

A first introduction into the application of
canopy exchange modelling systems:

MLC-CHEM

Multi-Layer Canopy CHemical Exchange Model

Laurens Ganzeveld

Meteorology and Air Quality
Wageningen University
Laurens.ganzeveld@wur.nl

MLC-CHEM: Analysis of reactive compound observations in terms of emissions, deposition, chemistry and turbulence

MLC-CHEM is a stand-alone multi-layer canopy exchange model for the simulation of the exchange of reactive compounds and aerosol inside and above vegetation canopies that also allows analysis of such observations, e.g., to infer emission fluxes from observed concentrations. A main specific feature of MLC-CHEM, distinguishing this model from other canopy exchange models, is that it can both be applied for site-scale analysis of observations but also for explicit simulation of atmosphere-biosphere exchanges in large-scale models such as regional air quality (AQ) models, e.g., WRF-CHEM, to global-scale atmospheric 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). This implies that the large-scale implications of newly gained insights in site-scale atmosphere-biosphere processes can rather easily be evaluated with the same model system being implemented in EMAC (or other large-scale models).

More details on the representation of processes included in the model are given in the manual but can also be found in some of the manual references. The main features that are included in the current model version are biogenic emissions of BVOCs according to Guenther et al. (1995, 2006) and soil-biogenic NO_x emissions according to Yienger and Levy (1995). Dry deposition of gases and aerosols is calculated according to Ganzeveld and Lelieveld (1995) and Ganzeveld et al (1998) whereas more details on the coupling of these processes including the role of turbulence and canopy chemistry is given in Ganzeveld et al. (2002a). The current implementation of gas-phase chemistry is based on a modified version of the Carbon Bond-4 mechanism (in future the coupling to the Kinetic Preprocessor Program, KPP, will allow more flexible consideration of gas-phase chemistry).

Note that some detailed process representations such as calculation of the canopy layer's energy balance, as being done in some of the other canopy exchange models, are not included in MLC-CHEM. This has also partly to do with the fact that MLC-CHEM is a model system also being deployed in large-scale models such as global tracer transport and chemistry models and chemistry-climate models, e.g., EMAC and which provide generally the information on main drivers of atmosphere-biosphere included in MLC-CHEM. In addition, including very detailed exchange models in those systems is sometimes too "expensive" in terms of required computing time. However, rather MLC-CHEM, in this so-called offline application introduced in this training activity, is driven by the observed micrometeorological and hydrological drivers of atmosphere-biosphere exchange. This secures that model simulations of atmosphere-biosphere exchange reflects the results for the actual observed field conditions. In addition, in contrast to most other canopy exchange modelling systems that are used for simulations of maximum some days/weeks, the implementation of this offline version of MLC-CHEM also allows to conduct very efficiently long-term (seasonal-annual) simulations of these exchange processes.

In this workshop, with the actual training activity, covering ~3 hours, we will introduce you in the application of MLC-CHEM, as an example canopy exchange modelling system, to assess a number atmosphere-biosphere exchange features. It entails conducting a number of experiments with the modelling system and analyses of a tropical forest measurement dataset with the model system. To get this done in an efficient manner we would like you to already go through the first instructions of this workshop manual ahead of the actual 3 hour training activity.

We are much aware that this one 3-hour introduction is definitely not sufficient to introduce you all the details of such a canopy modelling system as MLC-CHEM. However, the training aims to provide you a first introduction into how canopy-interactions and atmosphere-biosphere exchange processes are being represented in canopy exchange models and on their potential application to evaluate field observations and/or develop and evaluate canopy process representations relevant for atmosphere-biosphere exchange of reactive compounds and aerosols.

Workshop activities;

The workshop is built around a number of activities including the following:

To be done in preparation for the workshop:

- Installing and running the model under Windows/Linux/Mac (note that the application of MLC-CHEM at the Mac has not yet been tested); This installation step uses the provided zip file and comes with a detailed manual.
- Read the Manual; note that the provided manual is based on an earlier version of MLC-CHEM and where some differences might exist with the current version introduced in this training activity. However, most of the information should be still up-to-date and should help you on the actual use of MLC-CHEM and analysis of the output.
- Model settings; checking the namelist with model input parameters and switches
- Check out how MLC-CHEM is being constrained with prescribed and/or observed drivers of atmosphere-biosphere exchange

Activities done during the workshop:

- Conducting a number of different experiments with MLC-CHEM and analyze some first output on canopy interactions; we will as much as possible discuss with the group the various cases being analyzed in this activity.

