

# Table of Contents

<b>Boundary Conditions and Input Files for SOCOL.....</b>	<b>1</b>
Emissions.....	1
Regriding procedures.....	1
CO and NO <sub>x</sub> .....	1
Available files on Euler:.....	1
NMHC.....	2
Available files on Euler:.....	2
Methane.....	2
Available files on Euler:.....	2
Ozone Depleting Substances.....	3
Sulfur Species.....	3
Available files on Euler:.....	3
Tropospheric Species.....	4
Available files on Euler:.....	4
Energetic Particles and Ionization Rates.....	4
Available files on Euler:.....	4
Greenhouse Gases (GHG) and Ozone Depleting Substances (ODS).....	4
Available GHG files on Euler:.....	4
Available ODS files on Euler:.....	5
How to create input files following CCMI (=CMIP5) recommendations:.....	5
Nudging Files.....	5
Updates for downloading ERA5 data.....	5
Photolysis Rates.....	6
Available input files on Euler:.....	6
Quasi-Biennial Oscillation (QBO).....	6
Available QBO files on Euler:.....	6
How to create QBO input files based on wind observations:.....	6
Sea Surface Temperatures (SSTs) and Sea Ice Coverage (SIC).....	7
Available SST/SIC files on Euler:.....	7
How to prepare Hadley-SST input files:.....	7
Solar Irradiance.....	7
Stratospheric Aerosols.....	7
Available input files on Euler:.....	8
How to prepare stratospheric aerosol input files:.....	8
SOCOL-AER radiative lookup tables:.....	8
Tropospheric Aerosols.....	8
Available input files on Euler:.....	8
Other stuff.....	9


# Boundary Conditions and Input Files for SOCOL

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The boundary conditions are available for our standard model resolutions **T31L39** and **T42L39**. Most input data are also available in **T42L90**. A few data sets are further available in **T63L47** (note: SOCOLv3 never ran in this resolution).

Further information on CCMI-related boundary conditions can be found here:

[https://www.sparc-climate.org/fileadmin/customer/6\\_Publications/Newsletter\\_PDF/40\\_SPARCnewsletter\\_Jan2013\\_w](https://www.sparc-climate.org/fileadmin/customer/6_Publications/Newsletter_PDF/40_SPARCnewsletter_Jan2013_w)

 **NOTE:** Initial and boundary conditions for ECHAM5-MPIOM used in the FUPSOL project are stored here on Euler: `/cluster/work/climate/stenkea/echam5/input/`

## Emissions

Our input files include monthly mean emission fluxes at the surface. Units are usually  $[g/cm^2/s]$  or  $[kg/m^2/s]$  (**ATTENTION:** correct conversion factor to mixing ratio must be applied in `socol_boundary_conditions.f90`) (subroutine `set_socol_bcond_fluxes`). The emissions are assumed to be representative for the middle of the month. To avoid jumps from month to month, a linear interpolation in time between previous, present and next month is applied during a model simulation.

## Regridding procedures

For horizontal regridding of original emission fluxes to SOCOL's horizontal grid the tool `ncregrid` can be used. The source code, binary and several run scripts can be found here: `/home/stenkea/ncregrid/`

Details about how to use `ncregrid` can be found in the manual. An example script for regridding CO and NO<sub>x</sub> emission fluxes is given here.

For the final preparation of input files for SOCOL `ncf` can be used, e.g.

