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Geoscientific Model Development Discussions

A pre-processor of trace gases and aerosols emission fields for regional and global atmospheric chemistry models

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Abstract

The pre-processor PREP-CHEM-SRC presented in the paper is a comprehensive tool aiming at preparing emissions fields of trace gases and aerosols for use in regional or global transport models. The emissions considered are urban/industrial, biogenic, biomass burning, volcanic, biofuel use and burning from agricultural waste sources from most recent databases or from satellite fire detections for biomass burning. A plumerise model is used to derive the height of smoke emissions from satellite fire products. The pre-processor provides emission fields interpolated onto the transport model grid. Several map projections can be chosen. The way to include these emissions in transport models is also detailed. The pre-processor is coded using Fortran 90 and C and is driven by a *namelist* allowing the user to choose the type of emissions and the database.

1 Introduction

Atmospheric chemistry composition studies with numerical simulations have became largely used with the increasing availability of atmospheric-chemistry transport models and computational resources. Emission inventories of trace gases and aerosols provide surface as well as upper levels mass fluxes for the mass continuity equation (MCE), which are crucial needed information for these numerical studies. To fill up the lack of this information, several international programs and groups have been developing inventories of the most relevant atmospheric trace gases and aerosols.

The numerical simulation of the atmospheric chemistry composition is done with advanced models where MCE is solved on- or off-line (Zhang, 2008) on several spatial resolution and geographical projections, either regional or global scales. In this paper, we introduce a software tool, named PREP-CHEM-SRC, developed to provide gridded emissions of trace gases and aerosols on a flexible spatial resolution, several projections and suitable for regional and global models. Emission fields generated by this

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system have been used by CCATT-BRAMS (Freitas et al., 2009; Longo et al., 2010), WRF-CHEM (Grell et al., 2005), and the *F*low-following finite-volume *I*cosahedral *M*odel (FIM, Bleck et al., 2010). The emissions pre-processor is also under implementation at the Brazilian Center for Weather Forecasting and Climate Studies for their global circulation model.

This paper is organized as follows. Section 2 covers all emissions inventories of anthropogenic and biogenic sources as well as the chemical species available in the database of this software tool. In Sect. 3, we briefly describe possible way of how to introduce the emission contribution in the MCE. Section 4 describes the system and its functionalities. Our conclusions are discussed in Sect. 5.

2 Emissions inventories

This section is devoted to describe all types of emissions currently available within the PREP-CHEM-SRC system. Depending on the modeling system the user may select all or selected choices. WRF-CHEM, for example, has several other emissions pre-processors, depending on the location of the domain that the model will be run at. The user may choose to combine his or her own anthropogenic emissions preprocessor with only the biomass burning emissions from our system.

2.1 Urban-industrial emissions

One of the anthropogenic emission inventories used within the PREP-CHEM-SRC system is provided by the "REanalysis of the TROpospheric chemical composition over the past 40 yr" (RETRO, http://retro.enes.org), a long-term global modeling study of tropospheric chemistry funded by the 5th European Commission Framework Programme. The emission data has $0.5 \times 0.5^{\circ}$ of spatial resolution and global coverage, with monthly temporal resolution and it is based on the year 2000. The emission units are kg [specie] m^{-2} dy^{-1}. The Table 1 provides a list of chemical species available in the anthropogenic inventory.

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Anthropogenic emissions provided by the "Emission Database for Global Atmospheric Research" (EDGAR, http://edgar.jrc.ec.europa.eu, Olivier et al., 1996, Olivier et al., 1999) are also included. This program provides global past and present anthropogenic emissions of greenhouse gases and air pollutants. The species available are N_2O, CO_2, CO, CH_4, SO_2, SF_6, NO_x and NMVOC on $1\times1^\circ$ spatial resolution. The emissions do not have time variation and are associated to the year 2000. New recent released version of EDGAR, version 4, will be included in the data base of the PREP-CHEM-SRC system in an upcoming version.

For the South American continent, a regional urban emission inventory suitable either for the local and regional scale applications is also available. This database integrates information from local inventories of vehicle emissions using socio-economic data, extrapolation of emissions to cities lacking local inventories, and the geographic distribution of emissions at different spatial resolutions (Alonso et al., 2010, hereafter A2010).

Emissions of organic carbon (OC), black carbon (BC), SO_2 and DMS on $1\times1^\circ$ resolution on a monthly basis From the Goddard Chemistry Aerosol Radiation and Transport (GOCART) model database are also available.

2.2 Biogenic emissions

2.2.1 Biogenic emissions from GEIA Activity

Biogenic or natural emissions are based on the GEIA/ACCENT Activity on Emission Databases, http://www.aero.jussieu.fr/projet/ACCENT/description.php. Emission sources from land, vegetation and oceans are provided with $1\times1^\circ$ spatial resolution and monthly temporal resolution. Emissions for Acetone, CH_2H_4, C_2H_6, C_3H_6, C_3H_8, CO, CH_3OH, DMS, NO, Isoprene, Terpenes and NVOC are available. The emission units are kg [specie] m^{-2} dy^{-1}.

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2.2.2 Biogenic emissions from MEGAN

Biogenic emissions derived by the Model of Emissions of Gases and Aerosols from Nature (MEGAN, Guenther et al., 2006) are also available. MEGAN is a modeling system for estimating the net emission of gases and aerosols from terrestrial ecosystems into the atmosphere. Driving variables include land cover, weather, and atmospheric chemical composition. The data was provided by the GEIA/ACCENT Activity on Emission Databases, http://www.aero.jussieu.fr/projet/ACCENT/description.php. The data covers the entire world with spatial resolution of 0.5×0.5°. The temporal coverage is from January to December 2002 with monthly time resolution. Emission rates are provided for the following species: CO, CH_4, CH_2H_4, C_2H_6, C_3H_6, C_3H_8, CH_3OH, formaldehyde, acetaldehyde, acetone, other ketones, toluene, isoprene, monoterpenes and sesquiterpenes. The emission units are kg [specie] m^{-2} dy^{-1}.

