MEGAN version 2.10 User's Guide

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1 Introduction

1.1 How to use this document

This guide instructs both novice and experienced users on building and running MEGAN for climate and air quality applications. If you are a new user, we recommend that the introductory sections be read before moving onto other sections. This document is written so, as much as possible, individual sections stand on their own and the user's guide can be scanned and sections read in a relatively ad hoc order. In addition, the web version provides clickable links that tie different sections together and links to different processors and libraries that are required to run MEGAN 2.10.

Throughout the document, this presentation style indicates shell commands and options, fragments of code, namelist variables, etc. Where examples from an interactive shell session are presented, lines starting with ">" indicate the shell prompt.

Please feel free to provide feedback to MEGAN 2.10 about how to improve the documentation.

1.2 MEGAN Overview

The Model of Emissions of Gases and Aerosols from Nature (MEGAN) is a global emission model for estimating the net emission of gases and aerosols from terrestrial ecosystems into the atmosphere (Guenther et al., 2006, Sakulyanontvittaya et al. 2008, Millet et al. 2010, Stavrakou et al. 2011, Guenther et al., inreview). MEGAN is designed for both global and regional emissions modeling and has global coverage with 1km^2 or less spatial resolution. It can be also run at user defined spatial resolution. MEGAN is a semi-mechanistic model that accounts for the major known processes controlling biogenic emissions. MEGAN estimates only emissions of known compounds and includes additional compounds whenever they are identified as being of potential interest for the atmosphere. Emissions of 150 chemical species are included in MEGANv2.1 and the model can output individual compounds or categories associated with various atmospheric chemistry schemes. The 150 compounds are lumped into 20 categories based on how emissions vary in response to changes in environmental conditions. Emission variations are first estimated for the 20 categories and then speciated into the 150 compounds or output in chemical categories associated with common atmospheric chemistry schemes (e.g., CB4, CB05, CB6, SAPRC99, MOZART, SOAX). Driving variables include land cover, weather, and atmospheric chemical composition. The MEGAN code and input files are available at no cost. User's Guides, models and input files are provided at http://lar.wsu.edu/megan/guides.html MEGANv2.1 accepts PFT/LAI/EF MAP data in ASCII format and meteorological data in netcdf/ioapi format. The native outputs are in netcdf/ioapi format. The UAM-CAMx emission 2D format is optional with conversion processor. MEGAN can be run on a number of

32bit or 64bit LINUX/Unix operating system. Users may need to make changes in compliers and environmental settings to get it run on their own machines.

MEGAN was originally written as an ACCESS-VBA code by Alex Guenther. Jack Chen (Washington State University- now at NRC-Canada) developed the initial FORTRAN framework and I/O formats for MEGAN version 1.0. MEGAN Versions 2.00 to 2.04 were written in FORTRAN by Tanarit Sakulyanontvittaya (University of Colorado-now at ENVIRON). MEGAN version 2.10 was written by Xuemei Wang (Sun-Yat Sen University) and Tan Sakulyanontvittaya (ENVIRON).

1.2.1 MEGAN Software / Operating System Prerequisites

It should be noted that running this version of MEGAN requires both access to and knowledge of a LINUX/UNIX operating system and working knowledge of FORTRAN. Users who have never been exposed to Unix-type operating systems (i.e., if you are only familiar with Windows) unfortunately will find it difficult to run MEGAN. Although you do not need to be a computer programmer to run the model, you should have a basic understanding of computer programming and Unix (i.e., you should know how to unzip/untar files and other basic commands in Unix, install libraries and link files within Unix, and know basic FORTRAN commands such as how to invoke a code). If you need to regrid the MEGAN input files then you will also need either 1) knowledge/access to Python computer language and ESRI ArcMAP software or 2) use a FORTRAN based preprossor for regridding the input files. In summary, you should have a working knowledge of Unix and FORTRAN (and possibly ArcMap and Python for regridding input files) before attempting to use MEGAN.

The following are the system and software requirements for installing and running MEGAN 2.10:

- LINUX/UNIX operating system
- csh/sh scripting language
- FORTRAN 90 compiler, i.e. pgi
- It can only be run on a single processor, no MPI support
- Netcdf 3.6.0 or greater
- ioapi 3.1
- MCIP 3.6

It has been successfully tested on GNU/Linux x86_64 machine with PGI compiler.
The provided test case was also created on GNU/Linux x86_64 machine.

