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INTERIM REPORT IR-97-002/January

A Model for Optimizing Strategies for Controlling Ground-Level Ozone in Europe

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Abstract

In the preparation process for the Second Sulfur Protocol of the Convention on Longrange Transboundary Air Pollution, integrated assessment models have played an important role in identifying cost-effective strategies for reducing SO_2 emissions in Europe. Applying this effect-based approach to other environmental problems (e.g., photo-oxidants) seems appealing. In view of the timetable adopted for the current preparation of an updated Protocol on emissions of nitrogen oxides, an integrated assessment tool for ozone is required in the near future.

The paper presents some core elements of an integrated assessment model for tropospheric ozone in Europe, with elements on emissions, emission control technologies and costs, ozone formation and environmental impacts. The focus of the paper is on a 'reduced-form' model describing the relationships between the precursor emissions and long-term concentrations of ground-level ozone. This reduced-form model has been developed from a large sample of scenario runs from a more complex model of ozone formation in Europe. Differences of model results between the reduced form model and the full ozone formation model are typically within a few percent.

Based on the reduced-form model, an optimization problem has been formulated to identify the cost-minimal allocation of emission reductions to achieve prespecified constraints on regional ozone levels. The non-linear problem has been successfully solved with three alternative optimization software packages.

Finally, the report introduces a number of exploratory optimization scenarios, (i) asssessing the optimal response of NO_x/VOC control for increasingly stringent constraints on ozone levels, (ii) identifying the measures required to compensate for non-compliance of individual countries, and (iii) comparing the features of health-oriented and vegetation-related strategies.

Acknowledgments

This work was carried out as part of the activities of IIASA's Transboundary Air Pollution project and was supported solely by IIASA's core funds. The authors are grateful to the Institute for providing the financial basis for this work.

The successful completion of this initial model would not have been possible without the active participation and collaboration of many scientists. The authors of this paper would like to express their thanks to:

- David Simpson and Prof. Anton Eliassen from the Norwegian Meteorological Institute, Oslo, for providing the EMEP model and contributing thoughtful comments on the reduced-form model;
- Steffen Unger and Prof. Achim Sydow (GMD-FIRST, Berlin, Germany) for transferring the EMEP ozone model to parallel computers and producing the large number of scenario runs;
- Prof. Paul Crutzen (Max Planck Institute, Mainz, Germany), Prof. Manfred Deistler, Technical University Vienna, Austria, Dick Derwent from the UK Meteorological Office, Prof. Adolf Ebel (University of Cologne, Germany), Bill Stockwell from the Frauenhofer Institute, Garmisch-Partenkirchen, Germany for their thorough review of the reduced-form model of ozone formation;
- Piotr Zawicki, Pavel Bialon and Janusz Granat (Technical University of Warsaw and summer students at IIASA) for their practical contribution towards operationalizing the optimization software;
- Andreas Öhler (University of Stuttgart, summer student at IIASA) for assisting in the reduced-form model for the AOT60;
- Marina Baldi and Giuseppe Calori (former colleagues at IIASA) for their help in compiling the database on ozone monitoring results;
- Prof. Greg Carmichael from the University of Iowa (USA) for his useful hints during the search for appropriate reduced-form models;
- Arne Drud from ARKI Consulting and Development, Denmark, for making the CONOPT library available and for his helpful hints on the formulation of the optimization problem;
- Prof. Georg Pflug from the University in Vienna (Austria) for offering his experience in tackling difficult statistical problems;

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- Gary Wojcik from the University of Albany, New York, USA and summer student at IIASA for his analysis of the role of background ozone;
- Mike Wenborn and colleagues of AEA Harwell, UK, for supplying the preliminary VOC cost curves.

A Model for Optimizing Strategies for Controlling Ground-Level Ozone in Europe

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1. Introduction

This paper outlines the current stage in the development of an integrated assessment model for tropospheric ozone in Europe. Section 1 introduces the concept of integrated assessment of emission control strategies and provides a brief overview of the various elements of an integrated assessment model for tropospheric ozone. Focusing on the core element, Section 2 presents an approach for deriving simplified source-receptor relationships between precursor emissions and tropospheric ozone in Europe. The optimization framework is introduced in Section 3. Section 4 provides a preliminary analysis of first test runs of the optimization model, and conclusions are drawn in Section 5.

1.1 Integrated Assessment of European Emission Control Strategies

The RAINS (Regional Air Pollution INformation and Simulation) model (Alcamo *et al.*, 1990) was developed at IIASA as an integrated assessment tool to assist policy advisors in evaluating options for reducing acid rain. Such models help to build consistent frameworks for the analysis of abatement strategies. They combine scientific findings in the various fields relevant to strategy development (economy, technology, atmospheric and ecological sciences) with regional databases. The environmental impacts of alternative scenarios for emission reductions can then be assessed in a consistent manner ('scenario analysis'). A further refinement in developing strategies is the search for cost-effective solutions. Integrated assessment models also enable the

identification of those strategies that minimize the costs required to achieve a set of environmental targets ('optimization').

In recent years, the European implementation of the RAINS model has been used to support the negotiations on an updated Sulfur Protocol under the Convention on Long-range Transboundary Air Pollution. RAINS and other integrated assessment models indicated that flat-rate, source-oriented approaches, as used in earlier protocols, do not necessarily produce cost-effective solutions (UN/ECE, 1990). For the first time, the Second Sulfur Protocol made use of an alternative, effect-oriented approach, in which the extent of emission reductions is guided by the impacts that emissions from a given source have on sensitive ecosystems.

At the moment, highest priority is being given to the development of a strategy for a Second NO_x Protocol. Reducing nitrogen emissions based on environmental effects is a rather complex process. The interrelation of several environmental effects (acidification, eutrophication, tropospheric ozone, human health, etc.) constitutes a multi-effect, multi-pollutant problem. This paper outlines the development of an integrated assessment model for tropospheric ozone, which combines information on the emissions of ozone precursors, the available control technologies and abatement costs, the formation and transport of ozone, and its effects in Europe.

1.2 Integrated Assessment of Ground-level Ozone

The formation of ozone in the atmospheric boundary layer involves chemical reactions between nitrogen oxides (NO_x) and volatile organic compounds $(VOCs)^{\dagger}$ driven by solar radiation. Stated briefly, the aim of an integrated assessment model for tropospheric ozone is to describe the relationship between ozone exposure and the emissions of the NO_x and VOC precursors in such a way that the costs and effectiveness of emission reduction strategies within Europe can be quantified. To achieve this requires the integration of information from each of the following areas:

- current and future emissions of NO_x and VOCs, both man-made and natural;
- the abatement technologies available for NO_x and VOCs, and their costs;
- a concise description of the source-receptor relationships, taking account of meteorological influences on ozone formation;
- studies of the effects of ozone on agricultural crops, forests and human health, leading to the establishment of critical levels for ozone.

This information must be organized in such a way that scenario analysis (exploring the costs and environmental impacts of alternative emission reduction scenarios) and optimization (the systematic search for cost-effective solutions) will be possible.

[†] The term VOC is used in this paper to refer to all volatile organic compounds except methane

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Studies of the impacts of ozone indicate that critical levels to protect natural vegetation, agricultural crops and forests can be best established with long-term exposure measures, in particular, by the 'accumulated excess ozone' concept. Currently, a threshold of 40 ppb is proposed for plants. This exposure index is referred to as AOT40, the accumulated exposure over a threshold of 40 ppb (Fuhrer and Achermann, 1994). The accumulated exposure should be calculated for daylight hours. For natural vegetation and crops the accumulation period extends over three months, for trees over six months. Although most air quality standards to protect human health are defined as short-term concentrations, cumulative indices such as an AOT60 setting the threshold at 60 ppb, may be used as indicators for compliance with health guidelines.

Some of the elements necessary for the integrated assessment of ground-level ozone are already available in the acidification-focused version of the RAINS model. Figure 1 displays the enhanced structure of the model, taking into account ozone formation and thereby enabling the assessment of multi-effect, multi-pollutant strategies.

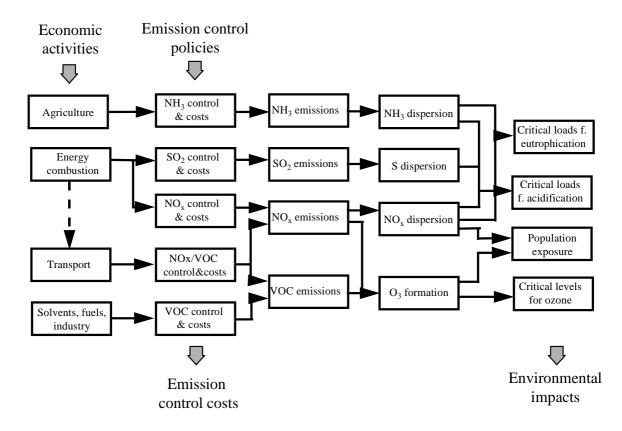


Figure 1: Structure of the RAINS Model

2. A 'Reduced-form' Model to Describe Ozone Formation

2.1 Source-Receptor Relationships

The formation of ozone involves chemical reactions between NO_x and VOCs driven by solar radiation, and occurs on a regional scale in many parts of the world. The time scale of ozone production is such that ozone concentrations build up in polluted air over several days under suitable weather conditions, and this pollutant and its precursors can be transported over considerable distances and across national boundaries. An integrated assessment model for ozone needs to be able to relate ozone exposure to changes in the emissions of ozone precursors.

For application in an integrated assessment model for ozone, the source-receptor relationships need to be valid for a variety of spatial patterns of emission sources and for a range of emission levels, and not restricted to the present-day situation alone. For this reason, attempts to define these relationships solely on the basis of recent ozone measurement data are likely to prove inadequate. Instead, the ozone formation description needs to be based on mathematical models that have gained widespread international acceptance.

Within the framework of an integrated assessment model, source-receptor relationships must be computationally efficient to enable the numerous scenario runs for analyzing costs and benefits from a wide range of control strategies. Furthermore, extended uncertainty and robustness analyses will be necessary to derive solid conclusions from the model, taking into account the gaps and imperfections of the available databases and models. In many cases, methodologies for such analyses require sufficiently simple formulations of the underlying models. In addition, optimization analysis has proven to be a powerful feature in the integrated assessment process for the Second Sulfur Protocol. Optimization of the entire chain from the sources of emissions, over the costs for controlling them, up to the regional impacts on ozone levels, however, also requires sufficiently simple source-receptor relationships.

