Evaluation of European emissions created with a modified version of the SMOKE model

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1. INTRODUCTION

Chemistry transport models (CTMs) are used for a variety of purposes (air quality modelling, source attribution, assessment of abatement strategies, etc.) with modeling domains reaching from global coverage down to local scales. In addition to the meteorological data, lack of knowlegde on emissions introduce a major uncertainty to the CTM modeling results (Russell, 2000; Seaman, 2000; Hanna and Davis, 2001; Anderson and Langner, 2005; Sofiev et al., 2009).
Besides proprietary emissions models which are not publicly available, there are several public models. Each of these models has its own restrictions: Compatibility to a certain CTM, temporal coverage, spatial resolution for regional modelling or the focus on a single nation or region. The EMEP emission data provided by MSC-W have a high temporal coverage for all of Europe with spatial resolution of 50x50km². Temporally disaggregated emissions are not published (Webdab, 2010). The Dutch CTM LOTOS-EUROS developed by TNO and RIVM as well as the French CTM CHIMERE have their own emission models producing suitable emission data (Schaap et al. 2005; Vautard et al. 2007). Yu et. al. adapted the SMOKE model to create emissions for the UK (2007). The Dutch TNO and the German IER emission models are two widely used emission models capable of producing high resolution emissions but are not public. (Friedrich and Reis, 2004; Visschedijk et al. 2007). However, the emission datasets calculated by TNO can be obtained free of cost. The EDGAR emission database contains emissions of air pollutants on a 1x1 degree grid for the years 1990, 1995 and 2000 (Olivier, 2001). The before mentioned models are only some examples and do not cover all European emission models. Looking at the variety of emission models available for Europe the question arises what benefit can be gained by an additional model. The reason to develop this emission model is to provide a flexible tool capable of creating consistent high resolution emission datasets for long term CTM runs over Europe based only on open source data. Flexibility means that the model can be easily altered concerning the input data and output format and that new species or different photochemical splits can be implemented with a minimum amount of work. Consistency means that emissions for each year are calculated using similar input data and the same algorithms. This consistency approach is in contrast to many emission models, which use the best available data for each new report year, with report years usually being every five or ten years. This approach leads to a steady improvement of the emission datasets but comes at the cost of inconsistency with older datasets since these older report years are not available with the new methodologies. The model introduced in this paper is specifically designed for long-term CTM runs and thus needs to overcome these problems.

2. MODEL OVERVIEW

The emission model SMOKE is the official emission model of the Unites States Environmental Protection Agency (US EPA) and is one of the most used emission models world wide (Houyoux et al., 2000; MCNC Environmental Modelling Center, 2008; UNC Carolina Environmental Program, 2005). SMOKE was originally created by the MCNC Environmental Modeling Center (EMC) and developed further by the US EPA. It is the official emission model of the Models-3 Community Modelling and Analysis System (CMAS) and creates emission data suitable for CMAQ (Byun and Ching, 1999; Byun and Schere, 2006). Anthropogenic emissions are calculated using the 'Top-Down' methodology while biogenic emissions are calculated by the Bottom-Up model BEIS3 (Guenther et. al., 2000; Pierce et. al., 1998; Schwede, 2005). Although

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SMOKE is highly specialized for usage with officially reported data in the US, there have been several successful attempts to use it for other regions. In Europe, for example, SMOKE has been adapted to use the national emission inventories of Spain and the UK (Borge et al., 2008; Yu et. al. 2008).

The SMOKE emissions model follows a modular setup (Fig.1). Area, point, mobile and biogenic sources are calculated by different modules and merged into a single output file. In order to run SMOKE, four kinds of data are needed for the different species: The bulk emission inventory, spatial surrogates, speciation profiles, and temporal profiles. For Plume in Grid (PiG) calculations and biogenic emissions certain meteorological input data are needed additionally (eg. temperature, radiation, wind, humidity).

2.1 Modifications

Since the SMOKE model has been under development for over a decade, it is highly specialized on the usage of official data of the US. Thus, this model setup is not directly compatible to European data reporting schemes and several adjustments need to be made for the use of SMOKE for Europe (SMOKE-EU).