Installing and running the model under Windows or Linux

For those that have not yet installed the model on their laptop/PC please do so following the instructions that you can find in the manual.

- Windows environment: You might need to install the required Fortran compiler on your Windows computer as indicated in the manual. If you happen to have another Windows Fortran compiler that you would like to use than you need to adjust the reference to the Fortran compiler in **Make.bat**. However, note that the model has been tested using the MinGW compiler (see manual) and it cannot be guaranteed that the model runs properly using other Windows Fortran compilers. You actually compile and build the model using the command **make**. You can do so by opening the command mode; go to **start** → **run** → type **cmd** (If your screen now turns black you can change to a small command mode screen using **Alt-Enter**)
- Linux environment: The model has been tested using the Intel Fortran compiler (referred to as **ifort**). If you want to use a different compiler make the required changes in the file **Makefile** with the main settings how to compile and build the model. You actually compile and build the model using the command **make**.
- Mac: still to be evaluated (in preparation of this workshop this has been initiated)
- If the model has been installed and compiled properly you can now test if the model runs properly using the command **emdep_xtsurf.exe** (Windows) or **./emdep_xtsurf.exe** (Linux).
- In running the model, it writes out quite some more detailed information on the various calculations being done. Carefully check this information also since it informs you already what processes are considered in the model simulations also dependent on the settings of the model simulation as defined in the namelist (see below). You could also check the manual on the model's main features and model infrastructure. This also informs you about where you can find the calculations of the various processes and which you might ultimately like to modify/improve based in potential future studies with MLC-CHEM.

Before actually conducting and analyzing yourself some first experiments with MLC-CHEM, it is needed to introduce you into the diagnostics you get from the current model implementation.

- You can check the manual's section on **Model output and diagnostics** to get a better insight in the currently available diagnostics on the model simulation. The model produces a number of output files that should all support analysis of the data on the drivers of atmosphere-biosphere exchanges, simulated concentrations and tracer fluxes and additional relevant output parameters.

The output files are all written in a format that allows to easily open them in Excel and plot the parameters. Other software such as Python can also be rather easily used for the actual plotting and analysis of the model results but such plotting programs are not (yet) provided with the modelling system.

- Note that the information provided in the manual on the model's output is also not fully up-to-date anymore with the actual list of output files and included parameters for the version of MLC-CHEM made available for this training activity.

Model settings; using a namelist with model input and switches

One feature of MLC-CHEM which should make its use much easier is the use of a file, a so-called namelist, that contains many input parameters and switches to control the set-up of the model system. This is done to avoid that you need to continuously change these parameters and switches in the model code itself and then recompile again (taking extra time..). You can easily do many different experiments by simply changing the values of the input parameters and switching on- or off particular processes.

- Check the namelist ***emdep.nml*** regarding the list of parameters and switches that you can manipulate in MLC-CHEM through changing the entries in this file. The parameter/switches names are selected such that these are as much as possible self-explanatory and there is also more information included in the comment line. However, for their actual use in the model and how they affect the various calculations of atmosphere-biosphere exchange you would ultimately need to check in more detail the modelling code.

Note that the namelist has three different sets of parameters/switches 1) the more general ones found under the block ***&CTRL*** 2) the ones specifically required for the emissions calculations; ***&CTRL_EMIS*** and 3) the ones used for the simulation of the actual canopy (surface) exchange processes; ***&CTRL_XTSURF***. We refer you to the manual to get more detailed information on the different parameters.

- Tip: whenever you introduce changes in the namelist settings, save the name of the original namelist under a different name so that you can always go back to the base simulation if problems show up for the new parameter settings. The model reads in default ***emdep.nml***.