2.3 Biomass burning emissions and the smoke plume rise model

Emissions from wild- or deforestation fires are provided using two methodologies. The first one is based on the Brazilian Biomass Burning Emission Model (3BEM, Longo et al., 2007). In this methodology, for each fire pixel detected by remote sensing the mass of the emitted tracer is calculated by the following expression, which takes into consideration the estimated values for the amount of above-ground biomass available for burning (α), the combustion factor (β), the emission factor (EF) for a certain species [η] from the appropriate type of vegetation, and the burning area (a_{fire}) for each burning event.

$$M^{[\eta]} = \alpha_{\text{veg}} \cdot \beta_{\text{veg}} \cdot \text{EF}^{[\eta]}_{\text{veg}} \cdot a_{\text{fire}} \quad (1)$$

A hybrid remote-sensing fire product is used to minimize missing remote sensing observations. The fire database actually used is a combination of the Geostationary Operational Environmental Satellite – Wildfire Automated Biomass Burning Algorithm (GOES WF_ABBA product, cimss.ssec.wisc.edu/goes/burn/wfabba.html; Prins

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et al., 1998), the Brazilian National Institute for Space Research (INPE) fire product, which is based on the Advanced Very High Resolution Radiometer (AVHRR) aboard the NOAA polar orbiting satellites series (www.cptec.inpe.br/queimadas; Setzer and Pereira, 1987), and the Moderate Resolution Imaging Spectroradiometer (MODIS) fire product (modis-fire.umd.edu; Giglio et al., 2003). The three fire product databases are combined using a filter algorithm to avoid double counting of the same fire, by eliminating additional fires within a circle of 1 km radius. The hypotheses assumed for the burnt area needed for Eq. (1) are detailed in Longo et al. 2007.

The fire detection maps are merged with 1-km resolution land cover data (Belward, 1996, Sestini et al., 2003) to provide the associated emission (EF) and combustion (β) factors through a look-up-table. The corresponding aboveground carbon density (α) is defined from the carbon in live vegetation data, estimated using Olson et al. (2000) and updated by Gibbs (2006) and Gibbs et al. (2007) using the Global Land Cover Database (GLC2000). For Amazon basin and neighbor areas the aboveground carbon density follows the estimation done by Saatchi et al. (2007) on 1 km spatial resolution. The land cover map for the Amazon basin was updated with data provided by the PROVEG project (Sestini et al., 2003) and it is based on the year 2000.

The emission and combustion factors for each biome are based on Andreae and Merlet (2001, hereafter AM2001) and Longo et al. (2009). These works provide emission factors for 110 chemical species emitted during burns of tropical forest, extratropical forest, savanna, pasture, charcoal production, agricultural waste, as well as emissions factors measured in controlled laboratory experiment. The mean combustion factor for each biome cited above is also provided. See AM2001 for a complete list of species available within the PREP-CHEM-SRC system.

The second methodology available for biomass burning emissions is based on Giglio et al. (2006) and van der Werf et al. (2006). These authors using burnt-area estimates from remote sensing, a biogeochemical model, and emission factors from the literature, estimated fire emissions during the 8-yr period from 1997 to 2004. This dataset, called Global Fire Emissions Database (GFEDv2), has $1\times1^{\circ}$ spatial resolution with 8-day

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and one-month time steps. Figure 1 illustrates the typical output of the PREP-CHEM-SRC system for biomass burning. It shows the spatial biomass burning CO emission estimation (mg m^{-2} dy^{-1}) averaged over 3 months (August-September-October 2002) at 35 km horizontal space resolution generated using this emission tool. Panel (A) shows the estimation obtained by 3BEM, on panel (B) is GFEDv2. This figure shows the good consistency between the two products but with a significantly finer resolution for 3BEM.

PREP-CHEM-SRC provides also data needed to drive the smoke plume rise model described in Freitas et al. (2006, 2007, 2010). This plume rise parameterization has been incorporated at CCATT-BRAMS, WRF-CHEM and FIM models, and is used to interactively determine the effective injection height of vegetation fires emissions during the flaming phase. The information comprises the mean fire size per biome type and per grid box as well as the partition of trace gases and aerosol mass emitted during the flaming and smoldering phases.

2.4 Volcanoes emissions and umbrella cloud characterization

2.4.1 Volcanoes eruption

For volcanoes eruption, the PREP-CHEM-SRC system is based on the Mastin et al. (2009, hereafter M2009) dataset. This work provides source parameters to model volcanic ash-cloud transport and dispersion during eruptions. There is information on 1535 volcanoes around the world comprising location (latitude, longitude and height) and the eruption source parameter (ESP). According to ESP of the volcano chosen by the user, the parameters plume height, mass eruption rate, volume rate, duration of eruption and the mass fraction of erupted debris finer than about 63 µm are provided. The emission tool provides the collocation of the volcano at the nearest grid box and the corresponding ESP parameters. To the user is left the work to implement the vertical distribution of the erupted mass within the specific transport model. Within our modeling transport system, 75% of the erupted mass is detrained in the umbrella

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cloud and 25% beneath. The base of the umbrella cloud is roughly located at 73% of the plume height (P. Webley, personal communication, 2009).

2.4.2 Volcanoes SO_2 degassing emissions

The data provided by the AEROCOM program (http://www-lscedods.cea.fr/aerocom/AEROCOM_HC/volc/, Diehl, 2009, Diehl et al., 2010) contains volcanic SO_2 emissions and other variables for all days from 1 January 1979 to 31 December 2007 for all volcanoes with historic eruptions listed in the Global Volcanism Program's database provided by the Smithsonian Institution. Each file contains the number of events for each day over the entire world. For each event are provided the volcano name, the date, the height, the cloud column height, longitude, latitude and the daily emission rate of SO_2. There is also a separation between eruptive and non-eruptive volcanic emissions.

For this type of emissions, PREP-CHEM-SRC collocates each volcano emission within the nearest grid box. The total emission will be calculated by the sum of emissions of all volcanoes which is within the grid cell and the effective column height will be given by weighted mean using SO_2 emission rate. The units are $\mathrm{kg\,[SO_2]\,m^{-2}\,dy^{-1}}$.

