# Manual for stand-alone version of the Multi-Layer Canopy CHemistry Exchange Model (MLC-CHEM)

**Version v5, June 2023: Updated version of MLC-CHEM compared to previously released version CANEXMIP training version (June 2017)**

Main modifications (see also main text changes compared to v2 and v1 indicated by *Italic text*) compared to v4/v3/v2/1:

1) **General bug fixes: Further experiences with application of the model in 1) MSc thesis projects (see references) 2) for the AQMEII phase 4 dry deposition model intercomparison initiative (Clifton et al., 2023, see references) and 3) PhD project studies by Auke Visser (see references), have revealed a couple of issues in the specific applications of MLC-CHEM for different sites. Below, the most significant changes are listed:**
   - **Modified calculation of friction velocity (see subroutine *emdep_xtsurf_calcra* in *messy_emdep_xtsurf.f90*); the previously calculated friction velocity (ustveg) from the read-in micrometeorology generally came out too small in comparison with the observed $u_*$. With the modified code, the simulated $u_*$ agrees much better with observations.**
   - **Modified calculation of time related parameters (*nstepinit*) used in the calculation of first-order estimates of the diurnal cycle in photolysis.**
   - **Modified calculations of in-canopy radiation profiles (*emdep_xtsurf_canrad2*) and proper use of of layer-averaged in-canopy radiation parameters such as fraction of sunlit leaves (*fsl*) for calculation of stomatal exchange (*emdep_xtsurf_ags*)**
   - **Modified calculation of some of the dry deposition terms also including extra diagnostics, e.g, stomatal contribution to total $O_3$ flux**

2) **Inclusion of atmosphere-biosphere exchange processes for carbonyl sulphide COS (Casse, L., 2020) and inclusion of ammonia ($NH_3$) exchange**

3) **Instead of having a 3 day dataset with observations for the tropical rainforest site ATTO (see below, v4), MLC-CHEM v5 comes with two example input datasets: 1) a simple example input dataset (4 tracers and precipitation data) and 2) a more detailed dataset with measurements collected at the Italian Bosco Fontana site (ECLAIRE, 2012). These data were applied in a study by Visser et al. (2022) relying on the use of MLC-CHEM on the role of canopy turbulence and soil NO emissions in $O_3$ deposition.**

4) **Option to use, instead of model calculated measured turbulent transport properties, e.g., the measured friction velocity and eddy-diffusivities (for different canopy layers), as done by Visser et al. (2021, 2022) for Ispra/Hyytiala and Bosco Fontana study.**

**Version v4, 16-6-2017: Updated version for the CANEXMIP training version**

**Main modifications (see also main text changes compared to v2 and v1 indicated by *Italic text*) compared to v2/1:**

1) Explicit calculation of stomatal resistance as a function of radiation, temperature, moisture and $CO_2$ based on an implementation of the AGS model system
2) Possibility to conduct simulations with > 2 layers. The default model system uses a crown- and understorey layer, similar to the application of MLC-CHEM in the global model system, but simulations can now also be conducted with many more canopy layers 1) to check the impact of increased resolution on atmosphere-biosphere fluxes and 2) for comparison of MLC-CHEM with in-canopy measurements at > 2 reference heights.

   The number of canopy layers is defined in the namelist with input parameters and switches (see below) where the parameter NVEGLAY_HR defines the number of layers for some of the high-resolution calculations of e.g. the canopy radiation profile and BVOC emissions. The parameter NVEGLAY actually defines the number of layers for which the calculation of the actual exchange is be done. In the default model this has a value of 2. Increasing this to more layers requires to also increase NVEGLAY_HR to an integer multitude of NVEGLAY.
3) For this training version of MLC-CHEM, the model uses as a default case simulations for the tropical rainforest using an input dataset that is inferred from the ATTO tower (Brazil) measurements. These simulations use the 2-layer exchange model version.

**Version v3, 14-06-2014**

**Main modifications (see also main text changes compared to v1 indicated by *Italic text*) compared to v1:**

4) Introduction of the option to consider a varying surface/mixed layer depth
5) Photolysis can be switched off
6) Added output to diagnose the role of processes; process tendencies (xttend.out) and NO, $NO_x$, isoprene, alpha- and beta-pinene and sesquiterpene emission fluxes and OH reactivity (included in veg_mlay.out)
7) Some modifications in the simulation of soil NO emissions
8) More obvious parameter names, e.g., "netrad" for net radiation and "tsurf" for the surface/skin/canopy temperature
9) Inclusion of example code to assign additional meteorological input parameters whenever you want to use your own input file with more observations compared to the example input file
10) Calculation of the date and time also being included in the output files to facilitate plotting; julian day is now calculated from the initial starting date and time
11) HONO and NOx emissions from leaf surface nitrate photolysis

This manual describes the main features and use of a stand-alone model version of a multi-layer canopy exchange model (MLC-CHEM) for the simulation of the exchange of reactive compounds and aerosol inside and above vegetation canopies. A main specific feature of this canopy model that distinguishes this model from other canopy exchange models such as CACHE (Forkel et al., 2006), CAFE (Wolfe et al., 2011) or FORCAsT (e.g., Asworth et al., 2015), is that MLC-CHEM can be applied for site-scale analysis of observations but also for explicit simulation of atmosphere-biosphere exchanges in large-scale models such as global chemistry and transport models. Actually, MLC-CHEM is based on the implementation of canopy exchange processes in the Earth system model EMAC (ECHAM5/MESSy Atmospheric Chemistry model, e.g., Ganzeveld et al., 2010).

