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# TransClim (v1.0): a chemistry–climate response model for assessing the effect of mitigation strategies for road traffic on ozone

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This document provides additional material to the article: *Rieger et al., TransClim (v1.0): A chemistry-climate response model for assessing the climate effect of mitigation options for road traffic*.

## S1 Implementation in EMAC: split-up of emission regions

To perform the emission variation simulations with EMAC, the simulation setup which is based on the model setup of *RC1SD-base-10a* (see Jöckel et al. (2016)) requires some adaptations. The file which contains the road traffic emissions for an EMAC simulation needs to be split up into the emission regions. This is done in such a way that each file describing one emission region only contains the road traffic emission data for its corresponding region. The rest is set to 0. However, to maintain the total emission amount, a residual file is created which includes the residual road traffic emissions. The abbreviation of the emission region (see below tab. S2) is appended to the name of the split emission file. Two examples are given for the emission region Germany "GER" and the residual file "RES":

```
CCMI_DLR1.0_AR5-RCP8.5_road_MISC_195001-201012_GER.nc
CCMI_DLR1.0_AR5-RCP8.5_road_MISC_195001-201012_RES.nc
```

In MESSy, the emission files are read in via the namelist structure `import.nml`. To consider the different emission regions, this namelist also needs to be modified:

```
! ROAD (LAND)
! (NO,CO,SO2,NH3,C2H4,C2H6,C3H6,C3H8,NC4H10,CH3CHO,CH3COCH3,CH3CO2H,
!  CH3OH,HCHO,HCOOH,MEK)

! emission region: Germany
!RG_TRIG(70) = 1,'months', 'first',0, 'ROAD_GER', 721,1,732,702,
'NML=./emregions/CCMI_DLR1.0_AR5-RCP8.5_road_MISC_195001-201012_regGER.nml',

! emission region: rest of the world
RG_TRIG(74) = 1,'months', 'first',0, 'ROAD_RES', 721,1,732,702,
'NML=./emregions/CCMI_DLR1.0_AR5-RCP8.5_road_MISC_195001-201012_regRES.nml',
```

For scaling the road traffic emissions, we explicitly introduce emission scaling factors for $NO_x$, VOC and CO emissions for each individual emission region in the MESSy run script `xmessy_mmd_TransClim_LUT`:

```
### Scaling factors of emission regions
sNOx_GER=1.0
sVOC_GER=1.0
sCO_GER=1.0
...
```

These emission scaling factors are passed to `offemis.nml`. Here, the emissions of each emission region are scaled with the emission scaling factors and then added to the corresponding chemical tracer. One example for the emission region Germany (GER) is given:

```
! emission region: Germany
EMIS_IN(110) = 'NO,$sNOx_GER;NOytra,$sNOx_GER',       'import_grid','ROAD_GER_NO',      'GP=1'
EMIS_IN(111) = 'CO,$sCO_GER;COtra,$sCO_GER' ,         'import_grid','ROAD_GER_CO',      'GP=1'
EMIS_IN(112) = 'SO2' ,                                'import_grid','ROAD_GER_SO2',     'GP=1'
EMIS_IN(113) = 'C2H4,$sVOC_GER;NMHCtra,$sVOC_GER' ,   'import_grid','ROAD_GER_C2H4',    'GP=1'
EMIS_IN(114) = 'C2H6,$sVOC_GER;NMHCtra,$sVOC_GER' ,   'import_grid','ROAD_GER_C2H6',    'GP=1'
EMIS_IN(115) = 'C3H6,$sVOC_GER;NMHCtra,$sVOC_GER' ,   'import_grid','ROAD_GER_C3H6',    'GP=1'
EMIS_IN(116) = 'C3H8,$sVOC_GER;NMHCtra,$sVOC_GER' ,   'import_grid','ROAD_GER_C3H8',    'GP=1'
EMIS_IN(117) = 'NC4H10,$sVOC_GER;NMHCtra,$sVOC_GER' , 'import_grid','ROAD_GER_NC4H10',  'GP=1'
!EMIS_IN(118) = 'CH3CHO' ,                            'import_grid','ROAD_GER_CH3CHO',  'GP=1'
```

```
EMIS_IN(119) = 'CH3COCH3,$sVOC_GER;NMHCtra,$sVOC_GER','import_grid','ROAD_GER_CH3COCH3','GP=1'
!EMIS_IN(120) = 'CH3CO2H',                          'import_grid','ROAD_GER_CH3CO2H', 'GP=1'
EMIS_IN(121) = 'CH3OH,$sVOC_GER;NMHCtra,$sVOC_GER' ,  'import_grid','ROAD_GER_CH3OH',   'GP=1'
EMIS_IN(122) = 'HCHO,$sVOC_GER;NMHCtra,$sVOC_GER' ,   'import_grid','ROAD_GER_HCHO',    'GP=1'
!EMIS_IN(123) = 'HCOOH' ,                            'import_grid','ROAD_GER_HCOOH',   'GP=1'
EMIS_IN(124) = 'MEK,$sVOC_GER;NMHCtra,$sVOC_GER' ,    'import_grid','ROAD_GER_MEK',     'GP=1'
EMIS_IN(125) = 'NH3' ,                               'import_grid','ROAD_GER_NH3',     'GP=1'
```