Most of the available models for ozone formation are process-oriented and contain a considerable degree of detail of the chemical mechanisms and meteorological factors relevant for ozone formation. Consequently, their computational complexity makes it impossible to use them directly within the framework of an integrated assessment model. In order to overcome this gap, an attempt has been made to construct a 'reduced-form' model, using statistical methods to summarize the reaction of a more complex 'reference' model.

The following sections describe the approach developed at IIASA to capture the important relationships between precursor emissions and long-term ozone levels using statistical techniques. It must be kept in mind that, in the overall context of an integrated assessment model, the aim of such an approach is solely to provide source-receptor relationships which are computationally efficient to enable cost- and optimization analysis of alternative emission reduction strategies. In contrast to

conventional, more detailed atmospheric models of ozone formation, a simplified approach of this sort does not try to explain the chemistry of ozone formation.

To this end, the work was carried out in collaboration with EMEP's Meteorological Synthesizing Centre - West, and the results of the EMEP ozone model (Simpson, 1993) provide the basis on which the reduced-form model has been built. The EMEP model has been selected for this analysis, i.a., because (i) it has repeatedly undergone extensive peer review and its structure and results have been compared with other ozone models, and (ii) the EMEP model is readily available for calculating ozone levels over all of Europe over a time period of six months, and the calculation of the necessarily large number of scenarios is a practical proposition with this model.

2.2 Ozone Isopleth Diagrams

Before starting the development of the simplified model, the EMEP ozone model was used to investigate the relationships in different areas of Europe between mean boundary layer ozone concentrations and changes in the emissions of NO_x and VOCs. A convenient way to illustrate the results of these investigations is by means of ozone isopleth diagrams. Such diagrams have been most commonly used, particularly in North America, to show how maximum ozone concentrations depend on the initial concentrations of NO_x and VOCs on a particular day at a specific location. Lines of constant value, or isopleths, of the maximum ozone concentrations are constructed by connecting points having the same ozone concentration but corresponding to various initial conditions. Ozone isopleth diagrams in this form provide a concise representation of the effect of reducing initial NO_x and VOC concentrations on peak ozone concentrations and, in the past, they have been used quantitatively to develop ozone control strategies as part of the U.S. EPA's empirical kinetic modeling approach (EKMA) (Gipson *et al.*, 1981).

The isopleth diagrams used in this section are constructed rather differently, although there are obvious similarities in appearance. Firstly, the ozone statistic depicted by the isopleths is the mean, over the six-month summer period, of the early afternoon ozone concentrations calculated by the EMEP model. Secondly, in the version used here, ozone is shown as a function of the percentage reduction in emissions of NO_x and VOCs across Europe. Thus, the top right-hand corner of each diagram represents the base case without any reduction in precursor emissions.

In areas with sufficiently high emission densities, i.e., in the north-west of Europe, the isopleths form a ridge dividing the diagram into two areas (Figure 2b). On the left of the ridge, corresponding to the greatest reductions in NO_x emissions, the system tends towards the NO_x -limited case (Figure 2a). On the right of the ridge, the NO_x / VOC ratio is relatively high and the NO_2 concentrations are sufficiently great that NO_2 competes with VOCs for reaction with the OH radical. In this region of the diagram, reducing VOC emissions results in lower ozone concentrations; to a large extent, ozone shows a linear dependence on VOC emission changes (Simpson, 1992). However,

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ozone concentrations may be increased, at least initially, by NO_x reductions in the absence of concurrent reductions in VOC emissions.

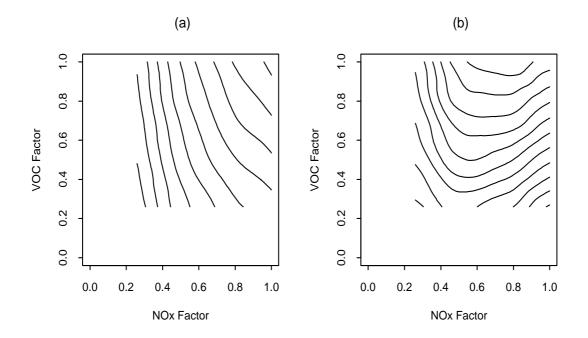


Figure 2: Typical patterns of ozone behavior in Europe

For regions with lower emission densities (Figure 2a), reductions in VOC emissions are seen to exert only a minor influence on mean ozone concentrations. In these regions the NO_x / VOC ratio is relatively low and there is an ample supply of peroxy radicals (RO_2 and HO_2) to convert NO to NO_2 and, thus, lead to ozone production. Decreasing the available NO_x leads directly to a decrease in ozone. In these circumstances, ozone formation is limited by the availability of NO_x , and the atmospheric chemistry system is said to be NO_x -limited. In such regions, reductions in emissions of NO_x are likely to be effective in reducing ozone concentrations, but ozone is relatively insensitive to reductions of VOC, and to changes in the VOC species distribution, at constant NO_x .

2.3 Sampling Design

The major task in developing a reduced-form model was to identify a simple functional relationship between the precursor emissions and the response of ozone exposure, which is capable of capturing the different and often non-linear characteristics of ozone formation as illustrated by the isopleth diagrams.

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The simplified model has been designed as a regression model that relates long-term ozone exposure, such as the mean of the daily maxima or the accumulated excess ozone (e.g., AOT40 and AOT60) over a six-month period to national, annual emissions of NO_x and VOCs. For this purpose the data sample, upon which the regression analysis is to be based, must also include cases with reduced emissions. Obviously, actual monitored data are available only for the current emission levels. To overcome this lack of data, the sample was constructed from numerous runs of the EMEP model, carried out using 1990 emissions data and meteorological data for the period April-September 1990. Consequently, the simplified model can be considered as a summary of the full EMEP model, limited to the response of mean ozone levels to changes in national NO_x and VOC emissions.

Although there exists a wide variety of statistical methods to fit optimally the overall response surface, for this analysis it was considered important that the model should be applicable to the non-linear behavior likely to be encountered as a result of realistic emission control policies. The experimental design of the EMEP model calculations used to provide a data set for the regression model determines the range within which the regression model may be applied. The reduced-form model is not intended to be used outside this range, i.e., no extrapolation is employed.

The range of model application in the present study was based on a consideration of the relevant emission sources, their applicable abatement technologies and potential control policies. It is likely that international cooperation among the member countries of the UN/ECE LRTAP Convention and their will to solve the problems arising from air pollution will result in an overall reduction of emissions. According to the countries' current reduction plans reported to the UN/ECE (UN/ECE, 1995), total European emissions of NO_x and VOC will decrease by the turn of the century by around 20-30 percent. Some countries indicate that reduction levels of 70-80% might be achieved by 2010 (compared to 1990 emissions). Only a few countries forecast a freeze of emissions at their current levels or a slight increase.

Consequently, the experimental design adopted in this work aims to represent the behavior of the EMEP ozone model as well as possible within the range between two points: (i) close to current emission levels, and (ii) at a point representing the maximum emission reductions considered technically feasible. Based on the considerations above, this second point was taken to be 70 percent reductions of both NO_x and VOC emissions.

With this goal in mind, the regression model has been built upon two "base" cases with uniform emission reductions across all European countries and, for each of the 40 emitter countries considered in this analysis, six scenarios in which emissions from single countries only have been reduced. In total, this design resulted in $2 + (6 \times 40) = 242$ scenario cases.

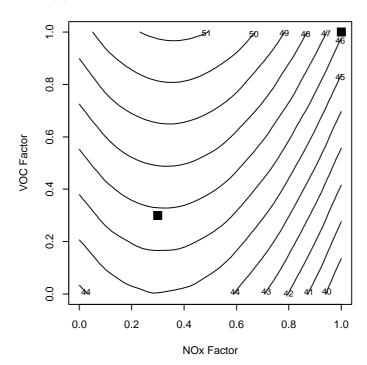
The emission reduction scenarios used to fit the model are shown on the ozone isopleth diagrams given in Figure 3. The two "base" cases are shown in Figure 3a as filled squares, superimposed on an isopleth diagram that has been calculated for uniform emission changes in all emitter countries. Three scenarios per country were calculated

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around the upper base case (which is indeed the 1990 base case), two involving NO_x emissions changes and one involving VOC. These scenarios are shown as filled diamond symbols in Figure 3c. The isopleth diagram in this figure shows the effect on ozone of emission reductions from just one emitter country (the most influential for this receptor grid), while emissions from all other sources are maintained at their 1990 base case level. The filled diamond symbols in Figure 3b indicate the corresponding three scenarios calculated for every emitter country around the lower base case. The background isopleth diagram for Figure 3b shows the effect of emission reductions from the same country for the same grid as Figure 3c, but now with both NO, and VOC emissions from all other countries reduced by 70 percent. The receptor grid used for the isopleth plots in these examples is rather extreme in showing a ridge in the isopleths at such low NO_x factors (i.e. large NO_x reductions). This illustrates why it was considered necessary to calculate an additional scenario involving 90 percent reductions of NO. from a small number of emitters in NW Europe, in order that the regression model could "see" over the ridge. This additional scenario is shown on Figure 3b by means of a filled triangle symbol.

Operation of the EMEP model on the mainframe computer used by the Norwegian Meteorological Institute is rather time- and resource-intensive. Carrying out the large number of scenario runs necessary for constructing the reduced-form ozone model is therefore an expensive undertaking. To simplify and accomplish this task, the EMEP model has been transferred to a parallel computing environment, which resulted in a significant decrease of computer time. This work was carried out for IIASA by GMD-FIRST (Institute for Computer Architecture and Software Technology of the German National Research Center for Information Technology) in Berlin.

To adapt the EMEP model to parallel computing, the computational tasks are subdivided into a number of subsets and distributed to individual parallel processors (nodes), where they can be carried out simultaneously. The results are then passed back to the host node (Unger, 1996).



(a) Uniform emission reduction scenarios - 'base cases'

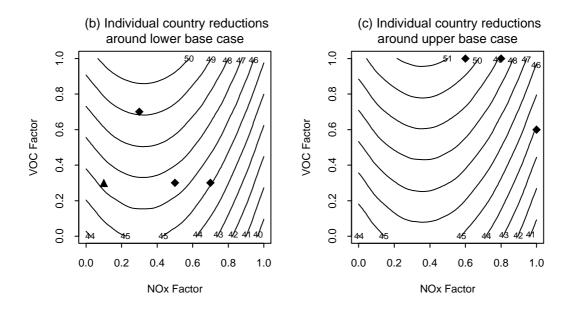


Figure 3: Ozone isopleth diagrams illustrating the emission reduction scenarios used in fitting the seasonal model

2.4 Model Design

This section outlines the development of the regression model designed to provide a simplified description of the source-receptor relationships between precursor emissions and the concentrations of ozone in the atmospheric boundary layer.