The model version is developed such that it can be run or on a Linux system or on a windows computer. The system can for example be applied to;

- use the model to analyze surface layer observations of tracer concentrations (and fluxes) as a function of the observed micro-meteorology and vegetation cover

- introduce new model representations of biogenic emissions, dry deposition, chemistry or turbulence and to evaluate the impact of these new models on the simulations of atmosphere-biosphere exchanges

- study the main set-up of the modeling system in support of the further deployment of the model in other large-scale models than EMAC

The model system includes an option to read in a file that contains observations of trace gas concentrations and other auxiliary atmospheric surface layer data such as measured radiation, temperature and surface cover properties. This allows to use the model to analyze these observations in terms of the role of biogenic emissions, dry deposition, in-canopy chemistry and turbulence. In addition the model provides diagnostics on simulated fluxes, in-canopy concentrations and the effective exchange fluxes between the canopy and the atmosphere. The latter is relevant for any chemical compound that is prone to chemical transformations or deposition occurring at a timescale shorter than that of turbulent transport.

MLC-CHEM has initially been developed and implemented in the Single Column chemistry and climate Modeling system SCM. Details about the development and evaluation of that model are found in Ganzeveld et al. (2002a). The canopy exchange model has then also be implemented in the global chemistry-climate modeling system ECHAM4 to conduct a study of the role of canopy processes in global soil biogenic $NO_x$ emissions (Ganzeveld et al., 2002b). Since then the SCM, including the canopy exchange model, has been further developed and used the following studies that focused on atmosphere-biosphere and boundary layer exchange processes:

- Impact of Amazonian deforestation on atmospheric chemistry (Ganzeveld et al., 2004)
- Atmosphere-biosphere exchanges of peroxides (Ganzeveld et al., 2006a and b)

- Analysis of surface and boundary layer exchanges observed during the Gabriel campaign over the Guyana's, South America (Ganzeveld et al., 2008)
- Atmosphere-biosphere $NO_x$ exchanges over Michigan forest (Seok et al., 2012).

If you are interested to get access to the SCM (which runs only under a Linux environment, contact laurens.ganzeveld@wur.nl).

## Stand-alone version of MLC-CHEM: Main features

MLC-CHEM consists of number of different sub-modules that are used to calculate the different relevant processes that ultimately determine atmosphere-biosphere fluxes of reactive compounds and aerosols. In most state-of-the-art chemistry and transport models atmosphere-biosphere exchange processes are represented by separate models of biogenic emissions and dry deposition without considering interactions that occur within the canopy. This commonly applied approach (the so-called "big leaf" approach) is applicable for compounds that are inert at the timescale of turbulent exchanges (seconds – minutes – hours), e.g., exchange of $N_2O$ and $CH_4$. However, for many more reactive species such as $NO_x$, VOCs and $O_3$ canopy interactions involving emissions, chemical transformations, dry deposition and turbulence ultimately determine the effective exchange between the canopy and overlying atmosphere.

The main processes considered in the simulations of atmosphere-biosphere exchanges in the box model version of the multi-layer exchange model are:

- Biogenic emissions of VOCs (Guenther et al., 1995, MEGAN, Guenther et al., 2006, will be implemented later on), $NO_x$ (Yienger and Levy, 1995), HONO and Radon. The latter is added since Radon is an extremely useful tracer to evaluate the turbulent transport in the model

- Dry deposition of gases and aerosols. The dry deposition of gases depends on their uptake resistances that are calculated according to Wesely's (1989) parameterization that estimates these uptake resistances based on the compounds solubility and reactivity. A number of these resistance estimates are replaced by updated resistance values according to Ganzeveld et al. (1995) and Ganzeveld and Lelieveld (1998). The model also includes the opportunity to consider the role of the compensation point. The latter is relevant for i.e. the leaf-scale exchange of $NH_3$ and $NO_2$ but also for a number of oxygenated compounds (methanol, acetone). Instead of having stomatal uptake, internal production in the leaf tissue can result in leaf-scale emissions for ambient concentrations smaller than the compensation point.
  Dry deposition of aerosols (Stier et al., 2005) is calculated explicitly from canopy turbulence properties and a selected typical aerosol size (distribution) considering Brownian diffusion, impaction, sedimentation and re-suspension. It is based on the aerosol dry deposition scheme that has been used to develop a parameterization of bulk sulfate aerosol dry deposition (Ganzeveld and Lelieveld, 1998) with a number of further modifications essential to canopy aerosol dry deposition.

- Gas-phase chemistry. The model offers the opportunity to also consider the role of gas-phase chemistry. The current implementation of canopy chemistry in MLC_CHEM is based on a well-tested implementation of the Carbon Bond 4 mechanism (CBM4) chemistry scheme. It considers in addition to standard methane photo-chemistry ($O_3$, $NO_x$, $CH_4$, $CO$) the role of non-methane hydrocarbons including isoprene ($C_5H_8$), and a selection of hydrocarbon oxidation products such as formaldehyde, higher aldehydes and acetone (Roelofs and Lelieveld, 2000). Some extension of this chemistry scheme have been introduced in a number of studies such as the extension of the peroxide chemistry (Ganzeveld et al., 2006b). In addition, the first-order destruction process of mono- and sesquiterpenes have been introduced to study the role of chemistry in the effective exchange of these VOCs. Note that the model can also be run without considering the role of gas-phase chemistry for the CBM4 tracer list (62 tracers in total; to study the sensitivity of the results to gas-phase chemistry, e.g., the role of OH oxidation in isoprene destruction) or for a model set-up that uses only a limited amount of tracers (16 tracers).

- Turbulent exchanges. The model calculates the turbulent exchange of tracers inside the canopy and between the canopy and surface/mixed layer based on the K-theory which means that fluxes are calculated from an eddy-diffusivity coefficient (K) and concentration gradients between the models layers. The eddy-diffusivity inside the canopy is estimated from the eddy-diffusivity in the surface layer using the surface layer wind speed and calculated wind speed profile inside the canopy which depends on canopy structure.

- Surface/mixed layer. The model would normally consider the exchange between the canopy layers and the surface layer of the atmospheric chemistry transport/climate model with a typical depth of this surface layer on the order of 64m (comparable to the surface layer depth in ECHAM5). However, this would result in a strong daytime accumulation of emitted species such as isoprene and other BVOCs, $NO_x$ and Radon which are also effectively diluted by mixing throughout the boundary layer. Consequently, the current model version also includes the option to define a maximum depth of a mixed (boundary) layer, for example ~1500m. This maximum depth of the assumed well-mixed layer is reached at noon with a simple function being used to scale between a minimum and this maximum mixed layer depth . The minimum mixed layer depth resembles the selected depth of the surface layer (two times the initial reference height) and reflects presence of an nocturnal inversion layer with suppressed turbulent mixing conditions.