A detailed description of the namelist structure and the file import in MESSy can be found in Kerkweg et al. (2006b) and Kerkweg and Jöckel (2015). The modified namelist setup for the emission variation simulations with EMAC is called `TRANSCLIMLUT` in the MESSy distribution.

## S2 Emission variation simulations with EMAC

### S2.1 List of submodels

Table S1 gives a detailed overview of the submodels which are used for the EMAC simulation setup described in sect. 2.4.1 of the main paper.

| Submodel | Description | References |
|---|---|---|
| AEROPT | aerosol optical properties | Dietmüller et al. (2016) |
| AIRSEA | air-sea exchange of tracers | Pozzer et al. (2006) |
| CH4 | methane oxidation and linkage to hydrological cycle | |
| CHANNEL | memory and meta-data management, data export | Jöckel et al. (2010) |
| CLOUD | cloud parametrisation | Roeckner et al. (2006), and references therein |
| CLOUDOPT | cloud optical properties | Dietmüller et al. (2016) |
| CONVECT | convection parametrisation | Tost et al. (2006b) |
| CVTRANS | convective tracer transport | Tost et al. (2010) |
| DDEP | dry deposition of tracers and aerosols | Kerkweg et al. (2006a) |
| E5VDIFF | land-atmosphere exchange and vertical diffusion | Roeckner et al. (2003) |
| GWAVE | non-orographic gravity waves | Baumgaertner et al. (2013) |
| IMPORT | import data from external files | Kerkweg and Jöckel (2015) |
| JVAL | determination of photolysis rates | Sander et al. (2014) |
| LNOX | lightning $NO_x$ production | Tost et al. (2007); Jöckel et al. (2010) |
| MECCA | chemistry in troposphere and stratosphere | Jöckel et al. (2010); Sander et al. (2011) |
| MSBM | multiphase chemistry in stratosphere | Jöckel et al. (2010) |
| OFFEMIS | offline emissions of tracers and aerosols | Kerkweg et al. (2006b) |
| ONEMIS | determination of online emissions | Kerkweg et al. (2006b) |

*Continued on next page*

Table S 1 – *Continued from previous page*

| Submodel | Description | References |
|---|---|---|
| ORBIT | Earth orbit calculations | |
| OROGW | orographic gravity wave drag | |
| PTRAC | testing with passive tracers | Jöckel et al. (2008) |
| QBO | Newtonian relaxation of the QBO (quasi-biennial oscillation) | Giorgetta and Bengtsson (1999); Jöckel et al. (2006) |
| RAD | radiative transfer calculation | Dietmüller et al. (2016) |
| RAD_FUBRAD | sub-submodel of RAD, high-resolution short-wave heating rate parametrisation | Nissen et al. (2007); Dietmüller et al. (2016) |
| SCALC | simple calculations | Jöckel et al. (2016) |
| SCAV | wet deposition and scavenging of tracers and aerosols | Tost et al. (2006a) |
| SEDI | aerosol sedimentation | Kerkweg et al. (2006a) |
| SURFACE | surface parameters | Jöckel et al. (2016) |
| TAGGING | attribution of source emissions to trace gases | Grewe et al. (2017) |
| TNUDGE | Newtonian relaxation of tracers | Kerkweg et al. (2006b) |
| TRACER | data and meta-data management of chemical tracers | Jöckel et al. (2008) |
| TROPOP | diagnostic calculation of tropopause height | Jöckel et al. (2006) |

Table S 1: List of submodels used for the EMAC simulation setup described in sect. 2.4.1 of the main paper.