2.5 Emissions by biofuel use and burning of agricultural waste

In addition to biomass burning emissions, biofuel use and agricultural waste burning inventories developed by Yevich and Logan (2003) are also available. This inventory covers the developing world with $1\times1^{\circ}$ of spatial resolution, and provides the amount of biomass burned per grid box in units of Tg dry matter annually. This information is evenly converted to daily biomass burned and then used calculate emissions of chemical species via AM2001 emission factors.

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3 Including emissions in a transport model

In this section we discuss how to include emissions in atmospheric chemistry transport models.

The advective form of mass continuity equation after Reynolds decomposition and neglecting molecular diffusion reads (e.g., Seinfeld and Pandis, 1998)

$$\frac{\partial \bar{s}_\eta}{\partial t} + \underbrace{\bar{u}_i \frac{\partial \bar{s}_\eta}{\partial x_i}}_{\text{I}} + \underbrace{\frac{1}{\bar{\rho}} \frac{\partial (\bar{\rho} \overline{s''_\eta u''_i})}{\partial x_i}}_{\text{II}} = \underbrace{\overline{Q_\eta}}_{\text{III}}, \tag{2}$$

where $\bar{s}_\eta$ is the grid box mean tracer mixing ratio of the specie η, term (I) represents the 3-D resolved transport term (advection by the mean wind, given by $\bar{u}_i$), term (II) is the sub-grid scale transport by the un-resolved flows ($\overline{s''_\eta u''_i}$ are the turbulent fluxes) and (III) is the forcing, respectively. The quantity $\bar{\rho}$ is grid box mean of the dry air density. The forcing is normally split in sink (R), emission (E) and the net production or loss by additional physical and/or chemical processes (PL):

$$Q_\eta = R + E + \text{PL}, \tag{3}$$

Here our focus is how to determine the emission (E) in terms of the mass fluxes described in Sect. 2.

3.1 Cold/low buoyancy emissions

Most of the emissions from urban processes, transportation (over the land and ocean), charcoal production, waste agricultural burning, biogenic, and others, typically have low buoyancy, when compared with its environment, being released into the atmosphere near of the surface. For this kind of emissions, with a prescribed flux (F_η, with units kg $[\eta]$ m^{-2} dy^{-1}) given by the corresponding inventories, the contribution for the mixing

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ratio tendency for a tracer η can be expressed as

$$\bar{E}_\eta = \begin{cases} \frac{F_\eta}{\bar{\rho}\ \Delta z_1}, & k = 1 \text{ (surface)} \\ 0, & k > 1 \text{ (above)} \end{cases}, \tag{4}$$

where Δz_1 is the vertical thickness of the first physical model layer where the tracer η will be released and k denotes the vertical layer. If the emission source is located above the first model vertical layer, as would be the case for tall chimneys with height is greater than the thickness of this layer, Eq. (4) must be changed accordingly. The unit of the emission in Eq. (4) is $\mathrm{kg}\,[\eta]\,(\mathrm{kg}\,[\mathrm{air}]\,\mathrm{dy})^{-1}$. To convert the emission per seconds, the user has two choices. If the diurnal cycle of the process that is emitting the tracer is constant during the time, Eq. (4) must be divided by $86\,400\,\mathrm{s\,dy}^{-1}$. However, several processes release tracers on non-homogenous rates during the day. Consequently, the user should develop a diurnal cycle function $r(t)$ which obeys with the following constraint

$$\int_0^{86\,400} r(t)\mathrm{d}t = 1, \tag{5}$$

In this case, the instantaneous emission rate will be given by

$$\bar{E}_\eta = \frac{F_\eta}{\bar{\rho}\ \Delta z_1} r(t), \tag{6}$$

with units of $\mathrm{kg}\,[\eta]\,(\mathrm{kg}\,[\mathrm{air}]\,\mathrm{s})^{-1}$. For emissions from mobiles sources in urban areas, $r(t)$ could, for example, be represented by a double Gaussian function with one peak in the morning and another one in the late afternoon, representing the typical rush hours in the cities, as illustrated in Fig. 2.

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3.2 Hot/high buoyancy emissions

One important example of hot and high buoyancy emissions are those from vegetation fires. This process emits hot gases and particles which are quickly transported upward due the positive buoyancy produced by the combustion (see Fig. 3). The entire fire process can be split in two main phases:

- smoldering with mostly of the emission released just above the surface,
- flaming with mostly of the emission directed injected in the PBL, free troposphere or even stratosphere.

In the methodology proposed by Freitas et al. (2006, 2007, 2010), a 1-D plume rise model is embedded in each column of 3-D low resolution atmospheric chemistry-transport models (the hosts) to provide interactively the smoke injection height, in which trace gases and aerosols, emitted during the flaming phase of the vegetation fires, are released and then transported and dispersed by the prevailing winds simulated by them. Following this approach, the total emission flux (F_η, in units of kg $[\eta]$ m^{-2} dy^{-1}) is first determined, followed by the partitioning of mass which is emitted during the smoldering (λ) and flaming (1-λ) phases. Finally, the plume rise model determines the smoke injection layer of the flaming phase (as illustrated by Fig. 3). From the above, the emission term of Eq. (2) can be expressed as

$$\bar{E}_\eta = \begin{cases} \lambda \frac{F_\eta}{\bar{\rho}\,\Delta z_1}, & k = 1 \\ (1-\lambda)\frac{F_\eta}{\bar{\rho}\,\Delta z_k}, & h - \frac{\Delta z_h}{2} < z(k) < h + \frac{\Delta z_h}{2} \end{cases} \quad (7)$$

where Δz_h is the vertical thickness of the smoke layer, and $\left[h - \frac{\Delta z_h}{2},\ h + \frac{\Delta z_h}{2}\right]$ the vertical domain of the injection layer prescribed by the smoke plume rise model. An example of the spatial distribution of biomass burning CO source emissions is given by Fig. 4a. It shows a vertical cross section of CO emissions at 18:00 UTC on 2 September 2002 along latitude 5.4° S (see Freitas et al., 2007 for more details), with surface emission

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associated with smoldering phase as well as elevated emissions layers associated with flaming phase.

