User guidance for the FLaMe (Fluxes of Lake Methane) model

This guidance is for the first version of FLaMe model (FLaMe v1.0), developed by the research group Biogeochemistry and Modeling of the Earth System (**BGEOSYS**), one of the three thematic research groups in the Department of Geosciences, Environment and Society (DGES) of the Faculty of Sciences at **Université libre de Bruxelles (ULB), Belgium**. The model codes and a testing example including four lakes (with input files uploaded) are publicly accessible, and the example corresponds to the evaluation of FLaMe model (section 3.2) in the accompanied manuscript, "*A new biogeochemical modelling framework (FLaMe v1.0) for lake methane emissions on the regional scale: Development and application to the European domain*". If you want to utilize the FLaMe model and have any problems with the model codes, please feel free to contact us through Maoyuan Feng (Maoyuan.feng@ulb.be or maoyuanfeng93@gmail.com).

1. Hardware and Software Requirement

The Fluxes of Lake Methane (FLaMe) model is written in the programming language Fortran (For) and runs well on PC or a clustering using a gfortran Compliler. The use of the cross platform Visual Studio Code, which can be downloaded for free from https://code.visualstudio.com/download, is recommended by the authors. A minimum random access memory (RAM) of 500 MB is required. A standard model simulation with 10 years can be finished in about several minutes on a regular PC, and the tests were performed successfully with Windows, Mac, and Linux operating systems. If users have problems or difficulties in compiling and running the model, please feel free to contact us for help.

2. Download FLaMe

A package named "FLaMe", containing the source code of FLaMe as well as the model project, is available as supplementary material. The package contains 2 sub-folders:

1) Subfolder named "INPUT_OUTPUT", which contains two subfolders of "input" and "output" for the model inputs and outputs, respectively.

2) Subfolder named "CODE", which contains 36 subroutines that are classified into two groups:

A) Subroutines inherited from Canadian Small Lake Model (CSLM):

- CLASSI.f

- CLASSL.f

- density.f
- DIASURFZ.f
- DRCOEF.f
- DRCOEFL.f
- EQNST.f
- FLXSURFZ.f
- FREECONV.f
- LKTRANS.f
- MIXLYR.f
- **RUNLAKE.f (main for a single run)**
- SCREENRH.f
- SLDIAG.f
- SNINFL.f
- SNOADD.f
- SNOALBA.f
- SNOALBW.f
- SNOVAP.f
- TLSPOST.f
- TLSPREP.f
- TMELT.f
- TSOLVE.f
- TSOLVL.f
- XIT.f

(B) Biogeochemical modules, **newly developed in this study:**

- area_layer.f
- CH4_module.f
- Clabile_module.f

- geometry_bgc.f

- initialisation.f

- O2_module.f

- oxidation.f

- search_zebmin.f

- transport.f

- Writing.f

3. Source Code Files Description

This section provides a brief description of the source code files of newly developed *biogeochemical* modules, and their correspondence in the model description in our manuscript:

area_layer.f

- Calculation of the area of different water layers in the lake, with the lake shape specified in section **2.2.1 Model Scope: Idealized representation of lake morphology.**

CH4_module.f

- This subroutine corresponds to the section **2.2.2.2 Methane module.**

- Detailed calculation of the methane production in sediment, the split of methane production into diffusive and ebullitive pathways, the methane oxidation in sediment, as well as the transit from sediment to water and further to atmosphere, and the methane exchange with atmosphere.

Clabile_module.f

- This subroutine corresponds to the section **2.2.2.1 Organic carbon module.**

- Detailed calculation of the dynamics of depth-integrated primary production, mineralization, and burial fluxes.

- The feedback of phytoplankton growth on the photic depth is determined in this subroutine.

geometry_bgc.f

- The adaption of the temperature field of the "bucket" shape solved by CSLM to the new "valley" shape lake.

initialisation.f

- Initialization of the biogeochemical modules

O2_module.f

- This subroutine corresponds to the section **2.2.2.3 Oxygen module**

- The oxygen production due to the photosynthesis, oxygen consumption in the sediment due to heterogeneous respiration, oxygen consumption in the lake water due to heterogeneous respiration, as well as the diffusive transport of oxygen within water column, and the oxygen exchange with atmosphere.

oxidation.f

- The oxidation of methane in the water column

search_zebmin.f

- Solution of $z_{eb,min}$ that split the methane production into diffusive and ebullitive pathways. This subroutine corresponds to the section **2.2.2.2 Methane module**, with details provided in the Supplementary Materials.

transport.f

- Numerical scheme for the diffusive transport of gas (oxygen and methane) in the water column, corresponding to section **2.2.2.2 Methane module** and **2.2.2.3 Oxygen module.**

Writing.f

- This subroutine prints the variables of interests to the output files.

4. Inputs and Output Files

4.1 Preparation of input files

We have prepared an example for the users in the "input" subfolder. There are two input files for the FLaMe model, one ("lake_characteristic.ini") for the lake characteristic information, and the other ("meteorological_data.met") for the meteorological forcings of the lakes.