## S2.2 Execution of emission variation simulations

The complete namelist setup of the emission variation simulations is found in the folder `/messy/nml/TRANSCLIMLUT` of the MESSy distribution (here indicated with `$MESSY`). The emission variation simulations were performed at the High Performance Computing system Mistral of the Deutsches Klimarechenzentrum (DKRZ). To perform and postprocess the emission variation simulations for the LUTs, the following steps need to be executed on DKRZ's Mistral:

1. create output folder (e.g. `GE_2.0_1.0_1.0`, naming convention see below) in the following folders:
   (a) `$SCRATCH/TransClim_LUT`
   (b) `$SCRATCH/TransClim_LUT/pp`
   (c) `$SCRATCH/TransClim_LUT/TMP`
   (d) `$SCRATCH/TransClim_LUT/SAVE`
   (e) `$WORK/TransClim_LUT`
   (f) `$WORK/TransClim_LUT/output`
   (g) `$WORK/TransClim_LUT/plots`

2. set emission scaling factors sNOx, sVOC and sCO for each emission region in the run script `xmessy_mmd_TransClim_LUT` in `$MESSY/messy/util`
3. run simulation: go to the output folder in `$SCRATCH/TransClim_LUT` and call `sbatch $MESSY/messy/util/xmessy_mmd_TransClim_LUT`
4. archive simulation
5. postprocess simulation: run `sbatch postprocessing_mm_sbatch.sh` in `$WORK/TransClim_LUT/output`

Note the nomenclature of the emission variation simulations is as follows:

`EmissionRegion_sNOx_sVOC_sCO`

`EmissionRegion` indicates the emission region abbreviated by two letters (see table S2). `sNOx`, `sVOC` and `sCO` stands for the emission scaling factors. For example, the simulation name `GE_2.0_1.0_1.0` indicates that in the emission region Germany the road traffic emissions of $NO_x$ are doubled while the emissions of VOC and CO are hold fixed (scaling factors 1.0).

| Emisssion region | Abbreviation | Abbreviation in MESSy namelist | reference simulation |
|---|---|---|---|
| Germany | GE | GER | ref_inst |
| Western Europe | WE | WEUR | ref_inst |
| Northern Europe | NE | NEUR | ref_inst |
| Eastern Europe | EE | EEUR | ref_inst |
| Southern Europe | SE | SEUR | ref_inst |
| North America | NA | NAM | ref_inst |
| South America | SA | SAM | ref_11 |
| China | CH | CHI | ref_11 |
| India | IN | IND | ref_11 |
| Southeast Asia | EA | SEA | ref_11 |
| Japan/South Korea | JP | JAP | ref_11 |

**Table S 2.** Abbreviation of emission regions and their corresponding reference simulations.

## S3 Simulations with TransClim

### S3.1 Settings

TransClim is implemented in Python. The current version runs with Python 2. The code is available at https://doi.org/10.35089/WDCC/TransClim_v01_chem-cl_response. All settings for a simulation with TransClim are conducted in the file `namelist.py`. The options are listed in table S3.