To convert the time unit of emission in seconds, it is convenient to introduce a diurnal cycle for the biomass burning emission. For South America fires a single Gaussian function centered at ~18:00 UTC is normally used. This curve is based on the typical diurnal cycle of fire occurrence over South America as reported by Prins et al. (1998). Figure 4b shows the diurnal cycle function $r(t)$ as used by CCATT-BRAMS model. For other tropical areas of the world, Giglio (2007) reports the diurnal fire cycles for 15 regions which can be used to describe the correspondent diurnal cycle functions $r(t)$.

4 System description and functionalities

4.1 The software

The PREP-CHEM-SRC emission tool is coded using FORTRAN 90 and C and requires HDF and NetCDF libraries. The code packed comprises FORTRAN 90 and C files routines and a README file for further instructions. Appendix A provides a list of the FORTRAN 90 files of the source code. We make intensive use of derived type data and modules, functionalities of FORTRAN 90, to provide clear, safe and easy understanding of the data structure. The grid configuration and emissions inventories desired to provide trace gases and aerosol fluxes are defined by a FORTRAN *namelist* file called "prep-chem-src.inp". Several options of map projection types (Polar-Stereographic, Gaussian, Lambert Conformal, Rectangular, Icosahedral horizontal grid of FIM model) for regional and global grids are available with flexible spatial resolution. The software has been tested with Intel and Portland Fortran compilers under UNIX/LINUX operational system.

The PREP-CHEM-SRC is ready to provide emissions for the chemical mechanisms RADM2 (Chang et al., 1989), RACM (Stockwell et al., 1991), CB07 (Yarwood et al.,

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2005) and RELACS (Crassier et al., 2000). The chemical mechanism is determined during the code compilation by providing the correspondent chem1_list.f90 file (see README file for further instructions).

The Table 2 provides a description of the parameters of the namelist file prep-chem-src.inp.

4.2 Some examples of regional and global emissions

For regional models with nested grids capability, emissions for both coarse and fine grids are provided. Local updates for mega-cities or inclusion of point and line sources are easily to be implemented. The product of this tool is a set of files with gridded daily emissions fluxes ($kg\,m^{-2}\,dy^{-1}$) and emission related information fields.

Figure 5 introduces the first example of the model output. In this case it is related to the anthropogenic emission of CO on the Southeast region of Brazil. The system was configured with 2 grids, the coarse one (showed at panel A) with 15 km horizontal resolution covering mostly of Sao Paulo State with Paraná State at South and Rio de Janeiro and Minas Gerais at North. The second and nested grid (panel B) has 3 km of horizontal resolution and covers the more densely urbanized areas of the Brazil, Sao Paulo and Rio de Janeiro Metropolitan Areas (MA), indicated by the letters SP and RJ on the panel. In this resolution is more discernible the emission rates within the SPMA and the shape of the emission field resemble much better the real urban island of this MA. Another remarkable feature in this resolution is the emission related to the main highways and roads of this area depicted by the red lines connecting SP and RJ and others urbanized locations. See A2010 for more details.

As an example of model output for regional grid covering the South America, Figs. 6 and 7 show SO_2 and NO emission estimates for a specific day, respectively. Figure 6 shows sources of SO_2 estimated for 27 August 2002 on a rectangular projection grid with spatial resolution of $0.2 \times 0.2^{\circ}$. The panel A shows SO_2 volcanoes emissions (in units $10^{-9}\,kg\,m^{-2}\,dy^{-1}$) along the Andes Mountains on the East side of South America. Panel B shows the emission associated to the biomass burning as estimated using the

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3BEM methodology, in this case fire counts from MODIS and WF_ABBA fire product was used. Finally, Panel C illustrates the SO_2 emission from urban and industrial processes as prescribed by the EDGAR inventory. For NO, Fig. 7 shows the biogenic emission (A) from GEIA, from biomass burning (B) from 3BEM and anthropogenic (C) from RETRO but updated with local sources of information according to A2010.

Emissions processed on global scale for an icosahedral grid of FIM model is showed on Fig. 8. In this case, anthropogenic and biomass burning emission (using MODIS fire product) of carbon monoxide is processed on grid resolution G5, approximately 250 km. On the left side, mostly of emission is associated to densely industrial and urbanized areas. On the right, besides the former kind of emission over the Europe, biomass burning emissions associated to the deforestation activities on the Northwest of Africa continent is also present.

5 Conclusions

In this paper we have described the functionalities of the new preprocessor of chemical species PREP-CHEM-SRC. PREP-CHEM-SRC was designed to prepare emissions fields from a large set of source types and databases to be used in global and regional transport models. Emissions fields are interpolated onto the model grid, with several options of map projections available and flexible spatial resolution. The types of emissions considered are: urban/industrial, biogenic, biomass burning, volcanic, biofuel use and burning from agricultural waste sources from most recent databases or from satellite fire detections for biomass burning. For urban/industrial emissions, the RETRO, EDGAR and GOCART databases can be used. Biogenic emissions are from GEIA and/or MEGAN databases. Biomass burning emissions can be provided by the GFEDv2 database or by the 3BEM model using satellite fire detection products. PREP-CHEM-SRC also provides the data needed to drive the plumerise parameterization used in CCATT-BRAMS, WRF-CHEM and FIM models. For volcanoes, ashes and SO_2 degassing are considered. The way to include both the low and the high buoyancy emission fluxes calculated by PREP-CHEM-SRC is also discussed.

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The main interests of this new pre-processor are:

- the easy use and grid configuration of the emissions fields on regional or global scales,
- the choice between different databases,
- the choice between different chemical mechanisms.

The code and mostly of the emission data base are available upon request to the 1st author, to the email address gmai@cptec.inpe.br or wrfchemhelp.gsd@noaa.gov.

