Manual PyLakeSMB

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1 Configuration of the model run

The configuration file config_model.yml is located in the main folder and it is used to set the different options of the model. See example below:

```
# ========================================================================
# Inputs path and filenames
# ========================================================================
path: 'Data'
path_res: 'Results'

# ========================================================================
# Model configuration
# ========================================================================
ConfModel:
  Kh_model: 'P' #('P' : Peeters 2005, 'L': Lawrence 1995)
  k600_model: 'kAVG' # ('VP : Vachon & Prairie, 'CC': Cole & Caraco)
  t_end: 30 # days
  dt: 0.005 # days
  dr: 1 # meters
  mode_model:
    mode: 'OPT'
    var: 'PNET'

lakes:
```

```
  Lake1: ['20180616', '20180902']
  Lake2: ['20180616']

Montecarlo:
  perform: True
  N: 10.1
```

1.1 Variable description

- `path:` Input data path (*default: Data*)
- `path_res:` Output data path (*default: Data_res*)
- `ConfModel:` Here is define some parameterizations options of the model.
  - `Kh_model:` String to choose the horizontal dispersion coefficient model. Options:

    `P`: Peeters & Hofmann[1] (*default*)

    `L`: Lawrence *et al.*[2]
  - `k600_model:` String to choose the k_{600} literature parameterizations. Options:

    `VP`: Vachon & Prairie[3]

    `CC`: Cole & Caraco[4]

    `MA-NB`: MacIntyre *et al.*[5] Negative-buoyancy.

    `MA-MB`: MacIntyre *et al.*[5] Mixed-buoyancy.

    `MA-PB`: MacIntyre *et al.*[5] Positive-buoyancy.

    `kAVG`: Average k_{600} extracted from flux chamber measurements (*default*).
  - `t_end:` Maximum time in days that define the pre-run time of the model to define the initial concentration. The pre-run stops when the concentration at time t and $t+1$ is lower than $1 \times 10^{-4}\,\mathrm{mg\,m^{-3}}$.
  - `dt:` Time interval in days to run the model.

  - dr: Distance in meters that define the spatial grid of the model.
  - mode_model: Here is defined the type of model to run.
    * mode: Options:

      OPT: Optimization option. Find the value of the variable defined in the var option until the model concentration best-fit the measured concentration along the transect.

      EVAL: Simulate the surface water concentrations using the inputs values.

    * var: Options:

      PNET: In-situ net production.

      FSED: Sediment flux.

      KH: Horizontal dispersion coefficient.

- lakes: List of lakes and dates (YYYYMMDD) to run the model associated to each lake.
- Montecarlo: Here is defined the Montecarlo simulations.
  - perform: Boolean to run or not the Montercarlo simulations.
  - N: Iteration number of the Montercarlo simulations.

2 Input files

All the data are located in the folder define in path. Each lake data are organized in a folder named as in the config_model.yml file section lakes. Each lake-folder needs to contain four files Data_inputs.csv, Data_transects.csv, Data_parameters.csv and Data_bubbledissolution.csv that are described below. In addition, all the metadata information are described on the files inside the metadata folder.

- **Flux data:** Flux data is found in *Data_ inputs.csv* file.

```
Column,Units,Description
----------,,
Dates,YYYY-MM-DD,Sampling date
Fa_avg,[mmolm-2d-1],Average diffusive flux to the atmosphere
Fa_std,[mmolm-2d-1],Standard deviation of the Fa_avg
Fs_avg,[mmolm-2d-1],Average diffusive flux from littoral sediment
Fs_std,[mmolm-2d-1],Standard deviation of the Fs_avg
Rd_avg,[umolm-3d-1],Average bubble dissolution into the water column
Rd_std,[umolm-3d-1],Standard deviation of the Rd_avg
Fz_avg,[mmolm-2d-1],Average vertical flux through the base of the surface mixed layer
Fz_std,[mmolm-2d-1],Standard deviation of the Fz_avg
P_avg,[umolm-3d-1],Average insitu production/consumption in the water column
P_std,[umolm-3d-1],Standard deviation of the P_avg
```

- **Transect data:** Transect data is found in *Data_ transect.csv* file.

```
Column,Units,Meaning
----------,,
Sample,,Sample name
Date,YYYY-MM-DD,Sample date
Depth,[m],Water depth at sample location
Distance,[m],Distance from closest shore
CH4,[mmolm-3],Surface CH4 water concentration
dCH4,[‰],Carbon CH4 isotopic signature
Tw,[°C],Surface water temperature at the sample location
pCH4atm,[Pa],Atmospheric CH4 concentration
U10,[ms-1],Wind velocity at 10m
Fa,[mmolm-2d-1],Diffusive CH4 flux to the atmosphere
```