The simplified source-receptor relationships need to be able to predict changes in ozone at a receptor grid resulting from emission abatement strategies adopted in various European countries. Emission estimates at a national level were considered to be the most appropriate for this purpose, and the regression model uses national, annual emissions of NO_x and VOCs as explanatory variables. Initial versions of the model discussed in this paper adopted the mean early afternoon ozone concentration over the six-month summer period as the response variable to be predicted. Subsequently, models of the same form were also developed for AOT40 and AOT60 measures.

Basic ideas about which terms should be included in the simplified model were developed from the published results of studies made using the EMEP ozone model and experience of this latter model's behavior gained during earlier efforts to develop a simplified model for calculating daily ozone concentrations.

Simpson (1992) investigated the relationship between mean ozone concentrations and VOC emissions and concluded that there is considerable linearity, in the sense that a 5x % reduction in VOC emissions from a given country results in five times the reduction in mean ozone that an x % reduction produces. He also showed that the change in ozone per unit VOC emission reduction depended on the extent of any simultaneous NO_x emission changes.

Ozone isopleth diagrams constructed from the results of EMEP model calculations, such as those in Figure 2, almost invariably show a relatively simple form. Earlier IIASA studies into the possibilities of developing a simplified regression model for predicting daily ozone concentrations (Heyes & Schöpp, 1995) made use of non-parametric methods. The results suggested that a multi-dimensional quadratic spline could be used to reproduce the main features of the relationship between ozone and the emissions of its precursors.

The simplified "daily" model also made use of the concept of "effective" emissions, suggested by studies with the EMEP model (Simpson, 1995) which showed that exchange processes between the boundary layer and the free troposphere could have a significant impact on the final ozone concentrations. The EMEP model includes two processes by which boundary-layer air can be mixed with free tropospheric air, *viz* day-to-day increases in mixing height and the venting effect of cumulus clouds. For some sites, at least, the consequent losses of ozone, NO_x and VOCs from the boundary layer could be considerable. To allow for these effects, emissions along the trajectory were weighted by the amount of dilution that subsequently takes place within the air mass (Simpson, 1995) to give the dilution-weighted or "effective" NO_x and VOC emissions used as variables in the regression model.

On the basis of the ideas outlined above a general formulation for the simplified "seasonal" model was developed. In subsequent sections the following abbreviations are used for model variables:

- v_i annual national emissions of non-methane VOCs from emitter country i
- n_i annual national emissions of NO_x from emitter country i
- ev_i "effective" emissions of VOCs, including natural sources, at receptor j
- en_i "effective" emissions of NO_x, including natural sources, at receptor j
- evn, "effective" natural emissions of VOCs at receptor j
- enn, "effective" natural emissions of NO_x at receptor j

The mean ozone concentration at receptor j, $[O_3]_j$, is assumed to be a function of the nmVOC and NO_x emissions, v_i and n_i respectively, from each emitter country i, and the mean "effective" emissions (of NO_x and VOCs), en_j and ev_j , experienced at the receptor over the period in question. The general model formulation adopted is:

$$\overline{[O_3]}_j = k_j + \sum_{i=1}^M (a_{ij}v_i + b_{ij}n_i + c_{ij}n_i^2) + \alpha_j \overline{en_j}^2 + g(\overline{en_j}, V) + \overline{en_j} \sum_{i=1}^M h_{ij}n_i (1)$$

where M is the number of emitter countries considered,

$$V = \{v1, v2, ..., vM\},$$
(2)

and the non-linear function g() is given either by:

$$g(\overline{en}_{j}, V) = \overline{en}_{j} \sum_{i=1}^{M} d_{ij} v_{i}$$
(3)

or by:

$$g(\overline{en}_{j}, V) = \beta_{j} \overline{en}_{j} \overline{ev}_{j}$$
(4)

The mean "effective" emissions are given by:

$$\overline{en}_j = \sum_{i=1}^M \overline{E_{ij}} n_i + \overline{enn_j}$$
(5)

$$\overline{ev}_j = \sum_{i=1}^M \overline{F_{ij}} v_i + \overline{evn_j}$$
(6)

where E_{ij} , F_{ij} depend on the meteorology and are obtained from EMEP model calculations, and enn_j and evn_j represent the "effective" natural emissions of NO_x and VOCs, respectively.

For the initial stages of evaluating this model, an heuristic approach was taken to decide which terms, if any, could be dropped from the model. Such experiments led to the conclusion that the following linear regression model contained sufficient information for the present purpose:

$$\overline{[O_3]}_j = k_j + \sum_{i=1}^M (a_{ij}v_i + b_{ij}n_i + c_{ij}n_i^2) + \alpha_j \overline{en_j}^2 + \overline{en_j} \sum_{i=1}^M d_{ij}v_i$$
(7)

In order to decide which emitter countries should be included in the model, the emitter countries were ranked (i) on the basis of their contribution to the "effective" NO_x emissions experienced at each receptor *j*, and (ii) by how great an ozone reduction was achieved for a given fractional VOC reduction. The most influential twelve countries were included in the equation, i.e. *M* was set equal to 12. This choice was based on an assessment of the EMEP model results for a small number of receptor sites, in an attempt to include in the simplified model all the most influential emitter countries (for a given receptor) yet exclude those which had very little effect.

The formulation of the reduced-form model given in Equation 7 above has been used in the construction of models for 598 European receptor grids.

It is of interest to relate the terms of Equation 7 to the physical and chemical processes that determine ozone formation in the atmosphere. Possible interpretations are:

- k_j includes the effects of background concentrations of O_3 and its precursors, and natural VOC emissions;
- $a_{ij}v_i$ provides the linear country-to-grid contribution from VOC emissions in country *i*, allowing for meteorological effects;
- $b_{ij}n_i$ provides the linear country-to-grid contribution from NO_x emissions in country *i*, allowing for meteorological effects;
- $\alpha_j e n_j^2$ takes account of the average non-linearity (in the O₃ / NO_x relationship) experienced along trajectories arriving at receptor *j* and any non-linear effects local to that receptor;
- $c_{ij}n_i^2$ serves essentially as a correction term to allow for non-linearities occurring close to high NO_x emitter countries;
- $d_{ij}en_{i}v_{i}$ allows for interactions between NO_x and VOCs along the trajectories.

The coefficients a_{ij} , b_{ij} , c_{ij} , d_{ij} and α_j are estimated by the linear regression, and n_i , v_i and en_j are used as variables. The coefficients a_{ij} and b_{ij} may also be regarded as a composite source-receptor matrix.

2.5 Model Selection

Since the proposed formulation is a linear regression model (containing quadratic terms) with many potential variables, the regressor selection was very important. For the selection, which had to be carried out for all receptor grids throughout Europe, a systematic selection process using the Akaike Information Criterion (AIC) was applied. Based on this criterion, the model with a minimum value of AIC was chosen among several competing models.

In practice, the 'step' function of the S-Plus statistical software package was used to automate the AIC-based regressor selection procedure (Venables & Ripley, 1994). Using this function a sequence of potential models is generated, each of which differs from its immediate neighbors by only one term; individual terms may be added or deleted during the search. The best candidate model is selected on the basis of the AIC statistic.

Although the experimental design described in the preceding section might easily lead to collinearity problems, no serious problems of this nature have been encountered in this particular case. However, for some receptor grids there have been indications of minor occurrences, as evidenced, for example, by instances of coefficients with the "wrong" sign. The following approach was adopted to deal with this problem:

- Initial models were constructed for each receptor grid including all the terms in Equation 7. The automated stepwise regressor selection procedure described above was implemented in order to remove 'unimportant' terms.
- Since a positive α coefficient is an indicator for potential collinearity, for such receptor grids the reduced-form regression models were recalculated with the term involving α omitted from the model. The regressor selection was also repeated.
- Finally, models were again recalculated for receptor grids where it was found that either the linear NO_x term (coefficient *b*) was negative or the quadratic NO_x term (coefficient *c*) was positive. This recalculation involved substituting data from the 90 percent NO_x reduction scenario for the corresponding 30 percent NO_x reduction scenario in the data set on which the revised regressions were based.

2.6 Validation

An earlier test version of the reduced-form model, calculated for seasonal mean ozone at 25 receptor grids and based on 1989 emissions and meteorological data (Heyes *et al.*, 1996), was extensively evaluated against the full EMEP model in several ways. The comparisons were performed for three kinds of emission reduction scenarios:

- uniform reductions of NO_x and VOC across Europe;
- increasing reductions of NO_x and VOC separately in individual countries;
- multi-national, non-uniform emission reduction scenarios.

Over a wide range of realistic emissions, the performance of the reduced-form model was found to be generally very good, giving results typically less than 1.3 percent different from the full EMEP model. Further details of the comparison results are presented in Heyes *et al.*, 1996.

For the full version of the reduced-form model discussed in this paper, an evaluation in terms of the AOT40 (accumulated excess ozone over a threshold of 40 ppb) measure was performed. The AOT40 model has exactly the same functional form as that for mean ozone:

$$AOT40_{j} = k_{j} + \sum_{i=1}^{M} (a_{ij}v_{i} + b_{ij}n_{i} + c_{ij}n_{i}^{2}) + \alpha_{j}\overline{en_{j}}^{2} + \overline{en_{j}} \sum_{i=1}^{M} d_{ij}v_{i}$$
(8)

where the AOT40 at receptor j (AOT40_{*j*}) is assumed to be a function of the nmVOC and NO_x emissions, v_i and n_i respectively, from each emitter country i, and the mean "effective" NO_x emissions experienced at the receptor over the period in question. M is the number of emitter countries considered.

The evaluation of this model concentrated on comparisons with EMEP model results for three non-uniform scenarios involving simultaneous reductions from all emitter countries. The three comparison scenarios were intended to represent (Cofala *et al.*, 1995):

- a) a 2010 "current legislation" (CLE) case;
- b) 1990 with road transport emissions removed;
- c) 2010 "CLE" with road transport emissions removed.

Clearly, these scenarios involve different percentage emission changes for different source sectors (and, of course, different countries). In the full EMEP model calculations used for comparison, different VOC species profiles were employed for each source sector. The EMEP model results will, therefore, include any effects due to varying VOC compositions inherent in the three scenarios. In contrast, the reduced-form model does not make any explicit recognition of VOC speciation, using a single v_i term (Equation 8) to represent the total annual VOC emissions from country *i*. Differences between the results from the EMEP model and the reduced-form model in the

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comparison presented here will include errors arising from this simplification in addition to those inherent in the regression calculation.

