OR 57/2000
E-91029D
NOVEMBER 2001
82-425-1225-6

## Evaluation of urban scale time-dependent dispersion model with subgrid elements in Oslo, Norway

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#### Summary

Hourly data on emission, wind and dispersion conditions are used to calculate hourly  $NO_x$ -concentrations in a 1 km grid system based on a time dependent finite difference dispersion model in three horizontal layers.

The local pollution contributions from roads and from point sources within 1 km distance are accounted for by a subgrid model based on Gaussian line source and point source models.

Results of concentration calculations are evaluated by using data from eight stations for four winter months (1.11.1991-29.2.1992) and from the three main stations for two summer months (1.5.-30.6.1992).

The time variation of calculated concentrations, as a result of variations in emissions and/or dispersion conditions, is compared with observed variations. On an hourly basis nearly all fluctuations are reproduced in the calculated values. The amplitudes of the fluctuations may be different as a result of inaccurate input data and model simplifications.

In the centre of the city the correlation coefficient is close to 0.8 during the winter months, 0.5-0.6 during the summer months. In the suburbs the correlation is lower (0.6-0.7) during the winter months.

The evaluation show a tendency to overestimate the  $NO_x$ -concentration by the calculation procedure. In particular the overestimation of monthly mean values is more than 100% during summer months.

- The subgrid-model overestimates maximum concentrations close to roads during low wind conditions.
- The finite difference model overestimates concentrations in the centre of Oslo.

The relative importance of processes affecting the  $NO_2$  -concentrations in an urban area as a function of advection time from a line source are discussed. A balance between NO,  $NO_2$  and  $O_3$  is found when the advection time is larger than 600-1000 s. The current calculation procedure leads to an overestimation of long-term averages of  $NO_2$  close to lane sources (roads). It is of importance to improve the model, since it affects the assessment of  $NO_2$  relative to the EU and Norwegian limit values.

The segregation between regional scale ozone and local scale NO has to be accounted for in a realistic  $NO_2$ -model. The combination of a subgrid line-source model and a grid model has been applied as a first approximation of the segregation process. The calculation procedure for  $NO_2$  was proposed by Yamartino and Wiegand in 1986.

#### 1. Introduction

Results from monitoring of air pollution concentrations in cities in Norway have shown that nitrogen dioxide (NO<sub>2</sub>) is one of the compounds which most often, and to the largest extent, exceeds current air quality guidelines (Hagen, 1992; Larssen and Røstad, 1993). This is the case both in city streets and in the urban atmosphere in general. In Norway, the highest NO<sub>2</sub> concentrations occur during the winter months, in connection with "episodes" with poor dispersion. In the general urban atmosphere, high 24-hour average values are of greatest concern relative to Air Quality Guideline (AQG), while in the street atmosphere, very high peak (hourly) concentrations may be the most important problem.

This paper describes the testing of an urban scale, time varying dispersion model under development at the Norwegian Institute for Air Research (NILU), to calculate, as a function of time and space,  $NO_x$  and  $NO_2$  concentrations in a grid (length 500 m-1 km) and in receptor points within the grid by means of integrated subgrid models. Input to the model are time-varying gridded fields of emissions and dispersion parameters.

The urban scale time dependent model has been used to describe the spatial distribution of air pollution in other urbanised areas (Grønskei et al., 1990, 1993), and the model has been further developed to account for subgrid variations as a result of emissions along roads and streets in Oslo. The subgrid model is based on HIWAY-2 (Petersen, 1980). This model has been modified to account for emission conditions in Oslo by Larssen et al., 1990.

The model evaluation is based on measurements of air quality, wind and dispersion conditions in Oslo in the period October 1991-June 1992 (Hagen et al., 1993).

The research carried out during the project, to develop and test the model with sub-grid elements, includes the following:

- Development of a data base for testing of the model for the city of Oslo, including an emission inventory and continuous measurement of NO, NO<sub>2</sub>, O<sub>3</sub> and dispersion parameters at a number of locations in Oslo during winter and summer periods (described further in chapter 2).
- Model development (described further in chapter 3).
- Model testing and modification (chapter 4).

#### 2. The establishment of the test data base

#### **Description of the Oslo area**

Oslo is situated at the end of the 100 km long Oslofjord (Figure 1). Surrounded by hills of height 200-500 meters, the city topography is bowl-like with valleys protruding between hills, the main valley rising from the fjord and city centre towards the Northeast. The area has a continental-type climate, normally with relatively cold winters (mean winter temperature: -3.9°C) and local drainage winds from the hill valleys, dominated in the city centre by the drainage down the main Northeast valley.

Oslo is largely a commercial city. There are only a few minor industrial emission sources and power plants. Car traffic is by far the dominating source of air pollution emissions, while space heating by oil (low-sulphur) and, in cold periods, wood burning, also contributes notably to the air pollution.

#### **Emission inventory**

The emission survey covers the urban part of Oslo, the eastern part of Bærum and the northern part of Nesodden, within a grid of  $22x18 \text{ km}^2$ . As the model is using data on area sources as well as subgrid point and line sources, it is important to present the emission data on different levels for the dispersion model. The main source of nitrogen oxides in the Oslo area is road traffic, so the major work was performed on the calculation of traffic emissions (Gram, 1994).

**Road traffic.** Data for traffic intensity for the main roads were available for the morning and afternoon rush, plus for "low traffic" conditions. The data were provided by the traffic authorities in Oslo by using the TRIPS model. (The "low traffic" corresponds to the period at noon, not night traffic.) The average daily traffic is calculated as (2\*morning+2\*afternoon+14\*low), assuming low traffic during 6 night hours. From these 3 data sets plus average traffic, emissions of CO, NO<sub>x</sub>, NO<sub>2</sub> and VOC within each km<sup>2</sup> were calculated, using routines from the NILU traffic model RoadAir (Torp and Larssen, 1993), with emission as a function of the driving conditions. Table 1 shows emission data for the main roads in Oslo in 1991. The driving conditions were different for the three scenarios, and for the average traffic. The total length of the main roads within the area was 458 km.

In addition to the emissions from the main roads, emissions were estimated for 954 km local roads to 1160 kg CO/h, 100 kg NO<sub>x</sub>/h, 7 kg NO<sub>2</sub>/h and 112 kg VOC/h. The emission of the nitrogen oxides from the small roads corresponds to the fraction of the traffic work, 10-12 %, but due to a lower speed on the local roads, the emissions of CO and VOC were about 25 % of the total.



Figure 1: The Oslo area with measurement stations.