- **Lake Parameters:** Lake parameters data is in *Data_ paraeters.csv* file.

```
Columns,Units,Description
----------,,
Date,YYYY-MM-DD,Sampling date
Aa,[km2],Surface lake area
Hsml,[m],Surface mixed layer depth
As,[km2],Littoral sediment area
Kz,[ms-1],Vertical diffusivity
Chyp,[mmolm-3],Concentration below the hypolimnion
```

- **Bubble dissolution:** Bubble dissolution information is found in *Data_ bubbledissolution.csv* file.

```
Column,Units,Description
,,
Date,YYYY-MM-DD,Sample date
Depth,[m],Depth
Radius,[m],Distance from center
DissPerDepth,[umolm-1-d-1],Bubble dissolution per depth
Diss,[umolm-3-d-1],Bubble dissolution
```

3 Theoretical background

3.1 1D lateral transport model

Using a modified version of the lateral transport model presented by Peeters *et al.*[6], In this study, the lateral transport model includes vertical diffusive CH_4 flux through the bottom of the SML and bubble dissolution:

$$\begin{aligned}\frac{\partial C}{\partial t} =& K_H \frac{1}{H(r)r}\frac{\partial}{\partial r}\left(H(r)r\frac{\partial C(r)}{\partial r}\right) + \frac{1}{H(r)}K_z\frac{C_{\text{hyp}} - C(r)}{\Delta z} - \frac{k_x}{H(r)}\left(C(r) - H_{\text{cp}}\text{pX}_{atm}\right) \\ &+ \frac{F_s}{H(r)} + R_{\text{dis}}(r) + P_{\text{net}}; \qquad [\text{mol}\,\text{m}^{-3}\,\text{d}^{-1}]\end{aligned} \tag{1}$$

The left side of the equation is the change of the concentration C in time. Then, the first term on the right is the lateral transport where K_{H} is the horizontal dispersion coefficient, r the radius of the lake and $H(r)$ is the spatially varying thickness of the SML. The second term is the vertical flux through the bottom of the SML, where C_{hyp} is the CH_4 concentration 1 m below the bottom of the SML, $\Delta z = 1\,\text{m}$ and K_z is the vertical diffusivity. The third term represent the diffusive flux to the atmosphere that is estimated using a mass transfer coefficient for the gas x (k_x) and the difference between the surface concentration and the saturation concentration of

that gas. The latter is calculated using the partial pressure of atmospheric concentration of the gas X (pX_{atm}) and its Henry constant at in-situ temperature (H_{cp}) [7]. Finally, F_s is the diffusive flux from littoral sediments, $R_{dis}(r)$ is the bubble dissolution rates in the SML as a function of the distance from the center and P_{net} is the in-situ production consumption term. This model considers that the surface layer is fully mixed in the vertical and, therefore, the vertical concentrations are homogeneous within the SML.

In the simulations of each lake, we assumed that the SML, sources and sinks are radially symmetric in the horizontal plane. Therefore, the development of the concentration can be described based on the radial distance r from the shore to the center of the lake ($r_{max} = \sqrt{A_a/\pi}$).

Two regions are defined in the model, the littoral zone ($r \leq r_s = \sqrt{(A_a - A_s)/\pi}$) and the pelagic waters ($r > r_s$). The SML thickness ($H(r)$) is equal to the mixed layer depth in the pelagic region and, within the littoral zone, $H(r)$ decreases linearly with r from the mixed layer depth to zero at the shore. The littoral sediment flux is zero in the pelagic zone ($r < r_s$) and equal to the measured average littoral sediment flux ($\overline{F_s}$) in the shallow region ($r \geq r_s$) as:

$$F_s(r,t) = \begin{cases} \overline{F_s} & \text{for } r \geq r_s \\ 0 & \text{for } r < r_s \end{cases} \qquad [\text{mmol}\,\text{m}^{-2}\,\text{d}^{-1}] \tag{2}$$

At the boundaries, horizontal fluxes were assumed as zero. This model can be used for any compound, but so fat it is implemented only for CH_4.

References

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6. Peeters, F., Encinas Fernandez, J. & Hofmann, H. Sediment Fluxes Rather than Oxic Methanogenesis Explain Diffusive CH_4 Emissions from Lakes and Reservoirs. *Scientific Reports* **9.** doi:10.1038/s41598-018-36530-w (2019).

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