## CO and NO<sub>x</sub>

The input files include CO and NO<sub>x</sub> surface emissions  $[g/m^2/s]$  as well as aircraft NO<sub>x</sub> emissions  $[molec/cm^3/s]$  on pressure levels. We assume a fraction of 90% NO in NO<sub>x</sub> emissions and 10% of NO<sub>2</sub>, respectively (parameters `nofracnox_bcond` and `no2fracnox_bcond` in `mo_socol_constants.f90`)

### Available files on Euler:

- `/cluster/work/climate/stenkea/echam5/data/SOCOL/T[31,42]/=co_nox`
  - ◆ SOCOLv3 description paper (Stenke et al., 2013), for 1949 to 2007, with anthropogenic emissions from RETRO and natural emissions from MOZART:  
`T42L39_co_nox_emiss_surf_aircr_socol_YYYY.nc`
  - ◆ Sensitivity with anthropogenic AND natural emissions from RETRO, for 1949 to 2000:  
`T42L39_co_nox_emiss_surf_aircr_socol_YYYY_RETRO.nc`
  - ◆ CCMI emissions, 1949 to 2000, based on ACCMIP dataset (download <https://eccad.aeris-data.fr/>):  
`T42L[39,90]_co_nox_emiss_surf_aircr_socol_YYYY_ccmi.nc`
  - ◆ Same as above, but for the different RCPs, 2000 to 2100:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/T[31,42]/co_nox/RCP[...].nc`
  - ◆ Lightning NO<sub>x</sub> climatology (used before interactive lightning parameterisation or if namelist parameter `interactivelnox = FALSE`):

T42L[39, 90]\_nox\_lightning\_socol.nc

- ◆ Scaling factor for interactive lightning NOx parameterisation:  
T42\_fac\_lightning\_socol.nc
- ◆ No emission files, but upper boundary condition for NOx VMR based on MIPAS data used for HEPPA project, Oct 2008 to May 2009: heppa/nox\_heppa\_YYYYMM.nc

## NMHC

NMHC emissions are lumped emissions and only used as an additional indirect source of CO, that is, a certain fraction of the NMVOC emission is directly added to CO. For the CCMI set up the conversion factors are 1.0 for anthropogenic NMHCs, 0.31 for biomass burning, and 0.83 for biogenic sources (Revell et al., 2015). The conversion factors are hard-wired in `src/socol_boundary_conditions.f90`.

### Available files on Euler:

- `/cluster/work/climate/stenkea/echam5/data/SOCOL/T[31, 42]/nmhc`
  - ◆ Anthropogenic emissions, 1949 to 2000, based on ACCMIP dataset (download <https://eccad.aeris-data.fr/>):  
ACCMIP\_emissions\_anthropogenic\_NMHC\_T42\_YYYY.nc
  - ◆ Biomass-burning emissions, 1949 to 2000, based on ACCMIP dataset (download <https://eccad.aeris-data.fr/>):  
ACCMIP\_emissions\_biomassburning\_NMHC\_T42\_YYYY.nc
  - ◆ Biogenic emissions, 1949 to 2000, based on ACCMIP dataset (download <https://eccad.aeris-data.fr/>): ACCMIP\_emissions\_biogenic\_NMHC\_T42\_YYYY.nc
- Same as above, but for the different RCPs, 2000 to 2100:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/T[31, 42]/nmhc/RCP[26, 45, 60]`
- Some older emission files used for the first test simulations: GFEDv2\_NMHC\_YYYY.nc for 1995 to 2007, and GEIA\_NMVOC\_\*\_1990\_T42.nc

## Methane

The default boundary condition for methane is prescribed surface mixing ratios. Methane emissions are only read, if namelist parameter `lch4flux = TRUE`. For details see PhD thesis of Ancelin Coulon.

