A Simplified Ozone Model Based on Fuzzy Rules Generation

Mina Ryoke[1]
Yoshiteru Nakamori[1]
Chris Heyes[2]
Marek Makowski[2]
Wolfgang Schöpp[2]

[1]*Japan Advanced Institute of Science and Technology, Ishikawa, Japan*
[2]*International Institute for Applied Systems Analysis, Laxenburg, Austria*

Research Reports, which record research conducted at IIASA, are independently reviewed before publication. Views or opinions expressed herein do not necessarily represent those of the Institute, its National Member Organizations, or other organizations supporting the work.

A simplified ozone model based on fuzzy rules generation

Mina Ryoke [a], Yoshiteru Nakamori [a], Chris Heyes [b], Marek Makowski [b,*],
Wolfgang Schöpp [b]

[a] *Japan Advanced Institute of Science and Technology, 1-1 Asahidai, Tatsunokuchi, Ishikawa 923-1292, Japan*
[b] *International Institute for Applied System Analysis, Schlossplatz 1, A-2361 Laxenburg, Austria*

Abstract

In this paper, simplified ozone models for potential use in integrated assessment are developed from the EMEP ozone model, which is a single-layer Lagrangian trajectory model. The simplification method uses fuzzy rule generation methodology to represent numerous results of the EMEP model as a response surface describing the source–receptor relationships between ozone precursor emissions and daily tropospheric ozone concentrations. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Modeling; Fuzzy sets; Environment; Tropospheric ozone

1. Introduction

Major concerns about the environmental impacts of air pollution exist in many parts of the world. In some cases, such concerns have led to the introduction of measures to reduce the emissions of air pollutants in order to limit their negative effects.

Within Europe interest in ground-level ozone has intensified in recent years, with increasing experimental evidence that ozone can have adverse effects on crops, trees, materials and human health. Studies of the impacts of ozone have resulted in the establishment of critical levels for ozone in order to protect agricultural crops and forests, using a long-term exposure measure, the 'accumulated excess ozone' concept described by Fuhrer and Achermann (1994). A threshold concentration of 40 ppb has been set for both crops and trees. This exposure index is referred to as AOT40, the accumulated exposure over a threshold of 40 ppb. In many parts of Europe the critical levels are exceeded and measures to reduce ozone concentrations in these areas will be needed to protect the relevant ecosystems.

* Corresponding author. Tel.: +43-2236-8070; fax: +43-2236-71-313.

E-mail addresses: ryoke@jaist.ac.jp (M. Ryoke), nakamori@jaist.ac.jp (Y. Nakamori), heyes@iiasa.ac.at (C. Heyes), marek@iiasa.ac.at (M. Makowski), schoepp@iiasa.ac.at (W. Schöpp).

In line with the revised World Health Organisation (WHO) Air Quality Guidelines for Europe (see WHO, 1997), a maximum 8-hour average concentration of 60 ppb has been proposed as the environmental objective relevant to the protection of human health. Because of current difficulties with the modeling of European abatement strategies for individual days over a multi-month period, which such an indicator implies, a surrogate AOT indicator (AOT60), analogous to AOT40 for vegetation, has been introduced. An AOT60 – i.e., the cumulative excess exposure above 60 ppb, for practical reasons over a six-month period – of zero is considered to be equivalent to the full achievement of the WHO criterion. Although the AOT60 has proved useful as a practical, surrogate indicator for risk to human health, an alternative method designed to handle shorter term, e.g., daily, ozone concentrations above 60 ppb remains a desirable objective.

The timescale 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. Consequently, measures to control ozone require international cooperation if they are to be successful and cost-effective. During the last decade several international agreements have been reached in Europe to reduce emissions – of sulphur dioxide (SO_2), nitrogen oxides (NO_x) and volatile organic compounds (VOC) – in a harmonized way. The negotiations leading to the more recent agreements have benefited greatly from the assistance given by integrated assessment models, which bring together in a consistent framework information on emission generation, emission control technologies and abatement costs, the long-range transport of pollutants and the environmental sensitivities of different areas of Europe. In addition to assessing the environmental impacts of alternative strategies for emission reductions, integrated assessment models can also be used in an 'optimization' mode to identify those strategies that minimize the costs required to achieve a given set of environmental targets. Such models

have now been developed further to take ground-level ozone into account.

An essential requirement of an integrated assessment model for ozone is a simplified but reliable description of the ozone formation process in order to represent the source–receptor relationships involved. It is possible to envisage several ways of condensing the results of more complex models of ozone formation to achieve this. One approach is to use statistical techniques to summarize the results obtained from a complex mathematical model for a large number of emission reduction scenarios. Two examples of this approach based on the EMEP photochemical model have been described, one using local regression techniques (Heyes and Schöpp, 1995) to model daily ozone concentrations, the other involving linear regression models of seasonal mean values (Heyes et al., 1996). The optimization problem related to the second of these methods is outlined by Makowski (2000) and it is this method that has been incorporated recently into the RAINS integrated assessment model described by Schöpp et al. (1999).

