

Simstrat

1D k-epsilon lake model

User Manual

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1. Introduction

Simstrat is a model for the physical simulation of water reservoirs, including basin morphology, interaction with the atmosphere, inflow and outflow.

A reservoir is simulated as a 1D vertical water column that is horizontally averaged. The column is composed of a certain number of layers, the evolution of which is driven by the atmospheric forcing, allowing the parameterization of stratification, energy transfers, turbulence effects, seiches, etc. Physically, water velocities, turbulent kinetic energy and its dissipation rate ($k-\epsilon$), temperature, salinity, seiche energy, stress and buoyancy are modeled.

This document is a user manual. For an in-depth description of how the model works (governing equations, numerical schemes, parameterization, etc.), the reader is referred to the paper by Goudsmit, G-H. et al. (2002): "Application of $k-\epsilon$ turbulence models to enclosed basins: The role of internal seiches." in *Journal of Geophysical Research: Oceans* (1978–2012) 107.C12: 23-1. Further changes to the physical model (i.e. which are not presented in this paper) are described in Chapter 2.

2. Changes up to version 3.0

2.1 Model changes

After the publication of the above-referenced paper, a few modifications have been performed on the algorithms governing the physical model.

Up to version 1.6

- The model tended to over-estimate wind-induced vertical mixing in winter (in non-stratified conditions), and to underestimate it during the stratified season. This is not surprising as one-dimensional models cannot account for horizontal gyres as well as two- or three-dimensional ones, and may give more energy to seiches than what really occurs in non-stratified conditions, when a basin is very difficult to excite vertically. It is now possible to feed the model with a time-series of pre-filtered wind, which will only be used for allotting seiche energy differently (equation 19 in Goudsmit et al., 2002). For example, it has been found that reducing the wind when it is not sufficient to trigger seiches motion (the duration of the wind event is small when compared to oscillation period of the basin) helps towards better modeling of the thermocline seasonal behavior. This setting can be enabled in the parameter file.
- Improved parameterization of heat fluxes according to Schmid and Köster (2016)
- Implementation of gravity driven inflows: one can let the inflow sink through the layers of the reservoir based on its density, entraining water with it and stopping when neutral buoyancy is reached. This can be particularly important because a one-dimensional model will first distribute an inflow across entire horizontal layers before it spreads vertically, therefore an arbitrary estimate of the inflow location can lead to great inaccuracies in compounds distribution and water column structure. This setting can be enabled in the parameter file.

Version 2.0

- Object-oriented Fortran 2003 architecture
- Implementation of a ice/snow model (based on MyLake)
- Implementation of surface bound in-/outflows: if the inflows are not gravity driven, one can either define them at a fixed spot in the morphology (i.e. subaquatic groundwater inflow) or let them vary with the water level (i.e. surface in- and outflows). The outflow is always placed manually and can be surface-bound or not.

Version 2.1

- Improved ice model with 3 layers and different formulation of light penetration

Version 2.2

- Water albedo is computed using the monthly Albedo data of Grishchenko in Cogley (1979)
- The seiche parameter α can have two different values, one for stratified and one for unstratified waters (stability threshold can be defined in the config file)
- Possibility to calibrate incoming short-wave and long-wave radiation separately using the scaling parameters p_{sw} and p_{lw} .

Version 2.4

- Possibility to start a simulation from a previously stored “snapshot” of the model. No need to run the whole model again from the very beginning for frequently updated simulations based on new meteo data for example.
- Possibility to define which variables will be written out
- Proper interpolation of model states when written to file at specific times

Version 3.0

- Coupling with the biogeochemical model “AED2” of the University of Western Australia (<https://github.com/AquaticEcoDynamics/libaed2>)

Version 3.01 (bug fix)

- Correct transfer of solar radiation from Simstrat to AED2

Version 3.02 (bug fix)

- Possibility to define the initial seiche energy in the configuration file.
- Addition of total seiche energy as output variable
- Possibility to switch off the progress bar
- Output of AED2 diagnostic variables (e.g. sediment and surface fluxes of variables) is possible now using a switch in the config file
- Elimination of a bug: the part of solar radiation which goes into the sediment is added back to the water column instead of disappearing

2.2 Changes to the configuration file

Version 2.0

- Addition of ice_albedo, snow_albedo and beta_snowice in ModelParameters
- Addition of switches for IceModel and SnowModel in ModelConfig

Version 2.1

- The ice/snow parameters are now defined in the model itself (strat_consts.F90) instead of the config file
- A few parameters were deleted in the config file by accident