In order to achieve a high spatial resolution SMOKE uses emission aggregates on county basis and distributes them using static surrogates for each region. This is done by the *Grdmat* module which creates a single, static gridding matrix for each year. When used with European emissions aggregated on the national level these static surrogates lead to a static spatial distribution for each country over the whole year. This is a sound assumption for sources that are spatially static like for example mobile emissions which are connected to the road network throughout the year. For emissions that are influenced by local events, such as combustion for heating, static surrogates in combination with large or inhomogeneous regions can lead to an unrealistic emission distribution. This is due to the fact that the spatial distribution of heating demand is not static throughout the year but changing depending on the temperature. Furthermore the temporal disaggregation in SMOKE is done via monthly, weekly and hourly profiles. This can lead to strong emission changes between the last day of a month and the first day of the next month. In order to overcome these restrictions of SMOKE, in SMOKE-EU a new module has been introduced. The new module uses external data, temperature in this case, to create new gridding matrices for each day of the year (Bieser et al. 2010). This leads to a more realistic spatial and temporal disaggregation of the emissions (Fig. 1).

2.2 Input datasets

The bulk emission inventory contains the annual total emissions of CO, NO_X, SO_2, NH_3, Non-Methane Volatile Organic Compounds (NMVOC), primary particulate matter (PM) as PM10 and PM2.5 aggregated over for each country. Additionally the emissions are distributed over 11 SNAP source sectors (Selected Nomenclature for sources of Air Pollution). SNAP is a standard defined by the CORINAIR guidebooks which ensures that emissions reported by different nations are comparable (European Environmental Agency, 2007). The bulk emission inventory is is created from two pan-European emission inventories. Point sources are taken from the European Pollutants Emission Register (EPER) (European Commission 2000) and are merged with the annual national total emissions of the European Monitoring and Evaluation Program (EMEP) (Vestreng, 2007; Webdab, 2010).

These annual total emissions are disaggregate in time and space using a variety of datasets. The temporal distribution is done via sectoral emission profiles from the LOTOS-EUROS emission model (Builtjes 2003). The vertical distribution is calculated via Plume in Grid (PiG) algorithms using average stack data for different industrial sectors (Pregger and Friedrich, 2009). The chemical speciation for compatibility with the photochemical mechanisms used by CTMs is done with NMVOC split factors obtained from Passant (2002). The spatial disaggregation is done with the help of spatial surrogates. Spatial surrogates, proxies used to disaggregate the national total emissions to the emissions model grid, are applied following Maes (2009). Data used for spatial surrogates are population density, land use, vegetation maps, road and railway networks as well as statistical data.

3. COMPARISON OF CTM CALCULATED CONCENTRATIONS TO OBSERVATIONS

The CTM CMAQ4.6 of the US EPA was used to simulate atmospheric concentrations of air pollutants for the year 2000 (US EPA, 2009). The spatial resolution is 54x54km² with 30 vertical layers, the photochemical mechanism used is CB-IV. Meteorological fields are taken from the COSMO-CLM model (Rockel and Geyer 2008; Rockel et al. 2008). Monthly average boundary conditions were derived from the MOZART global model (Horowitz et al., 2003; Niemeier et al., 2006). With this setup, four CMAQ runs using different emission datasets from widely used European emission models were calculated. The emission datasets used for this comparison are described in Bieser et al. (2010). The calculated atmospheric concentrations in the lowest model layer were compared to observations from EMEP measurement stations. From 242 available rural measurement stations those with more than 90% data coverage for the year 2000 were used for comparison. Six different compounds are used for comparison, three gaseous species (NO_2 SO_2, O_3) and three aerosol components (SO_4, NH_4, NO_3). Ozone concentrations are given as hourly values while all other values are reported as daily averages.

It could be shown that the vertical distribution has a strong influence on the simulated SO_4 and SO_2 concentrations (Table 1). Generally, SO_2 emissions in higher altitudes have lead to higher SO_4 concentrations near the surface and a better agreement with observations. The largest differences between the four CTM runs were found for NH_4 and NO_3 concentrations. NH_4 was systematically overestimated while NO_2 was strongly underestimated over the Spanish peninsula (Fig. 2).

A regional analysis showed that for Sulfate, correlations as well as the fractional bias are low over the Spanish peninsula (Fig. 3,4). Values over the Scandinavian region mostly have correlations higher than 0.6 but have a strong spread in the fractional bias. These results can be explained by the fact that many Scandinavian observation sites are located in extremely remote areas with measurements near the detection limit which can lead to a large fractional bias. Values for central European measurement sites on the other side tend to cluster between a fractional bias of -0.2 and +0.2. The regional analysis shows that the CMAQ runs for all four emission datasets give similar results.