The subject of this paper is an alternative method of representing the results of the EMEP model as a response surface using fuzzy rule generation methodology (Nakamori and Ryoke, 1994). The idea is to construct a number of fuzzy rules about the source–receptor relationships between ozone precursor emissions and daily tropospheric ozone concentrations. Actual ozone concentrations also depend on many local factors such as topographical location, local emissions and meteorological conditions. Taking account of such factors requires at least a daily model such as that provided by this approach. If developed for a sufficient number of receptor points, the set of fuzzy rules could be used as an alternative simplified ozone model.

Section 2 of the paper provides an outline of the salient features of ozone formation photochemistry, a brief description of the EMEP photochemical model and an explanation of the variables used in building the fuzzy model. As an example of the method, a fuzzy model developed for a receptor grid located in Austria is presented in Section 3.

2. Background

2.1. Ozone formation

The formation of ozone involves chemical reactions between NO_x (i.e., nitric oxide (NO) and nitrogen dioxide (NO_2) taken together) and VOCs driven by solar radiation, and occurs on a regional scale in many parts of the world. A complete description of the processes involved is beyond the scope of this paper; the following very brief outline serves only to highlight some of the important relevant features.

Ozone production requires the combination of atomic and molecular oxygen. In the troposphere, photodissociation of NO_2 is the only significant source of oxygen atoms. The ozone produced as a result of this photodissociation may then react with NO to regenerate NO_2, leading to the establishment of a photochemical steady state between O_3, NO and NO_2 in a relatively unpolluted atmosphere during hours with sunlight.

The photochemical steady state will be perturbed by any processes, other than reaction with O_3, which convert NO to NO_2, such processes resulting in the net production of ozone. This is made possible when VOCs are also present in the atmosphere. The essential first step in a potentially complex chain of reactions involving VOCs is attack by hydroxyl radicals (OH). Subsequent reactions can form peroxy and hydroperoxy radical species which are able to oxidize NO to NO_2, and therefore lead to enhanced ozone formation. Thus, NO_x and VOC species and the presence of sunlight are all necessary prerequisites for the production of ozone within the atmospheric boundary layer.

One of the main processes which removes free radicals, and therefore opposes ozone formation, is the combination of OH radicals with NO_2. When NO_2 concentrations are very high, as they may be in areas of high NO_x emission density, the NO_2 competes with VOCs for reaction with OH, and inhibits the production of ozone. Consequently, NO_x exerts a nonlinear influence on tropospheric ozone formation. This feature of ozone photochemistry has important implications for emission control strategies designed to reduce ozone concentrations.

While emissions of ozone precursors are clearly essential for ozone formation, meteorological factors also exert a crucial influence. The intensity of the incoming solar radiation must be high, and temperature is also important in influencing the rates of many of the chemical reactions involved. Other conditions favorable to ozone formation are low windspeeds and a persistent, well-defined atmospheric boundary layer. Other important factors in determining ozone concentrations at ground level are the rate at which ozone is removed by deposition to terrestrial surfaces and mixing processes occurring in the troposphere.

2.2. The EMEP ozone model

Within the UNECE European Monitoring and Evaluation Programme (EMEP) a Europe-wide ozone model has been developed at the Meteorological Synthesizing Centre-West in Oslo. This EMEP ozone model has been designed with the purpose of simulating ozone formation over long periods of time (one month to one year) and over the whole of Europe, so that the likely effects of emission control measures on long-term ozone concentrations can be estimated.

The EMEP ozone model (Simpson, 1992, 1993, 1995) is a single-layer Lagrangian trajectory model with a variable depth which extends from the ground to the top of the atmospheric boundary layer. The model calculates concentrations of photochemical oxidants every 6 hours for a set of up to 740 arrival points (on a 150 km × 150 km grid) covering the whole of Europe. Columns of air in the atmospheric boundary layer are followed along specified 96-hour trajectories, picking up emissions of NO_x, VOC, CO and SO_2 from the underlying grid. The height of the air column, the mixing height, containing the bulk of the polluted air is reset at 12 GMT each day from radiosonde data. Along each trajectory the mass conservation equations are integrated, taking into account emission inputs, photolysis and chemical reactions, dry and wet removal, and the influence of meteorological parameters. These equations are solved numerically, currently using

the quasi-steady state approximation method with a fixed time step of 15 minutes.

