MEGAN version3 User's Guide

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The latest version of this guide and any updates to the code and input data availability are described at https://sites.google.com/uci.edu/bai/megan.

The Model of Emissions of Gases and Aerosols from Nature version 3 (MEGAN3) modeling system shown in Figure 1 was developed to estimate time series of local, regional and global geogridded estimates of biogenic emissions. The MEGAN modeling system consists of three main components:

- Input Data (CSV and NETCDF) and pre-processor (FORTRAN code)
- MEGAN Emission Factor Processor (python code)
- MEGAN Emission Estimator (FORTRAN code)

This document describes the MEGAN3 Emission Estimator code. Additional User guides are available for the MEGAN data portal/pre-processor and the MEGAN Emission Factor Processor.

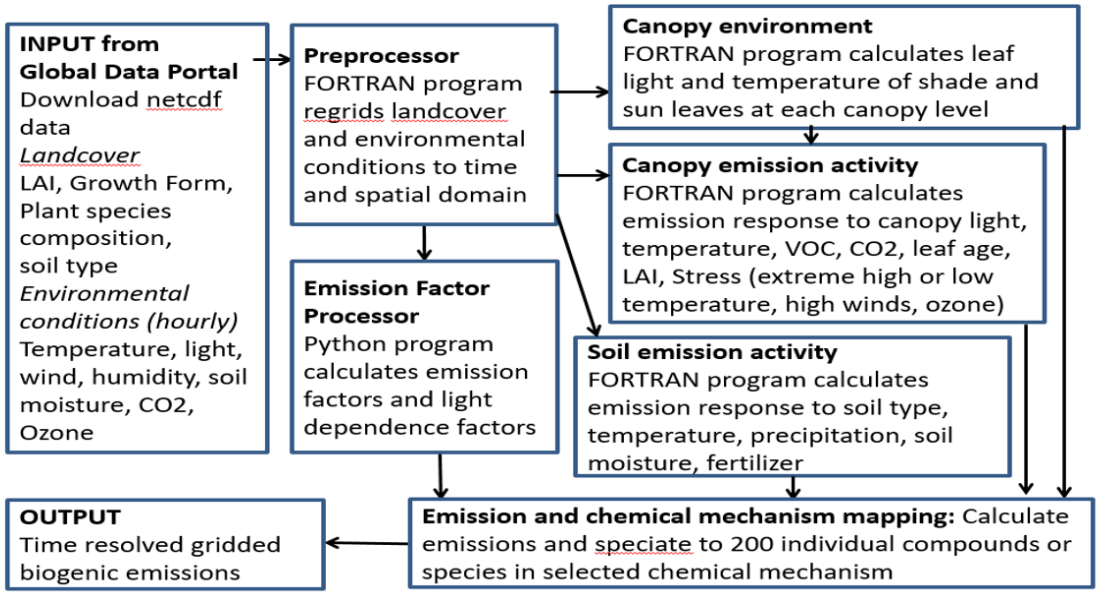

Figure 1. Schematic of the MEGAN3 modeling system.

MEGAN3 Data Portal and Preprocessor: Data sets required to drive MEGAN3 and MEGAN3EFP are provided in the MEGAN3 data portal. FORTRAN code for regridding the base data to provide the average values for each location within a user specified grid is also provided. Guidance for using MEGAN3 base data and regridding is given in the MEGAN3 Data Portal and Preprocessor User Guide.

MEGAN3 Emission Factor Processor (MEGAN3EFP): MEGAN3 driving variables includes estimates of emission factors (EF) and light dependence factors (LDF) for each of the 20

MEGAN3 emission categories (e.g., isoprene, monoterpene type 1, carbon monoxide, etc.) for each location in a model domain. The MEGAN3EFP generates these geogridded EF and LDF inputs using procedures described in this document (the MEGAN 3.0 Emission Factor Processor User Guide). The MEGAN3EFP also compiles lists of vegetation specific emission factors and light dependence factors that can be used for assessing the values used in a MEGAN3 simulation.

MEGAN3: This is a FORTRAN code that inputs driving variables and outputs biogenic emission rates. Guidance for running MEGAN3 simulations is given in the MEGAN3 Users 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 MEGAN3 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.

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.

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, Guenther et al., 2012). Emissions of reactive gases and particles from terrestrial ecosystems ("biogenics") drive atmospheric distributions of several constituents relevant for air quality and climate. Biogenic emissions tend to be highly variable and can vary more than an order of magnitude over spatial scales of a few kilometers and time scales of less than a day. This makes estimation of these emissions especially challenging and yet accurate quantification and simulation of these fluxes is a necessary step towards developing strategies for mitigating air pollution and climate change.

The MEGAN framework calculates biogenic emissions as the product of an emission factor, that represents the capacity of a vegetation type to emit a compound, and an emission activity factor that accounts for the response to environmental conditions. 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 uses simple mechanistic algorithms to represent the response of emissions to the major controlling variables. Emissions of 201 chemical species are included in MEGAN3 and the model can output individual compounds or categories associated with various atmospheric chemistry schemes. The 201 compounds are lumped into 20 categories based on emissions responses to changes in environmental conditions. Emission variations are first estimated for the 20 categories and then speciated into the 201 compounds or output in chemical categories associated with common atmospheric chemistry schemes (e.g., CB05, CB6, CBMZ, S07, RACM, CRIv2-R5). 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 available for download at https://sites.google.com/uci.edu/bai/megan.