Version 2.2

- The model parameters beta_sol (absorption of heat at the water surface), wat_albedo (user defined albedo of water), p_albedo (scaling factor for ice and snow albedo), freez_temp and snow temp are back in the configuration file
- New switch called "UserDefinedWaterAlbedo" is introduced to choose either internal calculation of water albedo or a use a user-defined constant.
- New model parameters a_seiche_w (winter seiche parameter) and strat_sumr (stratification threshold)
- New switch called "SplitSeicheParameter" to split the seiche parameter seasonally
- Name change p_radin to p_lw (scaling of long-wave radiation)
- New Modelparameter p_sw (scaling of short-wave radiation)

Version 2.4

- New switch "All" and parameter "Variables" in Output
- New switch "Continue from last snapshot"
- Unused ModelParameter "k_min" is removed

Version 3.0

- New config block "AED2Config" with AED2-specific parameters
- Name change of "InflowPlacement" to "InflowMode" and addition of the option of "InflowMode"=0 which disables all inflows. This means that InflowPlacement=0 maps to InflowMode=1 and InflowPlacement=1 to InflowMode=2.

Version 3.01

- Name change p_albedo to p_sw_ice (because this scaling parameter acts on the incoming short-wave radiation on ice and not on the albedo)
- Name change p_sw to p_sw_water

Version 3.02

- Name change “Start year” to “Reference year” because “Start year” is not the start of the simulation but the reference for the day count of the simulation.
- New switch “OutputDiagnosticVars” in AED2Config
- New parameter “seiche_ini” in ModelParameters
- New switch “Show progress bar” to switch progress bar on/off

3. Important hints

- Generally use a timestep ≤ 5 minutes (300 seconds) because the k-epsilon turbulence model requires a very small timestep.
- Use PressureGradient=2 for lakes close to the equator. Due to the lack of Coriolis force pressure gradients can become significant.

4. Model set-up

4.1. Physical

The physical model is run via its executable file, and is governed by a parameter file. The name of the parameter file can be given as first argument when calling the model executable; if nothing is given (or for example if the model is run with a double-click), then simstrat.par is the default (this will be the name used in the rest of this manual). This file specifies all input files, output locations, model settings and parameters. Table 1 shows an explanation of this file which is in JSON format. The model parameters (last part of Table 1) are better described in the above-referenced paper.

| JSON key | Description | Typical value |
|----------------------|--|---------------|
| Input | | |
| Initial conditions | Path to initial conditions file | |
| Grid | Path to grid file / vector of grid / grid resolution | |
| Morphology | Path to lake morphology file | |
| Forcing | Path to meteorological forcing file | |
| Absorption | Path to light absorption file | |
| Inflow | Path to inflow file | |
| Outflow | Path to outflow file | |
| Inflow temperature | Path to temperature inflow file | |
| inflow Salinity | Path to salinity inflow file | |
| Output | | |
| Path | Path result folder (is created if non-existent) | |
| OutputDepthReference | 1: Lake bottom, 2: Lake water surface | |
| Depths | Depths at which output is written: Path to file / vector of depths / output depth resolution | |
| Times | Path to file / vector of times / output time resolution | |
| All | True: all variables are written out, false: only selected variables in “Variables” are written out | |
| Variables | Vector of variable names (only used if “All”=false). | |

| | | |
|------------------------|---|-------|
| | Example: ["T","S"] | |
| ModelConfig | | |
| MaxLengthInputData | Maximum size of initial input data (initial conditions, morphology, grid...) | 1000 |
| CoupleAED2 | Switch to turn biogeochemistry model on/off (false = off, true = on) | |
| TurbulenceModel | 1:k-epsilon; 2:Mellor-Yamada | 1 |
| SplitSeicheParameter | True: use "a_seiche" if N^2 exceeds "strat_sumr" and "a_seiche_w" otherwise; false: always use "a_seiche" | false |
| StabilityFunction | 1:constant; 2:quasi-equilibrium | 2 |
| FluxCondition | 0:Dirichlet condition ; 1:no-flux | 1 |
| Forcing | 1:Wind+Temp+SolRad, 2:Wind+Temp+SolRad+VapP, 3:Wind+Temp+SolRad+VapP+Cloud, 4:Wind+HeatFlux+SolRad 5:Wind+Temp+SolRad+VapP+Incoming_long_wave | 3 |
| UserDefinedWaterAlbedo | True: Albedo is calculated internally according to Grishchenko tables; false: albedo has to be defined manually in the parameter block | true |
| UseFilteredWind | Use filtered wind to compute seiche energy (if "true", one more column is needed in forcing file) | false |
| SeicheNormalization | 1:max N^2 ; 2:integral | 2 |
| WindDragModel | 1:lazy (constant), 2:ocean (increasing), 3:lake (Wüest and Lorke 2003) | 3 |
| InflowMode | 0: no inflow; 1: manual inflow placement; 2: density-driven inflow | 2 |
| PressureGradients | Horizontal pressure gradients (0: off, 1: Svensson 1978 (not working), 2:bottom friction) | 0 |
| IceModel | 0: off, 1: on | 1 |
| SnowModel | 0: off, 1: on (needs IceModel=1 and an additional column in the forcing file: precipitation in [mm]) | 1 |
| AED2Config | | |
| AED2ConfigFile | Path to AED2 config file (*.nml) | |
| PathAED2initial | Path to folder with AED2 initial condition files | |
| PathAED2inflow | Path to folder with AED2 inflow files | |
| ParticleMobility | 0: off, 1: on | 0 |
| BioshadeFeedback | 0: off (light absorption is read from Simstrat file), 1: on (light absorption is computed in AED2) | 0 |
| BackgroundExtinction | Added to light absorption from AED2 (only used if BioshadeFeedback is turned on) | 0.2 |
| BenthicMode | 0: Only bottom most layer interacts with sediment, 1: flancs also interact with sediment (but sediment concentrations are not simulated) | 1 |
| OutputDiagnosticVars | True: AED2 diagnostic variables are written out; False: diagnostic variables are not written out | |
| Simulation | | |