| Variable | Type | Description |
|---|---|---|
| emission_regions | list | contains the emission regions for which the interpolation will be performed, emission regions are denoted as strings with the two letter abbreviations as indicated in table S2 |
| emScen | dictionary | contains emission scaling factors for emission scenario, key: emission region (abbreviated with two letters, string), value: list with emission scaling factors (1st index: sNOx, 2nd index: sVOC, 3rd index: sCO) |
| emRef | dictionary | contains emission scaling factors for reference scenario, key: emission region (abbreviated with two letters, string), value: list with emission scaling factors (1st index: sNOx, 2nd index: sVOC, 3rd index: sCO) |
| output_name | string | simulation name |
| pathIn | string | path of emission variation simulations (LUTs) |
| pathOut | string | path for output files (folder must already exist) |
| var | dictionary | contains variables and the resolution for which the interpolation will be performed, key: variable (string), value: resolution (string) |
| RFO3tra_scale_switch | boolean | True: switches on scaling of $O_3^{tra}$ radiative forcing with $NO_x$ emissions (further details see below) |
| RFO3tra_arg | dictionary | contains arguments which are necessary for scaling the radiative forcing of $O_3^{tra}$, keys: start_year, end_year, scale_year, pathNOx, fileNOx (for detailed explanation see below) |
| simRef | dictionary | defines reference simulation used for each emission region, key: two letter abbreviation of emission region (string), value: name of reference simulation, see table S2 (string) |
| simLUT | dictionary | defines the emission variation simulations per emission region which are used for the interpolation, key: two letter abbreviation of emission region, value: list with string of emission variaions (e.g. '0.0_1.0_1.0') |

Table S 3: Overview of settings in `namelist.py`. The column "Type" indicates the data type of the variable in Python. Detailed explanation of the different options is also found in `namelist.py` itself.

**Scaling of $O_3^{tra}$ radiative forcing**

The switch `RFO3tra_scale_switch` offers the option to switch on the scaling of $O_3^{tra}$ radiative forcing (True). This option scales the radiative forcing of $O_3^{tra}$ for a certain timespan with $NO_x$ emissions. `RFO3tra_arg` contains the necessary arguments. The $NO_x$ emissions are read in from file `fileNOx` in the folder `pathNOx`. `start_year` and `end_year` indicates the timespan for which is scaled. `scale_year` sets the year to which the radiative forcing RF($O_3^{tra}$) is scaled to. The scaled RF($O_3^{tra}$) and the corresponding years are written to the ASCII output file `output_name_RFO3tra` which can be read in by the response model AirClim (Grewe and Stenke, 2008).

### S3.2 Run simulation

Once all settings are determined in `namelist.py`, the simulation can be started by executing the script `main.py`. (In a unix shell the simulation is started with the command `python main.py`.) Then the default namelist `namelist.py` is used. Other namelists can be set as command-line argument: e.g. `python main.py namelist_scenario1.py`. The following output files are written in the folder determined in `namelist.py`:

– `output_name.nc`: netCDF-file containing all output variables in (level, latitude, longitude), (latitude, longitude), tropospheric or global mean (depending on the settings in `namelist.py`) for the emission and the reference scenario as well as the difference between the two. All possible output variables are listed in table S4.

– `output_name_eval.log`: a log file with all settings from the file `namelist.py`. Also global or tropospheric means of the interpolated variables for the emission and the reference scenario as well as the differences between emission and reference scenario are given.

– `output_name_RFO3tra`: is only written when `RFO3tra_scale_switch` is set to True. It contains the timespan and the corresponding RF($O_3^{tra}$) values. This output file can be read in by the response model AirClim (Grewe and Stenke, 2008).