The multi-layer exchange model calculates the interactions between dry deposition, biogenic emissions, chemistry and turbulence within the canopy distinguishing a canopy-crown and canopy-soil layer. Ganzeveld et al. (2002a) demonstrated, comparing different resolutions of the model, that distinguishing two canopy layers, coupled to an atmospheric surface/mixed layer, is generally sufficient to simulate realistic $NO_x$ and $O_3$ canopy-top fluxes. The advantage of having only two canopy layers is that the set of equations to calculate canopy concentrations and fluxes can

be solved analytically which makes the model very efficient in terms of CPU-use, a main pre-requisite to use the model also in large-scale chemistry models such as EMAC. However, because of a large sensitivity of simulated VOC emission fluxes to radiation gradients in the top of the canopy, for this two-layer set-up of MLC-CHEM biogenic VOC emissions are calculated from radiation profiles distinguishing four canopy layers and subsequently used to calculate the canopy-crown and canopy-soil VOC emission flux.

Alternatively to the default 2-layer set-up, MLC-CHEM can also be set-up with a larger number of canopy layers, e.g., to facilitate the comparison of the model simulated concentration profiles with measurements inside the canopy at 2+ reference heights. The higher resolution runs can also be used for sensitivity experiments, e.g., to evaluate impact of vertical resolution on effective canopy-top fluxes.

The calculations of surface exchange processes are constrained with surface parameters such as Leaf Area Index (LAI), roughness, canopy height, etc. which are provided to the model as input parameters defined in the models *namelist* (see below). In addition, the simulations use some simple initialization of the main micrometeorological drivers of canopy exchanges including some first-order estimates of the diurnal cycle in radiation, temperature, wind speed, etc. These parameter estimates can potentially be overwritten by the observed temporal variability in these parameters (see Model settings: Using observations to constrain the model).

## Model installation, infrastructure and running the model

The model code is mostly based on Fortran F90 code but includes some sub-modules that use an older (Fortran F77) programming code. The model runs on unix/linux based systems and has so far be used on a Linux X86-64 (Suse10.2) system. Specific requirements to run and diagnose the model are a Fortran compiler (on the Linux, the Intel ifort compiler has been used). Diagnostics is based on ASCII output files that can easily be read-in by excel (or other plotting software, python) for analysis.

### Installation of the model

The most straightforward way to install the model is to unzip the available zip file of the most recent model version in a subdirectory, e.g., called *models*. The unzip operations will result in installing the model system with the directory containing the following subdirectories *input, output, nml* and *src*. The subdirectory *input* contains two example input files (see below) whereas the model produces a number of output files for diagnostics. The subdirectory *nml* contains the namelists (with model settings) for the two different example case studies whereas the subdirectory *src* contains the source code files.

### Running the model (general instructions and some specific ones for Linux)

The model is default set-up to run under a Linux environment and in the Makefile there is a reference to the Intel Fortran compiler (ifort) being available as free software for application under Linux. If you would like to use another Fortran compiler feel free to do so but it cannot be guaranteed that the model will run without any errors. Modifications of the model code and settings might be needed based on those other compilers. Please let me know (Laurens.ganzeveld@wur.nl) if the model is being used

with different compilers so that I can keep track of those applications for other new users of the model system.

To compile the model, go to the subdirectory *src* where you can check/modify the compiler settings in the *Makefile*. Before actually compiling the model also secure proper use of the file *sfmakedepend* by using the command *chmod u+x sfmakedepend*. You can now compile the model by using the command *make*.

*Note that in the current version of the Makefile, the linux compiler settings for the intel compiler (ifort) are set as:*

*F90FLAGS = -cpp -i4 -r8 -O3 -align dcommons -check bounds -extend_source*

*Using the less extensive compiler settings (F90FLAGS = -cpp –O0) resulted in some running problems. Also note that changing the compiler settings, to secure that these are properly used in the modelling system, first do a **make clean** which removes all the \*.o and \*.mod files.*

When the compiling and linking is properly done, it produces the model's executable in the main model directory. Before running the model you first need to copy the *namelist* file *emdep_"xxxx".nml* of the case study you want to conduct from *nml* to the main directory, saving it with the name *emdep.nml*. Then you can run the model in that main directory using the command: *./emdep_xtsurf.exe*.

**Windows system**

The model can also be run on a Windows computer. This is basically following the same steps as installing, compiling and running the model under Linux. However, you need to secure access to a windows Fortran compiler. Here I provide you some instructions to install a free Fortran compiler for application under Windows:

- Download the Fortran MinGW compiler (MinGW refers to "Minimalist GNU for Windows); e.g., https://sourceforge.net/projects/mingw/

- This will prompt you to install the software where you can indicate the directory for installation, e.g., in C:\program files\fortran

- Do also install utilities and libraries as being requested

- Accept that the directory is being added to the PATH

This should do; to run the model you need to start the *command mode*; go to *start →  run →* type *cmd*. You screen will now turn black but you can change to a small *command mode* screen using *Alt-Enter*. Go to subdirectory *src* in the main directory where you installed the model. With the installed g95 Fortran compiler you can now compile the model by using the command *make.bat*. When the compiling and linking is properly done, it produces the model's executable in the main model directory. Before running the model you first need to copy the *namelist* file *emdep_"xxxx".nml*

of the case study you want to conduct from **nml** to the main directory, saving it with the name **emdep.nml**. Then you can run the model in that main directory using the command: **emdep_xtsurf.exe**.