### Available files on Euler:

- `/cluster/work/climate/stenkea/echam5/data/SOCOL/T[31, 42]/ch4`
  - ◆ Emissions from termites, climatology: `termite/CH4_TERMITES_T42_1974.nc`
  - ◆ Emissions from wild animals, climatology:  
`animal/CH4_WILDANIMALS_T42_1974.nc`
  - ◆ Degassing volcanoes, climatology: `volcano/CH4_VOLCANOES_T42_1974.nc`
  - ◆ Emissions from oceans, climatology: `ocean/CH4_OCEANS_T42_1974.nc`
  - ◆ Emissions from rice paddies, 1979 to 2010: `rice[_2, 3, 4]/CH4_RICE_T42_YYYY.nc`
  - ◆ Biomass burning emissions:
    - ◇ unknown dataset, 1960 to 2011: `bb/CH4_BB_T42_YYYY.nc`
    - ◇ 1960 to 2000, based on RETRO dataset (download <https://eccad.aeris-data.fr/>):  
`RETRO_CH4_BB_T42_YYYY.nc`
    - ◇ 1997 to 2009, based on GFEDv3.1 dataset (download <https://eccad.aeris-data.fr/>):  
`GFED3.1_CH4_BB_T42_YYYY.nc`
    - ◇ 1950 to 2000, based on ACCMIP dataset (download <https://eccad.aeris-data.fr/>):  
`T42_IPCC_emissions_CH4_BB_YYYY.nc`
    - ◇ Same as above, but for the different RCPs, 2000 to 2100:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/T42/ch4/rcp[26,`
  - ◆ Anthropogenic emissions:

- ◊ EDGARv4.1 for 1970 to 2005 (download <https://eccad.aeris-data.fr/>):
  - individual sources sectors: EDGAR\_anthropogenic/
  - combined emission files: EDGAR\_v41\_CH4\_anthrop\_T42\_YYYY.nc
- ◊ Modified EDGAR emissions for 2001 to 2009 based on Bergamaschi et al., (2013): Bergamaschi/
- ◊ Anthropogenic and ship emissions, 1950 to 2000, based on ACCMIP dataset (download <https://eccad.aeris-data.fr/>):
  - T42\_IPCC\_emissions\_CH4\_anthropogenic\_YYYY.nc and
  - T42\_IPCC\_emissions\_CH4\_ships\_YYYY.nc
- ◊ Same as above, but for the different RCPs, 2000 to 2100:
  - /cluster/work/climate/stenkea/echam5/data/SOCOL/T42/ch4/rcp[26,
- ◆ Wetland emissions:
  - ◊ unknown dataset, 1974 to 2010:
    - wetland[\_2, 3, 4]/CH4\_WETLANDS\_T42\_YYYY.nc
  - ◊ 1950 to 2006, based on MAIOLICA-1 (Hodson et al., 2011):
    - MAIOLICA\_CH4\_wetlands\_T42\_YYYY.nc
  - ◊ 1979 to 2010, from SDGVM vegetation model:
    - wetlands\_SDGVM/CH4\_WETLANDS\_SDGVM\_T42\_YYYY.nc
  - ◊ 1979 to 2011, from LPJ vegetation model:
    - wetlands\_LPJ/CH4\_WETLANDS\_T42\_YYYY.nc
- ◆ Sink by soil uptake: sink/CH4\_SINKS\_T42\_YYYY.nc

## Ozone Depleting Substances

The default boundary condition for ODSs are prescribed surface mixing ratios. The available emission fluxes of CFC-12, HCFC-22 and CH<sub>3</sub>CCl<sub>3</sub>? have been used for sensitivity simulations for the SPARC ODS-Lifetime assessment.

- Emissions in T42 for 1949 to 2100:
  - /cluster/work/climate/stenkea/echam5/data/SOCOL/T42/ods/T42\_ODS\_emiss\_surf
- Documentation:
  - [https://wiki.iac.ethz.ch/pub/Chemie/BoundaryConditions/ODS\\_Emission\\_Readme.pdf](https://wiki.iac.ethz.ch/pub/Chemie/BoundaryConditions/ODS_Emission_Readme.pdf)

## Sulfur Species

Emissions of sulfur containing species are only required for SOCOL-AER.