Met.stations O	Air quality stations D			
A. Fornebu Airport	1. Skøyen	(City regional)		
B. Bygdøy	2. Nordahl Bruns street	(City regional)		
C. Blindern (Norw. Met. Inst.)	3. Pilestredet	(Street)		
D. Bjølsen	4. Hovin	(City regional)		
E. Nordahl Bruns street (City centre)	5. Strømsveien	(Street)		
F. Hovin	6. Fyrstikkalleen	(50 m from street)		
G. Skøyen	7. Etterstadsletta	(City regional)		
	8. Holmlia	(Suburban residential)		

Tab	le	1:		Em	iss	sion	a	lata	for	•t	he	main	roaa	ls	in	Os	lo	1	99.	1.
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	Traffic work	CO	NO <sub>x</sub>	NO <sub>2</sub>	VOC
	10 <sup>3</sup> car-km/h	kg/h	kg/h	kg/h	kg/h
Morning	591	11 277	1 979	154	768
Afternoon	596	12 319	2 180	150	776
Low traffic	285	4 167	949	65	364
24 h-average	265	3 245	799	70	330

**Other traffic emissions.** The calculation of emissions from the harbour traffic and from Fornebu Airport was based upon detailed data about the traffic intensity, specially for the airport.

The harbour traffic is dominated by large ferries with a mean emission of 84 kg  $NO_x/h$ . The emission from Fornebu Airport was estimated in 1989 to 39.3 kg  $NO_x/h$  as a daily mean value. The airport was closed during the night giving a mean emission of 58.9 kg  $NO_x/h$  from 07-23.

**Heating.** The emissions from industry and the consumption of oil for heating purposes in Oslo are reduced substantially during the last decades, mainly due to low electricity prices, central heating and a fall in the industrial activity. The emission from point sources in Oslo 1991 was estimated to 93 kg  $NO_x/h$ , mainly from three incineration plants.

The emission from domestic use of oil and solid fuels was estimated to about 120 kg  $NO_x/h$ .

Table 2 shows mean hourly emissions from the Oslo-area for the winter 1991-92.

Traffic		Heating	
Main roads	798.7		
Local roads	99.6	Point sources	93.1
Harbour	84.0	Area oil heating	111.5
Airport	39.3	Solid fuels	8.2
Sum traffic	1 021.6	Sum heating	212.8

Table 2:Average hourly emissions of nitrogen oxides from traffic and heating<br/>for the winter 1991-92. Unit: kg/h as NO2.

#### Measurement program, NO<sub>x</sub>, NO<sub>2</sub>, O<sub>3.</sub>

A total of 9 measurement stations for nitrogen oxides and ozone were operated during the measurement period starting in October 1991 and ending in July 1992 (Hagen et al., 1993). All stations were not operated simultaneously. The location of the stations within Oslo city boundaries is shown in Figure 1. In addition to these a regional background station was operated, situated in a rural setting on the east coast of the Oslofjord, about 50 km south of Oslo.

The three main stations for testing of the model are the following:

•	Skøyen. Located in a park. Distance to surrounding main streets: about 1 km.	City regional station
•	Nordahl Bruns street. The location is inside a city block, in a built-up area, 4-8 stories buildings. Distance to streets surrounding the block: 30-50 meters.	City centre station
•	Hovin. Located in residential area with dispersed 4-stories apartment blocks. Distance to main roads: 250 m to the East, 500 m to the West.	City regional station

#### **3.** Description of the dispersion model

#### **General description**

The dispersion model is a gridded, 3-layer model, as shown in Figure 2.

The procedure for calculation and for specification of boundary values are described by Grønskei et al. in 1993.

The dispersion is partly caused by the time variation of the wind field and partly by turbulent exchange. Wind ( $V_h$  and w) and pollution concentrations ( $c_i$ ) are

divided in one average value in grid elements  $(\bar{})$  and deviations from the average values ('), i.e.

concentrations	$: c_i = \overline{c_i} + c'_i$
horizontal wind velocity	$: \mathbf{V}_h = \overline{\mathbf{V}_h} + \mathbf{v'}_h$
vertical wind speed	w = w + w'

For each of the pollution components, the following equation is solved:

$$\frac{\partial \overline{c_i}}{\partial t} = - \overline{\mathbf{V}}_h \cdot \nabla_h \overline{c_i} - \overline{w} \frac{\partial \overline{c_i}}{\partial z} - \frac{\partial (\overline{w'c_i})}{\partial z} - \nabla_h \cdot (\overline{\mathbf{v'}_h c'_i}) + Q_i. \quad (3.1)$$

$$\mathbf{I} \qquad \mathbf{II} \qquad \mathbf{III} \qquad \mathbf{IV} \qquad \mathbf{V}$$

Processes to be considered in the model are:

- () spatial average quantities
- I: horizontal advection,  $\overline{\mathbf{V}}_h \cdot \nabla_h \overline{c_i}$ II: vertical advection,  $\overline{w} \frac{\partial \overline{c_i}}{\partial z}$
- III: turbulent exchange vertically,  $\frac{\partial}{\partial z} \left( \overline{w'c'} \right)$
- IV: turbulent exchange horizontally,  $\nabla_h \cdot (\overline{\mathbf{v'}_h c'_i})$ V: emission,  $Q_i$ .

The computer codes are developed to include chemical reactions between different compounds, but in this presentation such reactions were not taken into account.

The vertical structure is shown in Figure 2.





When sodar measurements were not available in the current study, measurements from station F were used for wind direction in level three. Plume rise above layer three (200 m) was not taken into account.

#### Wind fields

Wind measurements close to the ground were used to define a two-dimensional wind field  $\mathbf{V}_{hl}(\mathbf{r})$  for layer 1. The wind field is calculated by statistical interpolation as described by Eidsvik (1982):

$$\begin{aligned} \mathbf{V}_{h1}(\mathbf{r}) &= a_1(|r - r_1|)\mathbf{V}_{h1}(\mathbf{r}_1) + a_2(|r - r_2|)\mathbf{V}_{h1}(\mathbf{r}_2) + a_3(|r - r_3|)\mathbf{V}_{h1}(r_3) + \\ &a_4(|r - r_4|)V_{h1}(\mathbf{r}_4) \end{aligned} \tag{3.2}$$

$$\begin{aligned} \mathbf{V}_{h1}(\mathbf{r}_1) \\ \mathbf{V}_{h1}(\mathbf{r}_2) \\ \mathbf{V}_{h1}(\mathbf{r}_3) \\ \mathbf{V}_{h1}(\mathbf{r}_4) \end{aligned} \qquad \text{observed velocities at four grid points.} \end{aligned} \tag{3.2}$$

$$\begin{aligned} a_1(|r - r_1|) \\ a_2(|r - r_2|) \\ a_3(|r - r_3|) \\ a_4(|r - r_4|) \end{aligned} \qquad \text{factors of proportionally, } a_k, \text{ are determined by spatial covariance functions of } |r - r_k|, \text{ the distances between the points of wind interpolation } (r) \text{ and the respective points of wind measurements } (r_k). \end{aligned}$$

Observed time series of wind at four wind stations were used to compute spatial covariance functions. The procedure was based on the "variate difference" method described by Kendall et al. (1983). The method is based on considering deviations from smoothed values of the hourly observations of wind.