**Model infrastructure**

The main program that calls all subroutines to calculate the exchange fluxes and canopy concentrations is called **messy_emdep_xtsurf_box.f90**. The first term, **messy**, reflects that the MLC-CHEM originates from an implementation of the canopy exchange model in the chemistry-climate model EMAC (ECHAM5/<u>MESSy</u> Atmospheric Chemistry model, e.g., Ganzeveld et al., 2010). The term **emdep** refers to the fact that this model is/was part of the **em**issions and **dep**osition simulations in EMAC whereas the term **xtsurf** expresses the combination of the parameter name of tracers in EMAC **xt**m and **surf**ace exchange simulations.

This main program, **messy_emdep_xtsurf_box.f90**, includes a call to a subroutine to initialize the model settings through reading a **namelist** file that contains all kind of model settings (**emdep_xtsurf_initialize**, see below).

This is followed by a call of the subroutine **emdep_xtsurf_vdiff** (**vdiff** is used in EMAC to refer to the vertical diffusion subroutine in which normally also the call to the emission/deposition routines is being done). In **emdep_xtsurf_vdiff** (found in **messy_emdep_xtsurf_box.f90**) a number of subroutines is called to;

1) Initialize tracers, their properties and some of required tracer settings (**emdep_xtsurf_tracer_init**). In the current set-up a distinction is made between a basic small number of compounds (16) for simulations that do not consider chemistry and a more extensive set of tracers (62+) whenever chemistry is being included in the simulations.

2) Calculate tracer specific photolysis rates (j-values) (subroutine **emdep_xtsurf_jval**, found in **messy_emdep_xtsurf.f90**)

3) Read in a file that contains observations of tracer concentration and/or other auxiliary data (see below for details on the format of the file) (subroutine **emdep_xtsurf_readdata**, found in **messy_emdep_xtsurf.f90**)

4) Calculate in-canopy radiation profiles (needed for biogenic VOC emissions and in-canopy photolysis rates) (subroutine **emdep_xtsurf_calcprof**, found in **messy_emdep_xtsurf.f90**)

5) Calculate biogenic VOC emissions (according to implementation of Guenther et al., 1995 algorithm, Guenther's et al. (2006) MEGAN algorithm will also be soon available) (subroutine **emdep_emis_bio_VOC**, found in **messy_emdep_emis.f90**)

6) Calculate biogenic NO emissions (according to implementation of Yienger and Levy 1995 emission algorithm) (subroutine **emdep_emis_bio_NO**, found in **messy_emdep_emis.f90**)

7) Calculate turbulent exchanges from wind speed, roughness and temperature data (subroutine **emdep_xtsurf_calcra**, found in **messy_emdep_xtsurf.f90**)

8) Calculate surface uptake resistances, used in the calculations of dry deposition, from the tracers chemical properties (subroutine **emdep_xtsurf_calc_rs**, found in **messy_emdep_xtsurf.f90**)

9) Calculate the in-canopy wind speed profiles (subroutine **emdep_xtsurf_wndprof**, found in **messy_emdep_xtsurf.f90**)

10) Calculate in-canopy photolysis rates (subroutine **emdep_xtsurf_rjveg**, found in **messy_emdep_xtsurf.f90**)

11) Calculate/assign tracer specific compensation points (the ambient tracer concentration above which (leaf) deposition occurs and below which emissions occur (subroutine **emdep_xtsurf_ccomp**, found in **messy_emdep_xtsurf.f90**)

12) Calculate canopy exchange fluxes, in-canopy concentrations and the ratio of the canopy-top to the emission fluxes (canopy reduction factor) and some additional atmosphere-biosphere diagnostics (subroutine **emdep_xtsurf_veg_mlay**, found in **messy_emdep_xtsurf.f90**)

## Model settings: namelist

Model run settings include a number of general model settings, e.g., latitude, canopy structure parameters and some micrometeorological parameters, emission settings and settings for the simulations of the actual canopy exchanges. The model uses two approaches to calculate the temporal variability in atmosphere-biosphere exchange fluxes and concentrations 1) it reads in a file that contains the information on the drivers of the exchange, e.g., based on the actually measured micrometeorology and concentrations or alternatively, 2) it uses first-order estimates of input parameters that drive the simulations of emissions, dry deposition, chemistry and exchange, e.g., using some sinus/cosines functions to impose a diurnal cycle in radiation, temperatures and wind speed, etc. (see **messy_emdep_xtsurf_box.f90**).
The model settings are provided as input to the model through reading-in a so-called namelist called **emdep.nml** (being done by **messy_emdep.f90**).