### Available files on Euler:

- /cluster/work/climate/stenkea/echam5/data/SOCOL/T[31, 42]/sulfur
  - ◆ SO<sub>2</sub> surface emissions, 1970 to 2009, based on ACCMIP dataset (download <https://eccad.aeris-data.fr/>): T42L39\_SO2\_surf\_emiss\_YYYY.nc
  - ◆ SO<sub>2</sub> surface emissions for RCP4.5, 2000 to 2100, based on ACCMIP dataset (download <https://eccad.aeris-data.fr/>): RCP45/T42L39\_SO2\_surf\_emiss\_RCP45\_YYYY.nc
  - ◆ SO<sub>2</sub> emissions from degassing volcanoes, GEIA dataset (download <https://eccad.aeris-data.fr/>): T42\_so2\_cvol\_emiss.nc
  - ◆ OCS surface emissions, 1970 to 2009 [**not used in SOCOL, tropospheric OCS is fixed to 500 pptv**]: T42L39\_OCS\_surf\_emiss\_YYYY.nc
  - ◆ CS<sub>2</sub> surface emission, climatology, 1 Tg S/yr, 52S 52N: T42L39\_CS2\_surf\_emiss.nc
  - ◆ DMS ocean concentrations, climatology based on Kettle et al. (1999) and Kettle and Andreae (2000): T42L39\_DMS\_sea\_concen.nc
  - ◆ DMS ocean concentrations, climatology based on Lana et al. (2011):
    - T42L39\_DMS\_sea\_concen\_lana11.nc

## Tropospheric Species

Emissions of isoprene ( $C_5H_8$ ?), formaldehyde ( $CH_2O$ ?) and acetic acid ( $CH_3COOH$ ?) required for the isoprene mechanism (MIM-1).

### Available files on Euler:

- `/cluster/work/climate/stenkea/echam5/data/SOCOL/T[31,42]/tropchem`
  - ◆ Historical emissions, 1949 to 2000, based on ACCMIP dataset (download <https://eccad.aeris-data.fr/>): `ACCMIP_emissions_Isoprene_T42_YYYY.nc`, `ACCMIP_emissions_Formaldehyde_T42_YYYY.nc`, `ACCMIP_emissions_CH3COOH_T42_YYYY.nc`
- Same as above, but for the different RCPs, 2000 to 2100:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/T[31,42]/tropchem/RCP[26,4`
- Some older emission files used for the first test simulations for the year 2000: anthropogenic: `IPCC_emissions_*_2000_T42.nc`, natural: `MEGAN_nat_*_2000_T42.nc`
- Photolysis rates for species in isoprene mechanism (no longer used since those species are included in regular photolysis files): `Photolysis_tropchem_T42.nc`

## Energetic Particles and Ionization Rates

The parameterisation for energetic particles have been developed with in the FUPSOL project within SOCOLv3-MPIOM and then transferred to the CCMI version of SOCOLv3. For details see PhD thesis of Julien Anet and PhD thesis of Pavle Arsenovic.

### Available files on Euler:

- `/cluster/work/climate/stenkea/echam5/data/SOCOL/energ_particles/`
  - ◆ MEE, GCR and SPE ion pair production rates [ion pair/g/s], 1960 to 2010: `particles_socol_YYYY.nc`
  - ◆ NOy flux at model top [ $cm^{-2}s^{-1}$ ], 1960 to 2010: `noy_abc_YYYY.nc`
- `/cluster/work/climate/stenkea/echam5/data/SOCOL/ionization/`
  - ◆ Ionization rates from Solar Proton Events (SEP) from Friedhlem Steinhilber [ $\#/cm^3/s$ ], 1990 to 2200: `YYYY_ionrate-nitrate.txt`
  - ◆ Ionization rates from Solar Proton Events (SEP) [ $\#/cm^3/s$ ], 1950 to 2006: `IonPair_Year-YYYY.dat`
  - ◆ Ap index used for Low Energetic Electrons (LEE): `monthly_mean_Ap_*`
  - ◆ For Galactic Cosmic Rays (GCR) the solar modulation potential (SMP) "Phi", geomagnetic latitude and altitude are used: `gcr_data_*`, `geomag_data_*.txt`, `phi_to_nc_*`
- `/cluster/work/climate/stenkea/echam5/data/SOCOL/CCMI_solar_data/ap_index/`
  - ◆ Ap index for REF-C1 and REF-C2 used for CCMI simulations
- `/cluster/work/climate/stenkea/echam5/data/SOCOL/CCMI_solar_data/ionrate/`
  - ◆ SPE ionization rates for REF-C1 and REF-C2, 1949 to 2012 / 2100