Appendix A

The FORTRAN files of the PREP-CHEM-SRC system

- Main routines
  - prep_chem_sources.f90
  - prep_chem_sources_utils.f90
  - chem1_list.f90
- Auxiliary routines
  - grid_dims_output.f90
  - var_tables.f90
  - io_params.f90
  - vtab_fill.f90
  - mem_grid.f90
  - node_mod.f90
  - rconstants.f90
  - lllc_utils.f90
  - adap_init_prepchem.f90
  - grid_dims.f90
  - gridset_prepchem.f90
  - rams_grid.f90
  - anheader.f90
- Utils/ Misc.
  - numerical routines
  - I/O routines
- Volcanoes emissions
  - volcanoes_emissions.f90
  - volc_degassing_emissions.f90
- Anthropogenic emissions
  - retro_emissions.f90
  - edgar_emissions.f90
  - fwb_awb_emissions.f90
  - cetesb_update.f90
  - convert_retro_to_racm.f90
  - extrapolacao_update.f90
  - gocart_emissions.f90
  - gocart_backgound.f90
- Biomass burning Emissions
  - AeM_emission_factors.f90
  - convert_AeM_to_racm.f90
  - emission_fields.f90
  - gfedv2_8days_emissions.f90
  - gfedv2_8days_plumerise.f90
  - gfedv2_emissions.f90
  - 3bem_emissions.f90
  - 3bem_plumerise.f90
  - fire_properties.f90
- Biogenic emissions
  - biogenic_emissions.f90
  - convert_bioge_to_racm.f90
  - megan_emissions.f90

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Table 1. List of chemical species available in the anthropogenic inventory developed by the RETRO program.

Acids	C_4H_{10}	Ethene	Other Aromatics
Alcohols	C_5H_{12}	Ethers	Other VOC
Benzene	C_6H_{14}_plus_higher_alkanes	Ethyne	Toluene
C_2H_2	Chlorinated Hydrocarbons	Ketones	Trimethylbenzene
C_2H_4	CO	Methanal	Xylene
C_2H_6	Esters	NO_x	
C_3H_8	Ethane	Other Alkanals	

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Table 2. Description of the parameters of the *namelist* file "prep-chem-src.inp".

Parameters and examples	Description and comments
grid_type= 'polar',	This parameter (character) defines the grid projection on which the emission fields will be generated. The options are: – "polar" = polar stereographic grid – "gg" = Gaussian grid – "ll" = rectangular projection grid – "lambert"= Lambert conformal grid – "FIM" = Icosahedral grid of FIM model
ihour=0, iday=12, imon=7, iyear=2004,	The date of emission using GMT time. All parameters are integers.
use_retro=1, retro_data_dir='./Emission/RETRO/anthro', use_edgar=1, edgar_data_dir='./Emission/EDGAR/anthro',	To select the anthropogenic sources datasets to be used (1=yes, 0=not) and to inform the directory path where the correspondent input data is. The parameters are integers and characters.
use_gocart=1, gocart_data_dir='./Emission/GOCART/emissions',	To define if GOCART emission of OC, BC, SO_2 and DMS will be used (1) or not (0) and the path where the raw data is.
use_bioge=1, bioge_data_dir='./Emission/biogenic_emissions',	To select the biogenic sources datasets to be used (0=not, 1=GEIA, 2=MEGAN) and the path where the original data is.

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Table 2. Continued.

Parameters and examples	Description and comments
use_fwbawb=0, fwbawb_data_dir='./Emission/ fwbawb ',	To define if the biofuel use and agricultural waste burning emissions will be used (1) or not (0), and the path where the raw data is.
use_gfedv2=0, gfedv2_data_dir='./Emission/GFEDv2-8days',	To define if GFEDv2 biomass burning inventory is to be used (=1) or not(=0) and the path where the raw data is.
use_bbem=1, use_bbem_plumerise=1,	To define if 3BEM biomass burning inventory and the smoke plume rise parameters will be used (=1) or not(=0).
merge_GFEDv2_bbem=0,	Define if the merging of GFEDV2 with 3BEM is desired (integer: 1=yes, 0=no). If yes, over South America 3BEM is used instead of GFEDv2.
bbem_wfabba_data_dir='./Emission/fires_data/WF_ABBA_v60/filt/f', bbem_modis_data_dir='./Emission/fires_data/MODIS/Fires.', bbem_inpe_data_dir='./Emission/fires_data/DSA/Focos', bbem_extra_data_dir='./Emission/fires_data/xx,	Fire products for 3BEM/3BEM-plumerise emission models: – Path of WF_ABBA fire product. The filtered fire product is recommended. The last letter "f" is the prefix of the file name. – Path of MODIS fire product and the prefix of the file name ("Fires"). – Path of INPE/DSA fire product and the prefix of the file name ("Focos"). – Additional fire product provided by the user.

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Table 2. Continued.

Parameters and examples	Description and comments
veg_type_data_dir='./surface_data/GL_IGBP_MODIS_INPE/MODIS	Only for 3BEM: Land cover data set (dir + prefix)
carbon_density_data_dir='./surface_data/GL_OGE_INPE/OGE',	Only for 3BEM: Carbon density data set (dir + prefix)
fuel_data_dir='./surface_data/fuel/glc2000_fuel_load.nc',	Only for 3BEM: fuel load data provided by the user (dir + full file name).
USE_GOCART_BG=1, GOCART_BG_DATA_DIR='./Emission/GOCART',	GOCART background data for H_2O_2, OH and NO_3 (only for WRF-Chem/FIM models with GOCART aerosol module)
USE_VOLCANOES=1, VOLCANO_INDEX=1450, USE_THESE_VALUES='NONE', BEGIN_ERUPTION='201004161200',	This section is to control emission of ASH by eruptive volcanoes. The data is based on M2009 paper. – USE_VOLCANOES:1=yes,0=no (integer). – VOLCANO_INDEX: the reference number (integer) of the volcano listed at M2009 database. This number will provide trough a look up table a set of default parameters for injection height, duration and emission of ash. – USE_THESE_VALUES: (character) if 'none', M2009 database will be used. If the user want to use a different set of numbers, them must be in text file with inj_height, duration, mass ash (units are meters – seconds – kilograms). As example, a file named 'values.txt' with the text line: 11000. 10800. 1.5e10 will replace the default values by these numbers by setting USE_THESE_VALUES='./values.txt'

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Table 2. Continued.