| | | |
|-----------------------------|---|-----------|
| Timestep s | Simulation timestep in seconds | 300 |
| Reference year y | Reference year (only used for Albedo calculation) | |
| Start d | Simulation start in [days] since 01.01. of reference year | |
| End d | Simulation end in [days] | |
| DisplaySimulation | Display in command window (0: off, 1:when data is saved, 2: at every iteration) | 1 |
| Continue from last snapshot | True: continue simulation from last saved simulation state ("snapshot" file) if available; false: Start simulation from initial conditions | 0 |
| Show progress bar | True: progress bar is shown; false: not shown | True |
| Save text restart | True: Save model state as text files, false: don't save models tate | False |
| Use text restart | True: Start model from text file with previous model state; false: use standard initial condition format | False |
| ModelParameters | | |
| lat | Latitude [°] | 47 |
| p_air | Air pressure [mbar] | 960 |
| a_seiche | Fraction of seiche energy to total wind energy [-] | 0.01 |
| a_seiche_w | Fraction of seiche energy to total wind energy [-] in winter (if $N^2 < \text{strat_sumr}$) | 0.001 |
| strat_sumr | Threshold for seiche parameter: if $N^2 < \text{strat_sumr}$, a_seiche_w is used instead of a_seiche (only used if SplitSeicheParameter = true) | |
| q_nn | Fit parameter for distribution of seiche energy [-] | 1.00 |
| f_wind | Fit parameter for wind speed at 10m [-] | 1.00 |
| c10 | Wind drag coefficient (a physical constant around 0.001 if wind drag model is 1; a calibration parameter around 1 if wind drag model is 2 or 3) [-] | 0.001 / 1 |
| cd | Bottom drag coefficient [-] | 0.002 |
| hgeo | Geothermal heat flux [W/m ²] | 0.10 |
| p_sw_water | Fit parameter for short-wave radiation from sky [-] | 1.00 |
| p_lw | Fit parameter for long-wave radiation from sky [-] | 1.00 |
| p_windf | Fit parameter for convective and latent heat flux [-] | 1.00 |
| beta_sol | Fraction of short-wave radiation directly absorbed as heat at the water surface [-] | 0.30 |
| wat_albedo | User defined water albedo [-] (only used if UserDefinedWaterAlbedo = true) | 0.08 |
| p_sw_ice | Fit parameter for short-wave radiation from sky in the presence of ice, snow-ice and snow [-] (only used if IceModel on) | 1 |
| freez_temp | Freezing temperature of water [°C] | 0.05 |
| snow_temp | Temperature of snow [°C] | 1 |
| seiche_ini | Initial seiche energy [J] (only used if InitializeSeicheEnergy=True) | 1e8-1e10 |
| snow_ini | Initial snow thickness (if snow model enabled) | |
| w_ice_ini | Initial white ice thickness (if ice model enabled) | |

| | | |
|-----------|--|--|
| b_ice_ini | Initial black ice thickness (if ice model enabled) | |
|-----------|--|--|

Table 1 – Simstrat configuration file (simstrat.par)

4.2. Biogeochemical (AED2)

Information for this section is available on

<https://aquatic.science.uwa.edu.au/research/models/AED/index.html> and a default AED2 parameter file can be found in the tests folder in the Simstrat repository.

5. Input files

The input files are opened and read by the model while it is running. For all these files, the given depths must be within the limits set in the lake morphology (depth is zero at the surface and negative as it decreases downwards), while the given times must fall in the frame set by the simulation start and end time. In files where a series of values is required, depths have to decrease monotonously while times have to increase monotonously.