## Greenhouse Gases (GHG) and Ozone Depleting Substances (ODS)

### Available GHG files on Euler:

- Text files containing global and monthly mean surface mixing ratios of  $CO_2$  [ppmv],  $CH_4$  [ppbv] and  $N_2O$  [ppbv] for past and future following different RCPs:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/GHG_ODS/*co2*.txt` or

\*ch4\*.txt or \*n2o\*.txt

## Available ODS files on Euler:

- Text files containing global and monthly mean surface mixing ratios of Bromine containing ODS family, short- and longlived Chlorine (CLS and CLL) containing ODS families [pptv]:  
/cluster/work/climate/stenkea/echam5/data/SOCOL/GHG\_ODS/\*odsbr\*.txt  
or \*odscls\*.txt or \*odscll\*.txt
- Text files containing global and monthly mean surface mixing ratios of individual ODS tracers as well as lifetimes and number of Cl and Br atoms:  
/cluster/work/climate/stenkea/echam5/data/SOCOL/GHG\_ODS/\*odsmem\*.txt

## How to create input files following CCMI (=CMIP5) recommendations:

- Original concentration data for before 2005, RCP2.6, RCP4.5, RCP6.0 and RCP8.5 downloaded from <http://www.iiasa.ac.at/web-apps/tnt/RcpDb/dsd?Action=htmlpage&page=about> : CMIP5\_CONC.tar
- Scripts for preparing input files for SOCOL: scripts\_ghg\_ods.tar

## Nudging Files

- Nudging files for SOCOL are based on ERA-Interim reanalyses [Dee et al., 2011]
- Get ERA-Interim analyses from ECMWF server:
  - ◆ Get access to ECMWF public data sets:  
<https://confluence.ecmwf.int/display/WEBAPI/Access+ECMWF+Public+Datasets>
  - ◆ edit python script: erai\_all.py
  - ◆ export PYTHONPATH=/home/stenkea/SOCOL/Nudging/ecmwfapi/
  - ◆ python erai\_all.py
- cdo scripts to create nudging files in T42L39? and T42L90?: cdo\_nudgfiles.csh, cdo\_nudgfiles\_L90.csh
- T42 Nudging files for L39 and L90 on Euler:  
/cluster/work/climate/stenkea/echam5/data/SOCOL/T42/nudge\_files/eraia\_T42L[39,90]\_netcdf/
- Available years 1980/01 to 2018/11
- Documentation: NudgingFiles-for-SOCOLv3.pdf

## Updates for downloading ERA5 data

- ERA-Interim is only available up to 31 August 2019, after which it has been superseded by the ERA5 analysis <https://www.ecmwf.int/en/forecasts/datasets/reanalysis-datasets/era5>. Therefore, nudging runs after August 2019 will require the use of ERA5 analysis to produce nudging files
- ERA5 can be downloaded from the Climate Data Store (CDS), with the full instructions shown here : <https://confluence.ecmwf.int/display/CKB/How+to+download+ERA5>
- The CDS API must be installed on your machine to download ERA5 data. For the IAC IT system, this can be done by creating a new environment and installing the CDS API package:  
[https://wiki.iac.ethz.ch/IT/PythonFAQ#How\\_can\\_I\\_create\\_my\\_own\\_environment](https://wiki.iac.ethz.ch/IT/PythonFAQ#How_can_I_create_my_own_environment)
- A new version of the python script to download the necessary ERA5 data programatically:  
retrieve\_ERA5.py
- Be aware of the long download times for the ERA5 data, due to the queueing system. One month of data required for nudging takes around 1-2 hours to download.
- A new version of the cdo script to create nudging files for T42L39?: cdo\_nudgfiles\_ERA5.csh