The six-hourly meteorological data required by the EMEP model are taken from the output of the Norwegian Numerical Weather Prediction model. Wind velocity data permit calculation of 96-hour back-trajectories to any point in the EMEP grid. The ozone model simulates the exchange of boundary layer air with free tropospheric air as a result of convective clouds. Photolysis rates are adjusted for cloud cover, and temperature data are used to calculate appropriate chemical reaction rates and in estimating natural VOC emissions. Other meteorological data are used in estimating deposition velocities, which are calculated as a function of atmospheric stability, latitude, time of year and time of day.

The anthropogenic emissions of NO_x, VOC, CO and SO_2 used in the model are based, as far as possible, on data supplied officially at a national level. For use in the ozone model, the emissions data are spatially disaggregated onto a 50 km× 50 km grid. Natural emissions of VOCs are represented in the EMEP ozone model by the emissions of isoprene from forests and agricultural crops (see Simpson, 1995). These are calculated at each time step using surface temperature data, land-use data for each grid square and published emission–temperature relationships.

The EMEP model uses a chemical mechanism in which each important VOC class is represented by one or two members whose chemical degradation is followed explicitly. The chemical mechanism comprises 136 reactions, including 25 photolysis reactions, and the model calculates explicitly the concentrations of 61 chemical species. Methane is treated in the model as a tropospheric background species. Initial concentrations of all species at the start of each 96-hour trajectory are taken from previous model calculations, if available; otherwise a set of assumed background tropospheric concentrations, based on appropriate measured data or tropospheric model calculations, is used.

2.3. Generation of input data

Input data for the fuzzy model are generated from EMEP model calculations carried out using 1990 emissions data and meteorological data for the period April–September 1990. The countries and regions contributing data of annual emissions of NO_x and VOC are shown in Table 1.

Two main scenarios are calculated: first is the 1990 'base' case with unabated emissions, second a scenario involving uniform emission reductions

Table 1
Emitter regions in the EMEP model

1	Albania	2	Austria	3	Belgium
4	Bulgaria	6	Denmark	7	Finland
8	France	9	East Germany	10	Germany
11	Greece	12	Hungary	13	Iceland
14	Ireland	15	Italy	16	Luxembourg
17	Netherlands	18	Norway	19	Poland
20	Portugal	21	Rumania	22	Spain
23	Sweden	24	Switzerland	25	Turkey
27	United Kingdom	29	Other land areas	30	Baltic Sea
31	North Sea	32	Remaining NE Atlantic	33	Mediterranean
35	Nat ocean emissions	36	Kola/Karelia	37	St. Peter/Novgo Pskov
38	Kaliningrad	39	Belarus	40	Ukraine
41	Moldova	42	Rest of the Russian Fed.	43	Estonia
44	Latvia	45	Lithuania	46	Czech Republic
47	Slovakia	48	Slovenia	49	Croatia
50	Bosnia Herzegovina	51	Serbia, Montenegro	52	Macedonia
53	Kazakhstan	54	Georgia		

across all European countries. In this second scenario, emissions of NO_x, VOC and CO are reduced, from all man-made emission sources, by 70%. In addition to these two main scenarios, numerous 'individual country' scenarios, in which emissions of a single pollutant from a single emitter country are reduced, are also investigated. The results from these model runs provide information on the influence of precursor emissions from individual countries on the results at a given receptor grid. Although there are many possible combinations for reducing precursor emissions, we have limited our study to the scenarios summarized in Table 2.

For this exercise, results from the EMEP model are obtained for three receptor grids, one in NW England, one in SW Germany and one covering the Upper Austria region of Austria. Results from this third grid, which includes the industrial towns of Linz and Wels as well as some remote areas such as the Salzkammergut, are presented by Ryoke (1996). In each of these three regions some nonlinear behavior with NO_x emissions is to be expected. The EMEP results provided data on ozone concentrations, photolysis rates of NO_2 and a dilution-weighted or 'effective' integrated emissions parameter which allows for losses of emitted species along an air mass trajectory.

In the EMEP ozone model, the emissions and meteorological input data are revised at 2-hour intervals, so that there are 49 time steps during

the four-day trajectory. Two processes are included in the model which lead to mixing of the boundary layer air parcels with free tropospheric air: the venting effect of cumulus clouds and day-to-day increases in mixing height. These exchange mechanisms operate at 2-hour intervals. If the emissions of an ozone precursor during time step i are denoted by E_i, and the exchange processes result in a dilution of the boundary layer air by a dilution factor d_i $(0 < d_i \leqslant 1)$, the contribution from time step i to the trajectory-integrated value of the precursor emissions, E, at time step $(i + 1)$ is given simply by

$$E_i \times d_{i+1}. \tag{1}$$

The integrated contribution from all 49 time steps, denoted by $\langle E \rangle$, is given by

$$\langle E \rangle = \sum_{i=1}^{i=48} \left(E_i \times \prod_{j=i+1}^{j=49} d_j \right) + E_{49}. \tag{2}$$

Such quantities are calculated for both NO_x and VOC emissions along each trajectory and investigated as predictor variables in regression models of the fuzzy model.

