

J5.3 Development and first results of a new photochemical model for simulating ozone and PM-10 over extended periods

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The ambient air quality framework directive 96/62/EC (FWD) of the European Commission provides an EU-wide framework for national, regional and local measures to improve or maintain air quality. According to the directive, the Member States have to assess air quality using measurements and/or air quality modeling. The requisite model should be capable of hourly predictions of O₃, CO, SO₂, NO₂ and PM₁₀ concentrations for periods of a year or more and be economical enough to permit repeated emissions scenario simulations.

This paper presents the first results of the new REM3/CALGRID model to assess European-wide O₃. A more complete description of the model and the year-long PM-10 results for 1997 can be found in the Stern & Yamartino (2001) reprint from the 5th GLOREAM Workshop (GLObal and REgional Atmospheric Modelling -- a subproject under EUROTRAC-II) at:

http://people.web.psi.ch/keller_j/GLOREAM/WS2001/WS01_frameset_proceedings.html

Rather than creating a completely new model, the urban-scale photochemical model CALGRID (Yamartino et al., 1992 and 1996) and the regional scale model REM3 (Hass et al., 1997) were used as the starting point for the development of the urban/regional scale model, REM3/CALGRID. The new model's features include:

- A new methodology to eliminate transport operator-splitting errors on a generalized-metric, fixed-/dynamic-layer grid, and ensure correct fluxes, mass conservation, and preservation of constant mixing ratio fields;
- Updated releases of the SAPRC-93 and CBM-IV photochemical reaction schemes

including a 1-product isoprene scheme and SO₂ oxidation to SO₄;

- Two equilibrium aerosol modules that treat the thermodynamics of inorganic sulfate, nitrate, ammonium and chloride aerosols and water; and
- An emissions interface that enables on-the-fly calculation of hourly anthropogenic and biogenic emissions, and greatly facilitates emissions reduction scenario studies.

Ozone was simulated for one year using the CBM-IV chemical mechanism on a domain that covers Central Europe with a resolution of 0.25° latitude and 0.5° longitude. The year 1997 was selected given the availability of O₃ background (Logan, 1998) data having a resolution of 5 by 4 degrees. The model was run with four vertical layers: a 20 m thick surface layer, two equal-thickness layers below the mixing height, and one above the mixing height and extending to the domain top at 2500m. Hourly meteorological data are provided by a Diagnostic Meteorological Analysis System (Reimer and Scherer, 1992). Hourly emissions are computed on-the-fly using CORINAIR annual data, and factors dependent on source group, month, day-of-week and hour.

Figure 1 shows reasonable agreement of the time series of modeled and observed hourly O₃ in August 1997 at a German rural station. Figure 2 shows the daily maximum-hourly O₃ over the year at two rural stations, one in Germany and one in Switzerland. Overall, the model is able to reproduce the observed O₃ time series rather well if a station is representative of the model scale. This good overall performance can be seen from the Figure 3. scatter diagram of predicted and observed daily maximum, 8h-average O₃ at 90 European rural stations.

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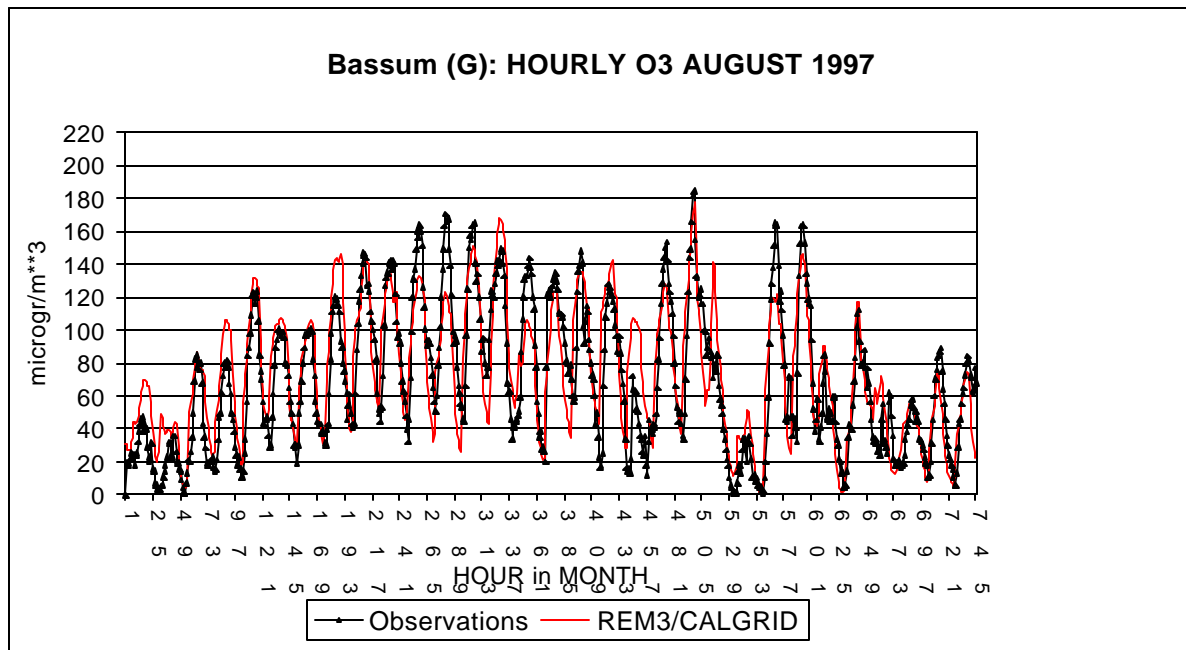


