EVALUATION AND VALIDATION OF THE OPS MULTI-SCALE DISPERSION MODEL USING LOCAL, NATIONAL AND INTERNATIONAL DATASETS

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INTRODUCTION

The Operational Priority Substances (OPS) model has been used since the late eighties for calculating high resolution atmospheric concentrations and depositions in the Netherlands. As such the model has become the *de facto* standard for deposition calculations on the national scale. Because of the wealth of available data, the validation of the model is historically based on comparisons with observations of the National Air Quality Monitoring Network (LML). This network consists of stations where primary (SO_2, NO_x, NH_3 on a hourly basis), secondary (SO_4^{2-}, NO_3^-, NH_4^+ on a daily basis) and wet deposition (SO_x, NO_y and NH_x on a monthly basis) compounds are measured since the mid 1970's. The set of data allows for an extensive comparison of measured and modeled time series and, due to the density of the network, also for a comparison of spatial differences. Together they give insight in the capability of the model to account for meteorological influences and terrain properties. Such a comparison, however, concerns the sum of the contribution of all sources, locally, nationally and internationally. It does not explicitly say anything about the influence of local sources or of a certain type of sources. It is therefore important, even for regional scale models, to test the performance of the model in relation to single source contributions and as a function of different source characteristics.
In this paper the results of comparisons with various datasets are presented among which the well known Prairie grass data and the Kincaid dataset.

MODEL CHARACTERISATION

The OPS model represents a combination of a plume model based on an analytical solution of the advection-diffusion equation for local-scale application and a trajectory model for long-range transport (*Van Jaarsveld*, 1995; 2004). This approach has the advantage that local contributions can be calculated and combined with background contributions in a single model run. The sum of these contributions can be compared directly with observations at (sub) urban sites as well as on rural sites. This multi-scale approach makes it easy to use a variety of existing observations for validation purposes.
Since acidification and eutrophication are basically long-term deposition problems the model was set up to produce long term averages (annual or monthly). An efficient method to calculate averages was found by means of arranging situations occurring in classes having similar properties and then calculating representative (short-term) concentrations for each of the classes. The average value will then follow from a summation of all concentrations, weighted with their relative frequencies. For long range contributions the most important classes are transport distance, transport direction, mixing height and transport speed. For local contributions additional classes for friction velocity and Monin-Obukhov length are used. All relations governing the transport and deposition process are solved analytically, allowing the use of non-gridded receptors and sources, and variable grid sizes.

Meteorological data

The basic meteorological data needed by the model is taken from the KNMI network in the Netherlands. The data includes wind, temperature, radiation and precipitation at 10m level at 14 sites and wind data at 200m level from the Cabauw meteorological tower.

Emission data

SO_2 and NO_x emission data for the Netherlands has been taken from the Dutch Emission Registration system (*Berdowski*, 1994). The basic resolution for the Netherlands is 5x5 km, but also data for a large number of individual point sources is available. For an area of approximately 400x400 km – including the Netherlands and parts of Belgium, along with former West Germany – emission of SO_2 and NO_x was inventoried by TNO (*Veldt*, 1981). Emission data for the rest of Europe is taken from the UNECE/EMEP database (*Webdab*, 2002).

VALIDATION

Comparison on the national scale

The basic model validation includes concentrations of sulphur dioxide and sulphate, nitrogen oxides and nitrate, ammonia and ammonium both in ambient air as well as in precipitation. Comparing with time series of measurements gives insight in the capability of the model to account for meteorological influences with emphasis on long-range transport. Figure 1 gives the results for SO_2. The highest monthly mean SO_2 concentrations occur during wintertime and are caused by the combination of (persistent) easterly winds, low mixing volumes and frozen or snow-covered soil. In these cases the low mixing volumes are combined with high emissions in Eastern Europe and low deposition losses. Similar (meteorological) episodes are presently not related with high concentrations anymore because of very large sulphur emission reductions in the so called 'black triangle'.

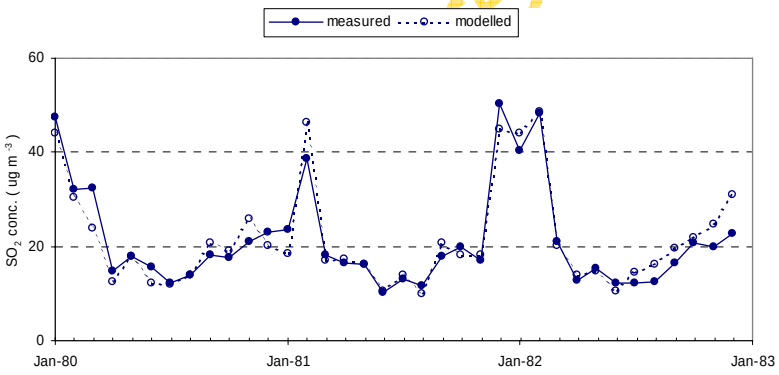

Figure 1; Calculated SO_2 concentrations compared with observations. Values represent spatial averages for the Netherlands (SO_2: 97 locations)