1.3 Downloading MEGAN2.10

1.3.1 Downloading the code and scripts

The latest version of User's Guide and MEGAN model, and input data files can be downloaded at http://lar.wsu.edu/megan/guides.html

1.3.2 Downloading required libraries and packages

netcdf 3.6.0 or greater can be downloaded at
http://www.unidata.ucar.edu/downloads/netcdf/index.jsp
ioapi 3.1 and MCIP 3.6 can be downloaded at
http://www.cmascenter.org/
Users will need to register before downloading these packages and user's guide for them. Users are highly recommended to refer to their user's guide for installing the packages.

You may also find the following links useful:

- FORTRAN tutorial: http://www.cisl.ucar.edu/tcg/consweb/Fortran90/F90Tutorial/tutorial.html
- UNIX tutorial: http://www.ee.surrey.ac.uk/Teaching/Unix/
- ArcGIS: http://www.esri.com/software/arcgis/index.html
- Python tutorials: http://python.org/

Below, we will provide a brief description about how to install and use these libraries and packages.

1.3.3 Downloading input data files and test case

Input datasets are needed to run the model. Input files for LAI, PFT and emission factors (EF) can be downloaded at http://lar.wsu.edu/megan/guides.html

A test case with these files and weather data can also be downloaded from this site. If users want to run the model for different time periods and at different spatial resolutions, they will need to use the input preprocessor, MCIP, and WRF/MM5 output to generate input files for MEGAN. A preprocessor using ArcGIS and FORTRAN to process LAI, PFT, and EF input files are also provided at the website.

2 Software Installation

2.1 Introduction

The MEGAN modeling system software installation is fairly straightforward on the supported platforms (i.e., GNU Linux). After you download the required libraries and packages following the above-provided links, you can refer to the simple steps listed below to install them. Installing MEGAN requires you to first install netcdf and ioapi libraries.

2.2 Installing libraries

2.2.1 Installing netcdf

There are two ways to install netcdf on LINUX/UNIX. One is to install the pre-built binary package. If you use pre-built netcdf, make sure you download the correct version for your operating system. The other is to install it from a tar.gz file.

Once you download it, untar it and go to the netcdf directory.
Type the following commands:

```
>./configure --prefix=/usr/bin/local
>make check install
```

Once the netcdf is installed, you need to set your environmental variables to the location where you installed it.

```
>setenv NETCDF path-to-netcdf-library
```

Please refer to the link below for the details about how to install the netcdf.
http://www.unidata.ucar.edu/software/netcdf/docs/netcdf-install/

2.2.2 Installing ioapi

Please refer to this link http://www.baronams.com/products/ioapi/AVAIL.html for installing ioapi 3.1.

2.3 Building the MEGAN2.10 code

- Unzip and untar the MEGAN code you downloaded from the MEGAN website,

```
>gunzip MEGANv2.10.tar.gz
> tar -xf MEGANv2.10.tar
```

it will create a MEGANv2.10 directory. This contains:

```
bin/            Directory for executable files linking to
                the locations where the files are.
Input/          Directory for input files including MAP
                (LAI, PFT, and EF), MET (weather), and PAR
                (radiation).
Output/         Directory for output files.
setcase.csh     Script to set up MEGAN environmental
                variables.
src/            Directory for main routines, Makefiles, and
                all executables after compilation. It
                includes five folders for different
                components of MEGAN.
work/           Directory for running the model, modeling
                domain information, and output log files.
```

- Go to MEGANv2.10 and make changes in `setcase.csh`.

```
>cd MEGANv2.10
```

The only thing you need to change is MGNHOME environmental variable. Reset the location of the MEGAN model in your computer:

```
setenv MGNHOME /data/home/MEGAN/MEGANv2.10
```

- Go to src directory and makes changes in `make_all_programs.scr`. This file is used to compile all MEGAN FORTRAN code files. Reset the location for `setcase.csh`:

```
source /data/home/MEGAN/MEGANv2.10/setcase.csh
```