The mean and variance of the differences between the two models for these three scenarios are summarized below:

a) CLE case in 2010 : mean difference = 0.37 ppm.h, variance = 0.26

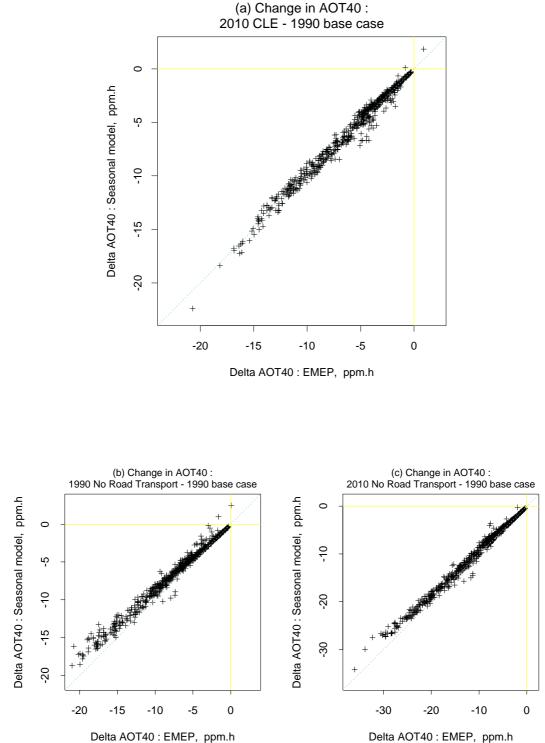
b) 1990, road transport emissions excluded : mean difference=1.20 ppm.h, variance=0.61

c) CLE 2010, road transport emissions excluded : mean difference=1.09 ppm.h, variance=0.74

Although the differences are not large, bias appears when the AOT40 approaches zero. This is a clear side-effect of using a linear regression model for a truncated problem (threshold of 40 ppb). However, as long as the interest is focused on exceedances above the critical level of 10 ppm.h, this problem can be neglected.

Figure 4 compares the results from the reduced-form model for each of the three scenarios with the corresponding EMEP model calculations. This figure provides scatter plots of the change in AOT40 between a particular scenario and the 1990 base case value, each point representing one receptor grid. The agreement between the models is seen to be generally very good, although for two of the scenarios, (b) and (c), the largest decreases in AOT40 are somewhat underpredicted by the reduced-form model.

The comparison is explored further in Figure 5, which shows for the 2010 CLE scenario the spatial distribution of differences between the two models for those receptor grids at which the 1990 base case AOT40 value - as calculated using the 1995 version of the EMEP model - exceeds 10 ppm.h. For the majority of European grid squares the differences lie within a range of \pm 5%. However, larger discrepancies are found in some areas, particularly in regions where the 1990 AOT40 value exceeds the 10 ppm.h threshold by only a small amount.



Delta AOT40 : EMEP, ppm.h

Figure 4: Comparison of the results from the reduced-form model for three scenarios with the corresponding EMEP model calculations

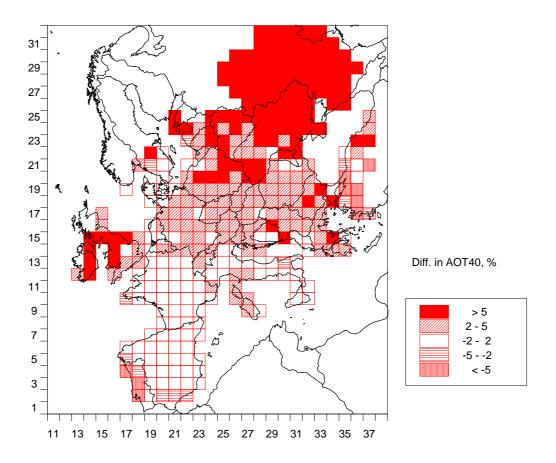


Figure 5: Spatial distribution of differences between the reduced-form and full EMEP models for those receptor grids at which the 1990 base case AOT40 value - as calculated using the 1995 version of the EMEP model - exceeds 10 ppm.h.

3. Optimization

The optimization mode of integrated assessment models can be a powerful tool in the search for cost-effective solutions to combat an air pollution problem. In the RAINS-acidification model, optimization techniques have been used to identify the cost-minimal allocation of resources in order to reduce the gap between current sulfur deposition and the ultimate targets of full critical loads achievement. The outcome of the optimization was used as a starting point for the political negotiations on the Second Sulfur Protocol. According to the nature of the problem (i.e., the linear source-receptor relationships for sulfur transport), linear programming techniques have been applied.

In the case of tropospheric ozone, a systematic search for cost-effectiveness appears even more attractive. The facts that several pollutants (NO_x and VOC emissions) are

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involved, and that important non-linearities between precursor emissions and ozone levels have been recognized, cut the likelihood of 'intuitive' solutions being identified in the scenario analysis mode. At the same time, these aspects also increase the complexity of the problem and, therefore, the demand for optimization techniques.

For simple cost-minimization, the objective function of the optimization problem can be formulated as

$$\sum_{i=1}^{N} Cf_i \longrightarrow \min$$
(9)

Cost curves providing emission control costs for varying levels of reductions can be converted into constraints for the optimization problem:

$$Cf_i = f(n_i, v_i) \tag{10}$$

A second set of constraints relates for each grid cell j emissions of NO_x and VOC with ozone exposure:

$$AOT40_j = f'(n_i, v_i, ...) \le f''(AOT40_{\lim}, ...)$$
 (11)

with *i* denoting emission sources (countries), *j* the receptor sites, n_i the emissions of NO_x, v_i the emissions of VOC, Cf_i the combined costs of reducing NO_x and VOC emissions in country *i*, $AOT40_j$ the ozone exposure (AOT40) at a receptor *j* and $AOT40_{lim}$ the critical level for ozone. Depending on the type of the function in Equation 8 and the number of emitter countries and receptor sites to be considered, the optimization task becomes a large-scale non-linear problem. To solve such a problem, the function derivatives (the Jacobian matrix) must also be available.

Using source-receptor relationships according to Equation 8, a test problem for 25 receptor sites (j) and 21 emission sources (i) was successfully solved with three alternative optimization packages (Zawicki & Makowski, 1995). The full-scale optimization feature, dealing with some 600 receptor grids and 38 emission sources, has now been successfully implemented for two of these optimization packages.

3.1 Cost Curves

Inputs to the optimization package include cost curves (Equation 10) providing, for the various pollutants under consideration, the costs of reducing emissions at the different source regions for a selected year.

The current implementation of the RAINS model contains modules for estimating emission control costs for SO_2 , NO_x and NH_3 . These estimates can be expressed in terms of cost curves, providing - for a given emission source (country) - the least costs for achieving increasingly stringent emission reductions. They are compiled by ranking the available abatement options according to their marginal costs. Consequently, this

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methodology produces piece-wise linear curves, consisting typically of about 30 segments.

For each of the pollutants (NO_x, VOC) and the countries, such piece-wise linear curves can be used as input to the optimization according to Equation 10. Although the solver softwares used for this exercise are capable of dealing with piece-wise linear constraints, for reasons of increased numerical stability a smoothed approximation of the cost curves has been developed and used. Analysis demonstrated that the given piece-wise linear cost curves could be best approximated with a second-order rational function

$$y_i = \frac{\mathbf{A}_i + \mathbf{B}_{i}x_i}{1 + \mathbf{C}_{i}x_i + \mathbf{D}_{i}x_i^2} + \mathbf{K}_i$$
(12)

with y_i as the total costs for one pollutant and x_i as the emission level. K_i is used to calibrate the no-control level at zero costs; A_i , B_i , C_i and D_i are determined through non-linear regression. The selected functional form guarantees that the curve is, within the selected interval, convex and monotonically decreasing, and shows asymptotic behavior at the maximum control level. For NO_x, the maximum deviation from the piece-wise linear curve is typically within a range of \pm 5 percent. Figure 6 displays a typical case (Germany) for a piece-wise linear cost curve and its approximation according to Equation 12 ($r^2 = 0.9993$).

The optimization runs presented in this paper used NO_x cost curves produced by the RAINS model for the Official Energy Pathway (i.e., for the officially projected levels of energy consumption) for the year 2010. Since at present the RAINS model does not yet contain cost curves for reducing VOC emissions, the calculations relied on the curves developed by Wenborn *et al.*, (1995). Work is underway to incorporate VOC cost estimates into the RAINS model.

A methodological problem arises from the fact that some emission reduction technologies (e.g., the three-way catalyst) simultaneously reduce NO_x and VOC emissions. Consequently, the costs of emission reductions for one pollutant are in reality not independent of the costs of the other. Initial work to develop multi-pollutant cost curves, using least-square techniques, has produced promising results.

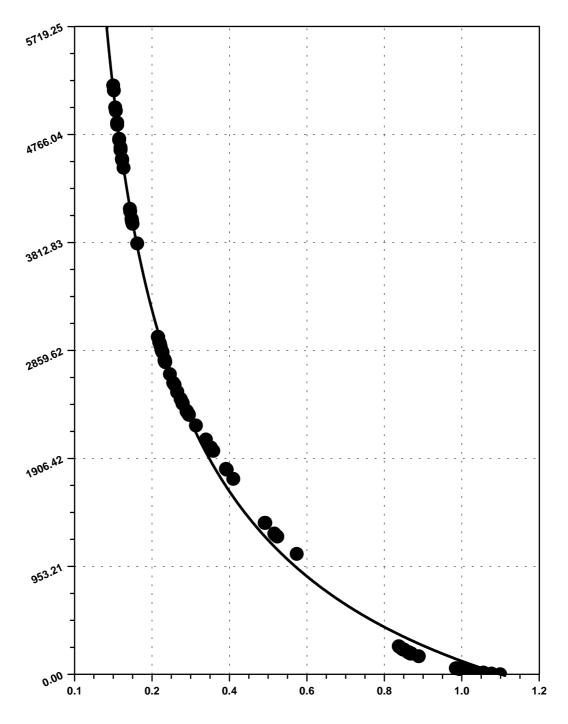


Figure 6: Comparison between the piece-wise linear cost curve for NO_x control for Germany (steps are indicated by dots) and the smoothed function

3.2 Solvers for the Non-linear Optimization Problem

The mathematical programming problem for the ozone optimization is a non-linear model which has about 1300 variables and 1800 constraints. It is known that non-linear models of this size may be difficult to solve, and that optimal solution may not be unique (more precisely, that there might be many very different solutions with very similar values of the goal function). Consequently, it is of utmost importance to aim at robust optimization techniques, if the model is to be applied for the examination of policy options. Furthermore, within the framework of an integrated assessment model the use of an optimization technique should be transparent also for users who are not specialists in mathematical programming.