# Photolysis Rates

SOCOL reads pre-calculated photolysis rates [1/s] for certain chemical species tabulated as function of 40 overhead O2 and 44 overhead O3 columns. The photolysis input files do not depend of vertical or horizontal resolution. For details contact: [eugene.rozanov@pmodwrc.ch](mailto:eugene.rozanov@pmodwrc.ch)

## Available input files on Euler:

- SOCOLv3 description paper (Stenke et al., 2013), for 1949 to 2007:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/sun/photolysis_socol_YYYY.`
- Same as above, but including sulfur species:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/sun_sulfur`
- The CCMI photolysis rates are supposed to be based on the solar irradiance data from the NRLSSI model (Lean et al., 2005)
  - ◆ CCMI REF-C1, for 1949 to 2011:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/CCMI_solar_data/photolysis_ref_c1_1949_2011.nc`
  - ◆ CCMI REF-C2, for 1949 to 2101:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/CCMI_solar_data/photolysis_ref_c2_1949_2101.nc`
  - ◆ Some photolysis rates for sensitivity tests:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/CCMI_solar_data/photolysis_sensitivity.nc`
    - ◇ the standard photolysis rates assume a surface albedo of 0.3 and a "surface cloud" of 50% cloud coverage
    - ◇ new\_lut\_C1.tar: REF-C1 photolysis rates assuming a surface albedo of 0.3, but no cloud coverage
    - ◇ new\_lut\_C1\_C0\_A0.tar: REF-C1 photolysis rates assuming a surface albedo of 0 and no cloud coverage
- CCMI photolysis rates, but including sulfur species:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/sun_ccmi_sulfur`

## Quasi-Biennial Oscillation (QBO)

### Available QBO files on Euler:

- Based on observations, 1949-2018 (continuously updated):  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/QBO/QBO_obs_YYYY.nc`
- Extended to 2110 following the approach described in Brönnimann et al. (2007):  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/QBO/QBO_socol_YYYY.nc`
- Note: QBO input files are independent of vertical or horizontal resolution

### How to create QBO input files based on wind observations:

- Data download from <https://www.geo.fu-berlin.de/en/met/ag/strat/produkte/qbo/index.html>
- Scripts for preparing netcdf input files for SOCOL: `qbo_scripts.tar`
  - ◆ `u_profile_198701-201812.f90`: F90 program to vertically extend observed u-wind profile
  - ◆ `compile_ifort`: script to compile F90 program with Intel compiler
  - ◆ `makeinput4SOCOL.ncl`: ncl script to create netcdf input files for SOCOL
- Further information on procedure (still, March 2019) available on CCMVal-1 webpage:  
[http://www.pa.op.dlr.de/CCMVal/Forcings/qbo\\_data\\_ccmval/u\\_profile\\_195301-200412.html](http://www.pa.op.dlr.de/CCMVal/Forcings/qbo_data_ccmval/u_profile_195301-200412.html)

# Sea Surface Temperatures (SSTs) and Sea Ice Coverage (SIC)

## Available SST/SIC files on Euler:

- Observation-based (Hadley data set), 1900-2018 (continuously updated):  
`/cluster/work/climate/stenkea/echam5/data/T[31,42]/hadley/`
- AMIP2, 1949-2000:  
`/cluster/work/climate/stenkea/echam5/data/T[31,42]/amip2/`
- CESM1-CAM5 simulations for CMIP5: past (1850-2005); RCP2.6, RCP4.5, RCP6.0 and RCP8.5 (2006-2100):  
`/cluster/work/climate/stenkea/echam5/data/T[31,42]/cesm1-cam5/`