Throughout the simulation, the given values will be linearly interpolated (in depth and time) to obtain values at the coordinates needed by the model. If these coordinates are outside the given range, the value of the nearest neighbor is used. The model does not tolerate missing values. The files can have an arbitrary extension but must be text files.

5.1. Numerical

Grid

The entry given to the json key “Input.Grid” can either be a string (path to a file), a vector containing the grid points (meaning the faces of the grid layers) or a value specifying the total number of grid points. If a file path is given, the file can contain again either a vector of values (mostly used for variable grid spacing) or a number specifying the total number of grid points. If the grid points are specified, one needs to make sure to include the top and bottom values as defined in the morphology file otherwise an error occurs and the simulation aborts.

Output depths

The Output.Depths key specifies at which depths the model results will be written. It can either be a string (path to a file), a vector containing the output depths in [m] or a value specifying output resolution in [m]. If a path to a file is given, this file can again contain either all output depths in [m] or an output resolution in [m]. The key Output.OutputDepthReference indicates whether the output depths should be interpreted as absolute height above sediment (“bottom”) or as depth below water level (“surface”). If the reference is “surface”, the depths are written as negative depths below water table. Conversely, if it is “bottom”, the depths are written as positive depths above lake sediment.

Output times

The Output.Times key specifies at which times the model results will be written. It can either be a string (path to a file), a vector containing the output times in [days] or a value specifying output time resolution in timestep units (i.e. if 100 is given, the output is written every 100 timesteps). If a path to a file is given, this file can again contain either all output times in [days] or the resolution [timesteps].

5.2. Physical

Morphology

The key Input.Morphology specifies the shape of the basin by giving its surface area (positive) at various depths. The values should cover at least the entire depth range of the reservoir: from the initial surface (0 m depth) to bottom (with ideally 0 m² surface area). During the simulation, water level will not be allowed to rise above the depth of the first given value which can be 0 or any positive number for which one knows the surface area.

The first line of the file is a header; the next lines are the depths in [m] in the first column and surface areas [m²] in the second column. An example of this file:

| z [m] | Area [m2] |
|-------|-----------|
| 0 | 500000 |
| -5 | 450000 |
| -10 | 410000 |
| -20 | 332000 |
| -40 | 175000 |
| -50 | 100000 |
| -60 | 0 |

Initial conditions

The Input.Initial conditions key specifies the state of the water column at simulation start time. Depth-dependent values for several variables can be given. Having initial conditions that are close to reality help the model to reach a physically consistent state faster. The depth values in the first column refer to the depth values in the morphology file. The first depth value is taken to be the initial water level of the reservoir (i.e. if -3 is chosen, the initial water level is set 3 meters below the 0 in the morphology file). The initial data values are extrapolated to the maximum depth in the morphology file in case not all the depths are given in the initial data file.

The first line of the file is a header, the next lines are the depths [m] in the first column and initial conditions in columns 2 to 7 (horizontal water velocity East U [m/s], horizontal water velocity North V [m/s], temperature T [°C], salinity S [‰], turbulent kinetic energy k [J/kg] and its dissipation rate ϵ [W/kg]). An example of this file (with initial water table at 0) :

| z [m] | U [m/s] | V [m/s] | T [°C] | S [‰] | k [J/kg] | eps [W/kg] |
|-------|---------|---------|--------|-------|----------|------------|
| 0 | 0.00 | 0.00 | 9.3 | 0.13 | 3e-06 | 5e-10 |
| -5 | 0.00 | 0.00 | 9.2 | 0.13 | 3e-06 | 5e-10 |
| -10 | 0.00 | 0.00 | 7.2 | 0.13 | 3e-06 | 5e-10 |
| -15 | 0.00 | 0.00 | 5.2 | 0.13 | 3e-06 | 5e-10 |
| -20 | 0.00 | 0.00 | 5.2 | 0.14 | 3e-06 | 5e-10 |
| -40 | 0.00 | 0.00 | 5.1 | 0.14 | 3e-06 | 5e-10 |
| -60 | 0.00 | 0.00 | 4.9 | 0.14 | 3e-06 | 5e-10 |

Forcing

The forcing file specifies the atmospheric conditions to be applied at the reservoir surface throughout the simulation. At various times (in days), several parameters are specified, depending on the forcing mode chosen by the key `ModelConfig.Forcing`.