*Below we show the namelist emdep_BoscoFontana.nml (see subdirectory nml). <u>In order to use this specific namelist, save it in the main directory as emdep.nml</u>. Hopefully the names of all the parameters/switches that can be modified are quite self-explanatory also checking the comments following the specific settings.*

```
! -*- f90 -*-

&CTRL
 casename  = 'BoscoFontana', ! Harvard forest simulations
 l_emis    = T,   ! switch for using emissions
 l_drydep  = T,   ! switch for considering dry depostion
 l_xtsurf  = T,   ! switch for exchange simulations
 ndtgstart = 2012062411, !
 ntimestep = 822,  ! number of timesteps (i.e., 31 days at 0.5-hour time steps)
```

```
dtimestep = 1800.,! length of timestep [s]
nwrite    = 1,   ! output frequency
zlatitude = 45.20,! latitude (for radiation calculations) [degrees]
zlongitude = 10.74,! longitude (needed to getting MEGAN emission factors [degrees]
zslf      = 1.,   ! surface land fraction [0-1]
zvegfrac  = 1.,   ! vegetation fraction [0-1]
zforestfr = 1.,   ! forest fraction [0-1]
zalbedo   = 0.12, ! surface albedo [0-1]
zlai      = 2.28, ! Leaf Area Index [m2 m-2]
zcanheight = 26., ! Canopy height [m]
zrheightsl = 81., ! reference height surface layer
zMLHmax   = 2500, ! Maximum mixed layer height
zroughness = 1.4, ! Roughness length for momentum [m]
ziladprof = 2,    ! Leaf Area Density profile (1=uniform, 2=top profile)
zqm1      = 0.012,! surface layer moisture [g H2O g-1 air]
zws       = 0.25, ! Soil moisture [g g-1]! NOTE the different units
zwsmax    = 0.465,! Field capacity [g g-1]! NOTE the different units, this wsmax is inferred from the read-in obs.
zprc      = 0.,   ! convective precipitation [m]
zprl      = 0.,   ! large-scale precipitation [m]
l_wetskinRH = T,  ! Calculates wet skin fraction as a function of RH
zwetskin  = 0.,   ! fraction of wetted surface [0-1]
l_fvpd    = T,    ! ESS_lg_20130424+ switch for water vapor pressure deficit impact
/
&CTRL_EMIS
l_emis_bio_NO    = T,   ! switch for biogenic NO emissions
l_emis_bio_VOC   = F,   ! switch for biogenic VOC emissions
l_emis_bio_VOC_MEGAN = T, ! ESS_lg_20130817+ added switch to use MEGAN model
l_emis_bio_jNO3  = F,   ! switch for foliage NOx/HONO emissions (nitrate photolysis)
l_emis_bio_NO_pls = F,  ! switch for considering pulsing in soil NO emissions
lcrfyl95         = F,   ! switch for using Yienger and Levy 1995 canopy reduction factor
iNOemclass       = 12,  ! MAQ_AV_20200416: changed from 8 (deciduous forest) ! soil NO emission class (see
messy_emdep_xtsurf_box.f90 for class names)
zisopemfact      = 16., ! isoprene emission factor [ug C g-1 hr-1]
zmonoemfact      = 0.4, ! MAQ_AV_20171003+ modified from 0.4, ! monoterpene emission factor [ug C g-1 hr-1]
zovocemfact      = 0.2, ! Other VOCs emission factor [ug C g-1 hr-1]
zfAPIN       = 0.45, ! fraction of monoterpene emission flux emitted as alpha-pinene
zfBPIN       = 0.45, ! fraction of monoterpene emission flux emitted as beta-pinene
zfSQTERP     = 0.1,  ! sesquiterpene emissions relative to total monoterpene emission flux
zradonemis   = 0.3e4,! radon emission flux [atoms m-2 s-1]
zco2emis     = 4.6e-6,! CO2 emission flux [mol CO2 m-2 s-1]
/
&CTRL_XTSURF
l_xtsurf_veg_mlay     = T, ! switch for using explicit canopy exchanges model
l_xtsurf_veg_mlay_ccomp = F, ! switch for using compensation points
l_xtsurf_veg_mlay_chem  = T, ! switch for considering gas-phase chemistry scheme with 62 tracers
l_xtsurf_veg_mlay_chem_reactions = T, ! switch for considering gas-phase rea ctions and photolysis
l_xtsurf_veg_mlay_chem_photolysis = T, ! switch for photolysis
l_xtsurf_AGS       = T, ! switch for using the AGS model to calculate the stomatal resistance considering CO2
Agstype            = 1,     ! Ags vegetation type, C3; Agstype=1, C4; Agstype=2, conifereous forest; Agstype=3, tropical
forest; Agstype=4
l_readdata         = T, ! switch for reading input data (observations)
infilename         = 'input/BFt_20120624_20120711.inp', ! dir/name of file with obs.
weight_pxtm1_obs    = 0.5, ! weight of observed concentrations in determining surface layer conc.
nveglay            = 2, ! number of canopy layers for exchange calc. being used (equidistant!, <=nveglay_hr)
nveglay_hr         = 4, ! number of canopy layers for high-resolution calc. (radiation, VOC emis., etc)
/
```

**Note:** when the switch l_xtsurf_veg_mlay_chem is set to true then the model uses the default CBM4 chemical mechanism to consider the role of gas-phase chemistry for 62+ tracers. Otherwise, the simulations are only done considering a limited set of 16 tracers. When you would like to test the sensitivity of the simulations to gas-phase chemistry for the model set-up with the 62+ tracers you can switch off the gas-phase reactions and photolysis for the 62+ tracers setting the switch l_xtsurf_veg_mlay_chem_reactions (which is default set at true) in &CTRL_XTSURF to false;

```
l_xtsurf_veg_mlay     = T, ! switch for using explicit canopy exchanges model
```

l_xtsurf_veg_mlay_ccomp = F, ! switch for using compensation points
l_xtsurf_veg_mlay_chem  = T, ! switch for considering gas-phase chemistry scheme with 62 tracers
**l_xtsurf_veg_mlay_chem_reactions = F**, ! switch for considering gas-phase reactions and photolysis

## Model settings: Using observations to constrain the model

One specific feature of using MLC-CHEM is that it can be constrained using observed meteorological and atmospheric chemistry parameters. In this way the model can be applied to evaluate those observations by conducting simulations to diagnose in-canopy concentrations, turbulent-, emission and dry deposition fluxes and canopy chemistry. In addition, through changing the model settings, e.g., by switching off and on the various processes, one can analyze the role of biogenic emission, dry deposition, in-canopy chemistry and turbulence in explaining the observed temporal variability in these observations. One could also analyze the sensitivity of the simulated concentrations and fluxes to assumptions about the canopy structure, e.g., changing the LAI and vertical distribution of biomass or changing relevant micro-meteorological parameters which are not always measured, e.g., soil moisture.

Constraining the model with the observations in the implementation of the canopy model coupled to the SCM is done using the so-called nudging methodology (Ganzeveld et al., 2006a and b). This methodology uses the difference between the actual observed and simulated parameter value to add implicitly the contribution by large-scale transport (e.g. advection of polluted air masses). This is done by adding a so-called advection tendency to other process  tendencies which are explicitly simulated in the SCM (turbulent and convective transport, emissions, deposition and chemistry) These tendencies are then used in the SCMs numerical scheme to calculate the new prognostic wind speed, moisture, temperature and tracer concentrations. However, in MLC-CHEM the temporal evolution in tracer concentrations does not use explicitly the tracer tendency in a numerical scheme. However, in MLC-CHEM you can also consider the role of advection of long-lived tracers and conduct simulations that resemble the actual observed conditions. This is done by simulating the changes in concentrations from the simulated and observed (surface layer) concentrations as a function of the selected weight assigned to the observed concentration. In the default version of the model this weight, called **weight_pxtm1_obs**, is assigned a value of 1 implying that the model results for the surface layer concentrations resemble the observed concentrations. But you can conduct experiments to assess the relative contribution by advection versus canopy vertical exchange processes by altering the value of this weight parameter in the **emdep.nml**.

