
This document briefly describes how to use the ebullition module based on bubble formation and growth described in Peltola et al. (2018).

The code can freely be used, on condition that this article is cited in publications. Please see the license.

1. COMPILING

The code is written in FORTRAN 90 and consists of the following files:

Makefile

| | |
|-----------------------|--|
| bubble_main.f90 | - Main program |
| bubble_parameters.f90 | - Contains model parameters and other control of the model run |
| bubble_geometry.f90 | - Controls the geometry of the grid |
| bubble_output.f90 | - Controls the output of the model |

The makefile is for compiling with gfortran. It is run with command make. This produces the executable file *model.exe*.

2. PARAMETERS

The set-up of the model runs is controlled via bubble_parameters.f90. It contains definitions of:

- constants (such as the gas constant)
- model parameter values
- the set-up of the run. Specifically, you can define:
 - peat depth
 - layer thickness
 - length of the model run, maximum is the length of the input data

3. INPUT FILES

The model requires as input three text files, named in the code *meteo.txt*, *Tprof.txt* and *CH4prof.txt*. Note that the locations of the input files on your computer are hard-coded in the code, modify them to match your folder structure.

- meteo.txt* contains three columns:

| Column # | 1 | 2 | 3 |
|----------------|-------|------------------------------|------------------------------------|
| Input variable | Day # | Air temperature *unit: °C | Atmospheric pressure *unit: hPa |

- Tprof.txt* contains the soil temperature profile in Kelvin. Its column number depends on the peat layer structure: there should be daily temperature values for each peat layer, starting from the top layer in column 1. No column for time is used. In the example file data in the first column corresponds to 0...0.2 m layer, the second 0.2...0.4 m and so on.

- c) *CH4prof.txt* contains the predefined pore water CH₄ concentrations in mol m⁻³. When the ebullition module is implemented in larger model this is of course solved dynamically by the model and hence this input is not needed, but for running the ebullition module independently, predefined CH₄ concentrations are needed. Note that when the ebullition module is run independently the exchange of CH₄ between the pore water and the bubbles does not alter pore water CH₄ concentration, but it matches always this input. Similarly as with the *Tprof.txt*, the file's column number depends on the peat layer structure: there should be daily concentration values for each peat layer, starting from the top layer in column 1. No column for time is used. In the example file data in the first column corresponds to 0...0.2 m layer, the second 0.2...0.4 m and so on.

4. OUTPUT

The model outputs the following text files:

1) *bubble_flux.txt*

- exchange of CH₄ between bubbles and pore water (mol s⁻¹) at different depths in the model
- first column is time, second column model layer closest to the surface (0...0.2 m), the third the model layer below that (0.2...0.4 m) and so on
- Negative values => pore water is losing CH₄
- Positive values => pore water is gaining CH₄ from the bubbles

2) *bubble_volumes.txt*

- Volume of free-phase gas (m³) at different depths in the model
- first column is time, second column model layer closest to the surface (0...0.2 m), the third the model layer below that (0.2...0.4 m) and so on

3) *methane_conc.txt*

- CH₄ concentrations in the pore water (mol m⁻³) at different depths in the model
- first column is time, second column model layer closest to the surface (0...0.2 m), the third the model layer below that (0.2...0.4 m) and so on

4) *output_fluxes.txt*

- CH₄ released in an ebullition event (mol m⁻² s⁻¹)
- first column is time, second column CH₄ released the surface and the third is the CH₄ released the lowest air layer below surface