## How to prepare Hadley-SST input files:

- Observed SSTs: **HadISST1** data set provided by the UK Met Office Hadley Centre [Rayner et al., 2003]
- Data download from <https://www.metoffice.gov.uk/hadobs/hadisst/data/download.html>
- Regrid data to model resolution and land-sea-mask: `remap_sst_sic_hadley.csh`
- Grid and land-sea-mask description files:  
<https://wiki.iac.ethz.ch/pub/Chemie/BoundaryConditions/grids.tar>

## Solar Irradiance

SOCOL reads a .txt files providing monthly mean spectral solar irradiance [W/m<sup>2</sup>] for the 6 short-wave spectral bands of MA-ECHAM5 (185 250nm, 250 440nm, 440 690 nm, 690 1190 nm, 1190 2380nm and 2380 4000 nm, Cagnazzo et al., 2007). These files are usually named `sun_irrad_*.txt`.

- SOCOLv3 description paper:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/sun/`
- CCMI:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/CCMI_solar_data/irrad_echa`

The next solar irradiance related input file provides data for the additional heating due to absorption by O<sub>2</sub> and O<sub>3</sub> in the Lyman-alpha line, the Schumann-Runge, Hartley and Huggins bands (see SOCOL source code `mo_socol_sun.f90`). These files are usually named `sun_par_*.txt`.

- SOCOLv3 description paper:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/sun/`
- CCMI:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/CCMI_solar_data/extra_heat`

⚠ The directory `/cluster/work/climate/stenkea/echam5/data/SOCOL/sun/` also includes the different solar irradiance data sets used in FUPSOL, `scaled`, `bestguess`, `constant`. For details see PhD thesis of Julien Anet.

## Stratospheric Aerosols

SOCOL reads short-wave (6 spectral bands) extinctions, single scattering albedo and asymmetry factor as well as long-wave (16 spectral bands) extinctions for the radiation scheme as well as surface area density and number densities or (CCMI and later) mean radius, volume density and H<sub>2</sub>SO<sub>4</sub>? mass for heterogeneous chemistry.



## Available input files on Euler:

- SOCOLv3 description paper (Stenke et al., 2013), for 1949 to 2011:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/T[31,42]/strat_aerosols/T[31,42].dat`
- CCM1, based on the SAGE-4l data set, for 1949 to 2100 (after 2011 set to year 2000):  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/T42/strat_aerosols/CCMI_SOCOL.dat`
- CMIP6v4, based on the SAGE-3l data set, for 1850 to 2014:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/T42/CMIP6_v4/T42L39_CMIP6_v4.dat`
- CMIP6v4\_PW: based on the SAGE-3l data set, with absorptivity coefficients in the solar NIR based on Palmer and Williams (Applied Optics, Vol. 14, 1975), for 1850 to 2014:  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/T42/CMIP6_pw_v4/T42L39_CMIP6_pw_v4.dat`

## How to prepare stratospheric aerosol input files:

- Script for preparing netcdf input files for SOCOL: `makeinputforsocol_CMIP6_T42.ncl`

## SOCOL-AER radiative lookup tables:

SOCOL-AER uses a lookup table approach to calculate the aerosol radiative properties (extinction coefficients, single scattering albedos, asymmetry factors) from the particle size distribution for 22 wavelength bands. The original lookup table for SOCOL-AERv1 is the file `band_echam5_aer_2012.dat`. A new lookup table was created for SOCOL-AERv2 since the aerosol size distribution is tracked with dry aerosol radius, and relative humidity is required to calculate the wet aerosol size distribution. Beiping Luo calculated a full lookup table with Mie theory at 95 temperatures and 1001 relative humidities (`band_echam5_pw_socol.dat`). Since the size of this file is rather big (3.6 GB), it slowed down the model significantly. Therefore the lookup table was condensed to only using 10 temperatures and 76 relative humidity values, chosen so that the change in aerosol sulfate weight fraction between subsequent relative humidity entries is at most 0.01 (`band_echam5_pw_socol_condense.dat`). The script used to do this file editing is `condense_lookup_T.sh`.