In terms of spatial variability the model produces similar patterns as the measurements (Figure 2). In this case annual average concentrations are compared in order to eliminate meteorological influences as much as possible. The spatial agreement between model and measurements is now to a large extent determined by the quality and spatial resolution of the emission data. Note that we are still comparing calculations on the basis of grid cell average emissions with point observations. In case of urban of semi-urban areas this may explain part of the differences. The problem of emission resolution is further addressed at the ammonia case. The model performance for NO_y species is similar to that of SO_x.

Comparison on the local scale

An example of a comparison on a local scale is given in Figure 3. This example is from a recent study in which it was investigated to what extend local emissions could explain local concentration levels (*Smits et al.*, 2005). Ammonia emissions within an area of 3x3 km were

inventoried on the farm level while measurements were carried out using a passive sampler method on a two weekly basis from august 2002 till august 2003.

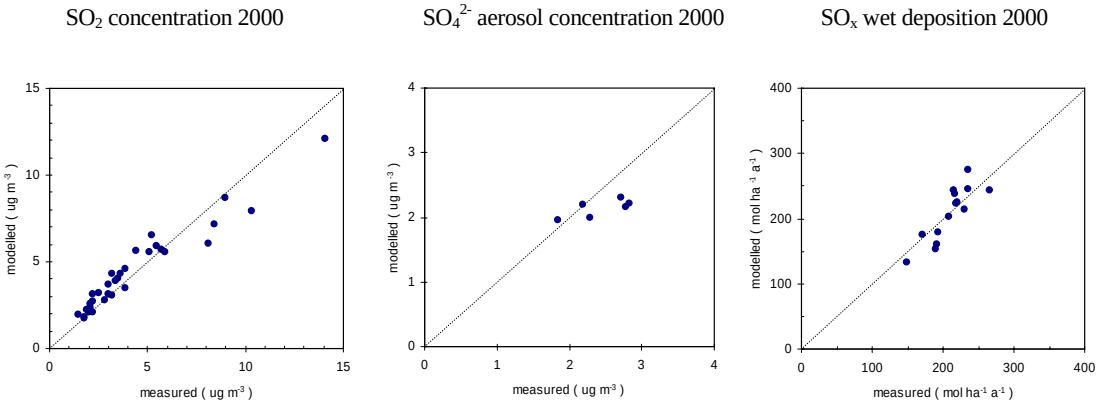

Figure 2; Comparison of the spatial distribution of annual mean measured and modelled SO_x concentrations, and wet deposition

The average concentrations within the 3x3 km area show a difference of a factor 3. Modeled levels are, on average, 15% lower than the observations. This underestimation is in agreement with earlier studies in the Netherlands and is known as the 'ammonia gap'. The reason for this gap is most probably a combination of uncertainties in the ammonia emissions and the parameterization of the dry deposition process in the OPS model (*Van Pul et al.*, 2004). More important is that the OPS model explains 75% of the spatial variations. This result supports the suggestion that the success of local model studies is mainly determined by the quality and detail of the emission data.

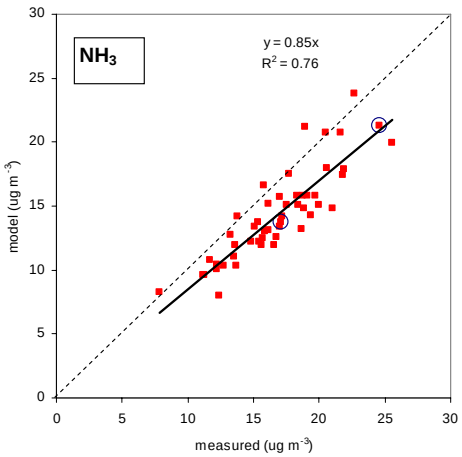

Figure 3; Comparison of measured and modeled NH_3 concentrations for 50 locations within a 3x3km area. The averaging period is from august 2002 to august 2003

Comparison for a single high stack source: the Kincaid case

The ability to calculate the contribution of single stacks to local concentration levels is demonstrated by a comparison with the Kincaid dataset. The Kincaid case concerns a 187 m

stack of a power plant in relatively flat terrain. In this case the long term version of the model is tested and therefore the comparison is carried out for two consecutive 4-week periods. In both cases more than 90% of the stations were within a factor 2 of the measurements, while the correlation was 0.7 and 0.6, respectively.