The interpolated values of horizontal wind velocities based on hourly average wind observations from four wind stations introduce uncertainties into the calculations of hourly pollution concentrations far from the wind stations, in particular close to the point sources.

The vertical wind component is specified by requiring a three-dimensional nondivergent and mass-consistent wind field in each level:

$$\nabla_h \mathbf{V}_h = -\frac{\partial w}{\partial z} \tag{3.3}$$

In the upper layer 3 homogeneous wind according to hourly averaged sodar measurements  $(V_{sod})$  is used for advection calculations:

$$\mathbf{V}_{h3} = \mathbf{V}_{sod} \ (150 \ m) \tag{3.4}$$

In layer 2 the following wind field is used for advection calculations:

$$\mathbf{V}_{h2} = 0.5 \left( \mathbf{V}_{h1} + \mathbf{V}_{h3} \right) \tag{3.5}$$

It may not be possible to describe the modes of motion that are important for vertical advection of pollution by using observations of horizontal winds only. Results of flow-field model calculations combined with wind measurements may improve the wind fields for calculation of advection terms considerably.

This source of error is probably more important for dispersion calculation in areas where vertical advection of pollution is important (Eidsvik, 1982).

#### Description of the diffusion process

Mean concentration distribution as a result of dispersion of emission from a point source may be approximated by a Gaussian plume formula. For the standard deviation in the vertical pollution distribution ( $\sigma_z$ ) the following formula applies:

$$\sigma_z = \frac{\sigma_w t}{\left(1 + t / 2T_L\right)^{1/2}} \tag{3.6}$$

 $\sigma_{\rm w}\!\!:$  the standard dviation of vertical wind fluctuations.

 $T_L$ : Lagrangian time scale

*t*: time of advection

The formulae is based on the assumption of stationary and homogous turbulence conditions locally (Csanady, 1973). The variation with respect to advection time is found by derivation of equation 3.6 with respect to time.

$$\frac{d\sigma_z}{dt} = \sigma_z \frac{4T_L + t}{t(4T_L + 2t)},\tag{3.7}$$

Venkatram (1984) described the length scale of turbulence (*l*) as a function of height above the ground (*z*) and temperature stratification  $(\partial \theta / \partial z)$  by equation (3.8):

$$\frac{1}{l} = \frac{1}{l_n} + \frac{1}{l_s},$$
(3.8)

where  $l_n = \alpha z$  provided  $z_0 \ll z \ll H$ ,

$$l_s = \gamma^2 \, \frac{\sigma_w}{N},$$

 $\alpha = 0.36$ ,  $\gamma = 0.52$  are empirical factors of proportionality,

$$N = \left(\frac{gd\theta}{\theta dz}\right)^{0.5},$$

$$T_L = \frac{l}{\sigma_w},$$

*l* : the length scale of turbulence

H : the mixing height

 $z_0$  : roughness length

- $l_n$ : the length scale of turbulence for neutral atmospheric temperature stratification
- $l_s$  : the length scale for stable temperature stratification
- N : the local value of the Brunt-Väisälä frequency at height z

Information on dispersion conditions based on the formula for plume development is used to determine hourly values of vertical exchange of pollution by turbulence (Equation 3.6). Sodar measurements of vertical fluctuations in the wind field  $(\sigma_w)$  at the levels separating the model layers (20, 50 and 200 m) were used in addition to observed values of the temperature variation with height at station A (Hovin) as a typical value for the definition of the Brunt-Väisälä frequency.

In the finite difference model the concentration within each layer is assumed to be constant with respect to height within each grid square.

In order to estimate turbulent mixing of pollution consistent with the subgrid plume models, it is assumed that the pollution in the layer between two levels in the grid model corresponds to a Gaussian plume with the same vertical extension. The following formulae is found for the first moment of a Gaussian pollution distribution  $(\bar{z})$ :

$$\overline{z} = \frac{\int_{H_0}^{\infty} z c_o \exp\left(\frac{z - H_0}{\sigma_z}\right) dz}{\int_{H_0}^{\infty} c_o \exp\left(\frac{z - H_0}{\sigma_z}\right) dz}$$

$$\overline{z} = \sqrt{\frac{2}{\pi}} \sigma_z$$
(3.9)

A reasonable value of the vertical extent of a subgrid plume when the further description of dispersion is carried out in the grid system would be:

$$\sigma_{z_{1-2}}(t_{o}) = \sqrt{\frac{\pi}{2}}\Delta z_{1-2}$$

It is assumed that the growth of Gaussian plumes on each side of the separation between the grid cells cause exchange pollution in accordance with the following formulae for the flux between the layers  $(F_{1,2})$ :

$$\mathbf{F}_{1,2} = -\frac{dz}{dt} (c_2 - c_1) \tag{3.10}$$

The exchange of pollution between layer 1 and layer 2 during the time step  $\Delta t$  is calculated by the following equation based on equations 3.10 and 3.9:

$$\frac{F_{1,2}\Delta t}{C_2 - C_1} = -\sqrt{\frac{2}{\pi}} \Big(\sigma_{Z_{1-2}}(t_o + \Delta t) - \sigma_{Z_{1-2}}(t_o)\Big)$$
(3.11)

It is assumed that the first moment of the vertical pollution distribution between the first and second levels grows with time, causing an exchange of pollution according to Equation (3.11). The exchange will be proportional to the difference in concentration between the levels. The third layer also exchanges pollution with the background air above the upper layer. The following fluxes are calculated:

 $F_0$ : dry deposition to the ground, (3.12)

 $F_0 = 0$  in this study.

$$F_{1,2} \cdot \Delta t = -\sqrt{\frac{2}{\pi}} (\sigma_{Z_{1-2}}(t_0 + \Delta t) - \sigma_{Z_{1-2}}(t_0)) \cdot (C_2 - C_1)$$

$$F_{2,3} \cdot \Delta t = -\sqrt{\frac{2}{\pi}} (\sigma_{Z_{2-3}}(t_0 + \Delta t) - \sigma_{Z_{2-3}}(t_0)) \cdot (C_3 - C_2)$$

$$F_{3,b} \cdot \Delta t = -\sqrt{\frac{2}{\pi}} (\sigma_{Z_{3-b}}(t_0 + \Delta t) - \sigma_{Z_{3-b}}(t_0)) \cdot (C_b - C_3)$$
(3.13)

The equations 3.13 are used to calculate pollution exchange between the layers in the grid system. Using K-theory would be an alternative.

