Scenario analysis of a summer smog episode in Berlin

P. Mieth, S. Unger, A. Sydow

GMD - Research Institute for Computer Architecture and Software Technology, Rudower Chaussee 5, 12489 Berlin, Germany

ABSTRACT

A mesoscale model (Eulerian type) including a meteorological and dispersion part was coupled with the chemical scheme of Carbon Bond IV to investigate the ozone production in the conurban area of Berlin. In cooperation with the Environmental Agency of the Senate of Berlin a realistic summer smog episode was simulated. In order to find strategies for an effective smog management scenario analyses were computed under different emission conditions. A dominant influence of ozone concentration and concentrations of precursor substances of ozone transported into the city on surface-near ozone concentrations is clearly visible. In case of typical meteorological conditions for the region of Berlin a traffic reduction leads to an increase of the ozone concentration in the city but to a decrease of ozone in the rural area. All scenarios always show regions with improved air quality and others suffering from negative tendencies.

INTRODUCTION

High ozone concentrations are among the hazardous environmental problems in regions with high solar radiation and anthropogenic emissions. But in Middle Europe ozone concentration can also reach considerable values under certain meteorological conditions. Under these circumstances the environmental agencies are demanded to take measures to limit critical amounts. But up to now they only have warned the population of an area to leave closed rooms, e.g., or they have asked them to reduce private traffic.

Before we can discuss effective measures against summer smog we have to consider and to understand all processes involved in the production of ozone. Obviously, the reduction of man-caused emissions always improves the air quality. But this is extreme hard to realise in a scale greater than regional one. It only seems to be possible for a more or less short time on a regional scale. But even in a regional scale it is very difficult to assess the effect of local emission reductions, especially because of the nonlinear character of the photochemical processes. Atmospheric models can help to identify different processes leading to critical ozone concentrations. In the last decades a lot of atmospheric models have been developed. Most of them are research models and hardly applicable for environmental agencies. Additionally, sophisticated models use a huge amount of computation time. In order to compute different scenario analyses a reasonable run time is essential. That is why we implemented an Eulerian meteorological and dispersion model with a relatively high level of
approximation. Nevertheless the model is able to describe the most important processes quite well. A parallel formulation of the program code helps to increase the computation speed.

In cooperation with the Senate of Berlin we simulated a lot of emission scenarios to find out possibilities to decrease ozone levels.

MODEL DESCRIPTION

For the computation of meteorological values and of the dispersion the Eulerian grid model REWIMET [1] is used. It is based on the conservation laws for impulse, mass, energy and passive constituents. According to the aim to determine the concentrations in a regional scale with a resolution of 2 km the model is formulated for the mesoscale. A hydrostatically stratified atmosphere is assumed, which is dry and incompressible. The model equations are expressed in three vertical layers. The first (surface layer) follows the ground level and has a fixed vertical thickness of 50 m above ground. It is turbulent mixed and its physical behaviour is strongly coupled with the surface characteristics. Emissions from traffic, from households, and from industrial sources with low emission heights are introduced into the surface layer. The second layer (mixed layer) reaches from the upper level of the surface layer to the upper level of the atmospheric boundary layer, up to the mixing height. This layer is also turbulently mixed and shows the characteristic diurnal variation of the thickness of the atmospheric boundary layer. Emissions from higher emission sources, for example high stacks from power stations, go into the mixed layer. The third layer (temporary layer) is located above the mixed layer. It is assumed to be free of turbulence. Since the atmospheric boundary layer can grow up to the suprascale inversion it is possible that the temporary layer disappears. It will be recreated when the atmospheric boundary layer sinks. No substances are emitted in this layer but it carries the suprascale background concentrations of ozone and ozone precursor substances above the atmospheric boundary layer.

The model REWIMET is driven by a time dependent geostrophic wind and an initial vertical temperature profile. The diurnal variation of surface temperature is determined by land utilization.

For a computation of the chemical reactions the Carbon Bond Mechanism IV (CBM IV) [2] has been chosen. This is a popular and sufficiently tested reaction scheme describing the most important chemical processes in the gas phase for the computation of ozone. CBM-IV is a condensed version of the extended CBM-version, a lumped molecule model. Carbon atoms with similar bonding are treated similarly. There is no need for the definition of an average molar weight so that this mechanism is mass balanced. Some species are handled explicitly because of their special character in the chemical system. The mechanism involves 34 species and 82 reactions and it contains 9 primary organic compounds.

In order to secure a high level of accuracy and stability the chemical module is executed every dispersion time step.

The program code has been developed to implement it on different hardware platforms. It runs on an UNIX-PC as well as on a supercomputer. But because of the high demand of computation time a parallel version of the program has been developed and tested on different parallel machines with distributed memory [3], e.g. on the CM-5, on the MANNA (a house intern parallel computer), on a PARSYTEC Transputer cluster, and on a cluster of SUN-Workstations. For the purpose of a parallel code the model area is subdivided into subareas according to the given number of processor nodes (method of geometrical decomposition). The efficiency increases as much as the number of grid elements.
The simulation system is embedded in a graphic environment and coupled with a small geographical data base.

