Description of the chemical transport model 'REM-CALGRID'

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Basic information [top]

Model name
REM-Calgrid

Full model name
Regional Eulerian Model - California Grid Model

Model version and status
Version 2.0

Latest date of revision
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Intended field of application [top]

Modelling of pollutants (photo-oxidants, aerosols) on different scales from Europe-wide domains down to urban domains.

Model type and dimension [top]

Eulerian, 3-D - Aerosol-Photochemistry-Transport-Model

Model description summary [top]

REM-CALGRID (RCG) is a chemical transport model development designed to fulfil the requirements of the ambient air quality framework directive 96/62/EC of the European Commission. It is an Eulerian grid model of medium complexity that can be used on the regional and the urban scale for short-term and long-term simulations of oxidant and aerosol formation.

The model includes the following features:

- A generalized horizontal coordinate system, including latitude-longitude coordinates;
- A vertical transport and diffusion scheme that correctly accounts for atmospheric density variations in space and time, and for all vertical flux components when employing either dynamic or fixed layers;
- A new methodology to eliminate errors from operator-split transport and to ensure correct transport fluxes, mass conservation, and that a constant mixing ratio field remains constant;
- Inclusion of the recently improved and highly-accurate, monotonic advection scheme developed by Walcek (2000). This fast and accurate scheme has been further modified to exhibit even lower numerical diffusion for short wavelength distributions;
- The latest release of the CBM-IV photochemical reaction scheme;
- The ISORROPIA equilibrium aerosol module, that treat the thermodynamics of inorganic aerosols;

- The SORGAM equilibrium aerosol module, that treats the thermodynamics of organic aerosols;
- Simple modules to treat the emissions of sea salt aerosols and wind blown dust particles;
- A simple wet scavenging module based on precipitation rates;
- An emissions data interface for long term applications that enables on-the-fly calculations of hourly anthropogenic and biogenic emissions.
- One-way-nesting capabilities

Resolution [top]

Temporal resolution
Variable internal time steps, output hourly

Horizontal resolution
Arbitrary resolution from ca. 1 km to 50 km

Vertical resolution

Arbitrary fixed grid or arbitrary dynamic layers coupled to the movement of the mixing height

Schemes [top]

Advection
For horizontal advection, RCG uses the highly-accurate, monotonic advection scheme developed by Walcek (2000). This fast and accurate scheme has been further modified to exhibit even lower numerical diffusion for short wavelength distributions. Vertical advection is treated with a Crank-Nicolson-scheme.

Turbulence
Vertical turbulent mixing formulation uses K-diffusion. Similarity theory for stable and convective boundary layer. Diffusion coefficients based on PBL scaling regimes.

Deposition
Dry deposition for gaseous species and particles is calculated using the resistance analogy. The deposition speed is described as the reciprocal sum of three resistances: the aerodynamic resistance, the viscous sub- layer resistance and the surface resistance. Surface resistances are parameterized following Erisman and Pul (1994).

Wet deposition

Wet deposition of gases due to in and below cloud scavenging is parameterized as a function of the species dependent Henry constant and the precipitation rate. Wet deposition of particles is treated in RCG using a simple scavenging coefficient approach with identical coefficients for all particles.

Gas-phase Chemistry
Updated CBM-4 with Carter's 1-product isoprene scheme; homogeneous and heterogeneous conversion of NO2 to HNO3; aqueous phase conversion of SO2 to H2SO4 through oxidation by H2O2 and O3; equilibrium concentration for SO2, H2O2 and O3 from Henry constants and assuming progressive cloud cover for relative humidity above 80%; effective rate constants for an average pH of 5 using acid/base equilibrium and kinetic data from Seinfeld and Pandis, 1998.

Aerosol treatment

Particle size distribution is represented with a two-mode bulk approach: a fine mode (PM2.5) and a coarse mode (PM10-PM2.5). The equilibrium between solid, aqueous and gas phase concentrations for inorganic ions and humidity is calculated as a function of temperature with the ISORROPIA thermodynamic module (Nenes et al., 1999). Production of secondary organic aerosol (SOA) from anthropogenic and biogenic VOC is treated with the SORGAM module (Schell et al., 2001) which calculates the partitioning of semi-volatile organic compounds produced during VOC oxidation between the gas and the aerosol phase.