There are a number of non-linear optimization techniques available and it is practically impossible to decide in advance, which technique is best for solving a given non-linear problem. Since the specifications and data for the ozone model come from different sources and because it cannot be excluded that the model formulation will need to be modified in the future, a specialized model generator has been applied which prepares the input files for a range of different solvers. The generator, composed of a library of C++ classes, combines the input data into one common HDF (Hierarchical Data Format) file. Up to now three different non-linear solvers have been tested:

- CFSQP (C Code for Feasible Sequential Quadratic Programming) developed by the University of Maryland,
- CONOPT developed by ARKI Consulting and Development, Denmark, and
- MINOS from Stanford University, California.

Two of the three solvers (CONOPT and MINOS) proved to be very efficient for the current formulation of the model. Generating and solving one optimization problem takes about one to five minutes on a SUN workstation.

Currently the problem is formulated for a single-criterion optimization. Multi-criteria analysis will be possible and can provide alternative ways to examine trade-offs, e.g., between a minimization of emission reduction costs and the ozone exposure in different parts of Europe. The goal function used as criterion for the (single-criterion) optimization (Equation 9) can be optionally augmented by a so-called regularizing term. This technique helps to remedy potential problems of non-uniqueness of the optimal solution.

4. Illustrative Examples of Optimization Runs

The subsequent sections present some illustrative examples of the results of a number of test optimization problems. It must be emphasized at the outset that these examples are provided solely as general illustrations of the optimization feature, to provide an indication of the reasonableness of the solutions found. However, at this stage, no conclusions whatsoever in terms of specific country emission reduction targets should

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be drawn from the results presented. Table 1 presents six important reasons why the optimization runs presented in this paper must be considered as exploratory, and why no quantitative conclusions on concrete abatement strategies should be drawn from it at the present time.

Table 1: Six important reasons for the preliminary nature of the optimization runs

- 1. The regression model <u>coefficients will need to be revised</u>. The full EMEP model runs to provide the data set from which the reduced-form model is derived were performed early in 1996 using a version of the EMEP ozone model (and emissions data) dating from August 1995. Since that time important revisions have been made to the EMEP model (EMEP, 1996), particularly with regard to ozone dry deposition velocities and the treatment of the temporal variation of emissions. The full EMEP model runs will be repeated in the near future so that the simplified model can be recalculated to take account of these improvements.
- 2. The regression model is currently based on the <u>meteorological conditions</u> of only <u>one particular year</u> (1990). It is of utmost importance to base robust conclusions on long-term meteorology in order to minimize the impacts of the inter-annual meteorological variability.
- 3. Country-specific <u>cost data</u> for controlling <u>VOC emissions</u> are not yet available for the optimization model. Testing has been carried out using surrogate cost data derived from available data for the UK. While appropriate for the purpose of testing the software, the use of these substitute data for other countries may clearly influence the actual solutions obtained from the optimization procedure. Furthermore, the cost curves for NO_x developed by IIASA have not yet been fully reviewed.
- 4. Both the VOC and the NO_x cost curves used for this initial analysis contain the costs for traffic-related measures, although some of them reduce NO_x and VOC emissions simultaneously. This means that the calculations presented in this report apply a <u>double-counting</u> of the costs for these measures.
- 5. The regression model used for this analysis relates only to the <u>critical level for</u> <u>forests</u> (i.e., the AOT40 for trees, accumulated over a six-month period). The critical level for natural vegetation and crops (AOT40 over a three-month period) might yield different results. The optimization tests were carried out using the simplified model derived for a six-month AOT40 response variable, where the AOT40 values were calculated in the standard way from the EMEP model ozone values for the 12 and 18 GMT trajectory arrival points.
- 6. All optimization runs start from a defined 'reference case', assuming the implementation of current emission control legislation in all European countries. The specific assumptions for this reference case are not yet reviewed in the context of the work of the UN/ECE Convention on Long-range Transboundary Air Pollution. Changing the baseline emission level will change optimization results.

This preliminary analysis follows the basic concept applied in recent international effect-based strategy discussions by exploring a number of variations of a so-called 'gap-closure' approach. Such gap-closure scenarios start from the current situation and aim at reducing the gap towards an ultimate target (e.g., the full achievement of critical loads or critical levels) everywhere (i.e., in all grid cells) by an equal percentage. To provide a basis for the following optimization analysis Figure 7 displays the AOT40 for trees as calculated by the August 1995 version of the EMEP ozone model. It was explained in Table 1 that the EMEP model has changed since then; however, the current coefficients of the reduced-form model, which provides the basis for the ozone optimization, have been derived from the 1995 version.

In the context of this paper a 'gap' for ozone is defined as the difference between the AOT40 values calculated for emissions in the 1990 base case and the AOT40 values calculated for the lower bound emissions employed in the optimization. For receptor grids where this gap closure gives targets below 10 ppm.h, the targets were reset to 10 ppm.h in line with the AOT40 critical levels for trees. Note that this concept is different from gap closure approaches used elsewhere: whereas in other studies (e.g., in the scenario calculations for the Second Sulfur Protocol and for the EU Acidification Strategy) the gap was related to the ultimate full achievement of critical loads or levels, this study defines for reasons of simplicity the gap as the practically achievable improvement (given by the maximum technically feasible emission reductions), which does not necessarily imply a full achievement of the critical levels.

Initial optimization runs showed that, using the full range of emissions, i.e., allowing countries to emit between the unabated level (zero percent reduction) and the maximum technically feasible reductions (60 - 80 percent), in certain cases numerical instabilities may occur. Limiting emissions to a range which could be expected for the real-world situation in the forthcoming negotiations on a NO_x protocol (i.e., excluding the already adopted measures to control emissions) eliminated the problem.

In practice, for these optimization tests the upper emission bound was set to a value midway between the uncontrolled emissions value and the maximum technically feasible emission reductions for each country. However, for countries where this value would then be lower than that to be expected from the Current Reduction Plans as compiled by the Secretariat of the Convention or from the implementation of the current national legislations on air emissions, such emission levels were used for the upper bound (see Table 2 and Table 3, 'upper bound'-columns).

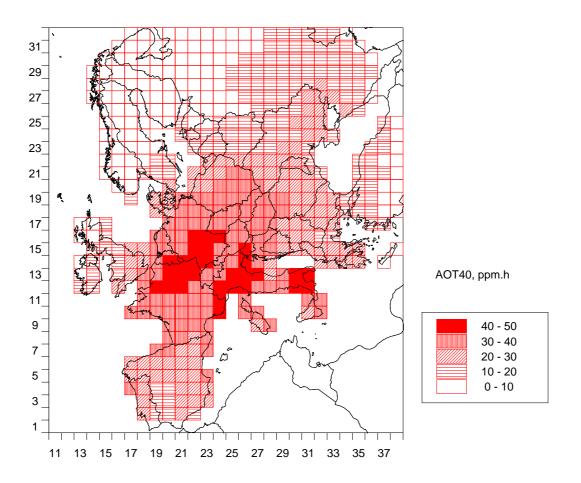


Figure 7: The AOT40 for trees as calculated for the year 1990. Note that this map is produced with the August 1995 version of the EMEP model and that the model has been changed since then!

4.1 Increasing the Stringency of Gap Closure Targets

A first set of scenarios explores the changes in optimized reductions for NO_x and VOC emissions in response to increasingly stringent gap closure targets. In practice, three cases aiming at a 25 percent, 50 percent and 75 percent closure of the gap have been analyzed. Results are presented in Table 2 and Table 3.

It should be mentioned that in this particular case the optimization starts from the emission levels expected after implementation of the current emission control legislation, as compiled for the study for the EU acidification strategy (Amann *et al.*, 1996). This means in particular, that for the EU countries measures proposed by the Auto/Oil program are assumed to be taken and are therefore not subject to the ozone optimization. As a consequence, only a limited set of measures for reducing NO_x

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emissions remains, and the marginal costs of these measures are much higher than the marginal costs of the available options for reducing VOC emissions.

Consequently, due to these differences in costs there is a tendency for the Member States of the European Union to prioritize additional VOC reductions for making the first step of a gap-closure strategy (i.e., the 25 percent gap closure scenario). As displayed in Figure 8b, only Central and Eastern European countries (Russia, St. Petersburg, Ukraine, Belarus, Lithuania and Latvia) take additional action to reduce NO_x, whereas all other countries restrict their measures to VOC control.

With the choice of a stricter target, such as a 50 percent gap closure objective, many more countries take further action to reduce their NO_x emissions. For most of the Central and Eastern European countries, VOC control will be matched by comparable reductions of NO_x . With the major exception of Denmark, NO_x control in Western European countries, however, will be on top of stringent reductions of VOC emissions (Ireland, UK, Germany, etc.), see Figure 8a.

Further tightening of the gap closure target will require significant NO_x and VOC reductions in most countries. As displayed in Figure 8c, a 75 percent closure of the possible gap leaves only very few countries with a single-pollutant task. The low obligations of Finland and Sweden have to be seen in the context of the forest protection objective of these example runs; in these countries there is hardly any excess of the critical level for trees in the base year. A focus on natural vegetation may produce different results.

Analyzing the sequence of scenarios with increasingly tight environmental targets, only one region (the Baltic countries) occurs where stricter targets are associated with less emission reductions. Whereas this effect can be explained with stricter control in a neighboring country relaxing the demand for a small country, the fact that this is not a frequent phenomenon should be noted.

Generally it can be noted that, for sufficiently stringent environmental targets which are however still above the critical levels, most countries will have to take measures to reduce emissions. In contrast to the acidification problem, where strict emission control is required for the north-west of Europe, controlling the ozone problem requires also substantial measures in Mediterranean countries, and less reductions in Scandinavia.

