Technical report

Biogenic VOC Emission Model GIS-BEM

University of Aveiro,

May, 2013

Ref. AMB-QA-01/2013

User's Guide to the GIS Version of Biogenic VOC Emission Model (GIS-BEM)

Version 1.1

Contributors:

Oxana Tchepel, Carlos Silveira, Joana Ferreira, Carlos Borrego

CESAM - Centre for Environmental and Marine Studies

Department of Environment and Planning

University of Aveiro

3810-193 Aveiro

Portugal

Reference:

AMB-QA-01/2013

Acknowledgements:

The Portuguese Foundation for Science and Technology (FCT) is acknowledged for the financial support of the project EMOSAT (PTDC/CTE-ATM/103253/2008, FCOMP-01-0124-FEDER-009305).

May, 2013

Contents

1. Introduction

Volatile organic compounds (VOC) are originated by anthropogenic and biogenic sources, and play an important role in atmospheric chemistry contributing to tropospheric ozone and secondary organic aerosol formation (Griffin et al., 1999; Kanakidou et al., 2005; Curci et al., 2009). On the global scale, the vegetation generates over 90% of VOC emissions (Guenther et al., 1995), and the isoprene is emphasized as the most abundant and highly reactive (Pacifico et al., 2009; Arneth et al., 2007). The emitted amount of biogenic VOC depends on interaction of environmental, biological, physical and chemical processes. However, direct measurements of VOC emissions are still scarce or absent for most ecosystems and vegetation types. In this context, modeling approaches able to quantify biogenic VOC emissions and to characterize their spatial and temporal variations are arising starting from leaf-level (Wilkinson et al., 2009; Niinemets et al., 1999) to the global scale models (Guenther et al., 2006). Using these tools, the quantification of the emissions for each type of vegetation may be performed based on definition of specific emission capacity under standardized conditions (standard temperature and light) and their further corrections for the actual environmental conditions.

2. GIS-BEM Overview

The GIS-BEM modeling system is an application developed in geographic information system (GIS) environment that allows users to estimate emissions of volatile organic compounds from biogenic sources (BVOC), namely isoprene and monoterpenes. Emissions are calculated on hourly basis, but the model is able to provide daily emission outputs. The use of GIS platforms has the advantage to provide greater flexibility in handling and analysis of input and output data. The implemented approach integrates a simple conceptual model adopted from several authors (Guenther et al., 1995, 2006; Oderbolz et al., 2013; Simpson et al., 1995) and based on empirical algorithms. Thus, the net emission of a compound from terrestrial ecosystems into the above-canopy atmosphere at a specific location and time is given as:

$$E = \varepsilon . M_A . [\gamma_L . LDF + (1 - LDF)] . \gamma_T . \gamma_{LAI} . \gamma_{NDVI} \quad (1)$$

Where:

E - Net emission of a compound [µg.m^{-2}.h^{-1}]

ε - Emission factor at standard conditions [µg.g^{-1}.h^{-1}]

M_A - Dry leaves mass per area unit [g.m^{-2}]

γ_L - Light correction factor

LDF - Light dependence fraction

γ_T - Temperature correction factor

γ_{LAI} - LAI correction factor

γ_{NDVI} - NDVI correction factor

More details on theoretical basis considered for the model are presented in Appendix A. A general concept of the modelling system is presented in Figure 1.

