Chemistry Emissions Module PALM4U

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1 Introduction

This report serves as a general overview of the chemistry emission module of PALM-4U and constitutes the reference for the technical developers of the chemistry model of PALM-4U. In the text that follows, detailed information concerning the module structure, the main subroutines and variables and possible discussion points will be presented.

2 Module Overview

The main function of the chemistry emissions module of PALM-4U is to read input values of chemistry emission species, that may be provided in different formats, and converting them to the format required by the chemistry model.

The user may select between three different operational modes when working with the emissions module of PALM-4U:

- PARAMETERIZED
- DEFAULT
- PRE-PROCESSED

In order to switch the chemistry emission module on, the namelist parameter **do_emis**, needs to be set to .TRUE. . The user may chose one of the above listed modes, by passing their names to the namelist parameter **mode_emis**.

Below, we try to provide a more detailed description of the 3 different emission modes, together with the required namelist parameters for each of the three cases.

As a general remark, for the DEFAULT and the PRE-PROCESSED mode, the user has to provide information relative to the emissions in a netcdf input file at the beginning of each simulation, while the PARAMETERIZED mode works with information provided via the simulation namelist.

For information regarding the format and the variable in each case when input emissions data are read from a netcdf file, refer to the PIDS (Palm Input Data Standards) documentation.

2.1 PARAMETERIZED Mode

The parameterized version of the chemistry emissions module is an easy straightforward solution for the users not particularly familiar with chemistry emissions.

All the information required for the PARAMETERIZED mode are provided in the simulation namelist.

In this case, the module reads-in a single emission value for each of the provided emission species. This value is then scaled by a street factor parameter, with a different value for main road and side road types. The scaling factors for each of the street types must be provided in the model simulations namelist, through the parameters **emiss_factor_main** and **emiss_factor_side**.

Finally, the emission values are additionally scaled by a factor for the daily cycle of the emissions, that is fixed inside the model (in the module netcdf_data_input).

Beside the ones already mentioned above, the namelist parameters necessary in the parameterized mode of the emissions module are the following:

1. **cs_surface_fluxes_names** with the names of all the species for which emission values are provided (separated by a comma) **IMPORTANT:** the chemical species provided as input in the parameterized mode, have to be one of the species of the specific chemical mechanisms selected in the simulation. If none of the input emission species matches the mechanisms spec

2. **cs_surface_fluxes** with the emission rates of the species declared through cs_surface_fluxes_names. **IMPORTANT:** The order of the passed values has to correspond to the ones of the species passed to cs_surface_fluxes_names.

3. **main_street_factor** indicating the value of a scaling factor for the emissions along a main street type.

4. **side_street_factor** indicating the value of a scaling factor for the emissions of species along minor street types.

In this case, the units of the emission inputs **MUST** be mole/(meters*day) for reactive components and kg/(meter*day). redreview

2.2 DEFAULT Mode

The DEFAULT mode works reading-in input data from a netcdf file, as designed in the PIDS (PALM Input Data Standard).

In this case, gridded (x-y) annual values of the emissions for different categories are scaled in time by means of pre-defined scaling factors. These will have the same values for each point of the domain and for all the emission species. Input would be in a reduced format. The DEFAULT mode of the emissions module, like in the PARAMETERIZED case, is also thought for users that are not particularly familiar with chemistry emissions. Nevertheless, it is a bit more sophisticated and precise than the simple PARAMETERIZED version, allowing to specify different time dependencies of the emissions, their values through different emission categories and several other aspects.

The DEFAULT mode of the emissions module may be activated with the namelist parameter **mode_emis** set to DEFAULT.

The namelist parameters used in the PARAMETERIZED mode are not necessary anymore. In this case, the important namelist parameters are:

1. **time_emis** allowing to select between two different time factors specification of the emissions:

   - **HOURLY** A scaling factor for the emissions has to be provided for each hour of a day of the considered year of the simulation
   - **MDH** A scaling factor for the emissions has to be provided for each month, day and hour of a single year, also differentiating between weekdays, holidays and weekends. In this case, the total number of scaling factors for a year would be:
     12(month of year) + 7(day of week) + 3x24 (number of days for the three mentioned cases) = 91.
     In order to distinguish among the different day types, in the MDH mode, the namelist parameter **daytype_mdh** has to be given one of the following values:
     - **workday**
     - **weekend**
     - **holiday**

2.3 PRE-PROCESSED mode

Also in the PRE-PROCESSED mode the emissions values are read from the netcdf file.

In this case, the inputs would be in the final format required by the model: a 5-dimensional array varying over each point of the domain, emission species and with a value for each hour. No time scaling factors would be required in this case. In the PRE-PROCESSED mode, the user needs to provide the values of the emissions of the specific chemical mechanism species for each hour of the simulation period.

IMPORTANT (ALSO FOR DEFAULT): It is not possible (at the moment) to assign values of the emissions for different vertical levels over the same grid box. Instead, values could be provided only to one surface layer for each grid box.

IMPORTANT: For the PRE-PROCESSED mode of the emissions, the input data contained in the netcdf may be on a single vertical level, even though information at each x-y could represent values at different heights.

IMPORTANT: At the moment the data on emissions in input for the PRE-PROCESSED mode have to be provided for each day. This means that each netcdf file has to contain at least 24 values, one for each hour of a day, or a multiple of 24. Additionally the simulation has to start on the same day for which emissions values are available in input.

2.4 Units Treatment

The emission values provided in input may have different units. The module will take care of their conversion to the model required units of surface fluxes for chemical sepcies: $ppm/(s)$ (kg/s). The units of the emissions species have to be declared in the netcdf input file as described in the PIDS. Nevertheless, for the PARAMETERIZED mode only certain values for the units are possible, as described in Sect. 2.1.

2.5 Time Treatment

Different modifications have been applied to the module date_time_mod for making the treatment of the time of the year more precise and, in particular, suitable for the update of the indices of the time factors of the emissions in the different modes.

The new changes applied to this routine, allow the model to know the exact date and time of the year.

Beside providing information on the day of the year through the previously employed namelist parameter time_of_year_init, it i now possible to specify the initial date of a specific year through the namelist parameter:

- **date_init**

The value of this variable has to be constituted of 8 digits, with the first 2 for the day, the following 2 for the month and the final 4 for the year:

DDMMYYYY

Knowing the actual date and hour of the simulation (time_utc)tion, the module is able to calculate the indices of the emission datasets according to the selected chemistry emission mode.

IMPORTANT: Only one between date_init and date_of_year_init should be given in a simulation namelist. If both are used, the value of date_of_year_init will be overwritten by the date_init.

At the moment, all the years have 365 days: no leap years considered.

2.6 List of Modified Modules

The following modules needed modification for the introduction of the chem_emis module

- time_integration.f90
- palm.f90
- parin.f90
- modules.f90
- init_3d_model.f90
- date_and_time_mode.f90
- surface_mod.f90
- chemistry_model_mod.f90
- netcdf_data_input_mod.f90
- chem_modules.f90