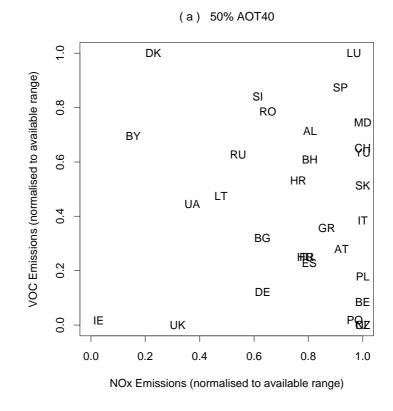
Summarizing the results of these initial test runs it can be stated that there is generally a logical and reasonable reaction of emission reductions in response to increasingly stringent environmental targets. Furthermore, the example runs demonstrate that costs are an important factor for allocating optimal reduction measures.

Country	Code	1990	Upper	25%	50%	75%	Lower
			bound	AOT40	AOT40	AOT40	bound
		kt	kt	kt	kt	kt	kt
Albania	AL	30	30	30	26	18	11
Austria	AT	222	205	205	196	142	80
Belarus	BY	285	260	218	105	105	77
Belgium	BE	343	248	248	248	102	94
Bosnia-H.	BH	54	48	48	41	30	15
Bulgaria	BG	376	290	290	212	152	79
Croatia	HR	83	64	64	54	31	24
Czech Republic	CZ	742	246	246	246	156	95
Denmark	DK	269	174	174	94	87	70
Estonia	EE	66	70	70	70	70	17
Finland	FI	284	187	187	187	187	62
France	FR	1584	1312	1312	1161	825	576
Germany	DE	3033	1903	1903	1375	795	469
Greece	GR	544	275	275	250	151	82
Hungary	HU	238	196	196	171	101	76
Ireland	IE	115	73	73	26	25	25
Italy	IT	2053	1238	1238	1238	845	454
Latvia	LV	54	93	89	93	93	36
Lithuania	LT	56	130	99	83	114	40
Luxembourg	LU	23	15	15	14	14	6
Moldova	MD	35	66	66	66	40	19
Netherlands	NL	570	346	346	346	170	132
Norway	NO	231	137	137	137	137	54
Poland	PL	1280	819	819	819	521	292
Portugal	PO	221	202	202	199	125	74
Romania	RO	883	442	442	327	204	113
Kaliningrad	KA	17	24	24	24	14	7
Kola/Karelia	KK	56	82	82	82	82	22
Rest of Russia	RU	2477	2388	2126	1606	1152	680
St. Petersburg	SP	124	160	153	150	160	41
Slovakia	SK	227	120	120	120	77	53
Slovenia	SI	53	35	35	26	15	12
Spain	ES	1256	888	888	778	531	330
Sweden	SE	398	254	254	254	219	80
Switzerland	CH	184	131	131	131	67	48
Ukraine	UA	1097	1403	1007	758	519	374
UK	UK	2860	1641	1641	922	725	585
F. Yugoslavia	YU	66	119	119	119	68	41
Total		22489	16312	15570	12753	8868	5344

Table 2: Optimized NO_x emissions for different AOT40 targets

Country	1990	Upper	25%	50%	75%	Lower
		bound	AOT40	AOT40	AOT40	bound
	kt	kt	kt	kt	kt	kt
Albania	30	30	30	25	22	14
Austria	430	310	310	224	209	190
Belarus	533	269	220	226	160	126
Belgium	365	248	211	138	128	128
Bosnia-H.	54	70	63	58	57	39
Bulgaria	217	217	202	133	121	93
Croatia	83	65	65	46	34	25
Czech Republic	534	253	226	118	118	118
Denmark	165	119	119	119	75	69
Estonia	94	50	50	50	50	16
Finland	209	112	112	112	96	59
France	2402	1672	1672	1025	950	810
Germany	3008	2019	1634	1212	1170	1101
Greece	325	318	318	180	148	104
Hungary	205	145	145	77	68	55
Ireland	180	138	138	78	78	77
Italy	2401	1909	1909	1283	1051	892
Latvia	130	49	41	49	49	12
Lithuania	187	111	88	83	98	58
Luxembourg	19	12	12	12	12	5
Moldova	116	114	112	98	86	49
Netherlands	451	324	200	191	191	191
Norway	251	189	189	189	189	109
Poland	951	819	723	500	487	431
Portugal	206	170	146	75	73	73
Romania	700	453	453	417	373	286
Kaliningrad	22	22	22	22	19	12
Kola/Karelia	75	64	64	64	64	39
Rest of Russia	3303	2573	2573	2169	2015	1489
St. Petersburg	166	196	187	185	196	108
Slovakia	146	108	108	87	80	66
Slovenia	35	25	25	23	21	11
Spain	1112	923	905	562	455	455
Sweden	533	308	308	308	218	164
Switzerland	297	208	208	177	164	119
Ukraine	1369	1366	884	895	759	518
UK	2612	1840	1194	1077	1078	1077
F. Yugoslavia	66	112	112	87	71	43
Total	23982	17929	15976	12375	11236	9230

Table 3: Optimized VOC emissions for different AOT40 targets



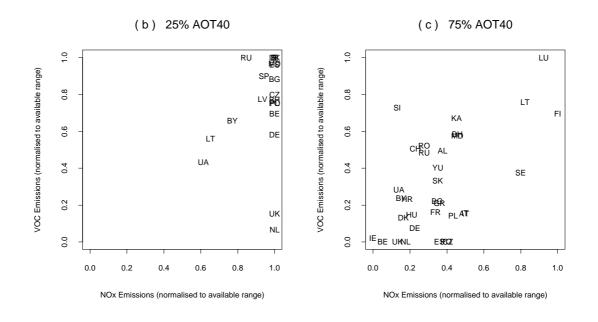


Figure 8: Comparison of optimized emissions for three AOT40 gap closure scenarios. The axes show the reductions of NO_x and VOC emissions. Countries are indicated by a two-letter code listed in Table 2.

4.2 Binding Receptors for the Ozone Optimization

It is often instructive to analyze the results of an optimization also in terms of its 'binding' constraints. Given a sufficiently large degree of freedom, optimizations with multiple constraints are usually driven by a few constraints, which are the most difficult to attain. In our case the constraints on the ozone exposure (AOT40) for the individual grids deserve special attention. As displayed in Figure 9, the 50 percent gap closure scenario is driven by about 20 'binding grids', where the AOT40s in the optimal case are exactly at the specified targets. At all other grids the resulting AOT40 is below the targets. It is worth mentioning that (i) these grids are rather evenly spread over Europe (with the exception of Scandinavia, where the AOT40 criteria for trees is not binding at all), and (ii) that there are about three times more binding receptors than in comparable runs for the acidification problem (e.g., in the runs carried out with the RAINS model for the EU acidification strategy). This means that the functional form of the ozone model leaves more flexibility for matching regional ozone targets at a finer scale than the 'broad-brush' atmospheric dispersion characteristics of acidifying pollutants.

Obviously, the optimal solution depends crucially on the targets specified for the binding grid cells. Any change in one of the targets at these grid cells will result in different emission reductions and costs.

It is interesting to realize that in Figure 9 in Mediterranean countries the grid cells containing the large cities (Athens, Lisbon, Madrid) show up as binding, if the gap closure for an AOT40 is to be optimized.

The concept of the EMEP model does not aim at modeling ozone levels in urban areas, but tries to capture the rural ozone on a larger scale. Comparison with monitoring results show that the EMEP model is in fact reproducing ozone levels around larger cities reasonably well, although it does not match urban concentrations, which are heavily influenced by local emissions. Although the EMEP model does not model ozone levels within urban areas, it takes stock of the high emission densities caused by the cities. This means that, also at the spatial resolution of the EMEP model, around such urban agglomerations high pollutant concentrations can activate different chemical schemes, which may modify the relevance of NO_x and VOC emission reductions from neighboring (rural) grids. To illustrate this effect, Figure 10 compares the ozone isopleths for Athens with some of its neighboring grid cells. There is clear evidence that the high emissions of Athens bend the shape of the curves in the Athens grid cell more towards a non-linear, VOC-limited type of isopleth.

Since the model apparently takes account of isolated high-emission areas, the question arises how dominating this 'city-effect' is for national emission reductions. In order to explore this further, a sensitivity case has been calculated in which the ozone constraints for the grid cells containing the major cities of the Iberian peninsula have been removed (but emissions from the cities are retained). Results from this variation in Table 4 demonstrate that there is only very little effect on optimized emissions from such an elimination of the urban areas. In the case when the three grids are excluded as constraints, neighboring grids become binding with only minor relaxation of emission reductions.

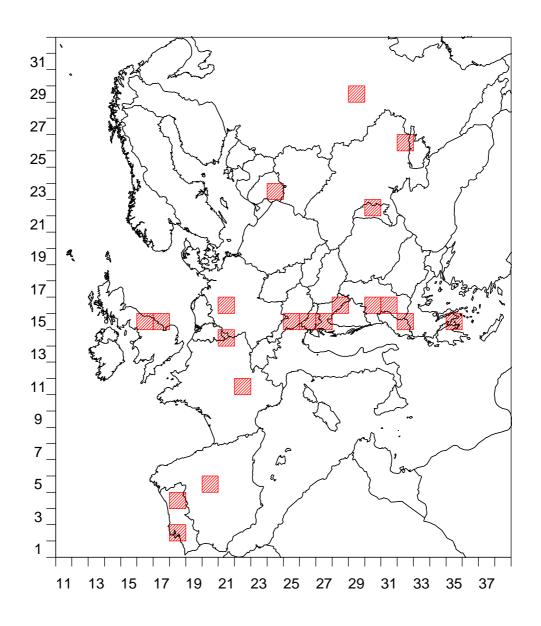


Figure 9: Binding receptor grids for an AOT40 50% gap closure scenario

Table 4: Emissions for	Spain and	Portugal i	f the	grid	cells	with	the	large I	berian	cities
are excluded from the op	ptimizatior	ı								

	NO	(kt)	VOC (kt)		
	Base case	ase case City grids		City grids	
		excl.		excl.	
Portugal	199	200	75	73	
Spain	778	807	562	555	