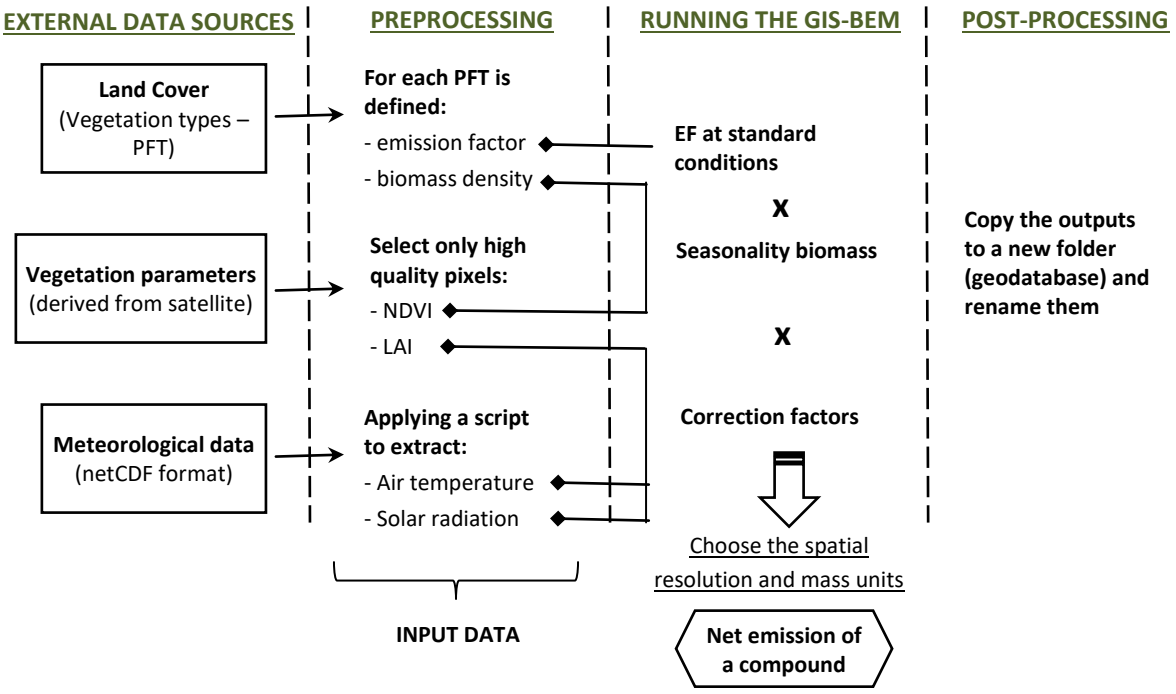

Figure 1. GIS-BEM modelling system flowchart.

3. Input data

The BVOC emission quantification requires several inputs, including land cover, vegetation parameters and meteorological data. For land cover, distribution maps of vegetation types are required, corresponding to each tree species or species group, a plant functional type (PFT). For each PFT, the specific emission rate under standard conditions (temperature=30ºC, PAR=1000 µmol.m^{-2}.s^{-1}) and the foliar biomass density

have to be defined. To characterize vegetation dynamics, satellite-derived products, specifically the Normalized Difference Vegetation Index (NDVI) and Leaf Area Index (LAI) are considered by the model. Thus, maximum-value composite images over several days are usually considered. Also the influence of meteorological variables, ambient air temperature and photosynthetically active radiation (PAR, represents a fraction of incoming solar radiation available to photosynthesis), is taken into account to correct the emissions to the current environmental conditions. The model is tested with the data provided by the Weather Research and Forecasting prognostic model (WRF). However, the outputs from this model generate very large files and to overcome this limitation, a script in python to extract only the needed variables must be applied (see Appendix B).

Before running the GIS-BEM, the following input data should be prepared for the study domain:

a) Emission factors

- A regular grid with emission factors for isoprene
- A regular grid with emission factors for monoterpenes
- Units required: [µg C. g^{-1}. h^{-1}]
- Data format: raster dataset

b) Biomass density

- A regular grid with the biomass density
- Units required: [g. m^{-2}]
- Data format: raster dataset

c) NDVI

- A regular grid with the actual NDVI
- A regular grid with the multiyear maximum NDVI
- Units required: dimensionless
- Data format: raster dataset

d) LAI

- A regular grid with the LAI
- Units required: dimensionless
- Data format: raster dataset

e) Meteorological data

- A file in NetCDF format that contains the ambient air temperature and incoming solar radiation.
- Units required: temperature [K], solar radiation [W. m^{-2}]
- Temporal resolution: hourly

All input data should be in the same geographic reference system, and whenever possible, one should choose fine resolution data in order to decrease the uncertainty sources in BVOC emission modelling. However, higher resolutions lead to an increase of the processing time to generate model outcomes.

4. Model requirements

4.1. Support software

ESRI ArcGIS software, version 10.0, is the GIS platform used to run GIS-BEM. To work with this model, basic knowledge on the ArcGIS software is required.

4.2. Installing the GIS-BEM

Inside the ArcToolbox window, right click on the empty space, choose “Add Toolbox”, and then browse to the GIS-BEM Toolbox and click “Open” (Figure 2).

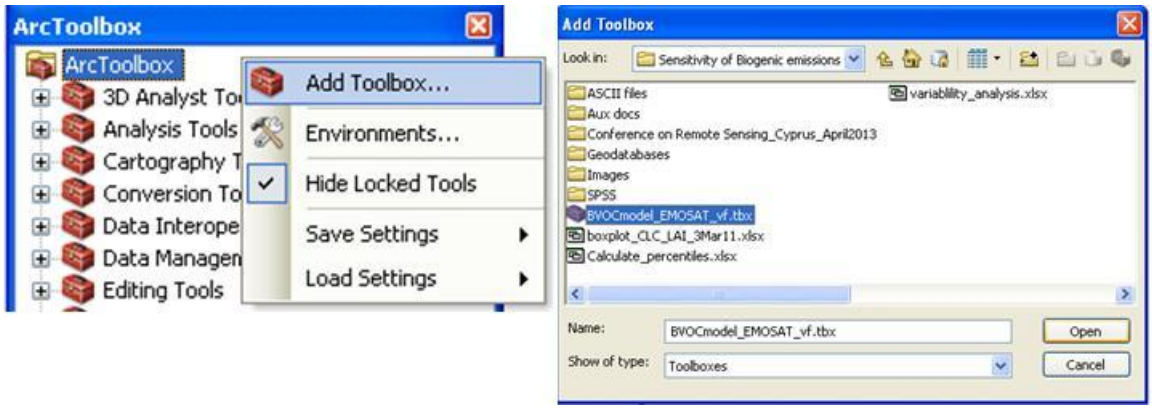

Figure 2. Procedures to install the GIS-BEM Toolbox.