The pollution fluxes calculated by 3.13 are consistent with the local subgrid models. The variation of the fluxes with grid distance and with meteorological conditions are automatically accounted for (eq. 3.6-3.13).

Measurements of vertical wind fluctuations ( $\sigma_w$ ) and temperature at two levels are used as input data for calculating pollution exchange between the layers. Hourly averaged sodar measurements were used for vertical wind fluctuations ( $\sigma_w$ ) and for measurements of temperature and temperature variation with respect to height (measurements from station A were used to determine temperature stratification). A further description of the vertical exchange including dry deposition is given by Grønskei and Gram (1984).

For the horizontal exchange process close to the source the method suggested by Irwin (1983) is applied using observed hourly values of horizontal wind fluctuations,  $\sigma_v$ , at each level (10, 35 and 150 m).

$$\sigma_y = \sigma_v t f_y \tag{3.14}$$

where  $\sigma_y$  is standard deviation of the pollution distribution perpendicular to the wind direction,  $\sigma_y$  is standard deviation of the fluctuations in the horizontal crosswind component:

$$f_y = 1.0 / (1 + a(t / t_0)^{0.5})$$
  
 $a = 0.9$   
 $t_0 = 1000 s$   
and t is advection time (s).

A procedure corresponding to Equation (3.13) could also be used for the horizontal exchange. The horizontal resolution (distance between grid points) in urban air pollution models is at least 10 times larger than the vertical resolution. The concentration variation in grid cells with time is not sensitive to turbulent exchange of pollution between grid cells in horizontal directions. In this study the horizontal fluxes were calculated by the K-theory in horizontal directions.

$$F_x = -K_h \left(\frac{\partial c}{\partial x}\right)$$

and in the y-direction

$$F_{y} = -K_{h} \left( \frac{\partial c}{\partial y} \right)$$

 $K_{h} = 0.1 \sigma_{v} \Delta x$   $\sigma_{v} = \text{standard deviation of horisontal wind fluctuations}$  $\Delta x = \text{horizontal grid distance.}$ 

Estimation of vertical exchange with the background atmosphere may cause errors underestimating concentrations in the lower layers of the model. This applies in particular to pollutants having the main sources in the third layer. The model could probably be improved by adding further layers of calculations above 200 m.

When a regional scale model is used to calculate background concentrations for the local scale model, the vertical fluxes in the large scale model may be used to specify the vertical exchange with the local scale model i.e.  $F_{3,b}$ 

The horisontal advection scheme is based on using Bott's 4<sup>th</sup> degree positive definite scheme. Vertically the advection scheme is based on using a standard upwind finite difference approach. This combined scheme approximately preserves a constant pollution field and the mass of pollutants emitted into the system. A more detailed description of the finite difference approximation is given in Bott (1989).

The initial distributions of concentrations are specified by measurements or given the homogeneous value of zero, when distributions are not available.

#### Subgrid model

Close to point sources and close to roads with high traffic intensity, data on subgrid gradients are needed to describe pollution concentrations at measuring stations and for estimating exposure.

A highway model, corresponding to HIWAY (Petersen, 1980) is used to estimate concentrations close to a set of roads with high traffic intensity within the square km<sup>2</sup> ( $\Delta C^{l}$ ). A puff trajectory-model is used to calculate the influence of point sources ( $\Delta C^{p}$ ). The emission intensity of local area sources are reduced accordingly.

#### 4. Evaluation of the NO<sub>x</sub> model

The dispersion model has been applied to calculate hourly  $NO_x$ -concentrations, based upon data for  $NO_x$ -emission (Gram, 1994), and meteorological measurements (Hagen et al., 1993).

(3.15)

Time series of observed and calculated  $NO_x$ -concentrations are available on request.

Station	$\overline{C_o}$ ( $\sigma_o$ )	$\overline{C_c}$ $(\overline{\sigma_c})$	Mo	M <sub>C</sub>	r	rmse	$(\overline{\Delta C_{*}^{2}}/\overline{\Delta C^{2}})^{0.5}$	IA	Ν
	µg/m³	µg/m³	µg/m³	µg/m³		µg/m³	%		
Winter									
Valle Hovin	296 (421)	303 ( 398)	2 694	3 012	0.79	269	40	0.88	2 499
Skøyen	195 (239)	177 ( 189)	1 264	1 026	0.80	146	38	0.88	1 355
Holmlia	94 (98)	146 ( 150)	541	909	0.48	144	40	0.62	842
Nordahl Bruns gt.	166 (196)	237 ( 277)	1 434	1 600	0.73	203	35	0.80	2 876
Pilestredet	476 (425)	427 ( 424)	2 319	2 410	0.76	299	39	0.87	1 264
Strømsveien	714 (629)	808 (1 079)	3 637	7 535	0.75	748	52	0.79	1 217
Etterstadsletta	216 (298)	333 ( 394)	1 865	2 776	0.64	328	23	0.75	1 239
Fyrstikkalleen	381 (467)	429 ( 544)	3 058	3 831	0.78	348	99	0.87	1 019
Summer									
Valle Hovin	53 (71)	119 ( 123)	732	1 038	0.48	127	53	0.56	1 340
Skøyen	30 (30)	62 ( 44)	223	292	0.63	48	67	0.63	353
Nordahl Bruns gt.	39 (31)	79 ( 66)	347	520	0.49	71	57	0.49	1 338

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Evaluation of the  $NO_x$ -model for the winter period 1.11.91-29.2.92 and the summer period 1.5.-30.6.1992. Table 3:

- $\frac{\overline{C_o}}{\overline{C_c}}$ = Average observed concentration
- = Average model calculated conc.
- $M_{a}$  = Maximum observed concentration
- $M_c$  = Maximum calculated concentration
- $\overline{(\Delta C_s^2}$  /  $\overline{\Delta C^2})^{0,5}$  = Percentage systematic rmse
- Ν = Number of observations

- = St. dev. observed concentration  $\sigma_{_o}$
- = St.dev. model calculated conc.  $\sigma_{c}$ 
  - = Correlation coefficient
- = Root mean square error rmse
- = Index of agreement IA

In the winter period the model works well to explain the values at the stations Valle Hovin, Skøyen and Pilestredet and reasonably well at the stations Strømsveien and Fyrstikkalleen. The indices of agreement at the three best stations are close to 0.9. The indices of agreement at Strømsveien and Fyrstikkalleen are 0.79 and 0.87 respectively. Good agreements at these stations as well as at Etterstadsletta are disturbed by an overestimation of the influence from neighbouring roads as a result of the subgrid model in low wind conditions. In particular the influence from Strømsveien is seriously overestimated in episodes i.e. the maximum observed concentration is only 50% of the calculated maximum value and standard deviations of the calculated values close to Strømsveien is 71% higher than the standard deviation of the observed values (see table 4).