The first line of the file is a header; the next lines are the input: the structure of the columns is shown in Table 2.

| Forcing mode | Column | | | | | | |
|--------------|----------|-----------------------|------------------------|--------------------------------|-------------------------------------|-----------------------|--|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
| 1 | Time [d] | Wind speed East [m/s] | Wind speed North [m/s] | Water surface temperature [°C] | Solar radiation [W/m ²] | | |
| 2 | Time [d] | Wind speed East [m/s] | Wind speed North [m/s] | Air temperature [°C] | Solar radiation [W/m ²] | Vapor pressure [mbar] | |
| 3 | Time [d] | Wind speed East [m/s] | Wind speed North [m/s] | Air temperature [°C] | Solar radiation [W/m ²] | Vapor pressure [mbar] | Cloud cover [-] |
| 4 | Time [d] | Wind speed East [m/s] | Wind speed North [m/s] | Heat flux [W/m ²] | Solar radiation [W/m ²] | | |
| 5 | Time [d] | Wind speed East [m/s] | Wind speed North [m/s] | Air temperature [°C] | Solar radiation [W/m ²] | Vapor pressure [mbar] | Incoming long wave radiation [W/m ²] |

Table 2 – Structure for forcing file

If the use of filtered wind is enabled, one more column has to be added after the standard ones. It contains the filtered wind speed [m/s] (norm value). If the snow module is enabled (not necessary for ice!), precipitation data [m/h] has to be added at the end (only possible for forcing modes 2,3 and 5).

An example of this file (with forcing mode “3” and without filtered wind and precipitation):

| t [d] | U [m/s] | V [m/s] | T [°C] | Sol [W/m ²] | Vap [mbar] | Cloud [-] |
|------------|---------|---------|--------|-------------------------|------------|-----------|
| 36556.0000 | -0.87 | -1.69 | 7.00 | 0.00 | 7.10 | 0.80 |
| 36556.0417 | -0.98 | 2.41 | 7.20 | 0.00 | 7.10 | 0.46 |
| 36556.0833 | 3.80 | -0.17 | 7.40 | 1.00 | 7.10 | 0.46 |
| 36556.1250 | 3.04 | -2.90 | 7.50 | 0.00 | 7.10 | 0.46 |
| 36556.1667 | 5.20 | 2.99 | 7.40 | 0.00 | 7.10 | 0.40 |
| 36556.2083 | 3.47 | 1.99 | 6.90 | 0.00 | 7.10 | 0.65 |
| 36556.2500 | -1.83 | 3.22 | 6.90 | 0.00 | 7.10 | 0.65 |
| 36556.2917 | -0.91 | 3.79 | 7.00 | 0.00 | 7.00 | 0.55 |
| 36556.3333 | -2.05 | -2.84 | 7.30 | 26.00 | 7.00 | 0.20 |
| 36556.3750 | 4.76 | 1.16 | 8.20 | 189.00 | 6.80 | 0.10 |

Light attenuation

The light absorption file specifies the attenuation coefficient of solar radiation as a function of depth and time. Here, the zero depth always represents the water surface (even if its absolute position varies during the simulation).

The first line of the file is a header, the second line gives the number of depths for which the attenuation coefficient is specified (say n), the third line represents these depths (with the first number being a dummy value), the next lines are times [d] in the first column and attenuation coefficients [m⁻¹] in columns 2 to n+1. An example of this file:

| t (1.column) | z (1.row) | Abs [m ⁻¹] |
|--------------|-----------|------------------------|
| 2 | | |
| -1 | 0 | -5 |
| 0 | 0.200 | 0.300 |
| 2130 | 0.212 | 0.331 |
| 2260 | 0.177 | 0.198 |
| 2390 | 0.667 | 0.668 |
| 10000 | 0.700 | 0.750 |

In this example, the light absorption coefficient on day 0 would be 0.2 m⁻¹ at the surface, then linearly increase to 0.3 m⁻¹ at 5 m depth, and remain constant below this depth.

Inflow and outflow

Four files define the flows entering and coming out of the simulated reservoir, as a function of depth and time: water inflow, water outflow, temperature input and salinity input. Their contents represent a different physical quantity, but their structure is similar.

There are two kinds of different inflows: “deep inflows” and “surface inflows”. The inflow depth of “deep inflows” is fixed relative to the bottom of the lake (i.e. does not vary with varying lake level), while the inflow depth of “surface inflows” is fixed relative to the water surface. If the key `ModelConfig.InflowMode` is set to “1”, both types of inflows will enter the lake at the depths given in the file. If this key is set to “2”, then the “deep inflows” will plunge and stratify according to their density (surface inflows still enter the lake at fixed depths). In the following, the structure of the inflow files is given for both inflow modes.

