pitlakq.py run [-h] project_name

run a project

positional arguments:
  project_name  name of project to be calculated
```

The subcommand `introspect` allows to explore internals:

```
pitlakq introspect
usage: run_pitlakq.py introspect [-h] [-w] [-p]

find out internals

optional arguments:
  -h, --help      show this help message and exit
  -w, --w2-names  show w2 names
  -p, --projects  show all projects
```

The option `-w` in short or `w2-names` in long form displays a long for named used in CE-QUAL-W2 (see CE-QUAL-W2 documentation) and their corresponding names in PITLAKQ.

The option `--projects` lists all projects in the in model path.

CHAPTER 4

Support

Please visit the PITLAKQ website for support options.

CHAPTER 5

Changelog

5.1 Version 1.6.0

- Update to Python 3.9
- Use *Loader* for reading *yaml* to avoid warning
- Add parallel PHREEQC calculations with processes on one machine
- Varies small typo and other fixes

5.2 Version 1.5.2

- Fix density calculation

5.3 Version 1.5.1

- Remove `raw_input`

5.4 Version 1.5.0

- Add linear gridding for bathymetry data

5.5 Version 1.4.2

- Fix missing conversion from list to NumPy array

5.6 Version 1.4.1

- Fix indexing of generator the new version `openpyxl` returns instead of a list
- Add changelog to documentation

5.7 Version 1.4.0

- Update to Python 3.6
- Use `m2w64-toolchain` from the channel `msys2` on Windows for C and FORTRAN compiler
- First conda package for Linux

5.8 Version 1.3.2

- `pip` installation without dependencies

5.9 Version 1.3.1

- Fix indexing in `phreeqc`
- Add `w2.pyd` to Windows release

5.10 Version 1.3.0

- Support Python 3.5
- Release as `conda` package
- Move output directory `balance` under `output`
- Turn user warnings into exceptions.
- Corrected for missing cos2sat values in netCDF file for high pH values
- Deep copy only needed data not whole input
- Add print out information for exceptions with small or wrong numbers
- Add deletion of input data that is already written to W2 readable files
- Correct time slots and reverse color map for pH values
- Corrected bathymetry preprocessing. Bottom is no always the second grid layer
- Allow three successive PHREEQC errors
- Add automatic saving of figures
- Add more specie names
- Use LLNL database as default
- Add tutorial for loading
- Add script to start Pyro servers for distributed PHREEQC runs
- Add script for charge balancing loading input data
- Add script to find date and concentration for a given water level

- Add script to calculate waterlevel-volume relation from W2 results
- Add script to convert balance files, so that relative time in days is used instead of date
- Add README
- Add W2 names for precipitation concentration
- Add some default concentration names to ‘‘ pitlakq/templates/precipitation_concentration.txt‘‘ Eventually, there need to be all names here
- Add equilibrium species to charge for preprocessing of charge for loadings
- Add cut of data below given heights
- Add all additional species to TDS.
- Remove `mx.DateTime` from project and use only `datetime`
- Add W2 manual for W2 version 2
- Add initialization script to automatically setup PITLAKQ
- Replace `optparse` with `argparse`
- Add option to show current project names

5.11 Version 1.2.0

- Include last day of month in groundwater time step
- Add print of error information if specie balance produces `inf` or `nan`
- Keep 10 old message files
- Ignore all sink/source terms for output per default
- Allow user-specified additional species and minerals
- Add check for defined constituents and mineral names
- Order of constituent flexible by for easier user input
- Add pit wall loading
- Constants are now input values
- Add more species to database
- PHREEQC database name is now an input parameter
- Keep 10 old copies of the PHREEQC output file for debugging
- Add Calcite and Siderite
- Enable parallel PHREEQC again
- Add PHREEQC executable for Mac OS X
- Add documentation for database extension and loading

5.12 Version 1.1.0

- Add help for command line options
- Support W2 compilation on Mac OS X
- Replace `pynetcdf` with `netCDF4`
- Set default algorithm for ice calculation to detailed

- Add preprocessing tool to allow user input of groundwater zones
- Added tool to find ice-free and freeze-over dates
- Add sub-module `gwh` for groundwater inflow based on lake water levels
- Add check for consistent names in distribution, flow, and concentrations
- Add commandline option to create new project.
- Add graphing for lake volume and area as function of water level
- Automation of Surfer to calculate volumes and planar areas for given levels
- Script to create waterlevel volume and area data and write them into a file
- Add `gwh` documentation

CHAPTER 6

Indices and tables

- genindex
- modindex
- search