Statistical parameters describing differences between observed and
calculated time series of concentrations.
Unit: per cent.

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1.00

	$\frac{\Delta \overline{C}}{\overline{C_o}}$	$rac{\Delta\sigma}{\sigma_o}$	$rac{\Delta C_m}{C_{mo}}$
Winter			
Valle Hovin	2	-5	12
Skøyen	-9	-21	-19
Holmlia	55	53	40
Nordahl Bruns gt.	43	41	12
Pilestredet	-10	0	4
Strømsveien	13	71	107
Etterstad	54	32	49
Fyrstikkalleen	13	20	25
Summer			
Valle Hovin	124	73	41
Skøyen	106	47	31
Nordahl Bruns gt.	103	113	50

 $\Delta \overline{C} = \overline{C}_c - \overline{C}_o$ : The difference between calculated and observed average values.

 $\Delta \sigma = \sigma_c - \sigma_o$ : The difference between the standard deviations in calculated and observed time series.

$$\Delta C_m = C_{mc} - C_{mo}:$$

The difference between maximum calculated and maximum observed concentration values.

In the summer period the observed values are seriously overestimated at the stations Valle Hovin, Skøyen and Nordahl Bruns gt. The discrepancies may be reduced in the following way:

- Improved subgrid model including suggested modification of procedures for dispersion calculations close to open roads and streets (Hertel and Berkowicz, 1989).
- Improvements in the procedure for calculating dispersion parameters during summer period.
- Improved description of wind and dispersion conditions in particularly in the suburbs (Holmlia).

The area source model as well as the line source model should be modified.

# 5. Deviation from photochemical balance on an urban scale in Norway

The concentrations of NO, NO2 and O3 varies as a result of

- emission and dilution,
- reaction between NO and O<sub>3</sub>,
- photodissociation of NO<sub>2</sub>,
- other chemical reactions.
- deposition

Within the framework of the project it has not been possible to describe in detail the complex interaction between emission, dispersion and deposition of nitrogen oxides and ozone and chemical reactions in the atmosphere over urban areas.

The basic photochemical cycle in an urban atmosphere are described by the following three reactions:

1)  $NO_2 + hv \xrightarrow{k_1} NO + O$ 

2)  $O + O_2 + M \xrightarrow{k_2} O_3 + M$ 

3)  $O_3 + NO \xrightarrow{k_3} NO_2 + O_2$ 

The reaction number 2 is fast and very low concentrations of atomic oxygen is found in the atmosphere. Ozone can be considered to be a result of reaction number 1.

In an urban area several scales of pollution are present explaining the spatial distribution of pollution components (see Figure 3). The descriptions of spatial distributions include non linear terms in areas where chemical reactions are important.

When the atmosphere is not well mixed, the effect of spatial fluctuations has to be accounted for estimating the reaction between NO and  $O_3$  i.e.

$$R_{NO,O_3} = k_3 [NO] [O_3]$$
$$= k_3 [\overline{NO}] [\overline{O_3}] + k_3 [\overline{NO}] [\overline{O_3}]',$$

where [NO]' and  $[O_3]$ ' are the deviations from the spatial average concentrations  $\overline{NO}$  and  $\overline{O_3}$ .

[NO]' and  $[O_3]'$  show negative correlation close to the source regions in an urban area, and the fluctuation term suppress the development of NO<sub>2</sub> from the reaction between NO<sub>2</sub> and O<sub>3</sub>.



Figure 3: A simplified NO<sub>2</sub>-model for exhaust emissions from a road in an urban area.
(X): distance from road
(U): urban scale concentrations
(B): regional (background) concentrations

In an air parcel the following equations for the individual derivatives with respect to time as a result of chemical reactions reads:

$$\frac{d_{h}\left[\overline{NO}\right]}{dt} = k_{1}\left[\overline{NO_{2}}\right] - k_{3}\left[\overline{O_{3}}\right]\left[\overline{NO}\right] - k_{3}\left[\overline{O_{3}}\right]'\left[\overline{NO}\right]' - \overline{w'}\left[\overline{NO}\right]' + Q_{NO} \quad (5.1)$$

$$\frac{d_{h}\left[\overline{NO}_{2}\right]}{dt} = -k_{1}\left[\overline{NO}_{2}\right] + k_{3}\left[\overline{O}_{3}\right]\left[\overline{NO}\right] + k_{3}\left[\overline{O}_{3}\right]'\left[\overline{NO}\right] - \overline{w'}\left[\overline{NO}_{2}'\right] + Q_{NO_{2}}$$
(5.2)

$$\frac{d_h[\overline{O_3}]}{dt} = k_1 [\overline{NO_2}] - k_3 [\overline{O_3}] [\overline{NO}] - k_3 [\overline{O_3}]' [\overline{NO}]' - \overline{w'} [\overline{O_3}]', \qquad (5.3)$$

where w is a measure for the vertical turbulent diffusion.

The marked concentration values show deviations from the spatial average value of the concentration within the air parcel (see chapter 3 and equation 3.1). The The  $O_3$ - and NO-concentrations in the atmosphere show negative correlations, and the nonhomogeneous mixing delays the reaction.