Fig. 1: Modeled and observed hourly O₃-time series at the rural station Bassum, Germany

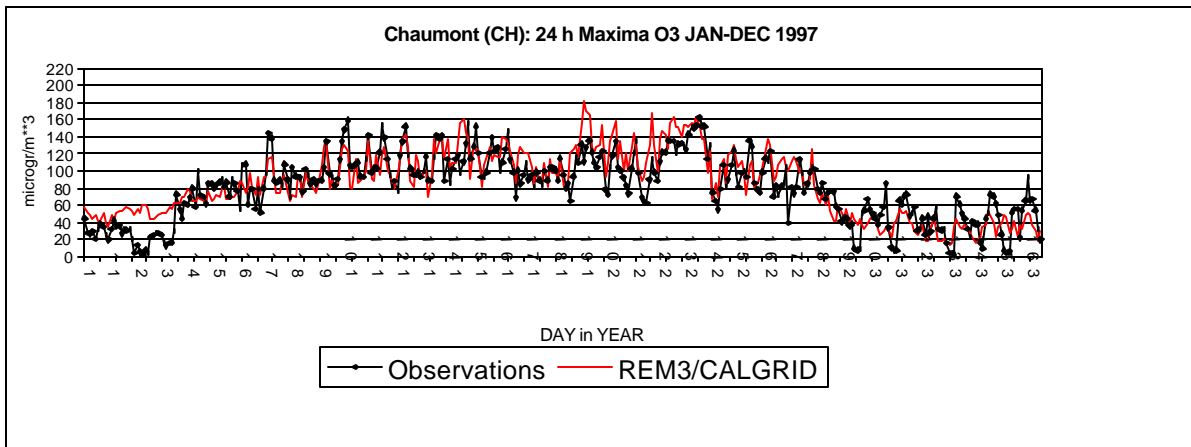
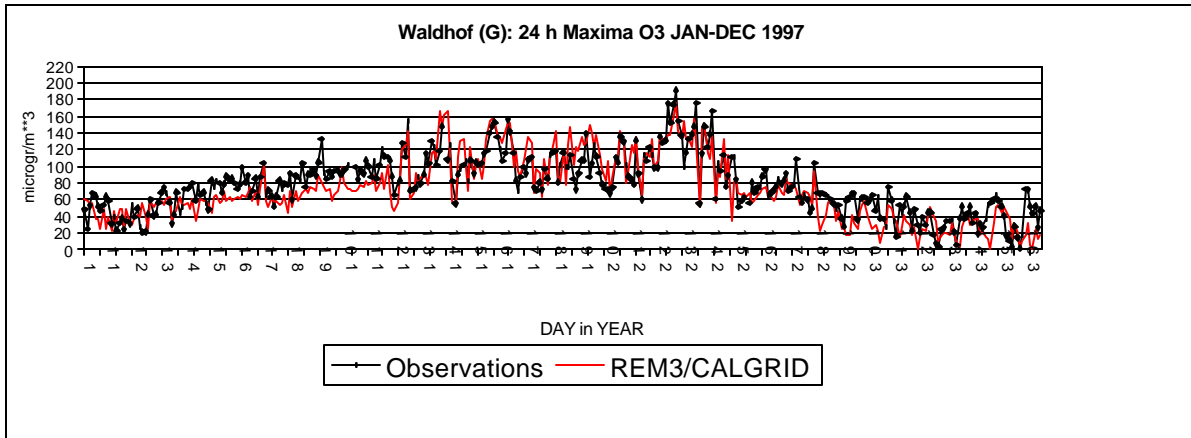


Fig. 2: Modeled and observed daily O₃-maxima at two rural stations: Waldhof, Germany, Chaumont, Switzerland

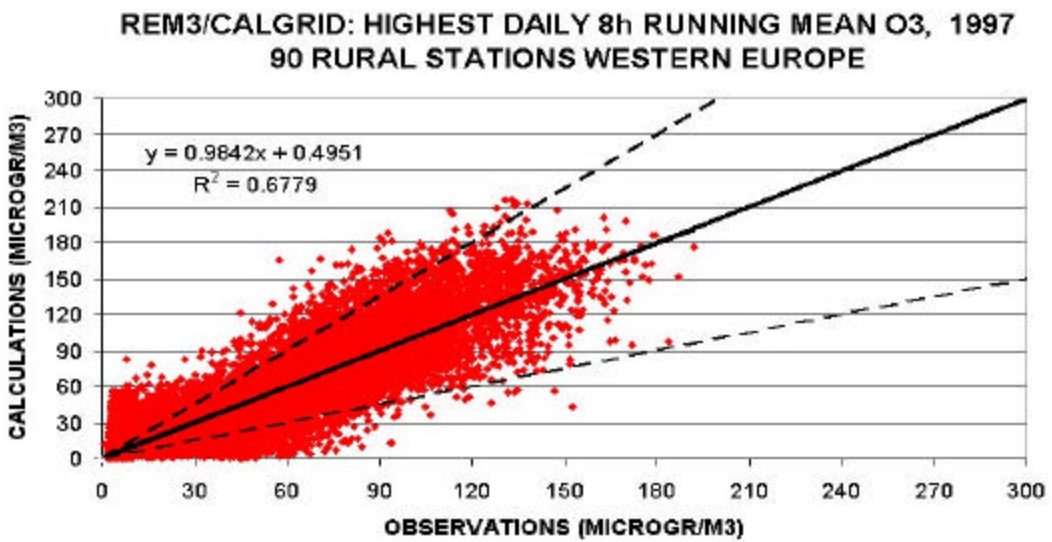


Fig. 3: Scatter diagram of observed and calculated highest daily 8h running mean O₃.