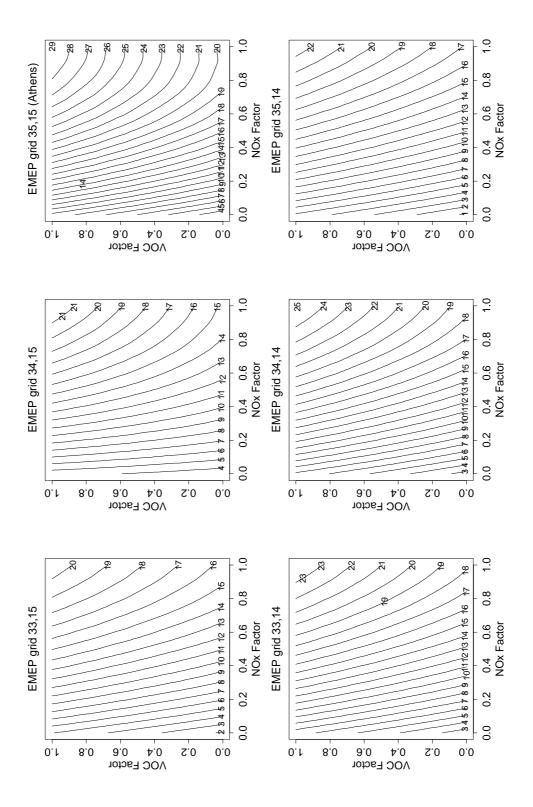


Figure 10: Ozone isopleths for Athens and surrounding grids

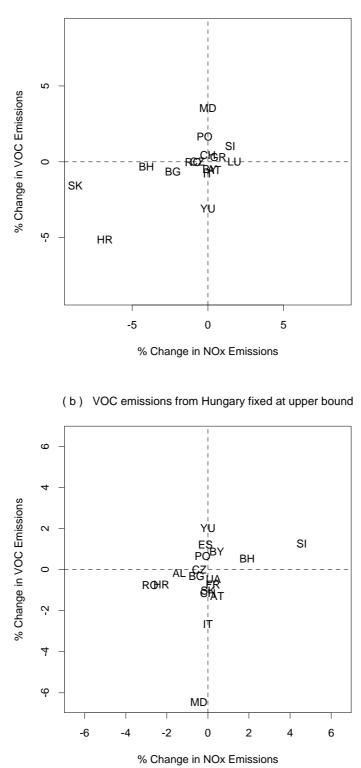
Another set of scenarios explores the effects of a hypothetical non-participation of a single country in the cooperative solution, or put differently, how other countries have to compensate for the absence of reductions in a given country. These scenarios are solely constructed in order to assess important structural aspects of the basic behavior of the ozone optimization, but should by no means bear any political implications. Furthermore, it must be kept in mind that all the arguments given in Table 1 apply also to this section.

It has been demonstrated elsewhere that ozone behavior shows distinct differences in different parts of Europe. Earlier work attempted to distinguish between 'NO_x-limited' and 'VOC-limited' regions, featuring the characteristic response of ozone levels towards changes in NO_x and/or VOC emissions. Although the preceding section demonstrates that such a concept can only be realized for a given situation (i.e., that the type of limitation will change, e.g., with reduced emissions) and also that emission control costs are a strong argument for allocating efficient control measures, it is still instructive to study the response in different parts of Europe.

As a first example three sensitivity cases assess the measures to be taken by other countries in order to compensate higher NO_x and/or VOC emissions in Hungary. With the above listed caveats in mind, Hungary could be attributed to the region where NO_x and VOC emissions are effective for reducing the AOT40. In the base case (the 50 percent gap closure scenario), Hungary would reduce its NO_x emissions by 13 percent and its VOC emissions by 47 percent below the upper bound.

As displayed in Figure 11a, keeping the Hungarian NO_x emissions at the upper bound (i.e., maintaining them 15 percent higher than in the optimal solution) would be compensated mainly by further reductions in neighboring countries, i.e., further cuts in NO_x emissions in Slovakia, in NO_x and VOC emissions in Croatia, and in VOC emissions in the former Yugoslavia. It is interesting to note a kind of second-order effect (a 'domino'-effect): the tightened control of the emissions of Hungary's neighbors enables a relaxation of measures in these more distant countries (e.g., Moldova). Furthermore, for a number of additional countries optimal emissions experience slight modifications, typically below two or three percent.

Maintaining Hungary's VOC emissions at the upper bound is mainly compensated by increased reductions of VOC in Moldova and Italy, and of NO_x and VOC in Romania and Croatia. The domino-effect becomes relevant for Slovenia and Bosnia-H. as neighbors of Croatia (Figure 11b).



(a) NOx emissions from Hungary fixed at upper bound

Figure 11: Changes in optimized emissions when emissions from Hungary are kept constant

The next set of scenarios examines the case if VOC emissions of Belgium are kept at the upper bound. Note that the optimal solution to reduce the AOT40 gap by 50 percent suggests for Belgium only further measures for VOC and keeps NO_x emissions constant. As displayed in Figure 12, the 44 percent (110 kt) increase in Belgium's VOC will be mainly compensated by a further decrease of NO_x emissions in neighboring countries (Denmark -15%, Luxembourg -10%, Germany -8%) and of VOC in Russia. These additional reductions allow in turn a relaxation of measures in other 'down-stream' countries, such as Austria, Hungary and Lithuania.

From these initial tests it can be concluded that it is difficult to predict (cost-optimal) measures necessary to compensate for missing volumes of optimized emission reductions. Generally, however, it can be stated that the number of involved countries is usually limited, which means that the non-participation of a single country does not influence the optimized abatement schedule for the majority of countries.

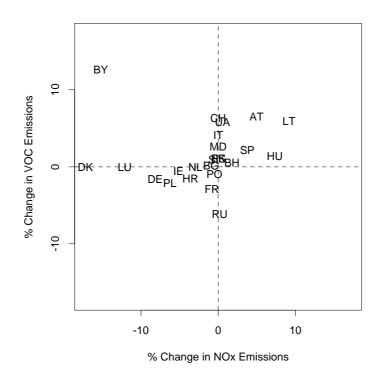


Figure 12: Changes in optimized emissions when emissions from Belgium are kept constant

4.4 Comparison between the 50% Gap Closure Target for AOT40 and AOT60

In this initial phase of model development a fourth set of optimization tests explored the differences between a gap closure aiming at the AOT40 for trees on the one hand and the AOT60 related to human health on the other.

It has been mentioned before that work has been undertaken to develop also a reducedform model for the AOT60. Although producing promising results, the work is not yet completed and all optimization results should be interpreted with great care. In particular a potential collinearity problem has not yet been entirely resolved.

Two optimization runs have been performed, one with the aim of reducing the gap of the AOT40 for trees by 50 percent, and the other aiming at a 50 percent gap closure of the AOT60 observed in the year 1990. Table 5 and Table 6 present the resulting emissions for NO_x and VOC. Not surprisingly, reducing the AOT60 generally involves less emission reductions than the AOT40.

Most interesting, however, is a structural comparison of the NO_x/VOC reductions for the individual countries (Figure 13). As can be concluded from this graph, for most countries the two solutions have significantly different structures (priorities for NO_x/VOC). Furthermore, what is most important, although the 50 percent gap closure of the AOT40 generally requires higher emission reductions than the AOT60, in several cases the optimization would suggest a reverse order for the NO_x emissions of some countries. For example, in the scenario aiming at a 50% gap closure of the AOT60 the Netherlands would reduce their NO_x emissions from 346 to 207 kt, whereas for achieving the AOT40 gap closure it would maintain them at the level of 346 kt. Similar effects occur for the Czech Republic, Bulgaria, Poland and for parts of Russia.

Figure 14 further illustrates the finding that reducing AOT40 for trees and AOT60 are structurally different problems by displaying the binding receptors for both optimization problems. Most striking is the fact that, out of the approximately 20 receptor grids which are binding in each problem, none is binding for both scenarios simultaneously.

There is a provisional conclusion to be drawn from this exercise: A concept using a reduction, or possibly a full elimination, of health-related ozone exposure levels (e.g., expressed in terms of an AOT60) as an interim target towards the ultimate target of full achievement of the vegetation-related critical levels does not appear to be a cost-effective way to approach the long-term goal. To what extent a strategy with a long-term aim of vegetation protection could maximize the benefits for health protection remains a subject for further analysis.

Country	1990	Upper	50%	50%	Difference	Lower
		bound	AOT40	AOT60		bound
	kt	kt	kt	kt	%	kt
Albania	30	30	26	30	13.96%	11
Austria	222	205	196	205	4.98%	80
Belarus	285	260	105	136	28.77%	77
Belgium	343	248	248	248	-0.10%	94
Bosnia-H.	54	48	41	48	15.47%	15
Bulgaria	376	290	212	147	-30.70%	79
Croatia	83	64	54	64	17.52%	24
Czech Republic	742	246	246	214	-13.21%	95
Denmark	269	174	94	164	74.73%	70
Estonia	66	70	70	70	0.00%	17
Finland	284	187	187	111	-40.45%	62
France	1584	1312	1161	1312	13.03%	576
Germany	3033	1903	1375	1903	38.35%	469
Greece	544	275	250	275	10.29%	82
Hungary	238	196	171	196	14.91%	76
Ireland	115	73	26	25	-5.15%	25
Italy	2053	1238	1238	1238	0.00%	454
Latvia	54	93	93	93	0.00%	36
Lithuania	56	130	83	115	39.10%	40
Luxembourg	23	15	14	9	-35.74%	6
Moldova	35	66	66	66	0.00%	19
Netherlands	570	346	346	207	-40.34%	132
Norway	231	137	137	137	0.00%	54
Poland	1280	819	819	620	-24.30%	292
Portugal	221	202	199	202	1.88%	74
Romania	883	442	327	442	35.17%	113
Kaliningrad	17	24	24	24	0.00%	7
Kola/Karelia	56	82	82	29	-64.87%	22
Rest of Russia	2477	2388	1606	2013	25.35%	680
St. Petersburg	124	160	150	63	-57.93%	41
Slovakia	227	120	120	120	0.00%	53
Slovenia	53	35	26	18	-30.13%	12
Spain	1256	888	778	888	14.11%	330
Sweden	398	254	254	254	0.00%	80
Switzerland	184	131	131	131	0.00%	48
Ukraine	1097	1403	758	831	9.67%	374
UK	2860	1641	922	1641	78.00%	585
F. Yugoslavia	66	119	119	119	0.00%	41
Total	22489	16312	12753	14405	12.96%	5344