Solution technique [top]

For transportable species the time dependent continuity equation is solved. The equation is solved by means of operator splitting, the solution technique includes

- a new methodology to eliminate transport operator-splitting errors on a generalized-metric, fixed- or dynamic-layer grid
- true mass conservation
- the preservation of constant mixing ratio fields.

Input data [top]

Necessary input data for a typical run with RCG are topography and land-use-data, emissions and meteorological data.

Emissions

RCG requires annual emissions of VOC, NO_x, CO, SO_2, CH_4, NH_3, PM10, and PM2.5, split into point and gridded area sources. Mass-based, source group dependent NMVOC profiles are used to break down the total VOC into the different species classes of the chemical mechanisms. Hourly emissions are derived during the model run using sector-dependent, month, day-of-week and hourly emissions factors. PM10 emissions are split into a PM2.5 and a coarse PM (PM10 – PM2.5, PM_{coarse}) part, the PM2.5 part is further split into mineral dust ($PM2.5^{prim}$), EC and primary OC (OC^{prim}).

Biogenic VOC-emissions are derived using the E94 emissions factors for isoprene and OVOC (Other VOCs) as described in Simpson et al. (1995) or Simpson et al. (1999). Terpene emission factors are taken from the CORINAIR emission hand-book. These biogenic calculations are based on the land-use data for deciduous, coniferous, mixed forests and crops. Light intensity and temperature dependencies are also considered.

Soil NO emissions are calculated as a function of fertilizer input and temperature following Simpson et al. (1995).

The sea-salt aerosol emissions (Na^+, Cl^-) are parameterized according to Gong et al. (1997) as a function of size and wind speed.

The aerosol scheme also includes resuspension of mineral aerosol as a function of friction velocity and the nature of soil; both the direct entrainment of small particles (Loosemore and Hunt, 2000) and saltation, i.e. the indirect entrainment due to large particles which fall back to the soil and entrain smaller particles (Claiborn et al., 1998) is taken into account.

Meteorology

Meteorological data needed by RCG at hourly intervals consist of layer-averaged 3-D gridded fields of wind, temperature, humidity and density, plus 2-d gridded fields of mixing heights, several boundary layer and surface variables, precipitation rates and cloud cover. In the operational version of the model, all this meteorological data is produced employing a diagnostic meteorological analysis system based on an optimum interpolation procedure on isentropic surfaces developed at Freie Universität Berlin. The TRAMPER system utilizes all available observed synoptic surface and upper air data (Reimer and Scherer, 1992). Alternatively, interfaces are existing for the output of the prognostic meteorological models MM5 or LM-COSMO.

Land use data

RCG can be run with any land-use data base that gives for each grid cell the fractional shares of the following land use classes:

- Urban areas
- Agriculture
- Grassland
- Deciduous forest
- Coniferous forest
- Mixed forest
- Water, marsh or wetland
- Sand, bare rocks
- Tundra
- Permanent ice
- Tropical forest
- Woodland scrub

Initial and boundary conditions

Initial and boundary conditions are derived internally using climatological background observations following the approach of EMEP (EMEP, 2003). Ozone background concentrations are taken from the ozone climatology derived by Logan (1998). Nested applications get their boundary conditions from the mother-domain.

Output quantities [top]

Four dimensional (x-y-z-t) concentrations fields in hourly resolution, dry and wet deposition fluxes of all active species in daily resolution.

Validation and evaluation [top]

RCG model evaluation was performed within many urban and regional applications and within the framework of several European model inter-comparison studies, see the following references:

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Hass et al., 2003
Van Loon et al., 2004
Van Loon et al., 2007
Stern et al., 2006
Stern et al., 2008
Cuvelier et al., 2007
Beekmann et al., 2007
Vautard et al., 2007
Thunis et al., 2007
Vautard et al., 2009

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