How to Install Run the SOCRATES Model

The following is an update of a guide to running SOCRATES, written by Rashid Khosravi in March, 2001 and updated by Anne Smith in 2006. It is intended to serve as a step by step guide on how to download, run, and view results of the NCAR 2-D model SOCRATES. This model was originally developed by Guy Brasseur and it has been improved and enhanced by several people over many years. The version of the model that is described here is the most recent (developed 1999-2001) and is called socrates3.

For detailed description of the physics, chemistry, I/O structure of the model, references and other pertinent information, see the file SOCRATES_description.pdf on this website:

https://cdp.ucar.edu/browse.do?uri=http://dataportal.ucar.edu/metadata/acd/software/Socrates/Socrates.thredds.xml

Downloading and Running the Model

To download the model fortran code, click on the link socrates3_updated.tar.gz from the above website. This is a tar file (~6 MB) containing all the model source code, a Makefile, all the data files, and a UNIX script to run the model. (Note: socrates_ver3.tar.gz is an older version that is very similar except that it has a few minor problems running on our computers.) To expand (untar) the file, do the following:

```
gtar xpzf socrates3.tar.gz
```

This will create the following directories and subdirectories:

```
socrates3/data
socrates3/in
socrates3/out/log
socrates3/out/divar
socrates3/out/save
socrates3/out/arch
socrates3/save
socrates3/src
```

The sample input file for a 10-year baseline atmosphere run is in the ‘in’ directory, and the script file to run this case is called runsoc and is in the main directory (socrates3). To make (using Makefile in ./src) and run the model, do the following

```
runsoc
```

This will create a log file of the run in the ./out/log directory, with the results in the output file (netCDF format) archived to ./out/arch.

For reference, a 10-year baseline-atmosphere output file that was run using socrates_ver3.tar.gz on a Linux workstation is also provided on the above website (arch.10yr.base.nc). This is a large binary file (~226 MB) that contains output for every month of the 10-year simulation. There may be small differences (a few percent) between this output and results from the more recent version.

Note that the Makefile provided in the 'src' directory is specific to the Linux operating system and Portland group fortran90 compiler. It should therefore be modified appropriately if the model is to be run on a different platform.

NOTE: It is highly recommended that after successfully downloading and making the model on your platform, a test case of the baseline atmosphere be run and the results compared with the above reference output. The test case does not need to be run for 10 years; for a quick test, it can be run for 1 month. See the 'Model Description' document for help with setting up the input file to specify the length of integration (with the parameter 'simulation end time') and the output dates or frequency. Some small numerical differences between your test baseline and the reference model should be expected.

Stability, Bugs, Portability, Etc.

The model has been stabilized numerically to a large extent so that running the baseline atmosphere case and the simulations described in the manuscripts listed below should proceed smoothly. However, it is possible that changing some constants or parameters in the model or making modifications such as changing some parts of the algorithm may cause the model to crash because of numerical instability in the overall algorithm that solves the thermodynamic equation for temperature (T). We have spent a lot of time trying to solve this problem but it has proven very difficult to do so. The region of the atmosphere where it occurs is usually the mesosphere, where numerical instability might cause T to be negative. It may help to make the desired change in increments to avoid this problem.

Generally the code is working well and no known bugs exist. However, this is not an "official" release of a software product. That is, no formal effort has been made to debug and/or test the code systematically according to software engineering principles. It is requested that any bugs or errors that are found be reported to Anne Smith (aksmith@ucar.edu). Also, even though most of the code is written in FORTRAN90, no formal effort has been made to make the code portable across all possible platforms. Any portability issues that may arise should be addressed by the user, but we encourage reporting these issues and their solutions to us.

Model Evaluation

Although we have not formally validated the version of the model released here, we have evaluated it and the model fields generally compare well with measured fields; they capture the features found in the observed atmosphere to within measurement uncertainties. See below for journal articles and other documents that present results from socrates3.

How to View the Results

A GUI program to view the model output (archive and diurnal variation) is provided on the website (view2d.tar.gz). The application is called 'view2d' and is written in IDL. To use the viewer, create a directory view2d, copy the tar file to that directory and untar using the following:

gtar xpzf view2d.tar.gz

Then edit the file 'preferences.pro' to change the I/O pathnames according to your setup. To run the program, run IDL and then type 'view2d'. The program will prompt you to select a directory from which to load a SOCRATES output file.

The application is generally intuitive and is easy to learn by playing with it. Also see the included files: README.txt, USAGE.txt, and BUGS.txt.

Publications and Documents Using SOCRATES 3

Huang, T. et al., *Description of SOCRATES – A Chemical Dynamical Radiative Two-Dimensional Model*, NCAR Technical Note, 1998.

Brasseur, G. P., A. K. Smith, R. Khosravi, T. Huang, and S. Walters, Natural and human-induced perturbations in the middle atmosphere: A short tutorial, in *Atmospheric Science Across the Stratopause,* edited by D. E. Siskind, S. D. Eckermann and M. E. Summers, pp. 7-20, 2000.

Chabrillat, S., *Modélisation du Changement Global dans L'Atmosphere Moyenne*, PhD thesis, Université Libre de Bruxelles, 2001.

Khosravi, R., G. Brasseur, A. Smith, D. Rusch, S. Walters, S. Chabrillat, and G. Kockarts, Response of the mesosphere to human-induced perturbations and solar variability calculated by a 2-D model, *J. Geophys. Res., 107*(D18), 4358, doi:10.1029/2001JD001235, 2002.

Chabrillat, S., G. Kockarts, D. Fonteyn, and G. Brasseur, Impact of molecular diffusion on the CO_2 distribution and the temperature in the mesosphere, *Geophys. Res. Lett.*, 29, doi:10.1029/2002GL015309, 2002.

Lee, H. and A. K. Smith, Simulation of the combined effects of solar cycle, QBO, and volcanic forcing on the stratospheric ozone changes in recent decades, *J. Geophys. Res., 108*(D2), 4049, doi:10.1029/2001JD001503, 2003.

Smith, A. K., Physics and chemistry of the mesopause region, *J. Atmos. Solar-Terr. Phys., 66,* 839-857, 2004.