- Manual inflow mode (`ModelConfig.InflowMode = 1`)

All values in the files must be given for a range of depths on a per-meter basis (Q/h), as they will be integrated over depth by the model. Water inflow values must be positive, water outflow values must be negative. Temperature and salinity input can be either, as it can be used as an independent source or sink of T and S . In order to specify temperature (resp. salinity) of the inflowing water, the given values must be the product of the water inflow (as in the water inflow file) and the inflow temperature (resp. salinity), and thus be positive. In addition, the depths and times must match.

The first line of the file is a header, the second line gives the number of deep inflows (the ones that don't move with the water level) and surface inflows (the ones that move with the water level). The third line represents these depths (with the first number being a dummy value), the next lines are the times [d] in the first column, values (water inflow [m^2/s], water outflow [m^2/s], temperature input [$^{\circ}Cm^2/s$] or salinity input [$\text{‰}m^2/s$]) in columns 2 to $nval+1$.

Note that the depths are given relative to the initial water level (for deep inflows) and relative to the changing water level (for surface inflows).

- Density-driven inflow mode (`ModelConfig.InflowMode = 2`)

For deep inflows, each column represents one density driven inflow with its input depth (from where it will move to its stratification depth) given in line 3 for inflow, temperature and salinity. For surface inflows and for the outflow (both deep and surface inflow), the manual syntax (see above) remains valid. From line 4 on, the actual inflows are given: times [d] in the first column, values (water inflow [m^3/s], water outflow [m^2/s], inflow temperature [$^{\circ}C$] or inflow salinity [‰]) in the second column.

An example of the water inflow file (left: manual inflow mode, right: density-driven inflow mode) for equal total inflow:

| t (1.column) | z (1.row) | | Q [m^2/s] | | | | | t [d] | z (1. row) | Q [m^3/s] / [m^2/s] | |
|--------------|-----------|-------|---------------|------|---|------|---|-------|------------|-----------------------------|---|
| 5 | 2 | | | | | | | 1 | 2 | | |
| -1 | -10.0 | -10.0 | -5.0 | -5.0 | 0 | -2.0 | 0 | -1 | -10.0 | -2.0 | 0 |
| 3084 | 0.000 | 0.5 | 0.5 | 0 | 0 | 1 | 1 | 3084 | 2.5 | 1 | 1 |
| 3098 | 0.000 | 0.55 | 0.55 | 0 | 0 | 1 | 1 | 3098 | 2.75 | 1 | 1 |
| 3112 | 0.000 | 0.6 | 0.6 | 0 | 0 | 1 | 1 | 3112 | 3.0 | 1 | 1 |

An example of the water outflow file with deep and surface outflow (for a neutral water balance with the inflow given above):

| t (1.column) | z (1.row) | OutflowQ [m2/s] |
|--------------|-----------|-----------------|
| 0 | 2 | |
| -1 | -2.0 | 0 |
| 3084 | -2.25 | -2.25 |
| 3098 | -2.375 | -2.375 |
| 3112 | -2.5 | -2.5 |

An example of the temperature input file for a deep inflow at a temperature of 5°C and a surface inflow at 10°C with the inflow given above (left, manual) and for the case of a deep, density-driven inflows with temperatures of 5 and a surface inflow at 10°C (right, density-driven).

| t (1.column) | z (1.row) | T [°C*m2/s] | | | | | | | | t [d] | z (1.row) | T [°C] / [°C*m2/s] | |
|--------------|-----------|-------------|------|------|---|------|----|--|--|-------|-----------|--------------------|----|
| 5 | 2 | | | | | | | | | 1 | 2 | | |
| -1 | -10.0 | -10.0 | -5.0 | -5.0 | 0 | -2.0 | 0 | | | -1 | -10.0 | -2.0 | 0 |
| 3084 | 0.000 | 2.5 | 2.5 | 0 | 0 | 10 | 10 | | | 3084 | 5 | 10 | 10 |
| 3098 | 0.000 | 2.75 | 2.75 | 0 | 0 | 10 | 10 | | | 3098 | 5 | 10 | 10 |
| 3112 | 0.000 | 3.0 | 3.0 | 0 | 0 | 10 | 10 | | | 3112 | 5 | 10 | 10 |

An example of the water inflow file (left: manual inflow mode, right: density-driven inflow mode), for an inflow at a salinity of 0.2‰ (both deep and surface inflows) with the inflow given above:

| t (1.column) | z (1.row) | InflowS [‰*m2/s] | | | | | | | | t [d] | z (1.row) | S [‰] / [‰*m2/s] | |
|--------------|-----------|------------------|-------|------|-----|------|-----|--|--|-------|-----------|------------------|-----|
| 5 | 2 | | | | | | | | | 1 | 2 | | |
| -1 | -10.0 | -10.0 | -5.0 | -5.0 | 0 | -2.0 | 0 | | | -1 | -10 | -2.0 | 0.0 |
| 3084 | 0.000 | 0.10 | 0.10 | 0.0 | 0.0 | 0.2 | 0.2 | | | 3084 | 0.2 | 0.2 | 0.2 |
| 3098 | 0.000 | 0.125 | 0.125 | 0.0 | 0.0 | 0.2 | 0.2 | | | 3098 | 0.2 | 0.2 | 0.2 |
| 3112 | 0.000 | 0.15 | 0.15 | 0.0 | 0.0 | 0.2 | 0.2 | | | 3112 | 0.2 | 0.2 | 0.2 |