### Example input file

Setting the switch **l_readdata = T**, the model will read-in the file being indicated in the namelist **emdep.nml** by the parameter **infilename**. This file can contain for example the observed tracer mixing ratios and some observed meteorological parameters. The model is provided with two example input files which you can find in the subdirectory **input**. Here we provide some more explanation of the example input file **example_run.inp**. The header of this formatted file (which can be manipulated using for example **wordpad** or **nedit**) is:

**NDTG     Starttime Endtime No. Day Dt [s]**

**2010062900 00.00  00.00  1    1800**

**Time NO[ppbv] NO2[ppbv] O3[ppbv] CO[ppbv] SO2[ppbv] Precip[mm]**

where **NDTG** refers to the reference time of the start of the simulation expressed in **yyyymmddhh**. The **Starttime** and **endtime**, number of days (**No. Day**) of observations and time between each observation (**Dt**, expressed in seconds) are also given. Then there is an open line. The next line starts with the reference time of each datapoint expressed in number of seconds relative to the **Starttime** followed by parameter names. Note that these parameter names are separated by a space and that there is not a space between the parameter name and it's units. So the file contains the NO, $NO_2$, $O_3$, CO and $SO_2$ mixing ratio, expressed in ppbv as well as the observed precipitation for 1 day covering the 29th of June, 2010, observed each half an hour (the parameter **time** reflects the time relative to the starting time with its value is here chosen to be in the middle of the measurement interval of 1800s. **The actual data points are produced in Excel saving the data in a tab delimited file**.

- Note that it is important that the start reference date/time (**ndtgstart**, see namelist) should be defined such that the model simulation start the simulation before the date/time of the first data point. Otherwise the model will stop giving a message that **NDTG < ndtgstart**

- Missing data points (NA) are indicated by the code -9999.999.

- Note that the subroutine does not only read the data but also conducts the time interpolation of data to correct for the differences in measurement- and model timestep

- The maximum number of read-in parameter is currently set at 100 parameters. If you want to read-in more parameters then change **nobs_max** in **emdep_xtsurf_vdiff**

- The actual use of the read-in observations is secured by assigning the parameter **observ** dependent on its index to the model specific parameters. This is done in the subroutine **emdep_xtsurf_vdiff** in **messy_emdep_xtsurf_box.f90** after the call of **emdep_xtsurf_readdata**. In case of reading in the example input file this assignment looks as follows:

```
! assigning the read-in observations to the specific model input data; in this case
! assigning the read-in NO, NO2, O3 and CO mixing ratios from the example input file
! to the parameter pxtm1_obs that is used to "nudge the calculated pxtm1" to simulate conditions
! close to the observed conditions
DO i=0,Nstep

  ! only assigned when not NA but also >= 0 (not using small negative concentrations)
  IF (observ(i,1) > 0.) pxtm1_obs(i,idt_NO)=1e-9*observ(i,1)  ! only assigning NO when NO > 0
  IF (observ(i,2) > 0.) pxtm1_obs(i,idt_NO2)=1e-9*observ(i,2) ! only assigning NO2 when NO2 > 0

  ! only assigning a value when not NA
  IF (observ(i,3) > -9999.) pxtm1_obs(i,idt_O3)=1e-9*observ(i,3)  ! observed O3 ppbv, only assigned when not NA
  IF (observ(i,4) > -9999.) pxtm1_obs(i,idt_CO)=1e-9*observ(i,4)  ! observed CO ppbv, only assigned when not NA
  IF (observ(i,6) > -9999.) prc(i)=1e-3*observ(i,6) ! assigning the read-in precipitation from the example file
```

! observ(i,6) is in mm whereas prc is in [m], only assigned when not NA  ENDDO

ENDDO

For example, if you would have the observed mixing ratios in pptv then use 1e-12 instead of 1e-9.

- *We have now also included another example input file, one actually used for the Bosco Fontana study by Visser et al. (2022). This input file can also be found in the input directory and being indeed read in by the model using the namelist file **emdep_BoscoFontana.nml** (see subdirectory **nml** and save that file as **emdep.nml** in the run directory). You can check the model code **messy_emdep_xtsurf_box.f90** specifically searching for **casename.EQ. 'BoscoFontana'** to find out how the read-in parameters have been applied to constrain the ~month of MLC-CHEM simulations for this site.*

- *When you produce another input file, then be aware that whenever observations are missing that the model then uses the first-order estimates of the input parameters. This can result in large changes in the parameter values of meteorological (and surface cover) drivers, dependent on the difference between the actual observed values and the first-order estimates. This can consequently result in unrealistic model results or even a model crash. In this case modify the first-order parameter estimates such that they are closer to the observed values. One should discard the model simulated output for those data points when there are missing observations in any comparison of the model simulations with the field observations.*

Since the subroutine is written specifically to read in this formatted file any new file that you would like to read-in should resemble this format. Of course you are free to read-in different files but this which would require editing the subroutine **emdep_xtsurf_readdata** (**messy_emdep_xtsurf.f90**). In the future, the model might be updated to include alternative subroutines to read-in and process alternative formats.

## Model output and diagnostics

NOTE: some output files of the provided version of the training activity contain more/slightly change output information compared to described below for each file. The list of output parameters given for most essential output, ***veg_mlay.out***, should though be reflecting the actual file being produced by the modelling system.

The model produces in the current version the following output for diagnosing the model simulations (*Note that all files now also include the date and time in a format that allows easy plotting as a function of time in programs such as Excel*):

***Avg_obs.out***: when ***l_readdata = T*** then the read-in and processed data are written to this file to allow checking for the proper reading and interpolation of the observations.