The following variables are considered in the fuzzy modeling approach:
- *Ozone concentration* (ppb): The dependent variable is taken as the daily O_3 concentration calculated for the 12 GMT trajectory arrival. This value is assumed to represent the early afternoon concentration when O_3 is expected to be at or near its daily maximum value.
- *Contributions to effective NO_x* (10^{10} molecules cm^{-2}): From the results of the individual country scenarios it is possible to calculate the contributions from individual emitter countries to effective emissions at a particular receptor grid. These data constitute weighted meteorological information. The individual country contributions to effective NO_x from the six most influential (usually neighboring) countries for the selected grid are used in the fuzzy modeling exercise. These combine information about the path taken by the air mass together with its atmospheric stability.

Table 2
Outline of scenario emission factors

	Individual countries		All (other) countries	
	NO_x	VOC	NO_x	VOC
Base Scenario1	–	–	1.0	1.0
Base Scenario2	–	–	0.3	0.3
Scenario1	1.0	0.6	1.0	1.0
Scenario2	0.8	1.0	1.0	1.0
Scenario3	0.6	1.0	1.0	1.0
Scenario4	0.3	0.7	0.3	0.3
Scenario5	0.5	0.3	0.3	0.3
Scenario6	0.7	0.3	0.3	0.3

- *Contributions to effective VOC* (10^{10} molecules cm^{-2}): These data are the VOC analogue of the effective NO_x contributions above; they are not used as the information they provide is similar to that from the effective NO_x contributions.
- *Effective NO_x* (10^{10} molecules cm^{-2}): The daily 12 GMT effective NO_x values at the selected grid, which include the contributions from all European countries and non-controllable sources, are used. This variable represents the total NO_x potentially available for reaction during the course of the four-day trajectory. At the arrival point some of this NO_x will have been lost through chemical reaction but is 'remembered' in the form of ozone or other species produced.
- *Effective VOC* (10^{10} molecules cm^{-2}): These data are again the VOC analogue of the effective NO_x values and include both man-made emissions from all the countries and natural VOC emissions.
- *NO_2 photolysis rate* (10^{-3} s^{-1}): The value used is the mean photolysis rate over the final 30 hours of the trajectory. This is used to represent solar radiation, which affects ozone formation, and is dependent on the cloud cover.
- *Mixing factor* ($0 <$ mixing factor $\leqslant 1$): The mixing factor describes the extent of mixing between the boundary layer and the troposphere. A value of 0 would indicate complete mixing, 1 no mixing.

The combination of individual country contributions to effective NO_x and the photolysis rate of NO_2 provides information about the meteorological conditions experienced by an air mass during the course of its travel to the selected receptor grid. It may be helpful, in some circumstances, to aggregate the contributions made by some countries when their patterns of influence are similar.

2.4. Implementation

We have developed a fuzzy modeling technique and corresponding modeling software with a highly interactive graphical user interface using the C-language and the Tcl/Tk toolkit. The objective function consists of two parts related to the regression errors and the data distances, respectively. Two dynamically changing parameters are introduced to make a balance of the above-mentioned two objectives. The software supports examination of the clustering results (for any two selected clustering variables), of the regression results with statistics for judging goodness of linear models, and simulation results by the developed fuzzy model.

3. Fuzzy model at a grid in Upper Austria

A previous pilot study presented by Ryoke (1996) showed that the fuzzy model provides a useful way to summarize results of the EMEP ozone model. It was found that the concept of effective precursor emissions is sufficient to model adequately the daily variation of ozone. However, the previous study was based on uniform emission control across Europe. The present study extends the work to include emission reduction scenarios for individual European countries.

3.1. Data and scenarios screening

The time period covers six months: April–September 1990. Daily values are provided, referring to 12 GMT air mass trajectory arrivals.

For each grid there are data for two 'base' cases involving the full set of countries considered. In such a scenario all countries make the same fractional changes to both their NO_x and VOC emissions. For these 'base' cases ozone concentration data are provided for all those days on which the following two conditions hold:
1. the solar radiation is considered high enough for reasonable ozone production to occur,
2. there is not so much mixing with the free troposphere that man-made emissions can have only very little influence on ozone concentrations.

In addition to the two base cases, there are six further country-specific scenarios for each of the six influential emitter countries, making a total of 38 ($= 2 + 6 \times 6$) scenarios for each receptor grid.

The combinations of emission reductions employed for these country-specific scenarios are outlined in Table 2.