Table 5: Optimized NO_x emissions for two 50 % gap closure targets

Country	1990	Upper	50%	50%	Difference	Lower
		bound	AOT40	AOT60		bound
	kt	kt	kt	kt	%	kt
Albania	30	30	25	30	17.81%	14
Austria	430	310	224	310	38.54%	190
Belarus	533	269	226	269	19.30%	126
Belgium	365	248	138	149	8.13%	128
Bosnia-H.	54	70	58	63	8.59%	39
Bulgaria	217	217	133	217	63.45%	93
Croatia	83	65	46	65	40.16%	25
Czech Republic	534	253	118	185	56.97%	118
Denmark	165	119	119	119	0.00%	69
Estonia	94	50	50	50	0.00%	16
Finland	209	112	112	112	0.00%	59
France	2402	1672	1025	1134	10.54%	810
Germany	3008	2019	1212	1256	3.62%	1101
Greece	325	318	180	318	76.42%	104
Hungary	205	145	77	145	87.38%	55
Ireland	180	138	78	138	77.10%	77
Italy	2401	1909	1283	1735	35.25%	892
Latvia	130	49	49	49	0.00%	12
Lithuania	187	111	83	111	33.59%	58
Luxembourg	19	12	12	12	0.00%	5
Moldova	116	114	98	114	17.12%	49
Netherlands	451	324	191	191	0.00%	191
Norway	251	189	189	189	0.00%	109
Poland	951	819	500	583	16.66%	431
Portugal	206	170	75	114	51.70%	73
Romania	700	453	417	453	8.51%	286
Kaliningrad	22	22	22	22	0.00%	12
Kola/Karelia	75	64	64	64	0.00%	39
Rest of Russia	3303	2573	2169	2573	18.61%	1489
St. Petersburg	166	196	185	196	6.00%	108
Slovakia	146	108	87	108	23.54%	66
Slovenia	35	25	23	25	9.44%	11
Spain	1112	923	562	809	43.91%	455
Sweden	533	308	308	308	0.00%	164
Switzerland	297	208	177	208	17.55%	119
Ukraine	1369	1366	895	981	9.62%	518
UK	2612	1840	1077	1107	2.74%	1077
F. Yugoslavia	66	112	87	112	28.80%	43
Total	23982	17929	12375	14623	18.17%	9230

Table 6: Optimized VOC emissions for two 50 % gap closure targets

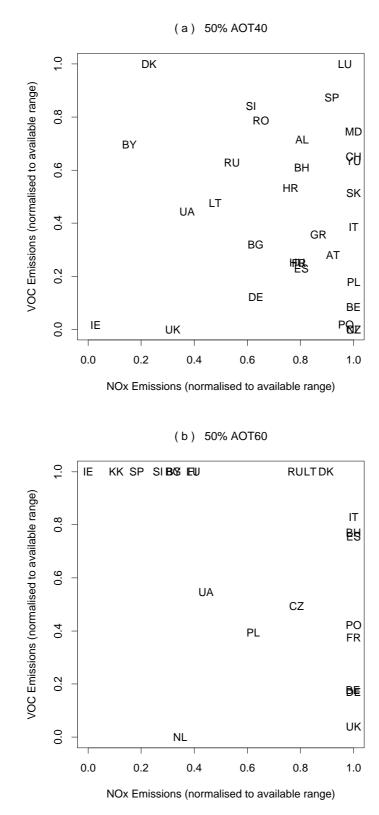




Figure 13: Comparison of optimized emissions for the AOT40 and AOT60 scenarios

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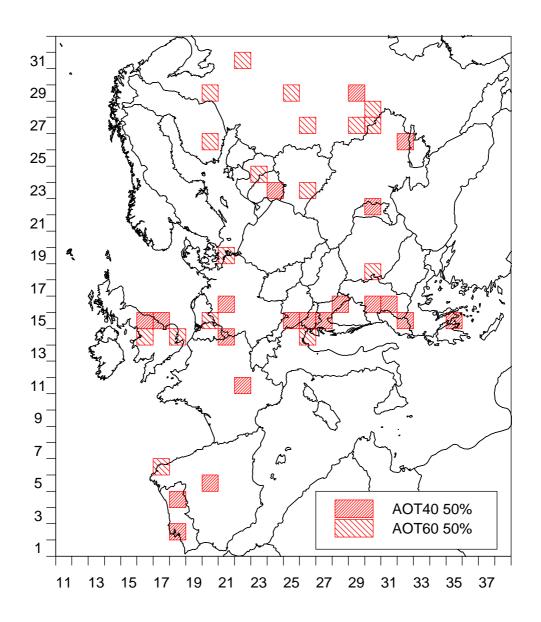


Figure 14: Binding receptor grids for the AOT40 and AOT60 50% gap closure scenarios

5. Conclusions

A first version of an optimization model for tropospheric ozone in Europe has been constructed. Although it is still premature to draw definite conclusions about concrete emission reduction strategies from the model, initial test runs suggest a reasonable response of the model framework towards changes in optimization targets and

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constraints. Operating in a realistic range of emission reductions, numerical instabilities do not occur as a major problem for the optimization software.

Based on current data and information, most European countries will have to control their emissions in order to achieve critical levels for ozone. For increasingly stringent sets of environmental targets, the relative importance of reductions of NO_x and VOC emissions changes, partly caused by the changing relevance of different chemical processes, partly caused by differences in emission control costs. Consequently, the concept of 'NO_x-' and 'VOC-limited' regions in Europe should be reconsidered in a dynamic context, in order to be useful for strategy development.

In the cases analyzed up to now the ozone optimization is driven by meeting the environmental targets of about 20 'binding' grid cells in Europe. This number is larger than for the acidification problem and indicates a higher flexibility in reaching regional environmental targets. For Mediterranean countries the test runs show clearly the influence of the large cities in the region. However, the initial runs suggest that a strategy would not experience significant modifications if it focuses more on rural areas in these countries.

The test runs demonstrate that for the ozone problem the optimal allocation of emission reductions is a rather complex task. It seems difficult to predict the optimal compensatory measures necessary to match non-participation of single countries without using the full framework of integrated assessment models.

There is some indication that optimizations aiming at reducing vegetation- and healthrelated exposure measures result in structurally different compositions of emission reductions. Consequently, it seems questionable to use, e.g., a health-related criterion as an interim target on the way towards a more stringent vegetation-related protection goal.

Further work will be necessary to improve the current model with latest information and to take into account some important aspects which have been ignored for the prototype optimization model. Particular attention should be devoted to the integration of the integration attention attention will be devoted to the integration of the free troposphere, and the modeling of health-related ozone exposure. Due to the preliminary nature of some elements of the integrated assessment framework, solid uncertainty- and robustness analysis will be essential for deriving credible conclusions.

The present analysis restricted itself to the ozone problem, focusing mainly on the critical levels for trees. Environmental policy, however, is in reality a multi-effect problem, with at least equal interest in protecting human health, natural vegetation and materials, taking into account also the implications on acidification, eutrophication and climate change. Considering these problems simultaneously will change the available space for efficient solutions and might therefore significantly change results obtained for a single-effect situation. Addressing this multi-effect problem (i.e., simultaneous consideration and optimization of acidification, eutrophication and tropospheric ozone) is envisaged within the next few months.

6. References

Alcamo J., Shah R., Hordijk L., eds. (1990) The RAINS model of Acidification. Science and Strategies in Europe. Kluwer Academic Publishers, Dordrecht, Netherlands

Amann M., Bertok I., Cofala J., Gyarfas F., Heyes C., Klimont Z., Schöpp W. (1996) Cost-effective Control of Acidification and Ground-level Ozone. First Interim Report to the European Commission DG-XI, International Institute for Applied Systems Analysis, IIASA, Laxenburg, Austria.

Cofala J., Heyes C., Klimont Z., Schöpp W., Amann M. (1995) The Contribution of the Transport Sector to the Achievement of Critical Loads and Critical Levels in Europe. International Institute for Applied Systems Analysis, Laxenburg, Austria.

EMEP (1996) MSC-W Status Report 1996 Part One; Estimated dispersion of acidifying agents and of near surface ozone. EMEP/MSC-W Report 1/96. Oslo, Norway.

Fuhrer J., Achermann B. (eds.) (1994) Critical Levels for Ozone, a UN/ECE Workshop Report. Swiss Federal Research Station for Agricultural Chemistry and Environmental Hygiene, Liebefeld-Bern, Switzerland.

Gipson G., Freas W., Kelly R., Meyer E. (1981) Guideline for use of city-specific EKMA in preparing ozone SIPs. EPA-450/4-80-027, US Environmental Protection Agency, Research Triangle Park, North Carolina, USA.

Heyes C., Schöpp W. (1995) Towards a simplified model to describe ozone formation in Europe. WP-95-34, International Institute for Applied Systems Analysis (IIASA), Laxenburg, Austria.

Heyes C., Schöpp W., Amann M. (1996) A Simplified Model to Predict Long-Term Ozone Concentrations in Europe. WP-96-12, International Institute for Applied Systems Analysis (IIASA), Laxenburg, Austria.

Simpson D. (1992) Long period modelling of photochemical oxidants in Europe : A) hydrocarbon reactivity and ozone formation in Europe. B) On the linearity of country-to-country ozone calculations in Europe. EMEP MSC-W Note 1/92, Norwegian Meteorological Institute, Oslo, Norway.

Simpson D. (1993) Photochemical model calculations over Europe for two extended summer periods : 1985 and 1989. Model calculations and comparison with observations. *Atmos. Environ.*, **27A**, No. 6, pp. 921-943.

Simpson D. (1995) Biogenic emissions in Europe: 2. Implications for ozone control strategies. *J. Geophys. Res.*, **100**, 22,891-22,906.

UN/ECE (1990) Integrated Assessment Modelling. EB.AIR/WG5/R.7, United Nations Economic Commission for Europe, Geneva, Switzerland

UN/ECE (1995) Strategies and Policies for Air Pollution Abatement. ECE/EB.AIR/44, United Nations Economic Commission for Europe, Geneva, Switzerland.

Interim Reports on work of the International Institute for Applied Systems Analysis receive only limited review. Views or opinions expressed herein do not necessarily represent those of the Institute, its National Member Organizations, or other organizations supporting the work.

Unger S. (1996) Parallelisation and Optimisation of EMEP's Transboundary Air Pollution Model. in Ruidervaart, J.C., Dekker L., Smit W. (eds.), Proceedings of the EUROSIM International Conference on HPCN Challenges in Telecomp and Telecom: Parallel Simulation of Complex Systems and Large-Scale Applications.

Venables W.N., Ripley B.D. (1994) Modern Applied Statistics with S-Plus. Springer-Verlag, New York.

Wenborn M.J., Marlowe I.T., Woodfield M.J., Passant N.R., Richardson S.J., Emmott M.A. (1995) VOC Emissions in Europe: An Assessment of the Potential for Abatement and an Estimate of the Associated Costs. AEA/CS/20011001/REMA-167, AEA Technology, UK.

Zawicki P., Makowski M. (1995) Software tools for generation, simulation and optimization of the simplified ozone model. WP-95-107, International Institute for Applied Systems Analysis, Laxenburg, Austria.