(1) lake_characteristic.ini: in each run, there could be multiple lakes in multiple grid cells

Here I use a "section" of an input template to explain the details in ***lake_characteristic.ini:***

===== Lake Classe 1 for (long,lat) = (8.98, 47.03)   =====

0   1.000 (Keep these two inputs unchanged)

21.40 (lake depth)   5.32 (lake shoreline)   0.0100 (total dissolved phosphorus)

10.00 (Initial temperature for different water layers)

(2) meteorological_data.met: The daily climate forcings are provided:

Variables in different columns:

Hour (here, all values are set as 0)

0

Day (e.g., 1,…,365 or 366)

Year (e.g., 2000,…, 2016)

rsds: Shortwave radiation (W m^{-1})

rlds: Longwave radiation (W m^{-1})

pr: Precipitation (mm s^{-1})

tas: Surface air temperature (°C)

huss: Near surface specific humidity (kg kg^{-1})

sfcWind: Surface wind speed (m s^{-1})

ps: Pressure (Pa)

As there may be several (representative lakes) in a single run, the climate forcings for different lakes in the same day are put in sequence. That's, in a single day, there should be *n* lines of climate forcing, with each line corresponding to a (representative) lake.

4.2 Postprocessing of output files

There are 14 output files named as "LAKE.of0–13", and we provide a matlab subroutine to extract the variables from these output files. Here we provide a brief description of the variables stored in each output file:

Lake.of0: I_max (number of lakes), dt (s; temporal resolution), DELZLK (m, water layer depth), and NLAKMAX_bgc (maximum number of layers of the valley shaped lake)

Lake.of1: NLAK_bgc (real number of layers of the valley shaped lake)

Lake.of2: YEAR (year), DAY (day of the year), HR (hour), MIN (minutes), I (lake index)

Lake.of3: HDTPH (m; photic depth), LKICEH (m, ice thickness), TSED (°C, sediment temperature, which is set as equal to the bottom water temperature)

Lake.of4: [Clabile] (g/m^3; concentration of labile carbon), FPP (g/m^3/dt; Flux of primary production), FRESP (g/m^3/dt, Flux of mineralization)

Lake.of5: [Clabile1] (g/m^3; labile carbon pool 1), [Clabile2] (g/m^3; labile carbon pool 2),

[Clabile3] (g/m^3; labile carbon pool 3), Fsed1 (g/m^3/dt; carbon flux that goes into labile carbon pool 1), Fsed2 (g/m^3/dt; carbon flux that goes into labile carbon pool 2), Fsed3 (g/m^3/dt; carbon flux that goes into labile carbon pool 3), FsCH41 (g/m^3/dt; methane production flux from labile carbon pool 1), FsCH42 (g/m^3/dt; methane production flux from labile carbon pool 2), FsCH43 (g/m^3/dt; methane production flux from labile carbon pool 3)

Lake.of6: [O2] (g/m^3; oxygen concentration in water), FatmO2 (g/m^3/dt; Oxygen exchange flux with atmosphere), FPPWC (g/m^3/dt; oxygen production flux due to the photosynthesis), Fw (g/m^3/dt, oxygen consumption due to heterogenetic respiration in water), Fsaer (g/m^3/dt, oxygen consumption due to heterogenetic respiration in sediment)

Lake.of7: FsCH4 (g/m^3/dt, methane production in the sediment), FsDiff (g/m^3/dt; Diffusion part of methane production), FsEbul (g/m^3/dt; Ebullition part of methane production)

Lake.of8: [CH4] (g/m^3, methane concentration in water), FatmCH4 (g/m^2/dt, methane exchange flux with atmosphere), FswDiff (g/m^3/dt, the diffusive flux of methane transfer from sediment to water)

Lake.of9: T_bgc (°C, the temperature field of valley shaped lake)

Lake.of10: k_diff (m2/s, the eddy-diffusive coefficient)

Lake.of11: ZPhotic (m, photic depth), ZRESP (m, maximum of the photic depth and mixing depth or thermocline), FRESPWC (g/m^3/dt, the respiration flux in the water column)

Lake.of12: FatmEbu (g/m^2/dt, Ebullitive methane flux)

Lake.of13: DELT_stor (s, time length with the occurrence of storage flux), Fstor (g/m2/dt, the storage methane flux), DELT (s, time length of the period), DELT_ice (time length with the appearance of ice)

5. Model compilation and run

(1) Before compiling and running the FLaMe model, the users need to modify the parameters in RUNLAKE.f, which is the **main** of the model.

The parameters need to be modified:

GEN_DIR and **FILE_DIR**: parameters for the directory where the codes are deposited.

SET: the scenario the users may use (the users may have multiple scenarios to test the model, so this parameter is used to set the scenario directory)

x_per_m: the number of printing the output per month, we have two choice for this parameter. i.e., 1 for monthly output and 4 for weekly output.

NLAT: Number of grid cells

NMOS: Number of representative lakes in each grid cell

(2) In the “CODE” subfolder, we provide a makefile to compile the FLaMe model, with the following commands:

rm *.o: remove all the previously compiled files

make -f Makefile_check: Compile the FLaMe model with a gfortran compiler

./RUNLAKE_check: Run the model, and you will find the new results in the “output” subfolder.