- Under src/, you will see five sub-directories, which are different components of the MEGAN model.

```
TXT2IOAPI/      Directory for converting comma delimited
                line input (LAI, PFT, and EF) to gridded
                netCDF-IOAPI format.
MET2MGN/        Directory for converting IO/API files with
                various meteorological variables to the
                format that can be read by MEGAN
EMPROC/         Directory for computing MEGAN biogenic
                emissions using input data generated by
                TXT2IOAPI and MET2MGN
MGN2MECH/       Directory for doing chemical speciation and
                MECHANISM conversion using MEGAN output.
IOAPI2UAM/
```

- Go to each of the five sub-directories to make changes in `Makefile.*.32bit/64bit` to set up new LIBS and INCLUDE locations. You may also need to change FC to the FORTRAN you are using. The default is pgf90. You will need to know if your machine is 32 bit or 64 bit before you go to the next step.

- Go back to src/ directory, and run the following command to build the MEGAN model if you are using a 32 bit machine. If you are using a 64 bit machine, you need to change 32 to 64.

```
> ./make_all_programs.scr 32bit
```

- After a successful compilation, you should have executables (`txt2ioapi, met2mgn, emproc, mgn2mech, and ioapi2uam`) created in the five sub-directories listed above under /MEGANv2.10/src. Now you have built MEGAN 2.10 and are ready to run it.

3 Weather Data Preprocessing (MET and PAR)

3.1 WRF/MM5 MET and PAR data

3.1.1 Installing the MCIP

Untar mcip_v3.6.tar.gz downloaded from http://www.cmascenter.org/
Go to src directory to make changes in Makefile to include correct paths for

```
NETCDF
IOAPI_ROOT
FC
LIBS
```

Type "`make`" to compile all the programs. After a successful compilation, you should see a file named "`mcip.exe`".

3.1.2 Obtaining MCIP weather input files

MCIP input meteorology files can be from WRF or MM5 output. You need to run WRF or MM5 to generate some input files.

3.1.3 Running the MCIP

Go to /`MCIP3.6/`, and make changes in `run.mcip` to include your meteorology files generated by WRF or MM5. WRF output files include `wrfout* and geo_em_d01.nc` (Terrain information). MM5 output files include `MMOUT_DOMAIN* and TERRAIN_DOMAIN*`

3.2 Satellite PAR data

MEGAN users have used satellite data (http://www.atmos.umd.edu/~srb/gcip/) to generate PAR inputs for MEGAN. Contact Tan Sakulyanontvittaya (tsakuly@environcorp.com) for more information.

3.3 Other MET and PAR data

MET and PAR data from other sources can be used to run MEGAN. For example, MEGAN users have used RAMS model output to generate MET and PAR inputs for MEGAN. Other data, including observations, could be used to run MEGAN but you will need to develop a preprocessor to convert these data into the format required for MEGAN.

4 Landcover Data Preprocessing (LAI, PFT, and EF)

4.1 Landcover data FORTRAN preprocessor

A FORTRAN based Landcover preprocessor is available for regridding the input data for a specific model domain.

4.2 Landcover data ArcGIS preprocessor

Landcover (LAI, PFT, and EF) input data can be regridded for a specific model domain using ArcGIS and python.

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5 Running MEGAN2.10

The scripts for running the MEGAN model are located under `/MEGANv2.10/work`. Before you execute the following steps, make sure you have a GRIDDESC file located under this directory. This file is generated by MCIP, including projection and domain information for your input files. A sample file is provided under this directory.

You can run the model by following the steps listed below:
1). Make changes in `run.txt2ioapi.v210.csh` to include `setcase.csh` and landcover input files generated in **Section 4**.
Execute the following command to convert csv format landcover data to ioapi format

```
>./run.txt2ioapi.v210.csh
```

2). Make changes in `run.met2mgn.v210.csh` to include `setcase.csh`, MCIP output files, and start and end dates of your case. You will also need to change "`GDNAM3D`" variable to be consistent with your MCIP output files.
Execute the following command to convert MCIP output files to MEGAN ioapi format.

```
>./run.met2mgn.v210.csh
```