- *Always carefully check this file to secure that the data are properly read-in and interpolated. You can do so, e.g. by plotting the interpolated data versus the observations. Also check for a proper synchronization of the data, e.g. with read-in incoming solar radiation peaking at 12LT.*

*Note that the following overview of available output files/parameters might not fully cover all the diagnostics of the most recent version of MLC-CHEM where more parameters have been included, also for some for the 2+ canopy layers, based on more recent experiences since v3/v4.*

***Radiation_canopy.out***: file that contains the output parameters of the simulations of the radiation regime inside the canopy including the following parameters:

***Net. rad.***: net radiation [W m-2]
***ldatltime***: date and time [dd:mm:yy hh:min]
***Rvd(1)***: Diffusive radiation term layer no. 1 (top of four canopy layers) [W m$^{-2}$]
***Rvd(2)***: Diffusive radiation term layer no. 2 [W m$^{-2}$]
***Rvd(3)***: Diffusive radiation term layer no. 3 [W m$^{-2}$]
***Rvd(4)***: Diffusive radiation term layer no. 4 (lowest of four canopy layers) [W m$^{-2}$]
***FSL-sum***: Canopy integrated fraction of sunlit leaves [0-1]
***FSL*LAI***: Canopy integrated total area of sunlit leaves [m$^2$ m$^{-2}$]

***soilNOxemis.out***: file that contains the output regarding the simulations of soil-biogenic NO$_x$ emissions. Also note that in the header information about the soil NO emission class and the wet and dry soil emission factors is included:

***Tsoil***: Soil temperature [K]
***Ws***: Soil moisture [m]
***no_slflux***: NO soil emission flux [molec. m$^{-2}$ s$^{-1}$]
***no_emflux***: NO emission flux (soil flux corrected with CRF) [molec. m$^{-2}$ s$^{-1}$]

***veg_mlay.out***: main output file with a lot of diagnostics from the canopy exchange model including micrometeorology parameters, canopy turbulence parameters, tracer concentrations, fluxes and the calculated canopy reduction factors (the ratio of the canopy-top flux to the total emission flux): Here I provide the extensive list of output parameters in case you run the model including canopy chemistry.
*Note that this is the output for the 2-layer version with a canopy height of 30m. When applying a 2+ layer set-up of the model, then many of the parameters being resolved for this 2+ layers (e.g., wind speed, concentrations), are being written to the output files indicating their specific reference heights.*

***u(81)l***: wind speed surface layer [m s$^{-1}$]
***u(22.5m)***: wind speed crown layer [m s$^{-1}$]
***u(7.5m)***: wind speed understorey/canopy soil layer [m s$^{-1}$]
***u*-veg***: friction velocity surface layer [m s$^{-1}$]
***netrad***: net radiation [W m-2]
***Tair***: air temperature [K]
***Tsurf***: surface temperature [K]
***RH***: relative humidity [0-1]
***RiB***: bulk Richardson number [-]
***ML-depth***: mixed layer depth [m]

***Kh(51.8m)***: eddy-diffusivity heat between surface and crown layer [$m^2\ s^{-1}$]
***Kh(15m)***: eddy-diffusivity heat between crown layer and understorey [$m^2\ s^{-1}$]
***stom. cond.***: stomatal conductance [$m\ s^{-1}$]
***ws***: soil moisture [m]
***f-ws***: soil moisture stress function [0-1]
***f-wetskin***: fraction of wet skin (wet surface) [0-1]
***jNO2(81m)***: photolysis rate $NO_2$, surface layer [$s^{-1}$]
***jNO2(22.5m)***: photolysis rate $NO_2$, crown layer [$s^{-1}$]
***O3(81m)***: $O_3$ mixing ratio in the surface layer [ppbv]
***O3(22.5m)***: $O_3$ mixing ratio in the crown layer [ppbv]
***O3(7.5m)***: $O_3$ mixing ratio in the understorey [ppbv]
Many more concentrations

*.....*

***VdO3(22.5m)***: $O_3$ dry deposition velocity crown layer [$cm\ s^{-1}$]
***VdO3(7.5m)***: $O_3$ dry deposition velocity understorey [$cm\ s^{-1}$]
Some more deposition velocities but not all for all layers; Vd_crownl is the top layer and Vd_sl is the lower layer (including soil deposition)

*.....*

***NO_slflux***: NO soil emission flux [molec. $m^{-2}\ s^{-1}$]
***emflx-NOx_cl***: NOx ($NO_2$) emission flux crown layer [molec. $m^{-2}\ s^{-1}$], comp. point + $NO_3$ photolsysis
***emflx-NOx_sll***: NOx ($NO_2$) emission flux understorey [molec. $m^{-2}\ s^{-1}$], comp. point +$NO_3$ photolsysis
***emflx-HONO_cl***: HONO emission flux crown layer [molec. $m^{-2}\ s^{-1}$], $NO_3$ photolsysis
***emflx-HONO_sll***: HONO emission flux understorey [molec. $m^{-2}\ s^{-1}$], $NO_3$ photolsysis
***emflx-ISOP_cl***: isoprene emission flux crown layer [molec. $m^{-2}\ s^{-1}$]
***emflx-ISOP_sll***: isoprene emission flux understorey [molec. $m^{-2}\ s^{-1}$]
***emflx-APIN_cl***: a-pinene emission flux crown layer [molec. $m^{-2}\ s^{-1}$]
***emflx-APIN_sll***: a-pinene emission flux understorey [molec. $m^{-2}\ s^{-1}$]
***emflx-BPIN_cl***: b-pinene emission flux crown layer [molec. $m^{-2}\ s^{-1}$]
***emflx-BPIN_sll***: b-pinene emission flux understorey [molec. $m^{-2}\ s^{-1}$]
***emflx-SQTP_cl***: sesquiterpene emission flux crown layer [molec. $m^{-2}\ s^{-1}$]
***emflx-SQTP_sll***: sesquiterpene emission flux understorey [molec. $m^{-2}\ s^{-1}$]
***atmbioflx-O3***: $O_3$ atmosphere-biosphere flux [molec. $m^{-2}\ s^{-1}$]
***atmbioflx-NO***: NO atmosphere-biosphere flux [molec. $m^{-2}\ s^{-1}$]
***atmbioflx-NO2***: $NO_2$ atmosphere-biosphere flux [molec. $m^{-2}\ s^{-1}$]
***atmbioflx-ISOP***: isoprene atmosphere-biosphere flux [molec. $m^{-2}\ s^{-1}$]
***atmbioflx-APIN***: α-pinene atmosphere-biosphere flux [molec. $m^{-2}\ s^{-1}$]
***atmbioflx-SQT***: sesquiterpene atmosphere-biosphere flux [molec. $m^{-2}\ s^{-1}$]
***CRF_NOx***: $NO_x$ canopy reduction factor [ratio]
CRF for more emitted compounds

