LEVCHEM_v1 files of Suciu et al. "A zero-dimensional view of atmospheric degradation of levoglucosan (LEVCHEM_v1) using numerical chamber simulations"

This document describes the LEVCHEM_v1 files used to generate the results presented in the revised manuscript of Suciu et al. (in review): "*A zero-dimensional view of atmospheric degradation of levoglucosan (LEVCHEM_v1) using numerical chamber simulations*" (https://gmd.copernicus.org/preprints/gmd-2020-189/).

The content of the archive "LEVCHEM_v1_files_02" consists of 7 directories as follows:

01_Main program. Contains the main program of LEVCHEMv1 "*boxmox_LEVCHEM_v1. f90*". This is the modified version of *boxmox.f90*, the main program of BOXMOXv1.7. Line 86 was added to call the subroutine "UpdateConcentration" developed by Suciu et al. to update the concentrations of chemical species due to gas-particle partitioning (evaporation/condensation). To compile the mechanism and run simulations using BOXMOXv1.7, *boxmox_LEVCHEM_v1.f90* must be renamed *boxmox.f90*.

02_Wrapper. Contains the *wrapper* of BOXMOXv1.7 that was modified by Suciu et al. to add the gas/particle partitioning mechanism (model lines 1056-1374). The modified version is called *wrapper_LEVCHEM_v1*. For running BOXOMOXv1.7 simulations, this file must be renamed *wrapper*. Note that for a particular simulation run (either used for model evaluation or sensitivity analysis as described by Suciu et al.) the parameters on lines 1337, 1362, 1363 and 1366 must be changed manually. Here, the changes have been made already and for each simulation run the respective *wrapper_LEVCHEM_v1* is provided in the content of the two subdirectories "Model evaluation" and "Sensitivity analysis". Note that the part "…F0004" in the LEVCHEM_v1_F0004 folder name, for example, refers to F = 0.004 (see Suciu et al. for details).

03_Mechanism files. Contains three mechanism files *LEVCHEM_v1.eqn*, *LEVCHEM_V1.def* and *LEVCHEM_v1.spc* for each simulation used for either model evaluation or sensitivity analysis. The structure of this directory is the same as above (02_wrapper) and the folder names have the same meaning. These mechanism files represent modifications of BOXMOXv1.7 mechanism files associated to two existing mechanisms (CB05TUCl_EPA and hetchem; see Suciu et al. for details). *LEVCHEM_v1.eqn* is an extension of CB05TUCl_EPA.eqn that includes reactions and reaction rate coefficient expressions for the added levoglucosan homogeneous gas-phase chemistry (lines 242-255), heterogeneous chemistry (lines 297-331) and equilibrium gas/particle partitioning (lines 333-356). *LEVCHEM_v1.def* represents a combination of CB05TUCl_EPA.def and hetchem.def of BOXMOXv1.7 to which lines (49-59) were added to code the function called on lines 336-343 and 349-356 of *LEVCHEM_v1.eqn.* Also, line 14 was added to code the FFACTOR to vary the F value (see Suciu et al. for details). *LEVCHEM_v1.spc* is the original CB05TUCl_EPA.spc file that was modified to include species used by LEVCHEM_v1 (see lines 87-124).

04_Compiled mechanism. Contains various compilations of LEVCHEM_v1 used to run the numerical chamber simulations described by Suciu et al. The structure of the directory is similar to those above and the folder names have the same meaning (see 02_wrapper). Note that the LEVCHEM_v1 must be compiled each time when FFACTOR (in *LEVCHEM_v1.def*) and other parameters (in *wrapper_LEVCHEM_v1*) are changed.

05_KPP file. Contains the mechanism-specific file *LEVCHEM_v1.kpp* needed to initiate the kinetic preprocessor (kpp) of BOXMOX1.7 to generate code and compile the mechanism.

06_Simulation input files. Contains the input files needed to run numerical chamber simulations for the compiled mechanisms using different conditions as described in Suciu et al. This directory contains two subdirectories “Model evaluation” and “Sensitivity analysis” and each contains subfolders with data for specific chamber experiments (see Suciu et al. for details).

06_Simulation experiments files. Contains the files used to run numerical chamber simulations (including the executable LEVCHEM_v1) for both model evaluation and sensitivity analysis based on conditions described by Suciu et al. See “02-wrapper” above for the meaning of the folder names containing the scripts and data.