4.3. Model structure and graphic interface

The Toolbox is structured in 4 modules, from which the separation in biogenic compounds and temporal resolution is performed (Figure 3).

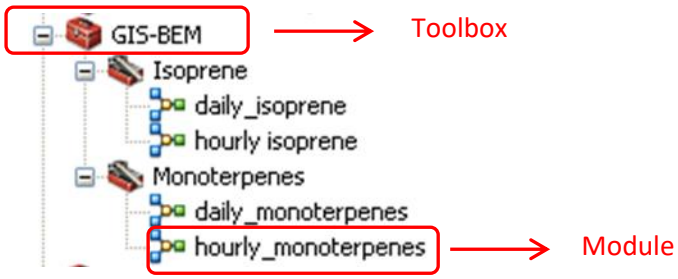

Figure 3. GIS-BEM Toolbox.

The modules that integrate the GIS-BEM Toolbox are:

Module 1 - *"hourly_isoprene"*: estimating hourly isoprene emissions.
Module 2 - *"daily_isoprene"*: estimating daily isoprene emissions.
Module 3 - *"hourly_monoterpenes"*: estimating hourly monoterpene emissions.
Module 4 - *"daily_monoterpenes"*: estimating daily monoterpene emissions.

For each module a window is opened to define user-control variables. Only a few differences in the graphic interface are displayed between modules that aim to get hourly and daily estimates. Nevertheless, daily values are obtained from an iteration applying the sum function on the hourly cycle.
Step by step instructions for using the modules within the GIS-BEM are presented below.

i) – Opening a module

Double click on the module;
or right click on the module and choose "Open" (Figure 4).

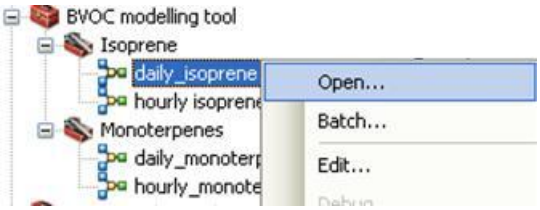

Figure 4. Opening a module.

ii) – User interface to estimate emissions for a single hour

Open the module *"hourly_isoprene"* or *"hourly_monoterpenes"*. The following window will opened and should be filled (Figure 5).