**DATA BASES**

The model domain is the conurban area of Berlin. This area of about 50x50 km extension is flat and shows a relatively weak orography. The topographical data base consists of a grid averaged altitude and the percentage of land utilization in a resolution of 2x2 km according to the computational grid size. Special solicitude has to be taken in order to obtain the emission data. Relatively accurate data are given for the big emittents, e.g. the power plants. But from the most emittents, e.g. the traffic, only the yearly emissions are roughly known. In addition, information about the hydrocarbon composition and dynamics is rare. Some statistical methods are used to improve the dynamical description of the emission process, e.g. vehicle countings. An averaged distribution of the hydrocarbons into the primary classes of the chemical module has been used.

An overview of the distribution of the emissions of NOx and VOC’s of five emission sources of the model is shown in Table 1. The main source for the hydrocarbon emissions is the traffic emitting into the surface layer, whereas NOx is mainly emitted by few power plants into the mixed layer.

<table>
<thead>
<tr>
<th></th>
<th>industry (emissions into the m-layer)</th>
<th>industry (emissions into the s-layer)</th>
<th>moving traffic</th>
<th>standing traffic</th>
<th>households (solvent emissions)</th>
</tr>
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<tbody>
<tr>
<td>VOC</td>
<td>4 %</td>
<td>20 %</td>
<td>38 %</td>
<td>22 %</td>
<td>16 %</td>
</tr>
<tr>
<td>NOx</td>
<td>66 %</td>
<td>4%</td>
<td>30 %</td>
<td>-</td>
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Table 1: Distribution of the emissions of different emission sources (in percentage of the yearly summary emission)

**DESCRIPTION OF THE EPISODE / STANDARD CASE**

Because of an accompanied measuring campaign of the Senate of Berlin we chose the 27.6.1990 as model episode. The measured wind lay between 3 and 5 m/s south-east, a temperature of 29 °C was reached and the sky was nearly clear. During the measuring campaign a maximum ozone concentration of about 180μg/m³ was determined in the rural area in the lee of the city, located approximately 50 km away from the city centre. Unfortunately, these locations are already out of our model domain. Despite of that, the computed distribution agreed very well with the measured values. The highest computed values lay in the rural area in the lee of the city (Figure 1). In order to achieve a greater effect of the anthropogenic emissions in the model area we assumed a lower geostrophic wind speed to define the standard situation. It can be considered as a case study with lower wind speed. In comparison with the original episode a remarkable increase of surface ozone concentration is determined. The reached maximum ozone level is about 1/3 higher and a lot of areas are polluted with high ozone concentrations.
Figure 1: Ozone concentration [μg/m³] in the area of Berlin on June 27, 1990, at 4 p.m.

SENSITIVITY STUDIES

The processes leading to high ozone concentrations are very complex. Mixing from stratospheric levels to the ground as well as the production of ozone from anthropogenic and natural ozone precursor substances, nitrogen oxides (NOₓ) and volatile organic compounds (VOC) can lead to high ozone concentrations even in considerable distances from the emission sources.

In order to study what is important for the formation of ozone a lot of simulation runs have been executed varying of different parameters (called sensitivity studies). The following parameters are varied:

meteorological parameters:
- geostrophic wind speed
- geostrophic wind direction
- cloudiness
- temperature
- humidity

other parameters:
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- deposition rates
- ozone and ozone precursor concentrations of inflowing air

Obviously, the geostrophic wind effects very strongly the obtained results. In nearly calm situations the ozone level is drastically increased especially in the plume in comparison to situations with medium wind speeds (Figure 2).

Figure 2: Diurnal variation of the maximum ozone concentration [\(\mu g/m^3\)]

- Standard : \(V_{geo} = 3 \, m/s\)
- Episode : \(V_{geo} = 11 \, m/s\)

Cloudiness reduces the photolytic reaction rates leading to a remarkable decrease of ozone concentrations in the whole model area. A considerable effect is determined in case of a reduction of the temperature. The humidity plays a relatively small direct role in the production of ozone but influences the energy budget.

The correct modelling of the ozone deposition is essential for the description of the strong diurnal variation of surface ozone concentration. Dry deposition is the main ozone destruction process during the night. If the dry deposition of ozone is neglected, the ozone concentrations in the night are overpredicted.

All parameters mentioned above are more or less known with a sufficient accuracy to obtain realistic simulation results. But generally very little is known about the ozone and ozone precursor concentrations of inflowing air and their diurnal variations during a given day. As simulation runs show, the quality of obtained results in a mesoscale model very strongly depends on these values. The main amount of ozone is transported into the model region or caused by the production of ozone from inflowing precursors (e.g. more than 80 percent except under calm conditions). If only a mesoscale model shall be used without nesting it in a suprascale model to obtain boundary values (which, of course, causes a lot of new difficulties and needs additional computation time), we propose to model the suprascale chemical values with the help of a huge chemical box in which the model area is embedded. In this case only the initial mean concentration of precursor substances with a certain vertical
resolution must be given. The diurnal variation of all species used in the chemical module is computed for the horizontal and vertical boundary elements. With the help of this method the ozone production in relatively small areas can be considered with no essential increase of computation time.