| **Variable** | | **Dimension** | **Unit** |
|---|---|---|---|
| | INPUT OF TRANSCLIM | | |
| ozone | `O3` | 3D, tm, gm | mol mol$^{-1}$ |
| road traffic ozone | `O3tra` | 3D, tm, gm | mol mol$^{-1}$ |
| str. adj. solar flux of $O_3$ at TOA | `flxs(rad02)` | 2D | W m$^{-2}$ |
| str. adj. thermal flux of $O_3$ at TOA | `flxt(rad02)` | 2D | W m$^{-2}$ |
| str. adj. solar flux of ($O_3$-$O_3^{tra}$) at TOA | `flxs(rad03)` | 2D | W m$^{-2}$ |
| str. adj. thermal flux of ($O_3$-$O_3^{tra}$) at TOA | `flxt(rad03)` | 2D | W m$^{-2}$ |
| hydroxyl radical | `OH` | 3D, tm, gm | mol mol$^{-1}$ |
| road traffic hydroxyl radical | `OHtra` | 3D, tm, gm | mol mol$^{-1}$ |
| methane | `CH4` | 3D, tm, gm | mol mol$^{-1}$ |
| methane loss | `CH4loss` | 3D, tm, gm | mol mol$^{-1}$ s$^{-1}$ |
| methane loss by $OH^{tra}$ | `CH4losstra` | 3D, tm, gm | mol mol$^{-1}$ s$^{-1}$ |
| methane lifetime | `tau_CH4` | tm | s |
| road traffic methane lifetime | `tau_CH4tra` | tm | s |
| | OUTPUT OF TRANSCLIM | | |
| ozone | `O3_emScen` | 3D, tm, gm | mol mol$^{-1}$ |
| | `O3_emRef` | 3D, tm, gm | mol mol$^{-1}$ |
| | `O3_diff` | 3D, tm, gm | mol mol$^{-1}$ |
| road traffic ozone | `O3tra_emScen` | 3D, tm, gm | mol mol$^{-1}$ |
| | `O3tra_emRef` | 3D, tm, gm | mol mol$^{-1}$ |
| | `O3tra_diff` | 3D, tm, gm | mol mol$^{-1}$ |
| str. adj. net flux of $O_3$ at TOA | `flxnO3_emScen` | 2D, gm | W m$^{-2}$ |
| | `flxnO3_emRef` | 2D, gm | W m$^{-2}$ |
| | `flxnO3_diff` | 2D, gm | W m$^{-2}$ |

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Table S 4 – *Continued from previous page*

| Variable | | Dimension | Unit |
|---|---|---|---|
| str. adj. net flux of $O_3^{tra}$ at TOA | flxnO3tra_emScen | 2D, gm | W $m^{-2}$ |
| | flxnO3tra_emRef | 2D, gm | W $m^{-2}$ |
| | flxnO3tra_diff | 2D, gm | W $m^{-2}$ |
| hydroxyl radical | OH_emScen | 3D, tm, gm | mol $mol^{-1}$ |
| | OH_emRef | 3D, tm, gm | mol $mol^{-1}$ |
| | OH_diff | 3D, tm, gm | mol $mol^{-1}$ |
| road traffic hydroxyl radical | OHtra_emScen | 3D, tm, gm | mol $mol^{-1}$ |
| | OHtra_emRef | 3D, tm, gm | mol $mol^{-1}$ |
| | OHtra_diff | 3D, tm, gm | mol $mol^{-1}$ |
| methane | CH4_emScen | 3D, tm, gm | mol $mol^{-1}$ |
| | CH4_emRef | 3D, tm, gm | mol $mol^{-1}$ |
| | CH4_diff | 3D, tm, gm | mol $mol^{-1}$ |
| methane loss | CH4loss_emScen | 3D, tm, gm | mol $mol^{-1}$ $s^{-1}$ |
| | CH4loss_emRef | 3D, tm, gm | mol $mol^{-1}$ $s^{-1}$ |
| | CH4loss_diff | 3D, tm, gm | mol $mol^{-1}$ $s^{-1}$ |
| methane loss by $OH^{tra}$ | CH4losstra_emScen | 3D, tm, gm | mol $mol^{-1}$ $s^{-1}$ |
| | CH4losstra_emRef | 3D, tm, gm | mol $mol^{-1}$ $s^{-1}$ |
| | CH4losstra_diff | 3D, tm, gm | mol $mol^{-1}$ $s^{-1}$ |
| $CH_4$ lifetime | tau_CH4_emScen | tm | s |
| | tau_CH4_emRef | tm | s |
| | tau_CH4_diff | tm | s |

Table S 4: Input and output variables of TransClim. The output variables are determined for the emission scenario (_emScen), the reference scenario (_emRef) and the difference between the emission and the reference scenario (_diff). All variables are annual means on model levels. The abbreviation 3D denotes levels, latitudes and longitudes, 2D stands for latitudes and longitudes. tm and gm denote tropospheric and global mean. The abbreviation str. adj. stands for stratosphere-adjusted. The dimension of output variables depends on the setting of the resolution (variable var in namelist.py, see tab. S3). All output variables listed in this table are written in a netCDF-file.

To run TransClim, following Python packages are required:

- sys
- os
- time
- copy
- math

- numpy
- scipy.interpolate
- netCDF4
- Ngl
- importlib

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