Parameters and examples	Description and comments
	– BEGIN_ERUPTION= begin time UTC of eruption YYYYMMDDhhmm
USE_DEGASS_VOLCANOES=0, DEGASS_VOLC_DATA_DIR='./Emission/VOLC_SO_2',	This section is to control emission of SO_2 by eruptive and non-eruptive volcanoes. The data is based on Diehl, 2009 and 2010 papers. – USE_DEGASS_VOLCANOES=1=yes, 0=no (integer). – DEGASS_VOLC_DATA_DIR: character designing the path of the directory where the raw data is**.**
GRID_RESOLUCAO_LON=0.1, GRID_RESOLUCAO_LAT=0.1, NLAT=320, LON_BEG = –170., LAT_BEG = 40., DELTA_LON= 90., DELTA_LAT= 40.,	This section is only for grid_type 'll' or 'gg'. The parameter "nlat" is integer, all others are real. – GRID_RESOLUCAO_LON and GRID_RESOLUCAO_LAT are the grid spacing in degrees. – NLAT is the number of grids on the latitudinal direction for a Gaussian grid. – LON_BEG and LAT_BEG are the longitude and latitude in degrees of the 1st grid box. The ranges are –180 to +180 and –90 to +90, respectively. – DELTA_LON and DELTA_LAT are the total extension of the domain in degrees. Set 360 and 180 degrees for global domains, respectively.

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Table 2. Continued.

Parameters and examples	Description and comments
NGRIDS = 1, NNXP = 275,50,86,46, NNYP = 250,50,74,46, NXTNEST = 0,1,1,1, DELTAX = 5000., DELTAY = 5000., NSTRATX = 1,2,3,4, NSTRATY = 1,2,3,4, POLELAT = 65., POLELON = –150., STDLAT1 = 65., STDLAT2 = 65., CENTLAT = 65., –23., 27.5, 27.5, CENTLON = –150., –46.,–80.5, –80.5,	This section is only for regional grids. – NGRIDS (integer) is the number of grids to generate emissions. – NNXP, NNYP (integer) are the number of x,y gridpoints for each desired grid. – NXTNEST (integer) is grid number which is the next coarser grid. – DELTAX, DELTAY (real) are the X and Y grid spacing (meters). – NSTRATX, NSTRATY (integer) are the nest ratios between this grid and the next coarser grid. – POLELAT, POLELON (real) are, if grid type is polar, the latitude (in degrees) of pole point. If lambert, lat/lon of grid origin (x=y=0.) – STDLAT1, STDLAT2 (real, only for Lambert-Conformal) are standard latitudes of projection in degrees. – CENTLAT, CENTLON are the center (latitude, longitude, in degrees) of each grid.

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Table 2. Continued.

Parameters and examples	Description and comments
PROJ_TO_LL='YES', LATI = –90., –90., –90., LATF = +90., +90., +90., LONI = –180., –180., –180., LONF = 180., 180., 180.,	This section is only for visualization using GrADS software. – PROJ_TO_LL (character) is to define if a rectangular projection is desired: "YES" or "NOT". – LATI, LATF, LONI, LONF (real, degrees) are the corners of the emission output domain for each grid.
CHEM_OUT_PREFIX = 'TEST-RACM', CHEM_OUT_FORMAT='vfm', CONVERT_TO_WRF = 'yes',	– CHEM_OUT_PREFIX: output file prefix (may include directory path) – CHEM_OUT_FORMAT: the format of the output: use "vfm" for CCATT-BRAMS, WRF-CHEM or FIM. Binary is also available by setting "bin". NetCDF is under implementation. – CONVERT_TO_WRF: convert to WRF/CHEM ("yes" or "not", character).

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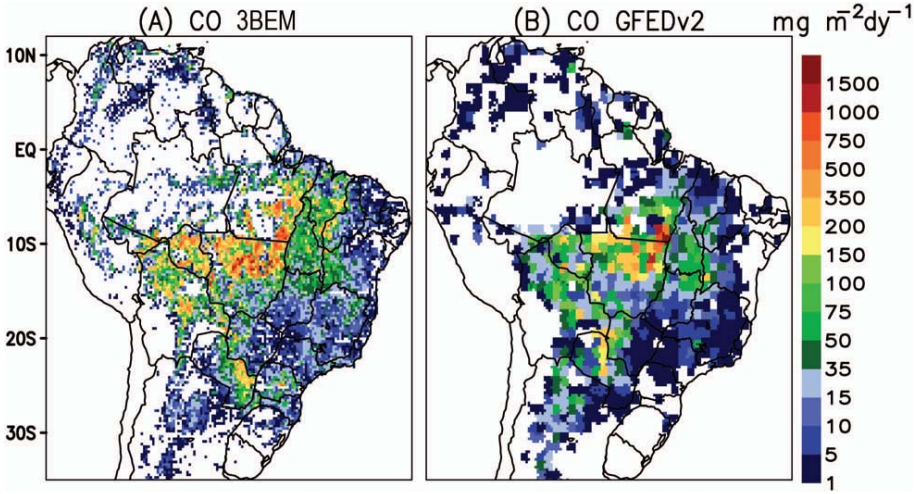

Fig. 1. Spatial distribution of the CO emission estimations in $mg\,m^{-2}\,dy^{-1}$ averaged over 3 months (AUG-SEP-OCT 2002) from the two biomass burning inventories available within the PREP-CHEM-SRC system: **(A)** 3BEM, **(B)** GFEDv2 (figure adapted from Longo et al. 2009).

