Project: **677**

Project title: **Evaluierung der Atmosphärenchemie in MECO(n)**

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Report period: **2021-01-01 to 2021-08-31**

This application for 2021 consisted of three major parts:

1. Development and evaluation of ICON/MESSy

   The development of ICON/MESSy progresses slowly

   A. due to time constrains of the people performing this development and
   B. due to the fact, that basic parts of the ICON model still change heavily with every (half-yearly) ICON release.

   Achievements in 2021:

   - The sub-submodel GRID-DEF has been built, to separate the information about the basemodel grid from other basemodel specific data.
   - The IMPORT-GRID submodel has been improved, which was also required for COSMO/MESSy and the MESSy DWARF.
   - The TENDENCY and TRACER submodel have been finally revised in a way, that the ICON convective and turbulent transport can also be used for MESSy tracers and that the tendencies calculated by these processes are directly dealt with as specific tendencies by the MESSy submodel TENDENCY.
   - The TENDENCY submodel has been expanded to also deal with "pseudo"-prognostic variables, i.e., TENDENCY accepts tendencies for temperature and the wind components u and v and organises the application of these tendencies to the ICON prognostic variables.

2. Investigation of impacts of the LSM-CLM coupling on the tracer distribution in the boundary layer

   To enable long-term simulations, the CCLM_SUBCHAIN and the OASIS setup for coupled MESSy simulations has been combined. In this way, externally coupled simulations can make use of the runtime environment which automates the provision of boundary data for the limited-area model and the post-processing of the COSMO models output.

   Again, this part of the project proves to be much more complicated than anticipated. The simulations with coupled COSMO and Community-Land-Model (LSM-CLM) via the MESSy submodel OASIS3MCT experience numerical instabilities after an arbitrary length of simulation (sometimes after months or even years). Until now, it was not possible to detect the reason for these instabilities as the intermediate outputs look very similar to the coupled COSMO-CLM^2 setup on which the MESSy development is based.

   Additionally, as land surface models require a spin up of at least a decade, a procedure for creating these spin-up of the LSM-CLM for arbitrary new domains within the MESSy environment is being developed.

3. Further MESSy developments and tests for collaboration within the CLM-Community:

   The MESSy community and the CLM-Community are interlinked since the start of the development of COSMO/MESSy. For the evaluation of the newest and last COSMO version v6.0, now also some MESSy diagnostic submodels are used. For this COSMO/MESSy was integrated into the CCLM_SUBCHAIN runtime environment. Furthermore, as COSMO-5.x is still being developed towards its final version COSMO 6.0, COSMO/MESSy needs permanent updates to new COSMO versions as long as COSMO v6.0 is not yet ready. This is important to guarantee that the MESSy interface, as implemented in the final version COSMO 6.0, will work correctly.

   A. Test COSMOv6.0/MESSy for COPAT2 setup,

COSMO v6.0 is still not finalised. Permanent updates to new intermediate COSMO model versions have been performed in 2020/2021. A version of COSMO/MESSy based on COSMO-5.09b has been provided to the colleagues of HEREON and BTU Cottbus who perform the COPAT2 evaluation simulations. The latest update integrated into MESSy is COSMO-5.11 (status 09/08/2021).

B. Prepare ICON-CLM/MESSy for COPAT2,

   No steps have been performed for this subproject so far, as the update of ICON/MESSy to the very last ICON release is still under development (responsibility of other colleagues at another institute).

C. Development of a MESSy-fied OASIS3-mct version for the CLM-Community using OASIS3-mct as coupler for further externally coupled models as NEMO or HD.

   The development is split into 2 parts:

   (a) COSMO/MESSy will be included in the well-established HEREON CCLM_SUBCHAIN setup for the coupling with OASIS3-mct as currently performed by the colleagues at HEREON.

   (b) The HEREON setup will be modified in a way, that the MESSy submodel OASIS3MCT is used for the OASIS coupling.

   The work on (a) started recently and will be finished for the HD coupling within the current application time. The coupling with NEMO in subproject (a) and subproject (b) need to be shifted to the next application period.

In addition to the projects listed in the applications some other developments and support of other MESSy users have been performed using up the computing time allocated by this project:

1. Development of the MESSy DWARF. A simplified MESSy model consisting purely of MESSy submodels i.e., without any legacy basemodel (as COSMO, ICON or ECHAM) has been developed. This required the implementation of a simple GRID definition, of an easy parallel environment setup and of some additional initialisation procedures. Similar to the ECMWF weather and climate dwarfs developed within the ESCAPE project (Müller et al., GMD, 2019, DOI: https://doi.org/10.5194/gmd-12-4425-2019), the MESSy DWARF enables to run individual MESSy submodels in a simple MESSy environment to work on their optimisation (e.g., porting to GPUs). Furthermore, it will be used to develop simplified physics or chemistry models, as column models for volcanic plume emissions or a chemical box model.
2. Use of MESSy DWARF as chemical box model: In a student's internship project first steps have been realized to run the MESSy DWARF as a chemical box model, which in the end, among others, should be used to interpret reaction chamber experiments or field campaign data.
3. Last but not least, a number of support requests w.r.t. the MESSy submodels of which the principal investigator of this application project is maintainer, have been issued. In order to answer the questions, understand and fix bugs in the code etc. numerous test simulations have been performed within the contingent of the computing time allocated by this project.