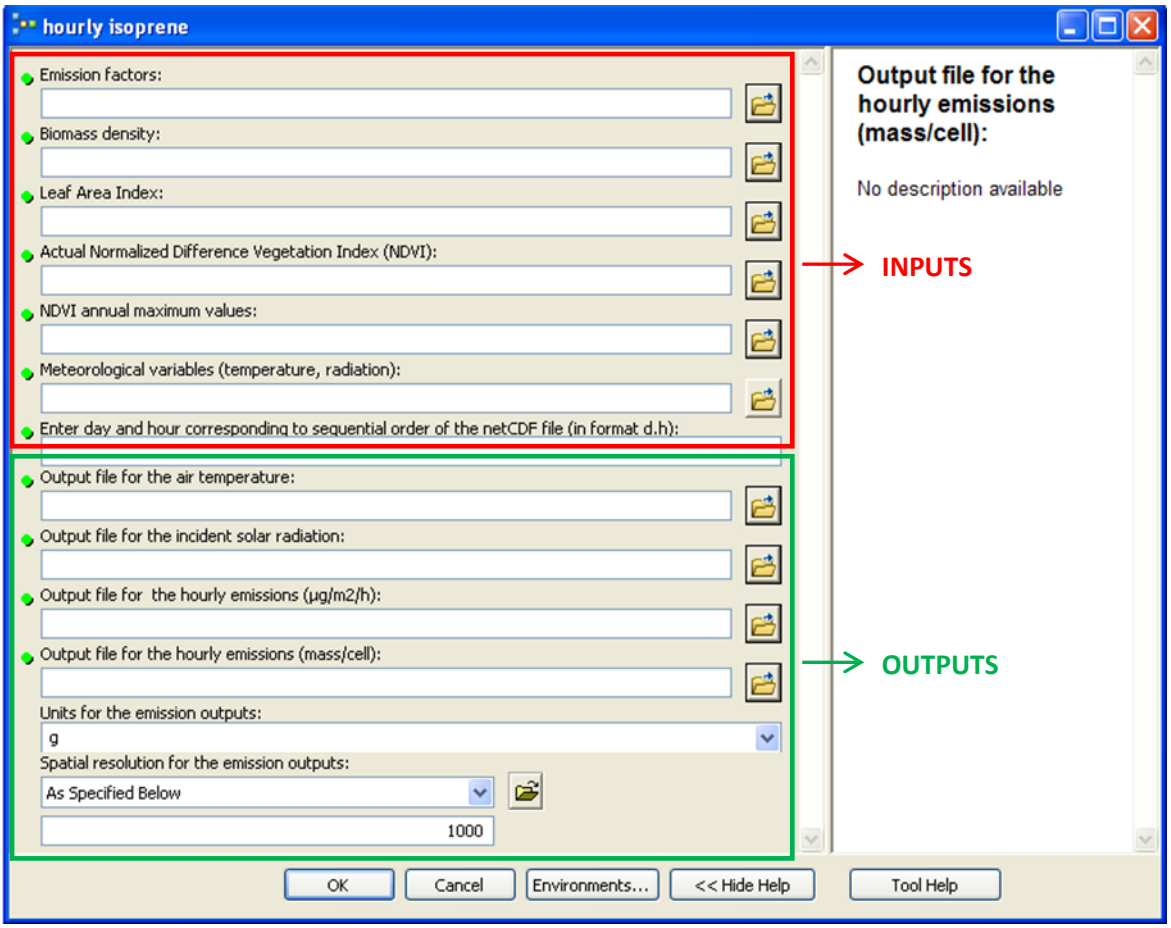

Figure 5. User interface for the module "hourly_isoprene".

To better understanding of the contents, a description about the required information is presented below.

→ **INPUTS:**

Emission factors

Name of the file that contains a regular grid with the emission factors for the selected compound (isoprene or monoterpenes) at standard conditions.

Biomass density

Name of the file that contains a regular grid with the biomass density for each PFT.

Leaf Area Index

Name of the file that contains a regular grid with the LAI corresponding to simulation date.

Actual Normalized Difference Vegetation Index (NDVI)

Name of the file that contains a regular grid with the NDVI corresponding to simulation date.

NDVI annual maximum values

Name of the file that contains a regular grid with the multiyear maximum NDVI resulting from a composition of overlapped NDVI images. These images should be available for different months of year, in order to capture the vegetation seasonality. Thus, to obtain the maximum regular grid within the ArcToolbox select Data Management Tools > Raster > Raster Dataset > Mosaic to New Raster. Opening this geoprocessing tool, add all NDVI images, and in Mosaic Operator choose "Maximum".

Meteorological variables (temperature, radiation)

Name of a NetCDF file corresponding to the simulation period which contains the meteorological variables needed in the modelling process to characterize the air temperature and incoming solar radiation. These files are composed by multiple layers, in which each one represents hourly data. To extract only these variables from the original NetCDF file, a script in python programming language should be used previously as describe in Appendix B.

Enter day and hour corresponding to sequential order of the netCDF file (in format d.h)

Within the temporal period covered by the netCDF file, select the day and hour (in format d.h) corresponding to sequential order of the file taking into account the simulation date. For example, the layer 60 in the netCDF file is equivalent to 3.12.

→ **OUTPUTS:**

Output file for the air temperature

Define the location and the name of the output file that contains a regular grid with the ambient air temperature for the simulation date.

Output file for the incident solar radiation

Define the location and the name of the output file that contains a regular grid with the incoming solar radiation for the simulation date.

Output file for the hourly emissions (µg/m2/h)

Define the location and the name of the output file that contains a regular grid with the hourly emission of a compound in [$\mu g.m^{-2}.h^{-1}$] for the simulation date. The spatial resolution is equal to the smallest cell size among all input datasets.

Output file for the hourly emissions (mass/cell)

Define the location and the name of the output file that contains a regular grid with the hourly emission of a compound per area unit. In a first step, emissions are calculated to the smallest cell size among all input datasets, and then can be aggregated for a larger cell size. This emission flux is dependent of the mass units and spatial resolution required by user.

Units for the emission outputs

Mass units to estimate hourly emissions. The following units can be chosen: micrograms (µg); milligrams (mg); grams (g); and kilograms (kg).

Spatial resolution for the emission outputs

Cell size (in meters) to estimate hourly emissions.

iii) – User interface to estimate daily emissions

Open the module *"daily_isoprene"* or *"daily_monoterpenes"*. The following window will opened and should be filled (Figure 6).