Constraining MLC-CHEM with drivers of atmosphere-biosphere exchange

MLC-CHEM simulates explicitly atmosphere-biosphere exchange having two different approaches 1) using some simple prescribed diurnal cycles in drivers such as net shortwave radiation, temperatures, moisture, wind speed, etc. 2) to read in a file with actual observations on these parameters. For this training activity we provide you a version of MLC-CHEM that reads in an input file with field observations collected at the Amazon forest Tall Tower Observatory (ATTO) site north of Manaus, Brasil. This input file is defined in the namelist:

Infilename = 'input/ATTO/O3_NOx_meteo_21092013_26092013_30min.inp',

Note that this file also contains, besides observations on the micrometeorology also the observed O₃ and NO_x concentrations and where the model has been constrained with the observed surface layer O₃ concentrations also to consider the role of advection of such a long-lived tracer. In the manual of MLC-CHEM you can find more details on how such an input file is put together (and how you could produce your own input file whenever you would like to use MLC-CHEM for your own specific field observations on tracer concentrations/fluxes).

The namelist settings further secure that the model conducts a simulation of 6 days with 144 timesteps of 10 minutes writing out data each third timestep. In addition, the model includes in these simulations of soil biogenic NO_x emissions for the emission class tropical forest (***iNOemclass = 11***) and uses an implementation of MEGAN to simulate BVOC emissions (***l_emis_bio_VOC_MEGAN = T***).

Besides the use of the prescribed or observed micrometeorological, hydrological and chemical drivers (e.g., surface layer O₃ concentrations) of atmosphere-biosphere exchange, MLC-CHEM also requires the definition of the basis biogeophysical properties of the canopy; this is also done in the namelist (***emdep.nml***). You can infer that for the tropical forest study of this training activity the model uses a canopy height (***zcanheight***) of 30m, an LAI (***zlai***) of 5 m² m⁻², a roughness length for momentum (***zroughness***) of 1m and a vertical distribution of LAI having the maximum in the top of the canopy defined by the Leaf Area Density (LAD) profile (***ziladprof***) in the model. The model also uses two canopy layers (***nveglay = 2***) for the exchange calculations whereas simulations of light dependent processes such as VOC emissions use a minimum resolution of 4 layers (***nveglay_hr = 4***). This higher resolution for these calculations is need to properly represent the large gradient in the canopy radiation profiles especially in the crownlayer.

With two layers for the simulation of the in-canopy and surface layer fluxes and concentrations and a canopy height of 30m, implying that the two canopy layers are 15m thick, the output is representative for a reference height of 22.5m (middle of the crownlayer) and 7.5m (middle of the understorey layer).

Conducting and analyzing some experiments with MLC_CHEM

Before start doing a number of different case studies you should do first an experiment using the default settings as defined in the provided namelist, saving those results in a subdirectory, e.g., called **default**, in the output directory. You can then use the results to compare those with those of the various case studies.

Before doing the various case studies, we strongly recommend you to first make a hypothesis on the expected results. You could also develop this hypothesis discussing this directly with your neighbor! To further trigger you developing such a hypothesis we have included in some of the case studies a number of questions that are indicated in italics.

Case #1: Ozone dry deposition as a function of moisture conditions

Dry deposition is calculated in MLC-CHEM from the turbulent transport, diffusion and uptake by the different surfaces found inside the canopy including leaf and soil surface. Leaf uptake is actually for most tracers controlled by stomatal uptake but for many more soluble and reactive compounds, there might also be significant non-stomatal removal dependent on specific conditions such as canopy wetness. Stomatal conductance is simulated in MLC-CHEM using two different parameterizations. With the settings of the namelist (**l_xtsurf_AGS = T**), the model uses actually the so-called **Ags** (Assimilation and stomatal conductance, **gs**) model in which stomatal exchange calculated as a function of radiation, temperature, CO₂, water vapor pressure deficit and soil moisture status.