## Tropospheric Aerosols

SOCOL reads mass mixing ratios of 10 tropospheric aerosol types as function of (TIME, LEV, LAT, LON) for radiation and heterogeneous chemistry (N<sub>2</sub>O<sub>5</sub>? hydrolysis): Methane sulfonate (MSA), Sulfate (SULFATE), accumulation mode dust (0-1  $\mu\text{m}$ ) (DUSTACCU), coarse mode dust (1-2  $\mu\text{m}$ ) (DUSTCOARSE), accumulation mode sea salt (0-1  $\mu\text{m}$ ) (SEASALTACCU), coarse mode sea salt (1-10  $\mu\text{m}$ ) (SEASALTCOARSE), hydrophilic and -hobic organic and black carbon (OCPHILIC, OCPHOBIC, BCPHILIC, BCPHOBIC)

## Available input files on Euler:

- Tropospheric aerosol climatology following Lohmann et al. (1999):  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/T[31,42]/tropo_aerosols/T[31,42].dat`
- Tropospheric aerosol record for 1995 to 2100 from a CAM3.5 simulation with a bulk aerosol model driven by CCSM3 (CMIP4) sea surface temperatures and the 2000–2100 CMIP5 emissions (S. Bauer, personal communication, 2011):  
`/cluster/work/climate/stenkea/echam5/data/SOCOL/T[31,42]/tropo_aerosols/T[31,42].dat`
- Script for regridding tropospheric aerosol data on SOCOL's horizontal grid by using `ncregrid`:  
`regrid_tropo-aerosols_t42.csh`
- The source code as well as binaries and several run scripts for **ncregrid** can be found here:  
`/home/stenkea/ncregrid/`

## Other stuff

- Initial file for chemical tracers, various vertical resolutions:  
/cluster/work/climate/stenkea/echam5/data/SOCOL/T[31,42]/chem\_initial/
- Input for interactive deposition scheme:  
/cluster/work/climate/stenkea/echam5/data/SOCOL/T[31,42]/misc/soilpH\_T42.nc  
and surf\_para\_T42.nc
- Various OH fields for running SOCOL with prescribed OH (namelist parameter loh\_ext = TRUE):  
/cluster/work/climate/stenkea/echam5/data/SOCOL/T42/misc/OHclim\_exp00060\_1  
and OH\_ACCENT\_T42.nc
- Input for interactive wetland emissions of CH4:  
/cluster/work/climate/stenkea/echam5/data/SOCOL/T42/misc/NPP\_T42.nc  
and HR\_T42.nc and global\_wetland\_frac\_T42.nc and  
30008\_1995\_tsurf\_annualmean.nc
- Emissions for synthetic CO tracer in CCMI simulations:  
/cluster/work/climate/stenkea/echam5/data/SOCOL/T42/misc/CCMI\_CO\_tracer\_T42.nc
- Definition of horizontal regions for ozone origin diagnostic:  
/cluster/work/climate/stenkea/echam5/data/SOCOL/T42/O3orig/
- Definition of emission regions for methane tracer tracking:  
/cluster/work/climate/stenkea/echam5/data/SOCOL/T42/ncmaps\_transcom/
- Methylchloroform (MCF) emissions as a proxy for tropospheric OH, 1979 to 2011, emission data from *TransCom-CH4 project*:  
/cluster/work/climate/stenkea/echam5/data/SOCOL/T42/mcf/
- NO and NO2 mixing ratio boundary condition for sensitivity run based on REF-C1 model output from CESM1-WACCM, 1990 to 2013:  
/cluster/work/climate/stenkea/echam5/data/SOCOL/T42/nox\_mbc/

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