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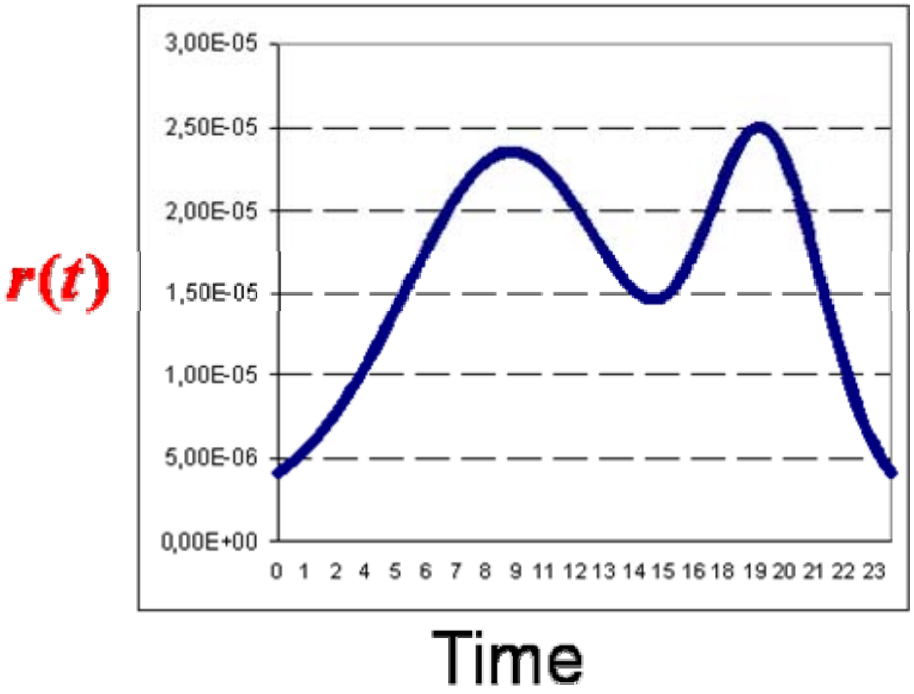

Fig. 2. A double Gaussian function used to determine the diurnal cycle of urban emission.

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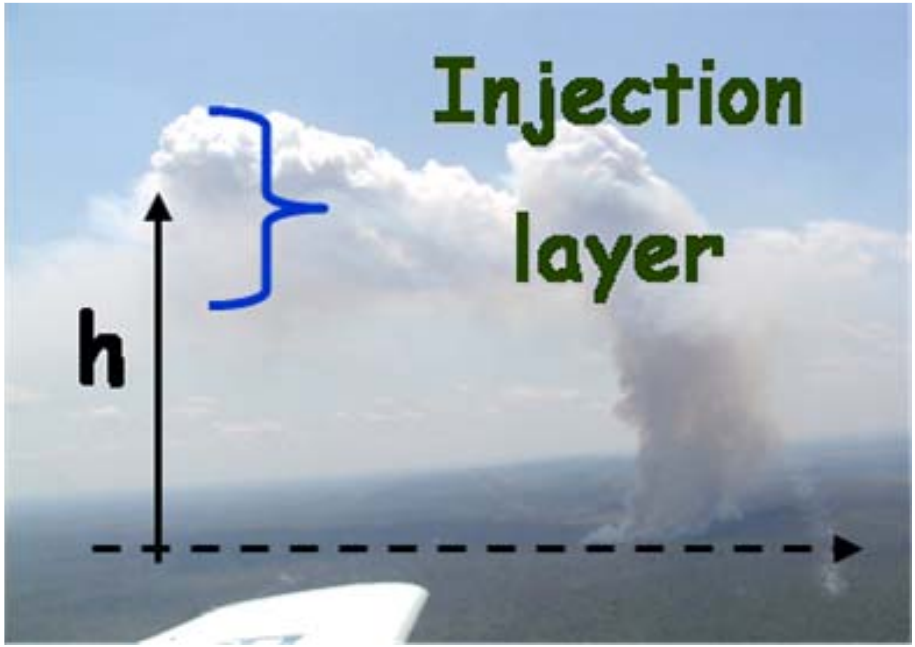

Fig. 3. Photograph of the smoke plume rise produced from a deforestation fire in the Amazon basin showing the injection layer at upper free troposphere associated to the flaming phase.

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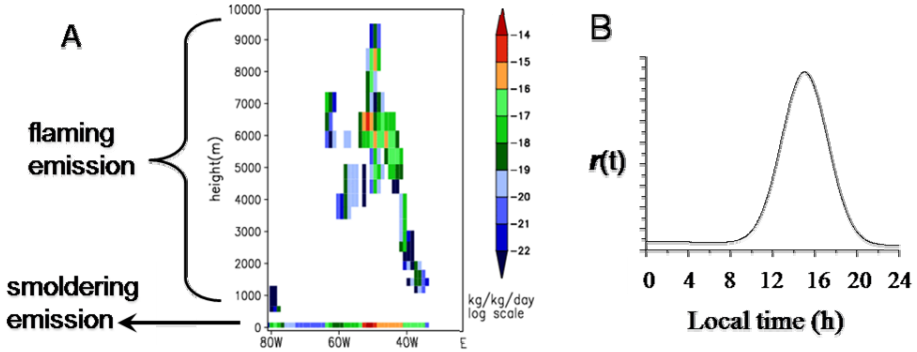

Fig. 4. **(A)** An example of a simulated vertical cross section of biomass burning CO source emission on 18:00 UTC 2 September 2002 at latitude 5.4° S (adapted from Freitas et al., 2007). It shows the surface emission associated to the smoldering phase as well as elevated emissions layers associated to the flaming phase. The panel **(B)** depicts a Gaussian function centered at 15:00 LT used to determine the diurnal cycle of biomass burning emissions on South America.

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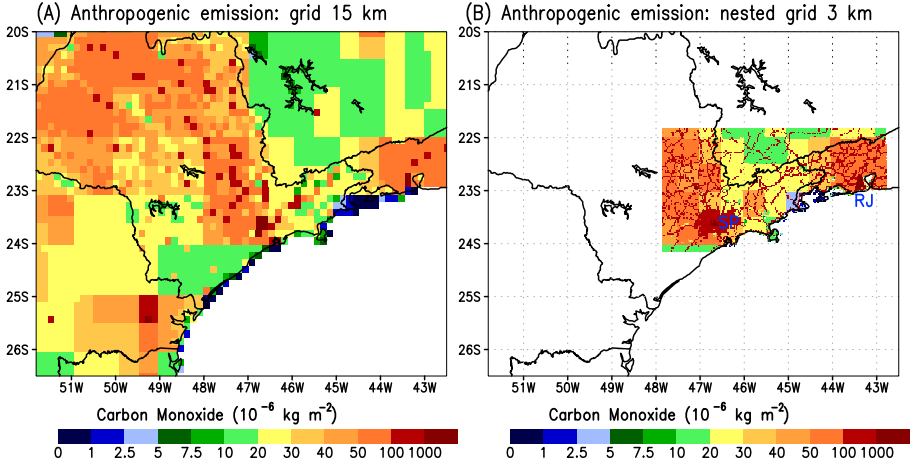

Fig. 5. Carbon monoxide anthropogenic emission field generated by the PREP-CHEM-SRC program: panel **(A)** for a regional grid with 15 km horizontal resolution, panel **(B)** for a nested grid with 3 km.