Ozone concentrations which are strongly influenced by the meteorology were almost identical for all datasets (Fig. 5)

4. CONCLUSIONS

The US-EPA SMOKE emission model has been successfully adopted and modified to use publicly available pan-European datasets in order to create high resolution emission data for Europe. Several preprocessors were developed which transform these datasets to create the input data necessary to run the SMOKE for Europe (SMOKE-EU) model.

CMAQ has been used to calculate atmospheric concentrations of air pollutants using the four different emission datasets. These are the TNO-GEMS dataset created by TNO, a dataset from IER purchased by GKSS and the official gridded EMEP emissions provided by the MSC-W. Comparison of simulated values with observations from EMEP measurement stations showed that each of the four CTM runs produced sound results.

By comparison with other emission datasets for the years 2000 and 2003 it could be shown that the project to create high resolution European emission data with the use of open source data only was successful. Emission data created by SMOKE-EU will now be used for European long-term CTM runs for the timespan 1970-2010. Being a very flexible tool, SMOKE-EU will be further enhanced in the future. Improvements planned are different temporal profiles for each country, implementation of further photochemical mechanisms and the implementation of additional species (benzo[a]pyrene, mercury).

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6. FIGURES AND TABLES

	SO_4	SO_2
EMEP 3D	0.61 ± 0.18	0.98 ± 0.83
EMEP 2D	0.58 ± 0.16	1.2 ± 1.18
TNO-GEMS 3D	0.55 ± 0.19	0.99 ± 1.03
TNO-GEMS2D	0.54 ± 0.16	1.06 ± 1.2

Table 1: Comparison of mean concentrations of SO_4 and SO_2 with and without vertical distribution. Values are averages over all measurement stations (51 stations for SO_4, 33 stations for SO_2) and their standard deviations.

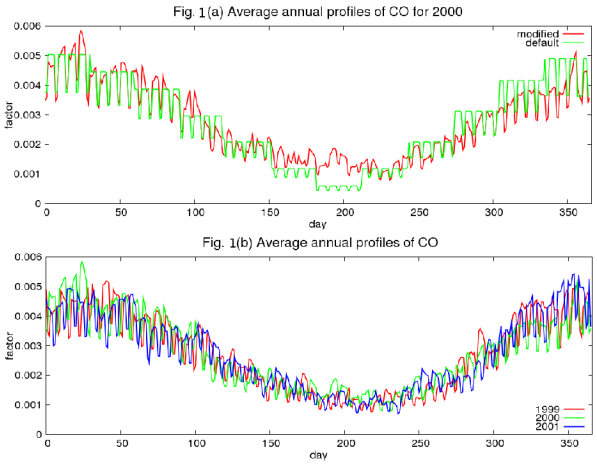

Fig. 1a: Annual average temporal profiles using the original SMOKE setup (default) and the modified version (modified). 1b: Comparison of temporal profiles of residential heating sector for three years using meteorological data for disaggregation (Aulinger et al. 2010).

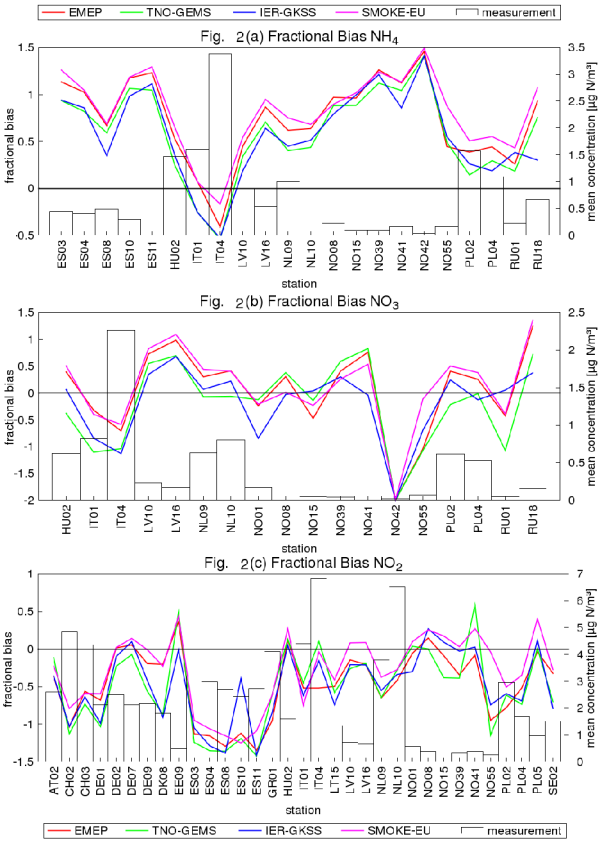

Fig. 2: Comparison of CMAQ calculated daily average air concentrations with observations from EMEP remote measurement stations. Colored lines indicate fractional bias of CMAQ runs using four different emission datasets. The black bars indicate the annual average concentrations measured at the site. a) NH_4, b) NO_3, c) NO_2

