MESSy StratO3Bud User Manual

for the MESSy StratO3Bud tool

Patrick Jöckel[1], Christoph Brühl[2], Hella Garny[1] and Stefanie Meul[3]

[1] Deutsches Zentrum für Luft- und Raumfahrt, Institut für Physik der Atmosphäre, Oberpfaffenhofen, 82230 Wessling, Germany

[2] Air Chemistry Department, Max-Planck Institute of Chemistry, PO Box 3060, 55020 Mainz, Germany

[3] Institut für Meteorologie, Freie Universität Berlin, 12165 Berlin, Germany

This manual is part of the electronic supplement of the article Meul et al., *Chemical Contribution to Future Tropical Ozone Change in the Lower Stratosphere*, submitted to Atmos. Chem. Phys.

The tool StratO3Bud is used to calculate (as post-processing step) the stratospheric ozone budget (production and loss via various reaction pathways).

History:

Original ferret-script	: Ch. Brühl, P. Jöckel (MPI-C, 2006)
Fortran90 code	: H. Garny, (DLR, 2011)
Adaption for MESSy2-MECCA	: P. Jöckel (DLR, 2011)
Extraction of rate coeff. from mecca.eqn	: P. Jöckel (DLR, 2013)
Documentation	: P. Jöckel (DLR, 2013), S. Meul (FUB, 2013)

Method:

The stratospheric ozone budgets are calculated using the model output for the temperature and a set of chemical tracers (see Data). The tool is based on the concept of chemical families which allows a reduction of the full chemical loss cycles to the rate limiting steps in the stratosphere. The ozone loss is calculated for the Chapman cycle ("LossOx") and the catalytic cycles involving the hydrogen ("LossHOx"), nitrogen ("LossNOx") and halogen radicals ("LossClOx"," LossBrOx"). The ozone production pathways are photolysis of oxygen ("Prod") and methane photooxidation ("ProdHO2", "ProdCH3O2").
At each gridpoint the reaction rate equations for the different loss and production pathways are integrated over one month. The corresponding reaction rate coefficients are automatically adopted from the chemistry module MESSy2-MECCA (../../mbm/caaba/mecca/mecca.eqn) or must be adapted by the user (see Application).

Content of the distribution:

strato3bud.tcsh	: wrapper-script
strato3bud.f90	: main program, calculation of the ozone loss and production pathways
readData.f90	: called by strato3bud.f90 to read and allocate the input data
writeData.f90	: called by strato3bud.f90 to write the output-file
eqn2f90.tcsh	: extracts the reaction rate coefficients (for MESSy users)
Makefile.m / main.mk	: for compilation (default: for MESSy users)

Data:

1) Input:
The program expects the required variables in ONE file per month. The input file can be tailor made via channel output redirection (Jöckel et al., 2010; Section 2 and MESSy2_channel_manual.pdf in corresponding supplement), or prepared with various netCDF tools (nco etc.). The time resolution of the input fields is recommended to be at least 10 hours to obtain reasonable results.

The required variables are:

Grid information:

float lat(lat) ;
float hyam(lev) ;
float hybm(lev) ;
float aps(time, lat, lon) ;

Temperature:

float tm1(time, lev, lat, lon) ;

Tracer:

float O3(time, lev, lat, lon) ;
float NO(time, lev, lat, lon) ;
float NO2(time, lev, lat, lon) ;
float O1D(time, lev, lat, lon) ;
float O3P(time, lev, lat, lon) ;
float HO2(time, lev, lat, lon) ;
float OH(time, lev, lat, lon) ;
float H(time, lev, lat, lon) ;
float CH3O2(time, lev, lat, lon) ;
float ClO(time, lev, lat, lon) ;
float BrO(time, lev, lat, lon) ;
float H2O(time, lev, lat, lon) ;

Photolysis:

float J_O2(time, lev, lat, lon) ;

Not required, but recommended are:

float lon(lon) ;
float lev(lev) ;
float geosp(time, lat, lon) ;
float gboxarea(time, lat, lon) ;
float tp_i(time, lat, lon) ;
float tp_f(time, lat, lon) ;

2) Output:

The output variables are:
LossOx(lev, lat), LossHOx(lev, lat), LossNOx(lev, lat), LossClOx(lev, lat), LossBrOx(lev, lat), Prod(lev, lat), ProdHO2(lev, lat), ProdCH3O2 (lev, lat)

The levels are model levels. The output fields are zonally averaged and averaged in time.

Application:

In order to apply this tool, you need to

1)

a) for MESSy users:
Compile it with "gmake tools" from the $BASEDIR of the distribution. This needs to be repeated, whenever the chemical MECCAnism has been modified. With "gmake tools", the script eqn2f90.tcsh extracts the rate coefficients from mecca.eqn and writes the Fortran90 include file rate_coeff.inc, which is included into strato3bud.f90 at compile time.

b) for other users:
Adapt the reaction rate coefficients in strato3bud.f90 to that you have used for your model integration. You have to remove the “include”-command and use the hard-wired definition. Adapt the Makefile.m and main.mk and compile it.

2) Edit the wrapper-script strato3bud.tcsh:
- set the experiment name (exp_name) to name the output file(s)
- set data path (datapath) to your (monthly !) data file(s)
- set the path to the executable (exepath) strato3bud.exe
- modify the loops for year and month according to your needs

The script creates a local link (tr_O3_sbud.nc) for input and processes an output file (stratO3bud.nc), which is renamed to ${exp_name}_stratO3bud_${year}${month}.nc.

Important notes:

The script eqn2f90.tcsh extracts the required reaction coefficients automatically from mecca.eqn (see above). If something goes wrong, the chance is high that this script is the cause. It it highly suggested to check manually the rate_coeff.inc.

Reference:

Jöckel, P., Kerkweg, A., Pozzer, A., Sander, R., Tost, H., Riede, H., Baumgaertner, A., Gromov, S., & Kern, B.: Development cycle 2 of the Modular Earth Submodel System (MESSy2), Geoscientific Model Development, 3, 717–752, doi: 10.5194/gmd-3-717-2010, URL http://www.geosci-model-dev.net/3/717/2010/ (2010).