

Supplement of

TransClim (v1.0): A chemistry-climate response model for assessing the effect of mitigation options for road traffic on ozone

Vanessa Simone Rieger¹ and Volker Grewe^{1,2}

¹Deutsches Zentrum für Luft- und Raumfahrt, Institut für Physik der Atmosphäre, Oberpfaffenhofen, Germany

²also at: Delft University of Technology, Aerospace Engineering, Section Aircraft Noise and Climate Effects, Delft, Netherlands

Correspondence: Vanessa Simone Rieger (vanessa.rieger@dlr.de)

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S1 Implementation in EMAC: split-up of emission regions

- 5 To perform the emission variation simulations with EMAC, the simulation setup which bases on the model setup of *RCISD-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
- 10 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,
- 15 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)
```

- 20 ! 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
```

```
25 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
```

```
30 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'  
40 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'  
45 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'  
50 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. 3.2.1 of
60 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)

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Submodel	Description	References
OFFEMIS	offline emissions of tracers and aerosols	Kerkweg et al. (2006b)
ONEMIS	determination of online emissions	Kerkweg et al. (2006b)
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. 3.2.1 of the main paper.

S2.2 Execution of emission variation simulations

The complete namelist setup of the emission variation simulation is found in the folder `/messy/nml/TRANSCLIMLUT` of the MESSy distribution (here indicated with `$MESSY`). The emission variation simulations were performed on 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 `NOx` are doubled while the emissions of `VOC` and `CO` are hold fixed (scaling factors

1.0).

Emission 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
China	CH	CHI	ref_11
India	IN	IND	ref_11
Southeast Asia	EA	SEA	ref_11
Japan/South Korea	JP	JAP	ref_11
South America	SA	SAM	ref_11

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

S2.3 List of emission variation simulations

Table S3 presents a list of all emission variation simulations performed with EMAC and which are currently available to create the LUTs for TransClim. The output of the emission variation simulations for the LUTs can be downloaded from [citation]. The list can be easily extended by more simulations with EMAC. Note that a new reference simulation might be needed.

Emission region	Emission scaling factors			Emission region	Emission scaling factors		
	NO _x	VOC	CO		NO _x	VOC	CO
Germany	0.0	0	0	Western Europe,	0.0	0.0	0.0
	0.5	0.5	0.5	Northern Europe,	0.5	0.5	0.5
	0.0	0.0	1.0	Eastern Europe,	0.0	0.0	1.0
	0.0	1.0	0.0	Southern Europe,	0.0	1.0	0.0
	0.0	1.0	1.0	China,	0.0	1.0	1.0
	0.0	1.0	2.0	India,	0.0	1.0	2.0
	0.0	2.0	1.0	Southeast Asia,	0.0	2.0	1.0
	1.0	0.0	0.0	Japan/South Korea,	1.0	0.0	0.0
	1.0	0.0	1.0	North America,	1.0	0.0	1.0
	1.0	0.0	2.0	South America	1.0	0.0	2.0
	1.0	1.0	0.0		1.0	1.0	0.0
	1.0	1.0	2.0		1.0	1.0	2.0
	1.0	1.0	3.0		1.0	2.0	0.0
	1.0	2.0	0.0		1.0	2.0	1.0
	1.0	2.0	1.0		1.0	2.0	2.0
	1.0	2.0	2.0		2.0	0.0	1.0
	1.0	3.0	1.0		2.0	1.0	0.0
	2.0	0.0	1.0		2.0	1.0	1.0
	2.0	1.0	0.0		2.0	1.0	2.0
	2.0	1.0	1.0		2.0	2.0	1.0
2.0	1.0	2.0					
2.0	2.0	1.0					
3.0	1.0	1.0					
Reference (ref_inst, ref_11)	1.0	1.0	1.0				

Table S 3. List of emission variation simulations performed with EMAC and used as LUTs for TransClim.

S3.1 Settings

TransClim is implemented in Python. The current version runs with Python 2. The code is available from [citation]. All settings for a simulation with TransClim are conducted in the file `namelist.py`. The options are listed in table S4.

Variable	Type	Description
<code>emission_regions</code>	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
<code>emScen</code>	dictionary	contains emission scaling factors for emission scenario, key: emission region (abbreviated with two letters, string), value: list with emission scaling factors (1st index: sNO _x , 2nd index: sVOC, 3rd index: sCO)
<code>emRef</code>	dictionary	contains emission scaling factors for reference scenario, key: emission region (abbreviated with two letters, string), value: list with emission scaling factors (1st index: sNO _x , 2nd index: sVOC, 3rd index: sCO)
<code>output_name</code>	string	simulation name
<code>pathIn</code>	string	path of emission variation simulations (LUTs)
<code>pathOut</code>	string	path for output files (folder must already exist)
<code>var</code>	dictionary	contains variables and the resolution for which the interpolation will be performed, key: variable (string), value: resolution (string)
<code>RFO3tra_scale_switch</code>	boolean	True: switches on scaling of O ₃ ^{tra} radiative forcing with NO _x emissions (further details see below)
<code>RFO3tra_arg</code>	dictionary	contains arguments which are necessary for scaling the radiative forcing of O ₃ ^{tra} , keys: <code>start_year</code> , <code>end_year</code> , <code>scale_year</code> , <code>pathNOx</code> , <code>fileNOx</code> (for detailed explanation see below)

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Table S 4 – *Continued from previous page*

Variable	Type	Description
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 variations (e.g. '0.0_1.0_1.0')

Table S 4: 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

95 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 $\text{RF}(O_3^{\text{tra}})$ is scaled to. The scaled $\text{RF}(O_3^{\text{tra}})$ and the corresponding years are written to the ASCII output file `output_name_RFO3tra` which can
100 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
105 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 S5.

- 110
- `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_RF03tra`: is only written when `RF03tra_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

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Table S 5 – Continued from previous page

Variable		Dimension	Unit
	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
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

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Table S 5 – *Continued from previous page*

Variable		Dimension	Unit
	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 5: 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 stratospheric adjusted. The dimension of output variables depends on the setting of the resolution (variable `var` in `namelist.py`, see tab. S4). All output variables listed in this table are written in a netCDF-file.

115 To run TransClim, following Python packages are required:

– sys

– os

– time

– copy

120 – math

– numpy

– `scipy.interpolate`

– netCDF4

– Ngl

125 – `importlib`

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