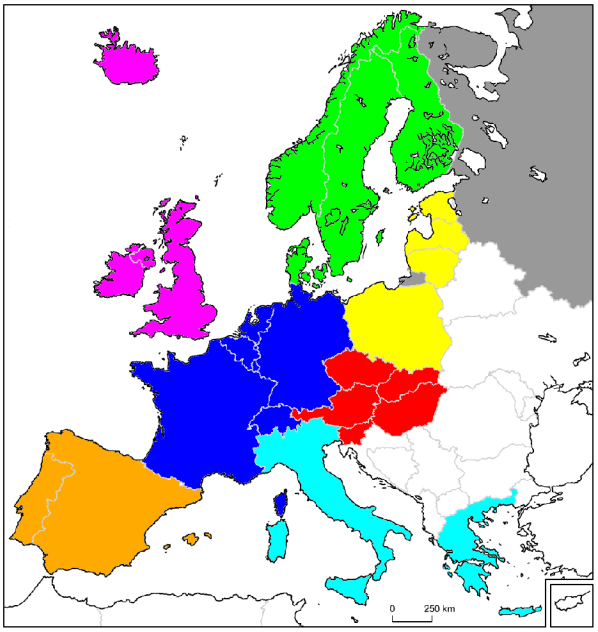

Fig. 3 Modelling domain covered by SMOKE for Europe. Colors indicate different regions used for a regional analysis (Fig. 4 and 5).

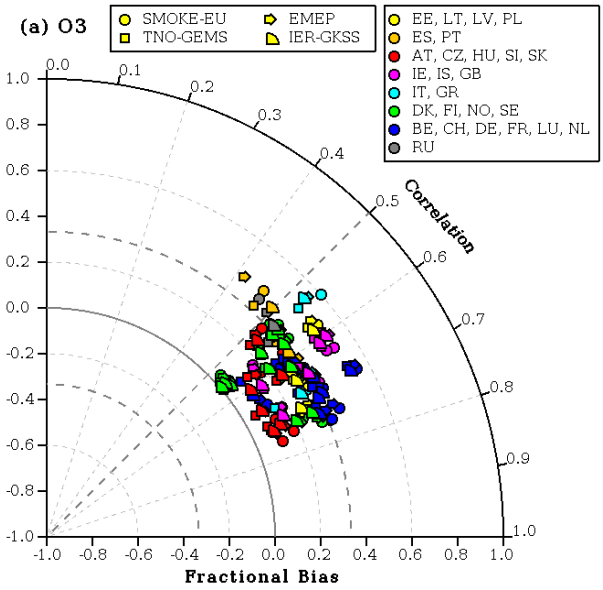

Fig. 5 Regional analysis of Ozone concentrations. Different shapes indicate the emission model used for CMAQ calculations. Different colors indicate regions of the measurements stations used (see Fig. 3).

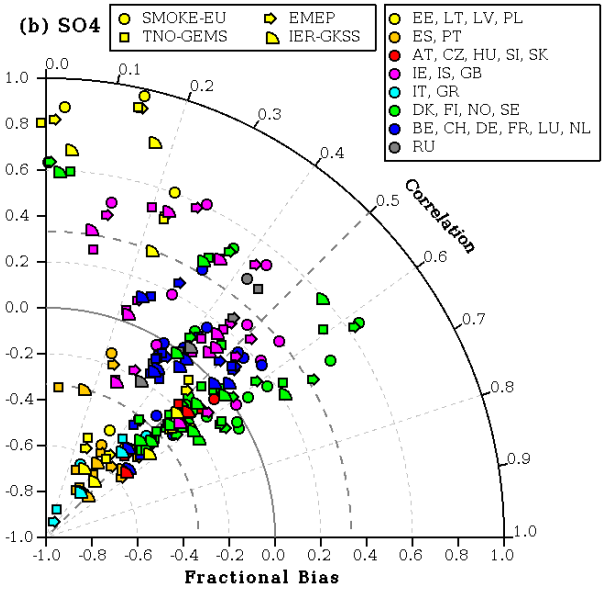

Fig. 4 Regional analysis of Sulfate concentrations. Different shapes indicate the emission model used for CMAQ calculations. Different colors indicate regions of the measurements stations used (see Fig. 3).