Data for these additional 36 scenarios are provided for days:

1. which meet the criteria given above for the 'base' cases (enough solar radiation and not too much mixing) and
2. for which the 'scenario' ozone concentration does actually differ from the appropriate 'base case' value.

That is, data are excluded for those days on which an emission change in one country has no effect on ozone concentration at the particular grid in question.

3.2. Fuzzy model

The model at the receptor j consists of c_j fuzzy rules. Let pv_{j1} be the effective NO_x from all countries to the grid calculated by the EMEP ozone model with scenarios. If pv_{j1} is very high, the concentrations of radicals which are necessary for ozone production will be distorted. Let pv_{j2} be the effective NO_x from countries excluding the country in which the grid j is located and calculated with the emissions of scenario 'Base Scenario1' in Table 2. If pv_{j2} is high, there is a larger long-range transport component. Let pv_{j3} be a mixing factor. If pv_{j3} is low, considerable mixing of free tropospheric air into the boundary layer takes place. Ozone concentration will very much depend on the free tropospheric ozone value. If pv_{j3} is high the boundary layer production is an important component for ozone. Let pv_{j4} be the photolysis rate of NO_2. When pv_{j4} is high, we have a lot of sunshine and a large ozone production capacity.

Rule R_j^p is given as follows:

If $(pv_{j1}, pv_{j2}, pv_{j3}, pv_{j4})$ is A_j^p (a fuzzy subset),

$$\text{then } oz_j^p = k_j^p + \sum_{i \in I_j} \alpha_{ij}^p n_i + \sum_{i \in I_j} \beta_{ij}^p v_i, \tag{3}$$

where $i \in I$ denotes emitters (countries), $j \in J$ the receptors (grids), I_j the highly influencing emitters to the receptor j, n_i the emission of NO_x from the emitter i, v_i the emission of VOCs from the emitter i, and oz_j is ozone concentration at the receptor j.

In the consequence part, the relation between consequence variables is independent of time t and scenario s explicitly. They are already given by the EMEP ozone model which considers trajectories for 96 hours. Actually, they are related to premise variables implicitly.

A_j^p is a fuzzy subset in the four-dimensional space spanned by $pv_{j1}, pv_{j2}, pv_{j3}$, and pv_{j4}. Let $f_j^p(x)$ be the membership grade in A_j^p, used to calculate the degree of confidence of a rule, which is a nonlinear function and $0 \leqslant f_j^p(x) \leqslant 1$. The degree of confidence of rules $f_j^p(x)$ is defined as follows. First of all, the membership function of a premise variable x_k is defined by using the subset Z_{jk}^p which corresponds to the data set to build Rule R_j^p.

$$
\mu_{jk}^p(x_k; \; q_{k1}^p, q_{k2}^p, q_{k3}^p, t_{k1}^p, t_{k2}^p)
$$
$$
= \begin{cases}
\exp\left\{ -\dfrac{(x_k - q_{k2}^p)^2}{2(t_{k1}^p)^2(q_{k1}^p - q_{k2}^p)^2} \right\}, & x_k \leqslant q_{k2}^p, \\[2mm]
\exp\left\{ -\dfrac{(x_k - q_{k2}^p)^2}{2(t_{k2}^p)^2(q_{k3}^p - q_{k2}^p)^2} \right\}, & x_k \geqslant q_{k2}^p,
\end{cases} \tag{4}
$$

where the first, second and third quartiles of the data subset p are denoted by q_{k1}^p, q_{k2}^p and q_{k3}^p, respectively. The second quartile corresponds to the medium of data distribution on the axis. The first and third quartiles are defined so that the first one is smaller than the third one. If two of them are equal, give one of them a small fluctuation to keep the restriction that $q_{k1}^p < q_{k2}^p < q_{k3}^p$. The tuning parameters t_{k1}^p, t_{k2}^p have default 1 and they are optimized in the identification of the fuzzy model (see Nakamori and Ryoke, 1994). Next, the membership function for Rule R_j^p is defined by

$$f_j^p(x) = \prod_{k=1}^{4} \mu_{jk}^p(x_k; \; q_{k1}^p, q_{k2}^p, q_{k3}^p; \; t_{k1}^p, t_{k2}^p). \tag{5}$$

Estimation of oz_j is done by the following formula: For a given $x = (pv_{j1}, pv_{j2}, pv_{j3}, pv_{j4})$,

$$\widehat{oz}_j = \frac{\sum_{p=1}^{c_j} f_j^p(x) \cdot oz_j^p}{\sum_{p=1}^{c_j} f_j^p(x)}. \tag{6}$$