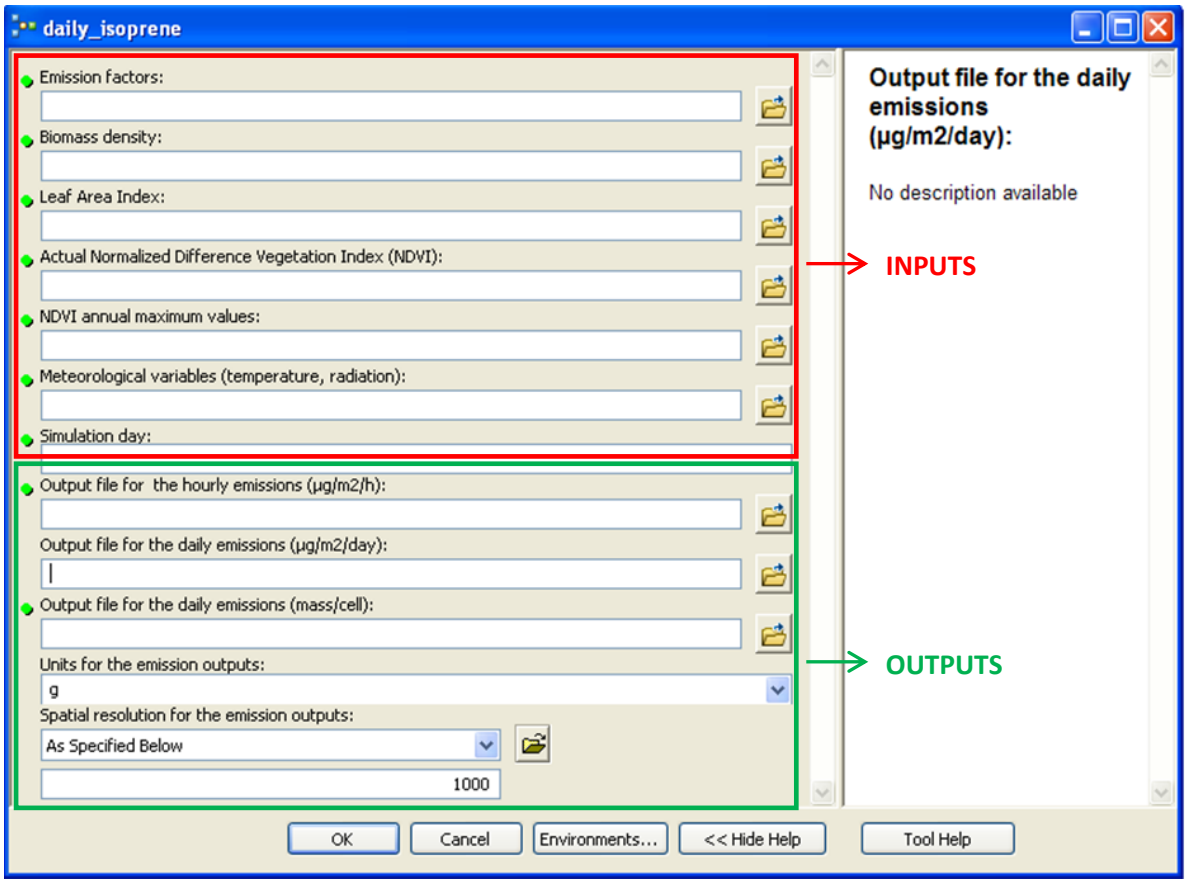

Figure 6. User interface for the module "daily_isoprene".

The differences found in relation to the user interface previously described are the following:

→ **INPUTS:**

Simulation day

Enter the day corresponding to sequential order of the netCDF file taking into account the file´s temporal coverage and the simulation date intended. For example, if the netCDF file is composed by 5 days considering meteorological model outputs from 9 to 13 of May and assuming that simulations for 10th of May are intended, the day 2 in the graphic interface should be specified.

→ **OUTPUTS:**

Output file for the hourly emissions (µg/m2/h)

Define the location and the name of the output files corresponding to regular grids with the hourly emissions of a compound in [ug.m^{-2}.h^{-1}] for the simulation day. The spatial resolution is equal to the smallest cell size among all input datasets. To store these files, a file geodatabase has to be created and output names should be defined. Follow these steps:

- In the bracket allocated for this field click "Open**"** ();
- and then click in "New File Geodatabase" on the desired location (Figure 7);

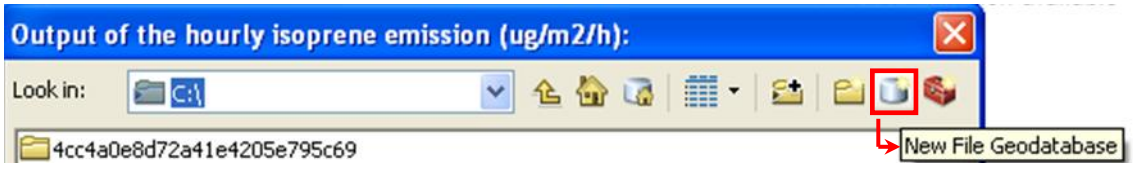

Figure 7. Create a geodatabase to store hourly emissions.