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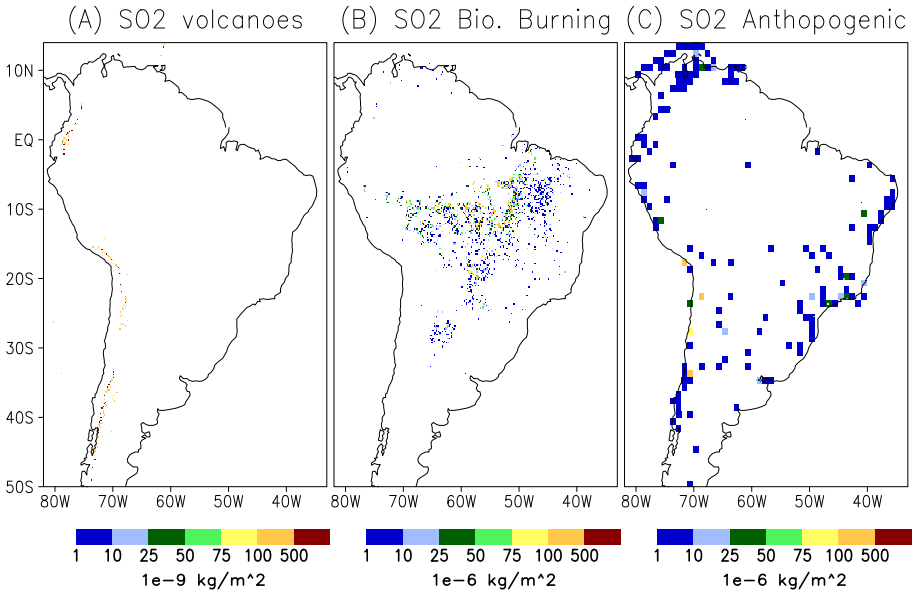

Fig. 6. Different sources of SO_2 estimated for 27 August 2002 on a rectangular projection grid with spatial resolution of 0.2×0.2°. Panel **(A)** represents volcanoes emission following Diehl, 2009 inventory, **(B)** biomass burning from 3BEM and **(C)** anthropogenic SO_2 using EDGAR.

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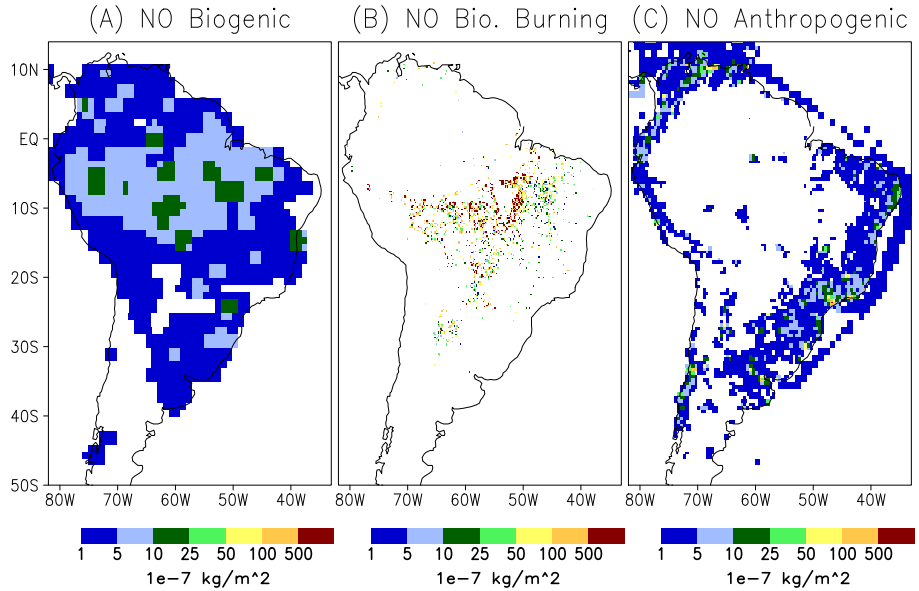

Fig. 7. Different sources of NO estimated for 27 August 2002 on a rectangular projection grid with spatial resolution of 0.2×0.2°. Panel **(A)** represents biogenic emission following GEIA inventory, **(B)** biomass burning NO emission from 3BEM and **(C)** anthropogenic NO using RETRO data but updated with local sources of information for the South American main cities.

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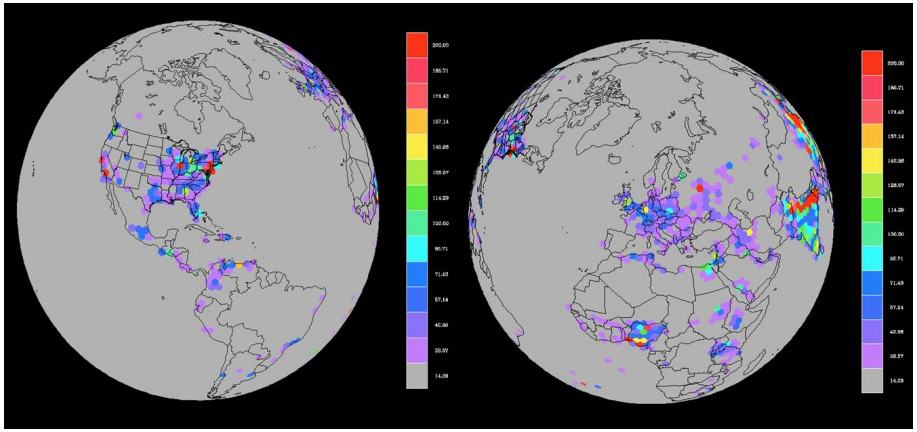

Fig. 8. Carbon monoxide emission field generated by the PREP-CHEM-SRC program for the icosahedral grid (level G5, resolution around 250 km) of FIM Model.

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