The sum of equations (5.1) and (5.2) and the sum of equations (5.2) and (5.3) show that the sum of nitrogen compounds  $[NO_x] = [NO] + [NO_2]$  and of oxidant compounds  $[O_x] = [O_3] + [NO_2]$  are not influenced by nonlinear chemical reaction terms.

$$\frac{d_h}{dt} \left( \boxed{NO} \right] + \left[ \overline{NO_2} \right] = -\overline{w'} \left[ \overline{NO} \right]' - \overline{w'} \left[ \overline{NO_2} \right]' + Q_{NO_x}$$
(5.4)

$$\frac{d_h}{dt} \left( \overline{NO_2} \right] + \left[ \overline{O_3} \right] = -\overline{w'} \left[ \overline{NO_2} \right] - \overline{w'} \left[ \overline{O_3} \right] + Q_{NO_2}$$
(5.5)

Further it is seen that

$$\frac{d_h \left( \overline{NO} \right) - \left[ \overline{O_3} \right]}{dt} = \overline{w}' \left[ \overline{O_3} \right] - \overline{w}' \left[ \overline{NO} \right]' + Q_{NO}$$
(5.6)

To study the relative importance of chemical and dispersion processes in the formation of  $NO_2$  the following equation is given

$$\frac{1}{[NO_2]} \frac{d[\overline{NO_2}]}{dt} = \frac{\overline{w'[NO_2]'}}{[\overline{NO_2}]} + k_3[\overline{O_3}][\overline{NO}] + k_3[\overline{O_3}]'[\overline{NO}]' - k_1 + \frac{Q_{NO_2}}{\overline{NO_2}} \quad (5.7)$$

$$[NO_2] = [\overline{NO_2}] + [NO_2]'$$

$$: \quad \text{concentrations}$$

$$[O_3] = [\overline{O_3}] + [O_3]'$$

- $k_3$ : reaction coefficient for production of NO<sub>2</sub> as a result of reaction between NO and O<sub>3</sub>. The plume containing NO from car traffic, mixes with ambient air containing O<sub>3</sub>
- $k_1$ : the photodissociation coefficient for NO<sub>2</sub> by absorption of short wave solar radiation

$$k_{1} = 0.01*(1-0.5*N/8)*(\exp(-0.39/\sin(\tau)) \qquad [s^{-1}]$$

$$k_{3} = (2.56/T) \exp(-1430/T) \qquad [s \cdot ppb]^{-1}$$
(5.8)

where

- N: the cloudiness given in octals (N = 0: clear sky; N = 8: overcast)
- $\tau$ : height of the sun above the horizon. Unit: degree
- T: temperature. Unit: °K

The cloudiness parameter N is taken from measurements every 6 hour at the meteorological station at Fornebu Airport.  $\tau$  is calculated for each hour depending on time of the day and day of the year.

To evaluate the importance of the different terms in Eq. 5.7 in the process of improving models, typical values and range of variation in cities are estimated. To study their relative importance the conditions are described as a function of advection time from a line source.

Figure 4 shows the specific rate of concentrations reduction for  $NO_2$  as a function of advection time from the road. Close to the road i.e. when the advection time is less than about 30-50 seconds, the dispersion of the plume is the most important term explaining the rate of concentration reduction for  $NO_2$ . When  $NO_2$  is diluted  $O_3$  is transferred from the background atmosphere and the reaction between NO and  $O_3$  is important as long as NO is observed in the atmosphere, i.e. close to the sources or when the dissociation of  $NO_2$  is important.

As the development of  $NO_2$  is suppressed, a chemical balance is not expected to be found in urban areas unless the  $O_3$ - or  $NO_2$ -concentration is very small.

When the advection time last longer than 100-200 seconds the photodissosiation of  $NO_2$  becomes important when the solar radiation is strong. At night and in winter the photodissociation of  $NO_2$  is negligible.

The scale analyses of the different terms in equation (5.6) indicate that chemical reactions as well as effects of small scale mixing have to be taken into account when NO<sub>2</sub>-concentrations are going to be described in an urban area. The time scale of small scale mixing is larger than the Lagrangian time scale (se eq. 3.6-eq. 3.8).



*Figure 4:* The relative importance of the processes affecting the NO<sub>2</sub>concentrations in an urban area as a function of advection time from a road with high traffic.

# 6. Evaluation of the chemical balance conditions at the different stations

As the plume moves from the road the contribution from dispersion becomes less important. Further away the reaction between NO and  $O_3$  and the photo dissociation of NO<sub>2</sub> may form a chemical balance far from local sources, i.e. when the advection time is larger than 1000s. The three chemical components were measured as hourly mean values on several stations, and deviation from a chemical balance at the different stations was studied.

$$\frac{d[NO_2]}{[NO_2]dt} \sim \frac{k_3[NO][O_3]}{[NO_2]} - k_1 \sim 0$$
(6.1)

Eq. 5.8 indicates that during the night and during the winter months the photodissociation of  $NO_2$  is slow compared to the other processes. In these situations either [NO] or [O<sub>3</sub>] values should be very small.

By substituting  $[NO] = [NO_x] - [NO_2]$  and  $[NO_2] = [O_x] - [O_3]$  in equation (6.1) this gives a second degree equation in O<sub>3</sub> to be solved

$$[O_3] = (b - sqrt(b*b - 4*a*c))/2*a$$
(6.2)

where  $a = -k_1$ ,  $b = k_1 ([O_x] - [NO_x]) - k_2$  and  $c = k_2 [O_x]$ .

Finally NO<sub>2</sub> concentrations are calculated by

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$$\left[NO_{2}\right] = \left[O_{x}\right] - \left[O_{3}\right] \tag{6.3}$$

According to Janssen et al., 1990 a chemical equilibrium exists locally in the plume when the advection time is larger than about 10 min. Close to sources (advection time less 10 min) the molecular diffusion affects the distribution of concentration flutctuations, and the rate of chemical reactions slows down as a result of incomplete mixing on molcular basis (eq. 5.1, 5.2 and 5.3).

Air quality guidelines are given for time average concentrations equal or larger than one hour, and description of short term fluctuations may not be required. One hour time average concentrations smooth out plumes with various scales in the urban area.

To study the deviation from hemical balance scatterplots of observed and calculated NO<sub>2</sub>-concentrations are considered. The calculated NO<sub>2</sub> concentrations are based on equation (6.1) using observed values of NO and  $O_3$  at the same station as observed NO<sub>2</sub>-concentrations.

Figure 5 shows plots for Valle Hovin for May and December. A typical advection time from a road with high traffic to the station is about 100 s. For hourly average concentration values these results are typical for the other stations too.

Very good correspondance is found for high and low NO<sub>2</sub>-concentrations in December. The NO<sub>2</sub>-concentrations based on observed NO and O<sub>3</sub>-concentrations in the chemical balance equation render slightly higher values than observed values in December. In May the scatterplot show larger deviations from the chemical balance condition. Further in May as well as in December observed concentrations around 40  $\mu$ g NO<sub>2</sub>/m<sup>3</sup> tend to be overestimated by the chemical model. The overestimation is probably a result of segragation between between NO and O<sub>3</sub> in the atmosphere.