Table 3
A regression model at a receptor located in Upper Austria

Ozone = 41.760		
$+1632. \times NO_x$ from Austria	($t\_ratio = +6.44$)	($correl. = +0.53$)
$+646.2 \times NO_x$ from France	($t\_ratio = +1.41$)	($correl. = +0.08$)
$+537.8 \times NO_x$ from East Germany	($t\_ratio = +1.78$)	($correl. = +0.25$)
$+119.2 \times NO_x$ from West Germany	($t\_ratio = +0.99$)	($correl. = +0.24$)
$+346.5 \times NO_x$ from Italy	($t\_ratio = +1.70$)	($correl. = +0.32$)
$+304.1 \times NO_x$ from Czech Rep.	($t\_ratio = +1.27$)	($correl. = +0.20$)
$+910.6 \times VOC$ from Austria	($t\_ratio = +3.64$)	($correl. = +0.53$)
$+621.2 \times VOC$ from France	($t\_ratio = +1.36$)	($correl. = +0.08$)
$+861.0 \times VOC$ from East Germany	($t\_ratio = +2.87$)	($correl. = +0.25$)
$+349.2 \times VOC$ from West Germany	($t\_ratio = +1.93$)	($correl. = +0.24$)
$+548.6 \times VOC$ from Italy	($t\_ratio = +2.71$)	($correl. = +0.32$)
$+25.19 \times VOC$ from Czech Rep.	($t\_ratio = +0.11$)	($correl. = +0.20$)
	$(R^2)^* = 0.4590,\quad T(2383, 0.05) = 1.961.$	

3.3. Model parameters and prediction result

Before going into fuzzy modeling, a regression model is developed by using all data. A regression model is determined by the least square method and shown in Table 3.

Here, $(R^2)^*$ denotes the coefficient of determination adjusted for the degree of freedom and $T(2383, 0.05)$ is the 5 percentile of the t-distribution with the degrees of freedom 2383. In the equation, the t_ratio of the regression coefficients and the correlation coefficients of explanatory variables with ozone are also shown. The correlation coefficient between predictions by EMEP ozone model and the traditional regression model is 0.6708. In Fig. 1, the prediction result by the linear regression model is shown.
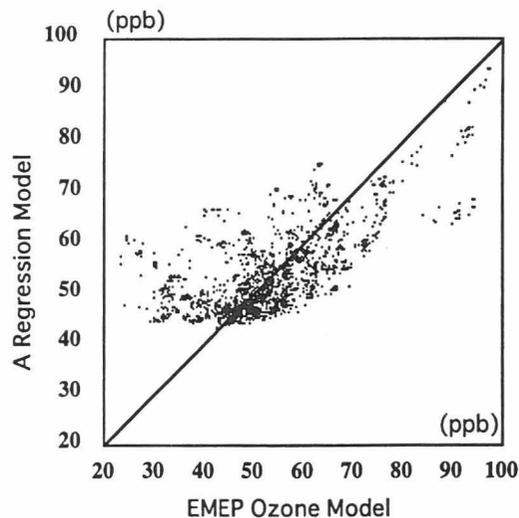

Fig. 1. Prediction result by a regression model.

Table 4
Clustering variables

Response variable	Ozone concentrations
Premise variables	pv_1
	pv_2
	pv_3
	pv_4
Consequence variables	NO_x from Austria
	NO_x from France
	NO_x from East Germany
	NO_x from West Germany
	NO_x from Italy
	NO_x from Czech Rep.
	VOC from Austria
	VOC from France
	VOC from East Germany
	VOC from West Germany
	VOC from Italy
	VOC from Czech Rep.

Table 5
Parameters of premise variables in Rule 1

Premise variables	min.	q_1	q_2	q_3	max.	t_1	t_2
pv_1	0.001917	0.004180	0.007426	0.01059	0.02363	3.4	4.1
pv_2	0.004594	0.01210	0.01623	0.02287	0.04126	1.0	4.7
pv_3	0.4008	0.4527	0.5102	0.5568	0.7498	4.6	3.4
pv_4	2.178	2.400	2.844	3.179	3.484	2.0	1.2

Table 6
Consequence coefficients in Rule 1

Consequence variables	Coefficient
NO_x from Austria	1512
NO_x from France	−1889
NO_x from East Germany	−111.9
NO_x from West Germany	−287.8
NO_x from Italy	186.8
NO_x from Czech Rep.	18.55
Constant	38.95
VOC from Austria	1534
VOC from France	993.8
VOC from East Germany	598.76
VOC from West Germany	360.1
VOC from Italy	706.9
VOC from Czech Rep.	−73.61

Now, we briefly summarize fuzzy models developed for one grid in Europe. First step of fuzzy modeling for the selected grid is provided by the adaptive fuzzy clustering presented by Ryoke et al. (1998) in order to obtain the classification and regressions in each rule. According to the above discussion, the clustering variables are given as in Table 4. Note, that the consequence variables NO_x and VOC specified in Tables 4, 6, 8 and 10 stand for the corresponding country contributions to effective NO_x and to effective VOC, respectively.