MEGAN3 inputs and intermediate files are in either ASCII or netcdf format. The native outputs are in netcdf/ioapi format. 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.

MEGANv0 was originally written as an ACCESS/VBA code by Alex Guenther in 2002. Jack Chen wrote the initial FORTRAN framework and I/O formats for MEGAN version 1.0. This framework was extended to MEGANV2 (and v2.04) by Alex Guenther in 2005 and the FORTRAN code written by Tanarit Sakulyanontvittaya. MEGAN version 2.10 was developed by Alex Guenther in 2010 with the FORTRAN code written by Xuemei Wang and Tan Sakulyanontvittaya. MEGAN3 framework was developed by Alex Guenther in 2016 and the FORTRAN code was written by Ling Huang.

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). In summary, you should have a working knowledge of Unix and FORTRAN before attempting to use MEGAN.

The following are the system and software requirements for installing and running MEGAN 3:

- 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 MEGAN3

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

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/

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. Information for doing this is found in the MEGAN Data and Preprocessor Guide.

A test case with these files and weather data can also be downloaded from the MEGAN website (https://sites.google.com/uci.edu/bai/megan). 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.

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 MEGAN3 code

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

```
>gunzip MEGANv3.tar.gz
> tar -xf MEGANv3.tar
```

it will create a MEGAN3 directory. This contains:

```
bin/            Directory for executable files linking to
                the locations where the files are.
Input/          Directory for input files including MAP
                (LAI, CT, EF, LDF, and W126 (optional)),
                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 MEGAN3 and make changes in `setcase.csh`.

```
>cd MEGAN3
```

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/MEGAN3
```

- 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/MEGAN3/setcase.csh
```

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

```
TXT2IOAPI/      Directory for converting comma delimited
                line input (LAI, CT, EF, LDF, and W126
                (optional))  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
DAYMET/         Directory for calculating daily
                meteorological variables that will be
                used by MEGVEA
MEGCAN/         Directory for converting above-canopy
                meteorology to within-canopy
                meteorology that will be used by MEGVEA
MEGSEA/         Directory for calculating soil moisture
                activity factor and soil NO emission
                activity factor
MEGVEA/         Directory for calculating various
                emission activity factors
MGN2MECH/       Directory for doing chemical speciation and
                MECHANISM conversion using MEGAN output.
IOAPI2UAM/      Directory for converting IO/API output
                files to CAMx low-level emission files
```

- Go to each of the eight 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, daymet, megcan, megsea, megvea, mgn2mech, and ioapi2uam`) created in the eight sub-directories listed above under /MEGANv3/src. Now you have built MEGAN3 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 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, CT, EF, LDF, and W126 (optional))

4.1 Landcover data FORTRAN preprocessor

A FORTRAN based Landcover preprocessor is available for regridding the input data for a specific model domain. The code and user guide are available at https://sites.google.com/uci.edu/bai/megan

4.2 Landcover data ArcGIS preprocessor

Some users may prefer to regrid the landcover (LAI, CT, EF, LDF and W126) input data for a specific model domain using a GIS program such as ArcGIS with python code (https://www.arcgis.com/).

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5 Running MEGAN3

The scripts for running the MEGAN model are located under `/MEGANv3/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.v3.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.v3.csh
```

Preparing/converting W126 data is optional. If user does not want to enable air quality-induced emission stress, you do not need to prepare W126 input data.

2). Make changes in `run.met2mgn.v3.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.v3.csh
```

3). Make changes as you did for 2). , and then execute the following command to generate daily meteorological variables. You will need to specify the start date and length of your simulation episode in the run script below.

```
>./run.daymet.v3.csh
```

4). Make changes as you did for 2)., and then execute the following command to

calculate soil moisture activity factor and soil NO emission activity factor.

```
>./run.megsea.v3.csh
```

5). Make changes as you did for 2)., and then execute the following command to convert above-canopy meteorology to within-canopy meteorology. If you wish to use alternative canopy model to generate within-canopy meteorology, you do not need to run this step. But you will need to prepare input files that have all the variables (e.g. SunleafTK, SunPPFD, etc.) that MEGAN3 needs.

```
>./run.megcan.v3.csh
```

6). Make changes as you did for 2)., and then execute the following command to run MEGAN3. It may take a while to finish running the model, depending on the length of your simulation and the domain size. User can specify which stress factors (e.g. air quality stress, high/low temperature stress, high wind stress, etc.) to include. Make sure you provide necessary input file if you enable specific stress factors.

```
>./run.megvea.v3.csh
```

7). Make changes as you did for 2)., and then execute the following command to convert MEGAN species to other speciation profiles. You can choose any one of fourteen chemical mechanisms to convert MEGAN species to by running this script.

```
>./run.mgn2mech.v3.csh
```

8). 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 `/MEGANv3/Output`. All the log files for running these scripts are under `/MEGANv3/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.