Figure 6 shows plots for stations located close to streets characterized by high traffic intencity.

The high  $NO_2$ -concentrations occur when the ozone values are close to zero. In these situations the calculated  $NO_2$  becomes equal to the observed values.

When ozone values are observed at the stations, the calculation procedure based on assumption of chemical balance overestimates the observed values. In Oslo the overestimation occurs when the concentrations are lower than about  $100 \ \mu g/m^3$ .

Chemical balance tends to overestimate the  $NO_2$ -concentrations and underestimate the  $O_3$ -concentrations at all stations within the Oslo-area. These observations may also be expected when the  $NO_2$ -model suggested by Yamartino and Wiegand in 1986 is used. Further it is seen that the difference from a local balance is small on all stations for high  $NO_2$ -values.



*Figure 5:* Observed and calculated hourly NO<sub>2</sub>-concentrations at Valle Hovin. The calculated NO<sub>2</sub>-concentrations are based on the chemical balance equations 6.2 and 6.3.





b) Strømsveien

*Figure 6: Observed and calculated hourly NO*<sub>2</sub>*-concentrations at Pilestredet (a) and at Strømsveien (b) in February 1992.* 

#### 7. Description of the NO<sub>2</sub>-model

The calculation procedure for  $NO_2$  was proposed by Yamartino and Wiegand in 1986, when  $O_x$  and  $NO_x$  are individually conserved in an urban area (see equation (5.4) and equation (5.5)).

The model calculations of  $[NO_x]$  at a given station is given by

$$[NO_x] = [NO_x]_{ij} + W \cdot [NO_x]_k + [\beta_{NO_x}]$$
(7.1)

where  $[NO_x]_{ij}$  is the km<sup>2</sup> grid concentration at the given station as calculated by the finite difference model, and  $[NO_x]_k$  is the subgrid contribution from individual roads as calculated by the subgrid model.

The background concentration  $[\beta_{NO_x}]$  is set equal to the measured value of  $[NO_x]$  at station Jeløya for each hour. Jeløya is located approximately 50 km south of Oslo. In the case of lacking data from the Jeløya station, the background value of  $[NO_x]$  is set equal to the respective average values of  $[NO_x]$  at Jeløya station in the two periods, which are 15 µg/m<sup>3</sup> in the winter period (1 Nov 1991-28 Feb 1992), and 10 µg/m<sup>3</sup> in the summer period (1 May-30 June 1992).

The calculation procedure for  $[O_x]$  at a given station is similarly given by

$$\left[O_{x}\right] = \left[O_{x}\right]_{ij} + W \cdot \left[O_{x}\right]_{k} + \left[\beta_{O_{x}}\right]$$

$$(7.2)$$

where  $[O_x]_{ij}$  is the contribution of  $[O_x]$  as a result of emissions within km<sup>2</sup>-squares at the given station as calculated by the finite difference model, and where  $[O_x]_k$  is the corresponding  $O_x$  contributions from individual roads as calculated by the subgrid model.

The background concentration  $\left[\beta_{O_x}\right]$  is set equal to the measured value of  $O_x$  at Jeløya for each hour. In the case of lacking data at Jeløya the background value of  $[O_x]$  is set equal to average values of  $[O_x]$  at Jeløya in the two periods which are 55 µg/m<sup>3</sup> for the winter period (1 Nov 1991-28 Feb 1992), and 95 µg/m<sup>3</sup> for the summer period (1 May-30 June 1992).

In Oslo the emission of ozone is very small, and the emission of  $O_x$  is equal to the primary emission of  $NO_2$  from the combustion processes, i.e. from car traffic and from home heating. The equation (7.2) reads

$$\left[O_{x}\right] = \left[NO_{2}\right]_{ii} + \left[NO_{2}\right]_{k} + \left[\beta O_{x}\right]$$

$$(7.3)$$

 $[NO_2]$  and  $[O_3]$  is then calculated based on the same balance equation as given in Eq. 6.2 and 6.3.

This gives hourly values of NO<sub>2</sub> and O<sub>3</sub> from the calculated hourly values of  $[NO_x]$  and  $[O_x]$  at each station in the area. Since O<sub>3</sub> is not emitted from the cars

$$\left[O_{x}\right]_{k}=\left[NO_{2}\right]_{k}$$

According to chapter 6 it is indicated that the relation between hourly values of NO, NO<sub>2</sub> and O<sub>3</sub> concentrations is described by reactions between NO and O<sub>3</sub>, photodissociation of NO<sub>2</sub> as well as small scale mixing in the atmosphere.

#### 8. Evaluation of the NO<sub>2</sub>- and O<sub>3</sub>-models

The results of the evaluations of the  $NO_2$ - and the  $O_3$ - models described in chapter 7 are shown in the tables 5 and 6.

Dispersion calculations of  $NO_x$  and specification of background values for  $O_3$  remain the most important sources of discrepancies between calculated and observed concentrations.

Close to streets with high traffic the highest discrepancies are observed. There are several systematic deviations to consider when the model is going to be improved.

- The deviation between observed and calculated concentrations close to line sources are particularly high in situations characterized by low wind and poor dispersion conditions.
- It is a tendency to calculate higher  $NO_2$  and lower  $O_3$  concentrations than observed. The development of  $NO_2$  as a result of chemical reactions between emissions of NO and the background concentrations of  $O_3$  in the urban atmosphere is delayed (10 min) as a result of small scale segregation of NO and  $O_3$ .

When a combination of dispersion calculations and chemical reactions are accounted for in detailed calculations it is seen that small gradients in the NO<sub>2</sub> concentrations may be found close to the roads in episodes with high background O<sub>3</sub>-concentration and poor exchange of air. The observations close to Fyrstikkalleen indicate similar results. The maximum NO<sub>2</sub> -value 50 m from Strømsveien reads only 3% lower values than the maximum NO<sub>2</sub> concentrations at the edge of the road.