*......*

***OHr(81m)***: OH reactivity in the surface layer [$s^{-1}$]
***OHr(22.5m)***: OH reactivity in the crown layer [$s^{-1}$]
***OHr(7.5m)***: OH reactivity in the understorey [$s^{-1}$]
***O3stfl(22.5m)***: $O_3$ stomatal flux for the crownlayer [molec $m^{-2}s^{-1}$]
***O3stfl(7.5m)***: $O_3$ stomatal flux for the understorey [molec $m^{-2}s^{-1}$]
***VdO3-canopy)***: inferred canopy-scale $O_3$ dry deposition velocity [$cm\ s^{-1}$], calculated from flux and $O_3$ surface layer mixing ratio.


## ***VOCemis.out***: data on biogenic VOC emissions:


***Net. rad.***: Net radiation
***Tsurf***: Surface temperature [K]
***isopflux(1)***: isoprene emission flux of crown layer [molec. $m^{-2}\ s^{-1}$]
***isopflux(2)***: isoprene emission flux of understorey layer [molec. $m^{-2}\ s^{-1}$]
***monoflux***: crown layer monoterpene emission flux [molec. $m^{-2}\ s^{-1}$]
***ovocflux***: crown layer other VOC emission flux [molec. $m^{-2}\ s^{-1}$]

***HONO-NOxem_jNO3.out***. *file that contains output on the simulated HONO and NO$_x$ emissions from the photolysis of nitrate on the leaf/needle surface:*

***ddNO3***: dry deposition flux of nitrate (HNO$_3$) to the surface [molec. m$^{-2}$ s$^{-1}$]
***NO3s***: amount of nitrate on leaf/needle surface [molec. m$^{-2}$]
***prec.***: total precipitation [mm]
***throughfall***: fraction of canopy being wetted by rain [0-1]
***Fslsum***: integrated fraction of sunlit leaves [0-1]
***HONO_em, cl***: HONO emission flux in crown layer [molec. m$^{-2}$ s$^{-1}$]
***HONO_em, sll***: HONO emission flux in understorey [molec. m$^{-2}$ s$^{-1}$]
***NO2_em cl***: NO$_2$ emission flux in crown layer [molec. m$^{-2}$ s$^{-1}$]
***NO2_em, sll***: NO$_2$ emission flux in crown layer [molec. m$^{-2}$ s$^{-1}$]

***xttend.out***: *file that contains the simulated contribution by the different controlling processes to the simulated temporal variability in concentrations for a selection of the tracers. This contribution is reflected by process tendencies expressed in ppbv hr$^{-1}$. NO$_x$ reflects here the tendencies of NO + NO$_2$. The emission and dry deposition tendencies are only given for the canopy layers whereas the chemistry and vertical diffusion tendencies are provided for all three layers.*

## Troubleshooting/issues to carefully checked!

Below you can find a list of issues that can occur when something goes wrong in setting up/conducting the simulations:

- Note that when it appears that the model does use properly the defined settings in ***emdep.nml*** that this can due to the fact that there has been an error reading in this namelist.

  *** ERROR: READ ERROR in NAMELIST 'CTRL'in FILE 'emdep.nml' !

  In this case carefully check your edits of the namelist to see if you entered wrong parameter settings (format).

- If you get the following error message: ./sfmakedepend --file=depend.mk messy_emdep.f90 messy_emdep_emis.f90 messy*….make: ./sfmakedepend: Permission denied, it means that the file *sfmakedepend* does not have the proper access settings. You can change this by securing that the file is also an executable. Under Linux use the following command: chmod u+x sfmakedepend. Under windows do a right click on the file, then go to Properties, then to Security where you can edit the Permissions of the file.

- When you get an error message regarding reading in the file that contains observations, you can check for the source of this error by printing the data to the screen. This is activated by uncommenting the following print statement in the subroutine ***emdep_xtsurf_readdata***:

  ```
  READ(NUNDATA,*,ERR=200,END=300)                          &
        TIME(I),(OBSERV(I,N),N=1,NPARAM)
  ```

! print *,'reading in observations: ',I,TIME(i),(OBSERV(I,N),N=1,NPARAM)

Having done so you get check the numbers as they have been read in but also, for example, the line number where the error occurs. One problem might be that NA (Not Available) values have not be replaced by the value -9999.999.

- *At the start of the model, a lot of information is written to the screen including the main settings but then also followed by the information on read-in data. Check carefully all that information to be sure that the experiments are properly initiated/set-up.*

- *Before analyzing in detail the simulated tracer fluxes, concentrations, other output, carefully check the main meteorological input parameters and directly related parameters of relevance for the simulations of atmosphere-biosphere exchange. Does the applied incoming radiation show the proper timing of sunrise, sunset and noon maximum? Does the calculated photolysis show a diurnal cycle that is consistent with the simulated diurnal cycle in radiation. Are other meteorological parameters such as wind speed, friction velocity but also canopy wetness (relevant for deposition) showing realistic diurnal behavior? For simulations covering multiple seasons, are seasonal changes in daylength properly represented? For multi-year simulations, check for the extra one day of the leap year.*

**Please report additional problems to [Laurens.ganzeveld@wur.nl](mailto:Laurens.ganzeveld@wur.nl) so that I can continuously improve the model and include these experiences in this particular section for other users of the model system.**

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