The reason why the adaptive fuzzy clustering proposed in Ryoke et al. (1998) is used, is that these clustering variables are highly correlated with each other. The number of clusters, determined by a trial and error approach, has been set to 3. In the next step, the tuning parameters of the premise variables have been optimized. The modeling system (outlined in Section 2.4) has been developed so that the modelers can carry out the fuzzy modeling interactively. The above clustering method and the tuning method for the premise parameters are also included in the system with graphical user interface.

The values of parameters in the developed fuzzy model are shown in Tables 5–10. The membership functions of the premise variables are illustrated in Figs. 2–5. The vertical axis means the grade of the membership function for each rule. The prediction result is presented in Fig. 6. The correlation coefficient between predictions by the obtained fuzzy model and the EMEP ozone model is 0.811.

4. Concluding remarks

This paper presents fuzzy models expressing relationships between precursor emissions of NO_x
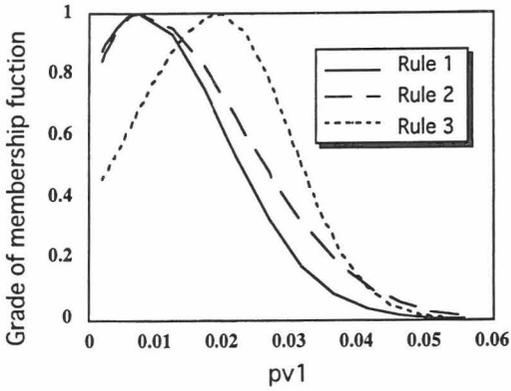
Table 7
Parameters of premise variables in Rule 2

Premise variables	min.	q_1	q_2	q_3	max.	t_1	t_2
pv_1	0.001844	0.005340	0.007384	0.01185	0.02463	4.6	3.6
pv_2	0.006268	0.01456	0.02013	0.02577	0.03717	4.0	2.3
pv_3	0.4097	0.4613	0.5148	0.6063	0.9701	4.8	3.9
pv_4	3.177	3.7462	4.1964	4.4047	4.644	0.7	3.7

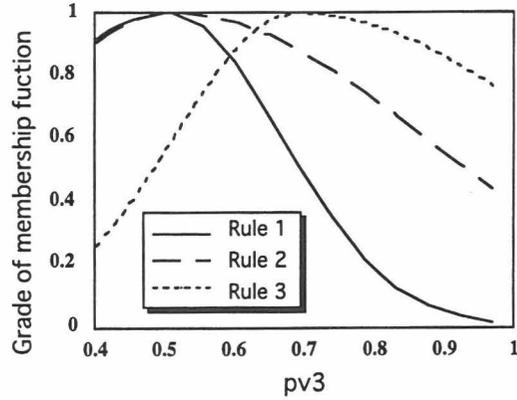Fig. 2. Membership function of pv_1.

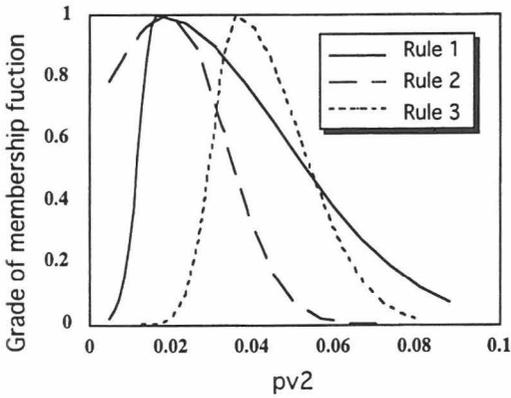Fig. 4. Membership function of pv_3.

Fig. 3. Membership function of pv_2.

Table 8
Consequence coefficients in Rule 2

Consequence variables	Coefficient
NO_x from Austria	1696
NO_x from France	652.2
NO_x from East Germany	157.8
NO_x from West Germany	311.7
NO_x from Italy	213.4
NO_x from Czech Rep.	342.5
Constant	45.19
VOC from Austria	908.4
VOC from France	269.6
VOC from East Germany	308.6
VOC from West Germany	229.7
VOC from Italy	340.4
VOC from Czech Rep.	43.40

and VOC and ozone concentrations developed for a grid located in Upper Austria. A comprehensive photochemical model (the EMEP model) and numerous emissions scenarios have been used for the development and verification of fuzzy models. It has been shown that the fuzzy model provides better predictions of ozone concentrations than the traditional regression model based on all data at each grid. Furthermore, the membership functions obtained appear to be sensible. Based on examination of meteorological data, the different fuzzy rules do seem to describe different meteorological conditions rather well.