- You can do an experiment with MLC-CHEM changing the assumptions on the amount of available soil moisture. You can do so changing in *emdep.nml* the soil moisture from its default value of 0.5m to something like 0.3m:

zws = 0.3, ! Soil moisture [m]

This parameter is used together with the maximum soil moisture, expressed by the field capacity, **zwsmax**, to calculate a correction function called **Fws** which value ranges between 0-1. Note that this function is actually commonly applied in Earth system models to consider the impact of reduced soil moisture on simulation of evapotranspiration.

For a soil moisture level at the field capacity its value is 1 and there is no soil moisture stress resulting in an uptake by the leaves at a maximum level. With a decrease in soil moisture, the value of **Fws** decreases and becomes 0 under a critical soil moisture level, called the permanent wilting point. In this case, there will not be stomatal uptake anymore. You could check the impact of having a reduced soil moisture by plotting (e.g., in Excel) the value of **Fws** and the dry deposition velocities of tracers such as O₃ written as output in the file **veg_mlay.out** (**VdO3(22.5m)** and **VdO3(7.5m)**) and comparing these with the results of the default simulation. You can also check how the differences in dry deposition affect the in-canopy O₃ concentrations (also found in **veg_mlay.out**).

This output file also contains the simulated O₃ stomatal fluxes (**O3stfl(22.5m)** and **O3stfl(7.5m)** expressed in molec m⁻² s⁻¹) and which can be compared with the actual canopy-top or atmosphere-biosphere flux of O₃: **atmbioflx-O3**. You could for example analyze how much of the canopy-scale deposition flux can be attributed to stomatal uptake (summing the crown- and understorey layer O₃ stomatal flux and dividing this by the canopy deposition flux) and how this changes with changes in soil moisture.

One specific useful feature of MLC-CHEM is that it also provides output on simulated process tendencies, expressed in ppbv/pptv/.. hr⁻¹, which is especially very useful to diagnose the role of different processes in determining the simulated change in concentrations (and fluxes). The process tendencies reflect the contribution by emissions, dry deposition, chemistry and turbulent transport to the simulated concentration changes inside the canopy and surface/mixed layer. In the current model implementation these data are given for a selection of tracers (to avoid getting too large files).

Question: Which process do you expect to dominate the changes in the O₃ concentrations inside the canopy?

- You can plot the O₃ process tendencies for the canopy crownlayer (22.5m) found in the output file **xttend.out** (for the default simulation). The file contains for O₃ the dry deposition tendency; **O3dd(22.5m)**, that for chemistry; **O3ch(22.5m)**, for turbulent transport (or diffusion); **O3df(22.5m)** and finally the total tendency which is the sum of those three individual tendencies; **O3tot(22.5m)**. This will help you to analyze which processes appear to control the simulated changes in the crownlayer O₃ mixing ratios.

This exercise should have made clear that for this particular simulation (the default case with soil moisture at field capacity), O₃ concentration changes are dominated by dry deposition of O₃, being an effective sink of O₃, and turbulent transport from the surface/mixed layer into the canopy to compensate for this strong pull of O₃ into the canopy. Chemistry plays a relative minor role in these concentration changes. These result stress that whenever there is a misrepresentation of simulated O₃ inside the canopy, e.g., based on comparison of the simulated and observed O₃ mixing ratios, that the #1 priority on explaining or solving this misrepresentation should be analysis of the simulated dry deposition and turbulence processes.

Case #2: Biogenic emissions and effective atmosphere-biosphere exchange: role of canopy interactions

If you would be interested to diagnose in more detail the simulations of soil NO and vegetation VOC emissions: More detailed output on these simulated emissions is found in the output files **soilNOxemmis.out** and **VOCemmis.out**. These files provide information on some of the basic drivers of these emissions and resulting emission fluxes.

In-canopy chemical destruction of the emitted reactive compounds such as NO and BVOCs and dry deposition of resulting reaction products such as NO₂ can be so fast/efficient that only a fraction of these emissions are actually being ventilated out of the canopy into the overlying mixed layer. This is one of the main reasons to consider canopy interactions in atmosphere-biosphere exchange of reactive compounds.