- A "New File Geodatabase" (GDB extension) is created. This name is attributed by default. To rename it, select this folder and click again.
- Open the geodatabase (double click) and defines the output names. Write "isop_hour**%Layer%**_ugm2", for isoprene emissions. Note that at least all characters between percentage symbols (inclusive) should be written in this way, because otherwise hourly data are not saved. The term "**%Layer%**" is a variable that corresponds to a layer number (equivalent to an hour) in the netCDF file. Data for each hour will be stored with a different file name, where only changes the layer

number. Thus, for a netCDF file composed by 72 layers (3 days x 24h), the information is organized automatically as follows:

First day: layers from 1 to 24

Second day: layers from 25 to 48

Third day: layers from 49 to 72

Assuming simulations for the third day, in the example above the hourly files will be saved as:

isop_hour49_ugm2; isop_hour50_ugm2; isop_hour51_ugm2; isop_hour52_ugm2; isop_hour…_ugm2; isop_hour72_ugm2.

Output file for the daily emissions (µg/m2/day)

Define the location and the name of the output file that contains a regular grid with the daily emission of a compound in [$\mu g.m^{-2}.day^{-1}$] resulting from the sum of hourly emissions. The spatial resolution is equal to the smallest cell size among all input datasets.

Output file for the daily emissions (mass/cell)

Define the location and the name of the output file that contains a regular grid with the daily emission of a compound per area unit. In a first step, emissions are calculated to the smallest cell size among all input datasets, and then can be aggregated for a larger cell size. This emission flux is dependent of the mass units and spatial resolution required by user.

To store the input and output files of the model, geodatabases must be created. For that, should follow the procedure previously explained or use the ArcCatalog, from which a right click on the empty space should be applied, selecting “New” and then “File Geodatabase”.

iv) – Running the model

After all the file names and parameters in the user interface have been filled, the model is ready to run. Click “OK”.

5. Post-processing and visualization

As post-processing step, the user might need to rename the output files, essentially the hourly emissions resulting from a simulation day, in order to correctly identify them. This task can only be performed inside the ArcCatalog, selecting the folder (geodatabase) that contains the files. Additionally it is recommended copy these files to a new geodatabase.
Once this stage is completed, the files may be opened in ArcMap environment allowing the user to make a spatial analysis of different layers.

References

Arneth, A., Niinemets, Ü., Pressley, S., Bäck, J., Hari, P., Karl, T., Noe, S., Prentice, I. C., Serça, D., Hickler, T., Wolf, A., Smith, B. (2007) Process-based estimates of terrestrial ecosystem isoprene emissions: incorporating the effects of a direct CO2-isoprene interaction. Atmospheric Chemistry and Physics, 7, 31-53.

Curci, G., Beekmann, M., Vautard, R., Smiatek, G., Steinbrecher, R., Theloke, J., Friedrich, R. (2009) Modelling study of the impact of isoprene and terpene biogenic emissions on European ozone levels. Atmospheric Environment, 43(7), 1444-1455.

Griffin, R. J., Cocker, D. R., Seinfeld, J. H., Dabdub, D. (1999) Estimate of global atmospheric organic aerosol from oxidation of biogenic hydrocarbons. Geophysical Research Letters, 26, 2721-2724.

Guenther, A., Karl, T., Harley, P., Wiedinmyer, C., Palmer, P. I., Geron, C. (2006) Estimates of global terrestrial isoprene emissions using MEGAN (Model of Emissions of Gases and Aerosols from Nature). Atmospheric Chemistry and Physics, 6: 3181-3210.

Guenther, A., Hewitt, C. N., Erickson, D., Fall, R., Geron, C., Graedel, T., Harley, P., Klinger, L., Lerdau, M., McKay, W. A., et al. (1995) A global model of natural volatile organic compound emissions. Journal of Geophysical Research, 100 (D5), 8873-8892.

Kanakidou, M., Seinfeld, J. H., Pandis, S. N., Barnes, I., Dentener, F. J., Facchini, M. C., Van Dingenen, R., Ervens, B., Nenes, A., Nielsen, C. J., Swietlicki, E., Putaud, J. P., Balkanski, Y., Fuzzi, S., Horth, J., Moortgat, G. K., Winterhalter, R., Myhre, C. E. L., Tsigaridis, K., Vignati, E., Stephanou, E. G., Wilson, J. (2005) Organic aerosol and global climate modelling: a review. Atmospheric Chemistry and Physics, 5, 1053-1123.

Niinemets, Ü., Tenhunen, J. D., Harley, P. C., Steinbrecher, R. (1999) A model of isoprene emission based on energetic requirements for isoprene synthesis and leaf photosynthetic properties for Liquidambar and Quercus. Plant, Cell and Environment, 22, 1319-1335.