The reported results illustrate how one can use a detailed model for the development of simple fuzzy models. The simple models can then be used for an analysis of many scenarios, which is practically impossible using a detailed (thus computation demanding) model. If further work is successful, then simplified fuzzy models for more grids within Europe could be developed and used for analysis of various emission reduction policy options. It remains to be seen if it will be possible to identify a relatively small number of clusters of grids and to develop a single model for all grids belonging to one cluster.

Table 9
Parameters of premise variables in Rule 3

Premise variables	min.	q_1	q_2	q_3	max	t_1	t_2
pv_1	0.004659	0.01254	0.01972	0.02415	0.05591	2.0	2.3
pv_2	0.01283	0.02851	0.03576	0.04547	0.08769	0.8	1.6
pv_3	0.4207	0.6025	0.691	0.7820	0.9701	2.0	4.2
pv_4	2.288	3.635	4.130	4.402	4.644	4.2	2.2

Fig. 5. Membership function of pv_4.

Fig. 6. Prediction result by the fuzzy model.

Table 10
Consequence coefficients in Rule 3

Consequence variables	Coefficient
NO_x from Austria	1403
NO_x from France	911.1
NO_x from East Germany	598.3
NO_x from West Germany	169.5
NO_x from Italy	401.1
NO_x from Czech Rep.	226.7
Constant	41.97
VOC from Austria	795.3
VOC from France	1013
VOC from East Germany	1028
VOC from West Germany	392.3
VOC from Italy	630.2
VOC from Czech Rep.	253.4

After developing fuzzy models in principal grids, interpolation is needed to predict the ozone concentrations in other grids in central and western Europe. One of the methods considered is to define a similarity measure between receptors.
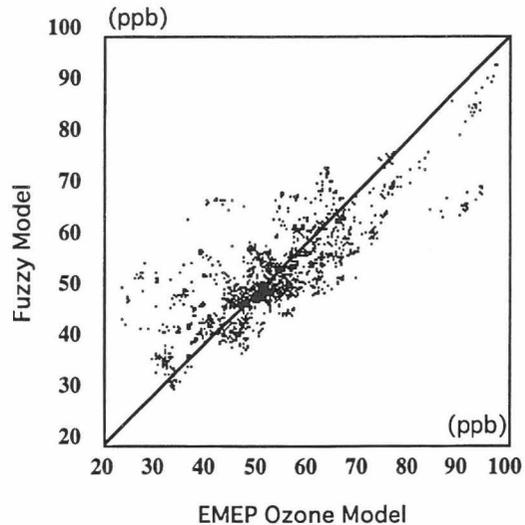
References

Fuhrer, J., Achermann, B., 1994. Critical levels for ozone. UN-ECE Workshop Report. FAC No. 16. Swiss Federal Research Station for Agricultural Chemistry and Environmental Hygiene, Switzerland.

Heyes, C., Schöpp, W., 1995. Towards a simplified model to describe ozone formation in Europe. Working Paper 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. Working Paper WP–96–12. International Institute for Applied Systems Analysis (IIASA), Laxenburg, Austria.

Makowski, M., 2000. Modeling paradigms applied to the analysis of European air quality. European Journal of Operational Research 122, this issue.

Nakamori, Y., Ryoke, M., 1994. Identification of fuzzy prediction models through hyperellipsoidal clustering. IEEE Transactions on Systems, Man and Cybernetics 24 (8), 1153–1173.

Ryoke, M., 1996. Fuzzy rule generation from the EMEP ozone model to examine source receptor relations. Working Paper WP-96-130. International Institute for Applied Systems Analysis (IIASA), A-2361 Laxenburg, Austria.

Ryoke, M., Nakamori, Y., Tamura, H., 1998. Dynamic determination of mixing parameters in fuzzy clustering. In: Proceedings of the Sixth Conference of the International Federation of Classification Societies (IFCS-98), Rome, pp. 111–116.

Schöpp, W., Amann, M., Cofala, J., Heyes, C., Klimont, Z., 1999. Integrated assessment of European air pollution emission control strategies. Environmental Modelling & Software 14, 1–9.

Simpson, D., 1992. Long-period modelling of photochemical oxidants in Europe, model calculations for july 1985. Atmospheric Environment 26A, 1609–1634.

Simpson, D., 1993. Photochemical model calculations over Europe for two extended summer periods: 1985 and 1989, model results and comparisons with observations. Atmospheric Environment 27A, 921–943.

Simpson, D., 1995. Biogenic emissions in Europe, 2, implications for ozone control strategies. Journal of Geophysical Research, 100.

WHO, 1997. Air Quality Guidelines for Europe, Second ed. WHO, Copenhagen.