3). Make changes as you did for 2). , and then execute the following command to run MEGAN2.10. It may take a while to finish running the model, depending on the length of your simulation and the domain size.

```
>./run.emproc.v210.csh
```

4). Make changes as you did for 2)., and then execute the following command to convert MEGAN species to other speciation profiles. There are nine mechanisms that you can convert MEGAN species to by running this script.

```
>./run.mgn2mech.v210.csh
```

5). The following command can be used to convert 1-D emissions files (I/O API) to CAMx low-level emissions files (UAM-IV).

```
>./run.ioapi2uam.csh
```

You can check your MEGAN output files under `/MEGANv2.10/Output`.
All the log files for running these scripts are under `/MEGANv2.10/work/logdir`.

6 Post-processing

Various techniques and tools are available for displaying MEGAN output data including NCL, ArcGIS, and IDL. Any tools that are capable of displaying the ioapi or UAM-CAMx 2D emission data format can be used for this purpose.

7 MEGAN Publications

- Guenther et al., J. Geophys. Res., 104, 30625-30639, 1999: This manuscript describes the canopy environment model used in MEGAN.
- Guenther et al., ACP 6, 3181-3210 (2006). Also read the Corrigendum which corrects typographical errors in some equations. This manuscript describes MEGAN isoprene emission algorithms, emission factors and landcover data.
- Guenther et al., Geosci. Model Dev., in review, 2012: This manuscript describes new updates for MEGANv2.10.
- Helmig, D., J. Ortega, T. Duhl, D. Tanner, A. Guenther, P. Harley, C. Wiedinmyer, J. Milford, T. Sakulyanontvittaya, Sesquiterpene emissions from pine trees- Identifications, emission rates and flux estimates for the contiguous United States, Environ. Sci. Tech., 41, 1545-1553, 2007. This manuscript describes regional sesquiterpene distributions estimated using MEGAN.
- Ortega, J., D. Helmig, A. Guenther, P. Harley, S. Pressley, and Christoph Vogel, Flux estimates and OH reaction potential of reactive biogenic volatile organic compounds (BVOCs) from a mixed northern hardwood forest, Atmos. Environ., 41, 5479-5495, 2007. This manuscript describes an application of a canopy scale version of MEGAN.
- Donkelaar, A., R. Martin, R. Park, C. Heald, T.-M. Fu, A. Guenther, Model evidence for a significant source of secondary organic aerosol from isoprene, *Atmospheric Environment* , 41, 1267-1274, 2007. MEGAN used to estimate biogenic VOC emissions.
- Guenther et al. Atmospheric Environment (in preparation for Atmos. Environ 50th anniversary special issue). This manuscript describes MEGAN emission algorithms and emission factors for compounds other than isoprene.

- Sakulyanontvittaya et al. Environ. Science and Technology, 42, 1623-1629, 2008. This manuscript investigates the sensitivity of MEGAN emission estimates to the monoterpene and sesquiterpene parameters.
- Stavrakou, T., A. Guenther, A. Razavi, L. Clarisse, C. Clerbaux, P. F. Coheur, D. Hurtmans, F. Karagulian, M. De Mazière, C. Vigouroux, C. Amelynck, N. Schoon, Q. Laffineur, B. Heinesch, M. Aubinet, C. Rinsland & J. F. Müller (2011) First space-based derivation of the global atmospheric methanol emission fluxes. *Atmos. Chem. Phys.,* 11**,** 4873-4898.
- Millet, D. B., A. Guenther, D. A. Siegel, N. B. Nelson, H. B. Singh, J. A. de Gouw, C. Warneke, J. Williams, G. Eerdekens, V. Sinha, T. Karl, F. Flocke, E. Apel, D. D. Riemer, P. I. Palmer & M. Barkley (2010) Global atmospheric budget of acetaldehyde: 3-D model analysis and constraints from in-situ and satellite observations. *Atmos. Chem. Phys.,* 10**,** 3405-3425.
- Heald, C. L., M. J. Wilkinson, R. K. Monson, C. A. Alo, G. L. Wang & A. Guenther (2009) Response of isoprene emission to ambient CO2 changes and implications for global budgets. *Global Change Biology,* 15**,** 1127-1140.