- Check on the role of canopy interactions in the effective exchange of NO_x and VOCs. You can do this by analyzing the fluxes of NO_x, isoprene and the monoterpenes for the different heights but also checking the simulated concentrations. The output file **veg_mlay.out** also contains the calculated so-called Canopy Reduction Factor (CRF) for a number of tracers, e.g., **CRF_NOx** (NO + NO₂), **CRF_ISOP**, isoprene **CRF_SQTERP**, sesquiterpenes). This CRF is calculated as the ratio of the canopy-top flux relative to the total soil/vegetation emission fluxes. A value of 1 for the CRF expressed that all the emitted mass is actually also ventilated out of the canopy into the surface/mixed layer whereas a value of 0 reflects that nothing of the emitted mass escapes the canopy. A negative value of the CRF actually reflects that there is a downward canopy-top flux.
- You could check on the role of gas-phase chemistry and dry deposition in the effective release of these reactive compounds from the canopy. You can do so by switching on/off the gas-phase chemistry and dry deposition using the switches:

I_xtsurf_veg_mlay_chem_reactions = T, ! switch for considering gas-phase..
I_drydep = T, ! switch for considering dry deposition

Question: What do you expect to be the differences in the NO_x and sesquiterpene canopy reduction factor when not considering in-canopy chemistry and/or in-canopy deposition?

You can also diagnose the impact of considering these processes in the effective exchanges of the reactive compounds comparing the process tendencies.

This analysis indicates about the role of the different processes in canopy interactions resulting in the occurrence of bi-directional exchange for a suite of reactive tracers. The fluxes can be downward or upward just dependent on the concentration gradient between the surface layer and the canopy, the latter being controlled by the continuously changing role of emissions, dry deposition, chemistry and turbulent transport. It results in a temporal variability in atmosphere-biosphere exchange fluxes quite different from how this is included in a large-scale model that ignore these canopy interactions (using the so-called “big-leaf” approach where the emissions and dry deposition processes are not coupled and the role of canopy chemistry and turbulence is being ignored).

Case #3: Compensation point: leaf- to canopy scale bi-directional exchange

Another exercise that you can perform with the model is to analyze the role of compensation points in atmosphere-biosphere exchanges. This refers to the fact that normally in the dry deposition calculations of many compounds it is assumed that the internal concentration (that of the substrate, e.g., the leaves) is ~ 0 implying that the exchange is dominated by the efficiency of uptake by the substrate, e.g., stomatal uptake, and the ambient concentration. However, it has been observed that for many reactive compounds, e.g., ammonia, NH_3 , oxygenated compounds such as methanol but also NO_2 , internal production mechanisms (e.g., inside the leaves or soil) result in internal concentrations comparable to or larger than ambient concentrations. This results in a substantial decrease in the dry deposition fluxes for internal concentrations $<$ the ambient concentration and even in a change from deposition/uptake to emissions in case that the internal concentration becomes larger than the ambient concentration. The concentration at which this switch from uptake to a release happens is called the compensation point.

- In the current model version we have included the role of an NO_2 compensation point of 0.5 ppbv. You can conduct a simulation with and without consideration of this compensation point using the switch:

`l_xtsurf_veg_mlay_ccomp = T, ! switch for using compensation points`

You could analyze how this affects the simulated in-canopy and surface layer NO_x concentrations as well as the atmosphere-biosphere fluxes, e.g., by comparing the sum of the **`atmbioflx_NO/NO2`** for the simulation with and without inclusion of this NO_2 compensation point. You can also check on the role of this NO_2 compensation point by plotting the differences in the concentrations and, potentially, the process tendencies, e.g., those of NO_x for the crown- and understorey layer.

Question: You will see that actually the differences in the simulated atmosphere-biosphere NO_x fluxes are quite small although, instead of having NO_2 , we have now in the simulation of this case an actual extra source of NO_2 due to the direct emissions by the leaves; do you have any explanation for this?

Case #4: Biogenic emissions, concentrations and mixed layer depth

In the current version of MLC-CHEM the model uses a surface/mixed layer with a depth that can be modified by changing the value of the parameter:

`zMLHmax = 750, ! Maximum mixed layer height`

This parameter is used to introduce a diurnal cycle in the mixed layer depth using a simple sinus-shape scaling function. This results in that the nocturnal mixed (or inversion) layer depth resembles the prescribed depth of the surface layer and that during the day it increases to this maximum depth being reached around noon.