Oderbolz, D. C., Aksoyoglu, S., Keller, J., Barmpadimos, I., Steinbrecher, R., Skjøth, C. A., Plab-Dülmer, C., Prévôt, A. S. H. (2013) A comprehensive emission inventory of biogenic volatile organic compounds in Europe: improved seasonality and land-cover. Atmospheric Chemistry and Physics, 13, 1689-1712.

Pacifico, F., Harrison, S. P., Jones, C. D., Sitch, S. (2009) Isoprene emissions and climate (review). Atmospheric Environment, 43, 6121-6135.

Sakulyanontvittaya, T., Duhl, T., Wiedinmyer, C., Helmig, D., Matsunaga, S., Potosnak, M., Milford, J., Guenther, A. (2008) Monoterpene and Sesquiterpene Emission Estimates for the United States. Environmental Science & Technology, 42, 1623-1629.

Simpson, D., Guenther, A., Hewitt, C. N., Steinbrecher, R. (1995) Biogenic emissions in Europe: 1. Estimates and uncertainties. Journal of Geophysical Research, 100(D11), 22875–22890.

Wilkinson, M. J., Monson, R. K., Trahan, N., Lee, S., Brown, E., Jackson, R. B., Polley, H. W., Fay, P., Fall, R. (2009) Leaf isoprene emission rate as a function of atmospheric CO2 concentration. Global Change Biology, 15, 1189-1200.

Appendix A

Methodology description

According to implemented approach, the net emission of a compound from terrestrial ecosystems into the above-canopy atmosphere at a specific location and time is given as:

$$E = \varepsilon . M_A . [\gamma_L . LDF + (1 - LDF)] . \gamma_T . \gamma_{LAI} . \gamma_{NDVI} \quad (1)$$

Where:

E - Net emission of a compound [µg.m^{-2}.h^{-1}]

ε - Emission factor at standard conditions [µg.g^{-1}.h^{-1}]

M_A - Dry leaves mass per area unit [g.m^{-2}]

γ_L - Light correction factor

LDF - Light dependence fraction

γ_T - Temperature correction factor

γ_{LAI} - LAI correction factor

γ_{NDVI} - NDVI correction factor

BVOC emission factors (ε) under standardized environmental conditions (T=30ºC, PAR=1000 µmol.m^{-2}.s^{-1}) and leaves biomass (M_A) are associated with the vegetation type.

In order to estimate BVOC emissions at current environmental conditions, correction factors are applied to the standard emission rates. Based on the Guenther et al. (1995) algorithms, the light and temperature influence are analyzed. Also the dependence of the BVOC emission on vegetation parameters (NDVI and LAI) is considered.

Light influence on BVOC emissions

$$\gamma_L = \frac{C_L \times \alpha \times PAR}{(1 + \alpha^2 \times PAR^2)^{0.5}} \quad (2)$$

PAR - Photosynthetically active radiation at leaf level [µmol.m^{-2}. s^{-1}] – can be estimated from solar radiation and sun angle or applying a correction factor (0.45*4.6 = 2.07)

→ Percent of the radiation that is the PAR spectrum based on observed data = 0.45

→ Conversion factor to convert radiation of W.m^{-2} to µmol.m^{-2}. s^{-1} = 4.6

C_L = 1.066 (scaling constant to force the function to 1.0 at the standardized value of PAR - commonly taken as 1000 µmol.m^{-2}.s^{-1})

α = 0.0027 (apparent quantum yield of isoprenoid emission)

The LDF modulates BVOC emissions taking into account the fractions assigned to each compound or category. Sakulyanontvittaya et al. (2008) assume that 5 to 10% of monoterpene emissions occur through the light and temperature dependent route. In the current approach was considered the upper threshold, that is, LDF equal to 0.1. For the isoprene the LDF is assumed to be 1, since this compound is only emitted in the presence of light.

Temperature influence on BVOC emissions

Equation 3 is applied for the isoprene.

$$\gamma_T = \frac{\exp\left[\frac{C_{T1} \times (T_L - T_S)}{R \times T_S \times T_L}\right]}{C_{T3} + \exp\left[\frac{C_{T2} \times (T_L - T_m)}{R \times T_S \times T_L}\right]} \quad (3)$$

T_L - Absolute leaf temperature [K] ⟶ Assume as air temperature

T_S - Leaf temperature at standard conditions (typically 303.16 K) at which γ_T =1

T_m = 314 K (optimum temperature that describes the temperature response function for BVOC synthesis)

R - Gas constant (8.314 J.mol^{-1}.K^{-1})

C_{T1} = 95 000 J.mol^{-1}
C_{T2} = 230 000 J.mol^{-1}
} Parameters that describes the activation and deactivation energies of the emissions

C_{T3} = 0.961

The equation parameters, C_{T1} and C_{T2} are typically chosen to yield γ_T = 1

For monoterpenes the temperature response function is given as:

$$\gamma_T = exp\left[\beta\left(T_L - T_S\right)\right] \quad (4)$$

β is a temperature dependence parameter, estimated through the combination with temperature dependence information from different plant species. The resulting value for monoterpenes (n = 59 plant samples) is β = 0.13±0.07 K (Sakulyanontvittaya et al., 2008). This value was considered in the current approach.