If `ModelConfig.InflowMode` = 0, the calculation of vertical advection is deactivated. This is in particular useful in case inflows are negligible for the dynamics of the reservoir.

5.3. Biogeochemical (AED2)

Initial conditions

In contrast to the initial conditions of the physical model (Simstrat), each biogeochemical variable needs its own file for the initial conditions. The reason for this is that AED2 modules can be turned on or off individually and thus the number of biogeochemical variables

simulated can be highly variable. The names of the AED2 initial condition files are “AED2MODULE_variable_ini”, for example the file for CH₄ of the AED carbon module would be “CAR_ch4_ini”. These files need to be placed into the folder defined by AED2Config.PathAED2Initial. The structure of the AED2 files is very similar to the Simstrat initial condition file:

| z [m] | ch4 [mmol/m3] |
|-------|---------------|
| 0 | 0 |
| -5 | 0 |
| -10 | 0 |
| -15 | 0 |
| -20 | 5 |
| -40 | 10 |
| -60 | 30 |

Inflow and outflow

The structure of AED2 and Simstrat inflow files is identical. For every simulated AED2 variable, there needs to be an inflow file named according to “AED2MODULE_variable_inflow” (for example for CH₄ of the carbon module: CAR_ch4_inflow) placed into the folder in AED2Config.PathAED2Inflow. For more details, the reader is referred to the “inflow and outflow” section for the physical model (4.2).

6. Output

The output is written to a separate text file for each output variable and stored in the location defined by Output.Path. If the output folder does not exist, it will be created automatically. The files are named according to the variable they contain var_out.dat, where var is the short name of the variable (see Table 4). Output depth and times are used as defined in section 3.1. If Output.All is “true”, all variables in Table 4 are written out, if it is “false”, only the variables defined in Output.Variables are written out.

The output depth and time resolution can be specified using the keywords “Depths” and “Times” in the “Output” block. “Depths” can either be i) a number (interpreted as depth interval in [m]), ii) a list with output depths or iii) a path to a file. The file again contains either a number or a list of output depths. Similarly, “Times” is either i) a number “n” (interpreted as output every “n”th timestep), ii) a list of output times or iii) a path to a file. The file again contains either a number or a list of output times.

The AED2 variables are written into the same output folder.

| Short name | Description | Grid | Units |
|------------|--|--------|-------------------|
| U | Water velocity (East direction) | Volume | m/s |
| V | Water velocity (North direction) | Volume | m/s |
| T | Temperature | Volume | °C |
| S | Salinity | Volume | ‰ |
| Qvert | Vertical advection | Face | m ³ /s |
| k | Turbulent kinetic energy | Face | J/kg |
| eps | Dissipation rate of turbulent kinetic energy | Face | W/kg |
| nuh | Turbulent diffusivity of temperature | Face | J·s/kg |
| num | Turbulent diffusivity of momentum | Face | m ² /s |
| NN | Brunt-Väisälä frequency (stratification coefficient) | Face | s ⁻² |
| B | Production rate of buoyancy | Face | W/kg |
| P | Production rate of shear stress | Face | W/kg |
| Ps | Production rate of seiche energy | Face | W/kg |
| HA | Long-wave radiation from sky | - | W/m ² |
| HW | Long-wave radiation from water | - | W/m ² |
| HK | Sensible heat flux | - | W/m ² |
| HV | Latent heat flux | - | W/m ² |
| Rad0 | Solar radiation penetrating lake | - | W/m ² |
| TotalIceH | Total ice thickness | - | m |
| BlackIceH | Black ice thickness | - | m |
| WhiteIceH | White ice thickness | - | m |
| SnowH | Snow height above ice | - | m |
| WaterH | Water depth (positive height above sediment) | - | m |
| Qvert | Vertical advection | Face | m ³ /S |
| Eseiche | Total seiche energy | - | J |

Table 3 – Current Simstrat Output variables

7. Restart Simstrat from a previous model run

There are two possibilities to save a model state and use it to restart a new model run:

