User Manual

The H2I model (v1.0) allows to simulate species concentrations in indoor environments, taking into both homogeneous chemistry and heterogeneous reactions. In this version, the VOCs compounds are fixed to experimental records provided by user, while the inorganic compounds are modelled thanks to parameters fixed by user.

Compilation

The H2I model is written in the programming language FORTRAN. To compile this code, the construction tool SCONS must be installed. The compilation can be done by typing the command scons in the same directory as the main program.

Files and Folders

The H2I model main program is photochemistry.f ; the rest of the routines are stored in the directories Chem. The input files are stored in folder CONTROL, and the output files in folder RESULTS.

The CONTROL folder contains the following files :

- species-racm2.dat and species-list-racm2.dat : list and features of the RACM2 compounds. These files should not be modified by user.
- critical_constants.dat :
    - number of possible reactions with surfaces (including simple deposition)
    - critical molar volumes (Vc) and critical temperatures (Tc) of the species that can undergo surface reactions. These variables are required to compute diffusion coefficient. Sorbed species are given the values Tc = 0 and Vc = 0, since no deposition coefficient is considered for them.
- which_exp.dat : user here specifies the name of the modelled experiment (e.g. *demo_Exp*), time step of the main loop, name of the output folder (to be placed in folder RESULTS) and name of the output simulation files (run name).

The input data are provided in the folder named after the modelled experiment (here *demo_Exp*), in the CONTROL directory. In this folder, can be found :

- config.dat : contains all of the parameters featuring the experiment (location, light, room volume and surfaces), the name of the file containing the temperature and humidity profiles (to be placed in the same folder), the name of the files containing the initial concentrations assessed from simulations (to be placed in the same folder), the start time and the end time.
- init.dat : contains the initial concentrations of the compounds which were measured experimentally.
- param.dat : contains the tunable parameters and sorbed species initial concentrations. Note that the uptake values are listed separately in surface_reactions.dat.
- surface_reactions.dat : provides the following parameters for each reaction listed in critical_consants.dat
    - *k_react* : type of reactivity with surfaces
        - -1 : surface reaction inactivated (no deposition)
        - 0 : deposition fully controlled by transport (no limitation by uptake)

        - 3 : deposition both controlled by transport and uptake.
    - *uptake_ref* : uptake coefficient of the room surfaces in reference conditions
- outdoor.dat : contains the variable *omeas* referring to outdoor measurements. If greater or equal to zero, the *omeas* value is a permanent outdoor concentration; otherwise, the -1 value indicates that outdoor profile is available. Outdoor profiles are stored in folder outdoor_conc. In this version the *omeas* variable is set to zero for all measured VOCs, since their concentrations are fixed to experimental records provided as input.
- records : contains the indoor concentrations measured experimentally. VOCs_conc.txt provides the VOCs concentrations, and VOCs_time.dat the corresponding measurement times. These records are used to compel species to follow their experimental variations.

Simulation outputs

The simulation outputs are written in a folder chosen by user, placed in the directory RESULTS. The output file names are constructed with the name of the experiment, followed by a suffix, followed by the name of the simulation test. The three possible suffix are param, light and shade. The param file contains the list of parameter values fixed by the user. The light and shade files contain the concentrations in the sunlit and shaded boxes computed in the main loop, i.e. the evolution of all the simulated species concentrations throughout the simulation.

Contact

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