LAI influence on BVOC emissions

LAI is used to characterize structural properties of plant canopies in terms of the amount of foliage at a given location. It is defined as the green leaf area per ground surface unit. The LAI correction factor is implemented based on Guenther et al. (2006):

$$\gamma_{LAI} = \frac{0.49 \times LAI}{\left[\left(1 + 0.2\ LAI^2\right)^{0.5}\right]} \quad (5)$$

NDVI influence on BVOC emissions

NDVI is considered as an indicator of the foliar greenness. In the current model, the NDVI was implemented to derive a correction factor for BVOC emission quantification using the ratio between a pixel actual value and its multiyear absolute maximum value (eq. 6). NDVI values are in the range of -1 to 1 (dimensionless). Positive values are indicative of vegetated surfaces.

$$\gamma_{NDVI} = \frac{NDVI_{act}}{NDVI_{max}} \quad (6)$$

Appendix B

Python script to extract meteorological variables from netCDF files

Script in python (using the version 2.7.2) to extract the ambient air temperature and incoming solar radiation from netCDF files provided by WRF model.

To apply the script below should follow these steps:

1) – Within the python version select “IDLE”;
2) – In the File menu, choose “New Window”;
3) – Copy the script code for this window, changing only the fields referred in the code (identified in red);
4) – Save the script code on the desired location;
5) – In the Run menu, choose “Check Module”. If there aren´t errors, the model is ready to run. Click “F5” or in the Run menu, choose “Run”.

Script Code

```
import os
import sys
from netCDF4 import Dataset #import the dataset of the netCDF module
import numpy as np

direc='C:/'
```

→ Indicate the directory or the path where is the original netCDF file. Write between quotation marks.

```
os.chdir(direc)

ficheiro='original_netCDF_name.nc'
```

→ Write between quotation marks the name of the original netCDF data file.

```
dados=Dataset(ficheiro)

#View all variables in the original netCDF file and select those that are required:

print dados.variables

Time=dados.variables['XTIME']
Latitude=dados.variables['XLAT']
Longitude=dados.variables['XLONG']
Temperatura=dados.variables['T2']
Radiacao=dados.variables['SWDOWN']

#View the shape of the required variables (n layers, n rows, n columns) in the original netCDF file:

print 'Hora =',Time.shape
print 'Latitude =',Latitude.shape #Latitude = (n layers, n rows, n columns)
print 'Longitude =',Longitude.shape
print 'Temperatura =',Temperatura.shape
print 'Radiação =',Radiacao.shape
```

#Create a new netCDF file:

```
print 'Create a new netCDF File "novo_netCDF"'

novo_netCDF=Dataset('C:/new_netCDF_name.nc','w',format='NETCDF3_64BIT')
```

Write between quotation marks the path and the name to give the new netCDF data file.

#Create the dimensions and variables for the new netCDF file:

```
Tempo = novo_netCDF.createDimension('Time',None)
north_south = novo_netCDF.createDimension('north_south', n rows)
east_west = novo_netCDF.createDimension('east_west', n columns)
```

Write the number of rows and columns according to shape of the variables in the original netCDF file.

```
print novo_netCDF.dimensions

Times=novo_netCDF.createVariable('Time','i4',('Time',))
Latitudes=novo_netCDF.createVariable('Latitude','f4',('Time','north_south','east_west',))
Longitudes=novo_netCDF.createVariable('Longitude','f4',('Time','north_south','east_west',))

Times.units='hour'
Latitudes.units='degrees_north'
Longitudes.units='degrees_east'

Temperaturas=novo_netCDF.createVariable('Temperatura','f4',('Time','north_south','east_west',))
Radiacoes=novo_netCDF.createVariable('Radiacao','f4',('Time','north_south','east_west',))
```

#Define the units and the geolocation of the meteorological variables:

```
Temperaturas.units='k'
Temperaturas.coordinates='Time Latitude Longitude'
Radiacoes.units='W/m2'
Radiacoes.coordinates='Time Latitude Longitude'

print novo_netCDF.variables
```

#Copy the values of the meteorological variables from the original netCDF file to the new netCDF file:

```
Temperaturas[:,:,:] = Temperatura[:,:,:]
Radiacoes[:,:,:] = Radiacao[:,:,:]

dados.close()
novo_netCDF.close()
```

NOTE: In python, comments start with a hash mark (#).