- The “snapshot” functionality: If “continue from snapshot” is set to “true”, Simstrat produces a binary file called “snapshot” containing the total state of the simulation. The same switch is used to restart the simulation from a “snapshot” file (if available). The snapshot functionality is easy to use and works for any Simstrat simulation. However, it does not allow to change the saved model state, i.e. does not allow updating the model state based on field observations for example.
- The “text restart” functionality: If “save text restart” is set to “true”, the model saves a txt file called “text_restart_1” which includes the model state variables U, V, T, S, k, eps, num and nuh at the internal depth resolution (on a staggered grid). In addition, a second txt file called “text_restart_2” is generated containing information about snow/ice thickness and total seiche energy. The file “text_restart_1” can be used as initial conditions for a new run and the information in “text_restart_2” can be used in the configuration file (initial conditions of snow/ice thickness and seiche energy). This functionality allows changes to the saved model state because it is written as text file. **However, this functionality is not intended to be used for simulations where the lake level changes!**

8. Parameter estimation

8.1. Introduction

Parameter estimation is performed through the software package PEST¹, which allows state-of-the-art model calibration and uncertainty analysis. More information about how the software works can be found in the PEST User Manual. In order to install PEST, one first has to download the archive containing all required files, and unzip it. The path to this directory must then be added to the PATH environment variable.

PEST requires several inputs that configure the parameter estimation for Simstrat:

- A control file (simstrat_calib.pst) that specifies the parameter estimation setup: optimization settings, parameter values and ranges, field data, references to the other files, etc.
- A template file (simstrat_par.tpl) that mimics the simstrat.par file, but with parameter names instead of values. Throughout the optimization process, PEST will fill it in with the values it wants and provide this new file to the model.
- A batch file (simstrat.bat) which takes care of the execution of the model.
- Field data that can be used to calibrate the model (e.g. temperature profiles, salinity profiles, ice thickness measurements).
- Model results that can be directly compared to the field data (i.e. in the same units, at the same times and depths).
- An instruction file (simstrat_obs.ins) that tells PEST how to relate the field data to the model results.

PEST can run in parallelized mode and operate much faster (using several CPUs, or several computers).

8.2. Set-up

The Python script PEST.py contains all the functions to prepare the whole PEST configuration and run calibration of Simstrat. As the single necessary input, it requires a configuration file (JSON format), which provides (i) the paths to the model, Simstrat configuration, observation files, and output directories/files, (ii) the number of CPUs to use in case of parallel calibration, (iii) the fixed and calibrated parameters.

The structure of the PEST configuration file is as follows:

| JSON key | Description |
|-------------|--|
| files | |
| model | Simstrat executable |
| configFile | Simstrat parameter file |
| (obsFile_X) | Observation file(s) for variable X; the name X must correspond to the Simstrat output file X_out.dat. Examples: obsFile_T, obsFile_S, obsFile_IceH |

¹ <http://www.pesthomepage.org/>

| | |
|---|--|
| refDate | Reference Simstrat date (corresponding to time=0), e.g.: "1981.01.01" |
| pestDir | Output directory for PEST to use as a working directory (PEST creates many files) |
| configFile_out | Output file to write the Simstrat parameter files with optimal parameters |
| results_out | Output directory to write the Simstrat results using optimal parameters |
| PEST | |
| nCPU | Number of CPUs to use (= 1 for single-threaded calibration, >1 for parallel calibration) |
| parameters | |
| (name of parameter as in Simstrat parameter file; max. 12 characters) | Fixed parameter(s): give a single value, e.g.: 1.0 |
| (name of parameter as in Simstrat parameter file; max. 12 characters) | Calibration parameter(s): give a vector as [starting value, lower bound, upper bound], e.g.: [1.0, 0.5, 2.0] |

An example of such a PEST configuration file is given on the GitHub: "Simstrat_v2/testcase/TestCase_LakeZurich.json".

In order to launch parameter estimation, one has to run the function `runPEST(configFile)` from within Python, where "configFile" is the PEST configuration file. For our test case, the series of commands on a Windows command prompt would be as follows (assuming the working directory is at the location of both PEST.py and the PEST configuration file):

- > python
- > import PEST
- > PEST.runPEST('TestCase_LakeZurich.json')

8.3. Output

When running, PEST outputs several text files useful to understand (and possibly correct and improve) the calibration procedure. The set-up file (`simstrat_calib.pst`) contains the configuration used by PEST. The record file (`simstrat_calib.rec`) contains the whole log of calibration, for example the evolution of the performance as different parameter values are tested. If calibration succeeded, the parameter file (`simstrat_calib.par`) contains the final (calibrated) value of the parameters. The residuals file (`simstrat_calib.res`) contains the final residuals for all observations used for calibration. The run management record file (`simstrat_calib.rmr`) contains a log of the interactions between the processors (in the case of parallel calibration).