Question: with a decrease by a factor 2 in the mixed layer depth to 750m do you expect to see a linear or a non-linear response expressed by a factor 2 increase in NO_x/isoprene concentrations? Also try to already hypothesize what might explain the expected behavior.

- You can check the sensitivity of the simulated NO_x and isoprene concentrations to the assumptions made on the maximum mixed layer depth. You could do this by assuming a significantly shallower mixed layer or a deeper mixed layer. The mixed layer depth of a very wet vegetation cover can be low as 750m whereas very deep mixed layers, > 2500m, might occur over very dry vegetated/bare soil surfaces. You could conduct these experiments making consistent and simultaneous changes in soil moisture and the maximum mixed layer depth (less soil moisture > less transpiration > more sensible heat > deeper mixed layer depth)

Similar to the issue on soil moisture, measurements on boundary evolution and depth are not commonly included in campaigns that focus on atmospheric chemistry and chemical exchange processes. MLC-CHEM can thus also be used to analyze the sensitivity of the observed concentrations and fluxes to these assumptions on mixed layer depth and which can have quite different impacts on the concentrations of emitted compounds but also on depositing compounds.

Other Cases:

Other experiments/analyses you can perform with the model are:

- Check the vertical radiation profiles inside the canopy; if you happen to have observations of photolysis rates, possible at multiple heights, you could compare the simulated J-values above and inside the canopy with the simulated J-values.
- Analyze the concentration of other relevant reactive compounds, e.g., OH, peroxides (H₂O₂, methylhydroperoxides), VOC oxidation products and some of the oxygenated compounds that are also included in the chemistry scheme, e.g., methanol and acetone.
- Check how the stomatal O₃ stomatal uptake is affected by the assumptions on the BVOC emissions; how do for example stress-induced increases in BVOC emissions affect the atmosphere-biosphere flux of O₃ and stomatal contribution to this flux?
- Check the sensitivity of the model simulations of atmosphere-biosphere exchange to some basic biogeophysical properties, e.g., sensitivity to the amount of biomass expressed by the Leaf Area Index (LAI), surface roughness or canopy height. In this case the changes in concentrations, fluxes and canopy reduction factors are the complex expression of all induced changes in emission, dry deposition, chemistry and turbulent mixing.
- Referring to case #1; there are two other links between the hydrology and atmosphere-biosphere exchange of reactive compounds and aerosols are 1) the role of water stress on short, diurnal timescales associated with the occurrence of a water vapor pressure deficit (vpd) and that results in

stomatal closure for very warm conditions, mainly occurring the afternoon 2) differences in uptake efficiency by dry and wet leaf surface (wet skin).

You can do some additional experiments with MLC-CHEM, e.g., considering 1) the role of the VPD in stomatal closure by setting:

`l_fvpd` = T

2) the impact of differences in dry versus wet leaf surfaces. In the default model the deposition to wet leaf surface is actually considered having set:

`l_wetskinRH` = T, ! wet skin fraction calculated from RH

In this case the model estimates the wet skin fraction from the (measured) relative humidity and by setting this switch to false, the model uses the prescribed constant wet skin fraction of 0:

`zwetskin` = 0., ! fraction of wetted surface [0-1]

You can compare the results on O₃ dry deposition flux simulations with these different settings of the model and the default model run but you could also, for example, check how there would be differences in the dry deposition velocities of some of the other reactive compounds.

Further application of MLC-CHEM

The model can obviously be modified by any user and it would be nice if its application will ultimately result in substantial improvements of the system by integration of newly developed emission, dry deposition, chemistry or turbulent transport representations. If you are interested to indeed apply MLC-CHEM for some of your scientific activities, please contact me at laurens.ganzeveld@wur.nl. I would be keen to help you on getting started using the modelling system and where I would then also provide you with the most up-to-date version of the modelling system that already contains quite some new features compared to the version we introduced in this training activity. Also, changes introduced in the system will be recorded using a version control system so that modifications can rather easily be traced and further exchanged within the user community.