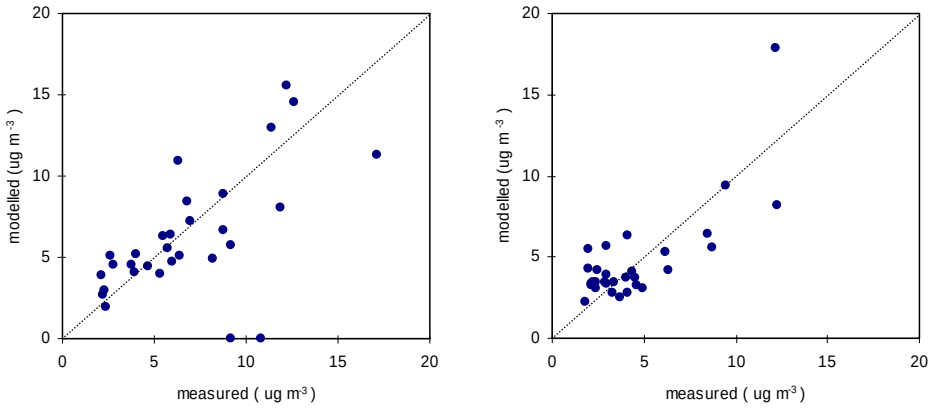

Figure 4; Comparison of measured and modelled SO_2 concentrations around the 187-m Kincaid stack. Left: 26 April-23 May 1980. Right: 23 May-23 June 1980.

Comparison for a single low stack source: the Prairie grass case

The Prairie grass experiment concerns the release of SO_2 at 0.46 m above the surface while at 3 distances (50, 200 and 800 m) arc-wise concentrations are measured. This experiment is especially suited to test the dispersion from near surface emission sources such as ammonia evaporating from manure. For the comparison the cross-wind integrated concentrations of *Van Ulden* (1978) are used and also the secondary meteorological parameters as friction velocity and Monin-Obukhov length. The results in Figure 3 show a good agreement for all down-wind distances. Also, if a distinction is made in atmospheric stability, the agreement is good (not shown). Strictly speaking, with the present comparison on the basis of cross-wind integrated concentrations, only aspects of horizontal transport and vertical diffusion are tested. Nevertheless, the performance of the OPS model for near-surface sources seems comparable or even better than more dedicated models.

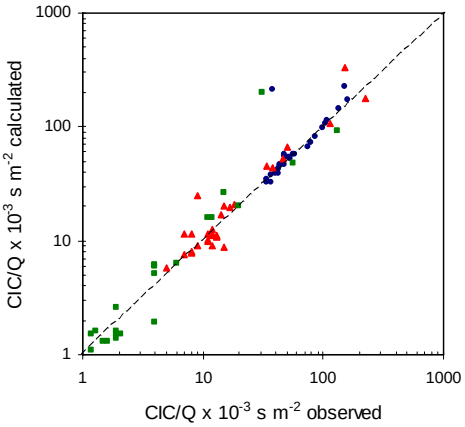

Figure 3; Comparison of calculated and measured cross-wind integrated concentration (CIC) divided by the source strength for three down-wind distances. Circles: 50 m. Squares: 200 m. Triangles: 800 m.

Comparison with other models

The most important product of a dispersion and transport model within the acidification issue is not the atmospheric concentration but the deposition flux. Measured fluxes, however, are seldom available. In such a case with little hard data available one can also compare results with results of other models. A first intercomparison of model results was carried out by *Derwent et al*., (1989). Recently, a selected set of analyses has been performed with the OPS model as part of the evaluation of the EMEP Unified (Eulerian) model (*Tarrason et al.,* 2003).The analyses concentrated on the concentration and deposition of SO_x, NO_y and NH_x species in the Netherlands and on the source-receptor relations for the Netherlands and surrounding countries (*Velders et al*., 2003). In terms of total deposition to the Netherlands the models agree rather well. Part of the differences between the models can be explained by different dry deposition parameterizations.

CONCLUSIONS

From the comparisons given it can be concluded that local dispersion from individual low and high sources under various meteorological conditions is modeled satisfactorily. A further conclusion is that spatial differences in concentrations can be simulated very well, provided that emissions are known with high spatial detail. Finally, the dynamics of monthly mean concentration variations are shown to be well simulated. High concentrations of SO_2 and NO_x in the Netherlands appear to be related to specific source-receptor directions, low mixing volumes and enhanced emission rates, but a dominant parameter may be also the (temporarily) low dry deposition rate.

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