SCENARIO ANALYSIS

The computation of scenario analysis is the main tool to prove the effect of emission reduction measures in comparison to a standard case. The following examples are computed on behalf of the Senate of Berlin:
- traffic reduction and increase in different levels
- modification of the composition of the emitted hydrocarbon- mixture
- closing of the inner city for private traffic
- introduction of catalysts for all cars
- reduction of solvent emissions from households
- variation of emissions of industry
- measures effecting only one group of emitted substances

Under typical meteorological conditions for summer smog in the area of Berlin most of these local measures increase ozone levels in the city but decrease the ozone values in the lee side of the town. Some results should be presented for a hundred percent reduction of the emissions of the moving traffic. In Fig. 3 the decrease of the number of grid elements polluted with values greater then 180 µg/m³ (which serves as a limit for warning the population in Berlin) is considerable. In comparison to the standard case only one third of the former high polluted areas show ozone values greater than 180 µg/m³. So the reduction of traffic might be effective in order to avoid locally high values of ozone. But the results of reducing emitted values of ozone precursors for a

![Number of Grid Elements vs Time Graph](image)

**Figure 3: Number of grid elements with ozone concentrations greater than 180 µg/m³**

- **Standard**: without emission reduction
- **Scenario**: with a complete stop of the traffic
fixed amount are neither uniform in time nor in space. E.g. a complete stop of the traffic leads to an increase of higher polluted areas from morning till midday, but then it starts to decrease. The most positive effect is determined at the moment when the maximum ozone concentration is reached (about 4 p.m.).

Analysing the local distribution of ozone concentrations at 4 p.m. in comparison to the case without any emission reduction always shows regions with improved air quality and others suffering from negative tendencies relating to ozone (Figure 4).

Figure 4: Difference plot of ozone concentrations [μg/m³] at 4 p.m. without emission reduction and under the condition of a complete stop of the traffic; positive values express a decrease of ozone.

In the city centre as well as in some parts of the pollutant plume of the city the ozone level increases. These areas show a high concentration of nitrogen oxides in relation to the hydrocarbon concentration. It is well known that NOx-control under these circumstances leads to an increase of ozone, and emission reduction of traffic causes a reduction of both classes of precursor substances. Besides of these comparably small areas the ozone concentration decreases in a broader range. Especially in the former extremely high ozone polluted areas the air quality improves considerably. A reduction of hydrocarbon emissions only, which also has been computed, causes always and everywhere a decrease of ozone, but generally to a much lower extent. If
we do not only focus our interest on ozone, we will have to bear in mind that all emission reduction measures always lead to a decrease of primary air pollutants and, additionally, to a reduction of some other probable hazardous secondary substances like peroxyacetyl nitrate. It seems to be very difficult to reduce ozone levels with regional limited emission reduction in summer smog situations in the model area of Berlin but it should be possible to improve the integral air quality.

CONCLUSIONS

Because of the complexity and nonlinearity of the involved processes the results can hardly be generalized. Nevertheless, some facts should be mentioned:
- The formation of ozone concentrations in the model area is mainly caused by ozone and ozone precursor substances from outside. To reduce the ozone concentration in the centre of Berlin large scale emission reduction measures are necessary.
- Especially under meteorological conditions with low wind speeds, high solar radiation and high temperatures anthropogenic emissions in Berlin cause a considerable ozone production in the lee side of the town (up to 50 percent of the ozone level in certain areas). Obviously, these especially high ozone concentrations can be reduced quite well due to lower emissions in Berlin.
- Emission reduction measures usually reduce emissions of hydrocarbons and nitrogen oxides as well. In areas with a high level of nitrogen oxides these reduction measures mostly lead to an increase of ozone. In locations with relatively low concentrations of nitrogen oxides and high concentrations of hydrocarbons emission reduction measures help to decrease ozone concentrations quite effectively. Practically imaginable measures always cause areas with improved air quality and others suffering from an increase of ozone. But these areas showing higher ozone concentrations under emission reduction conditions formerly were not high polluted with ozone, and areas showing a decrease of ozone used to be the most ozone polluted ones. Additionally, ozone is not the only air pollutant. Despite of a probably weak increase of ozone in the city centre as a consequence of local emission reduction measures the integral air quality as valuation of a lot of primary and secondary air pollutants improves.
- Although good results have been achieved by REWIMET some questions have remained unsolved. Especially the rough vertical resolution has to be improved. In a second version of a model environment (in progress) a more sophisticated and fully 3-dimensional meteorological model called GESIMA [4] will be used. Additionally, an enlargement of the model area and the incooperation of emissions in the surroundings of Berlin are in progress.

REFERENCES