Station	$\overline{C_o}$ ( $\sigma_o$ )	$\overline{C_c}$ $(\overline{\sigma_c})$	Mo	M <sub>c</sub>	r	rmse	$(\overline{\Delta C_s^2} / \overline{\Delta C^2})^{0.5}$	IA	Ν
	µg/m <sup>3</sup>	µg/m <sup>3</sup>	µg/m <sup>3</sup>	µg/m <sup>3</sup>	µg/m <sup>3</sup>	µg/m <sup>3</sup>	%		
Winter									
Valle Hovin	49 (33)	69 (37)	283	261	0.74	33	65	0.78	2 498
Skøyen	39 (21)	57 (27)	136	180	0.73	26	70	0.74	1 355
Holmlia	31 (18)	53 (26)	111	178	0.48	32	70	0.55	842
Nordahl Bruns gt.	44 (24)	66 (29)	194	178	0.64	32	72	0.68	2 876
Pilestredet	66 (29)	83 (33)	210	244	0.76	28	63	0.80	1 264
Strømsveien	76 (42)	109 (77)	324	554	0.62	69	48	0.64	1 217
Etterstadsletta	45 (32)	73 (34)	246	258	0.66	39	76	0.68	1 239
Fyrstikkalleen	57 (35)	82 (43)	313	328	0.68	41	63	0.73	1 019
Summer									
Valle Hovin	29 (22)	68 (35)	117	197	0.43	51	62	0.47	1 340
Skøyen	19 (14)	50 (26)	63	117	0.63	37	84	0.48	353
Nordahl Bruns gt.	30 (19)	56 (30)	137	182	0.55	37	73	0.55	1 338

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Table 5: Evaluation of the  $NO_2$  model for the winter and summer periods.

 $\frac{\overline{C_o}}{\overline{C_c}}$ = Average observed concentration

= Average model calculated conc.

 $M_o$  = Maximum observed concentration

 $M_{c}$  = Maximum calculated concentration

- $\left(\overline{\Delta C}_{s}^{2} / \overline{\Delta C}^{2}\right)^{0,5}$  = Percentage systematic rmse
- = Number of observations Ń

- = St. dev. observed concentration  $\sigma_{o}$
- = St.dev. model calculated conc.  $\sigma_{_c}$ 
  - = Correlation coefficient
- = Root mean square error rmse
- = Index of agreement IA

Station	$\overline{C_o}$ ( $\sigma_o$ )	$\overline{C_c}$ $(\overline{\sigma_c})$	Mo	M <sub>C</sub>	r	rmse	$(\overline{\Delta C_s^2} / \overline{\Delta C^2})^{0.5}$	IA	N
							-		
	µg/m <sup>3</sup>	µg/m <sup>3</sup>	µg/m <sup>3</sup>	µg/m <sup>3</sup>		µg/m <sup>3</sup>	%		
Winter									
Valle Hovin	15 (17)	9 (17)	62	71	0.81	12	57	0.88	1 602
Skøyen	19 (23)	11 (18)	102	75	0.79	16	75	0.84	1 451
Holmlia	20 (26)	13 (20)	83	70	0.68	25	81	0.75	1 243
Nordahl Bruns gt.	10 (11)	8 (15)	59	70	0.77	10	24	0.85	1 453
Pilestredet	13 (17)	2 (6)	74	35	0.54	18	96	0.56	1 271
Strømsveien	7 (15)	2 (6)	52	36	0.46	10	87	0.61	1 243
Etterstadsletta	9 (8)	5 (10)	39	38	0.54	10	53	0.71	1 151
Fyrstikkalleen	12 (17)	3 (8)	80	36	0.50	18	92	0.59	1 019
Summer									
Valle Hovin	29 (13)	35 (27)	80	122	0.53	24	30	0.62	1 335
Skøyen	30 (16)	53 (30)	98	126	0.67	32	72	0.60	1 163
Nordahl Bruns gt.	36 (14)	45 (27)	97	119	0.58	24	39	0.64	1 338
$\overline{C_o}$ =	$\overline{C_o}$ = Average observed concentration $\sigma_o$ = St. dev. observed concentration								
$\overline{C_c}$ =	Average model calculated conc. $\sigma_c$ = St.dev. model calculated conc.								

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*Table 6:* Evaluation of the  $O_3$  model for the winter and summer periods.

 $\overline{C_o} = \text{Average observed concentration}$   $\overline{C_c} = \text{Average model calculated conc.}$   $M_o = \text{Maximum observed concentration}$   $M_c = \text{Maximum calculated concentration}$   $\left(\overline{\Delta C_s^2} / \overline{\Delta C^2}\right)^{0.5} = \text{Percentage systematic rmse}$  N = Number of observations

- Correlation coefficient
- rmse = Root mean square error
- IA = Index of agreement

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Appendix A

### **Description of model evaluation parameters**

#### Introduction

US EPA has given guidelines on procedures to be followed in evaluating air quality models (EPA, 1984), and a list of recommended model evaluation performance parameters. In this study statistical parameters have been selected in accordance with these recommendations (Fox, 1981, 1984). Selecting the parametes, results of Willmott (1982) were also taken into consideration.

#### **Description of model evaluation performance parameters**

Let T denote the number of data, and let  $O_t$  and  $P_t$  denote the observed and calculated (predicted) values at time t, t = 1,..., T. For each station the following model evaluation parameters are defined:

 $\overline{O}$ : Mean value of observations  $\overline{P}$ : Mean value of predictions : Standard deviation of observations  $\sigma_0$ : Standard deviation of predictions  $\sigma_p$ NMD : Normalized mean difference : Root mean square error RMSE RMSE<sub>s</sub> : Systematic RMSE RMSE<sub>11</sub> : Unsystematic RMSE : Intercept and slope of regression line a, b : Correlation coefficient r IA : Index of agreement

The parameters are defined through the following set of equations:

Mean values:

$$\overline{O} = \frac{1}{T} \sum_{t=1}^{T} O_t \tag{A.1}$$

$$\overline{P} = \frac{1}{T} \sum_{t=1}^{T} P_t \tag{A.2}$$

These denote the usual arithmetical average values of the time series  $O_t$  and  $P_t$ .

Standard deviations:

$$\sigma_o = \left(\frac{1}{T-1}\sum_{t=1}^T \left(O_t - O\right)^2\right)^{0.5}$$
(A.3)

$$\sigma_{p} = \left(\frac{1}{T-1}\sum_{t=1}^{T} \left(P_{t} - \bar{P}\right)^{2}\right)^{0.5}$$
(A.4)

These denote the usual standard deviations of the time series  $O_t$  and  $P_t$ .

Normalized mean difference:

$$NMD = \left(\overline{O} - \overline{P}\right) / \overline{O} \tag{A.5}$$

This dimensionless parameter is a measure of the bias of P versus O. Ideally it should be zero, or close to zero.

Root mean square error:

$$RMSE = \left(\frac{1}{T} \sum_{t=1}^{T} (O_t - P_t)^2\right)^{0.5}$$
(A.6)

The RMSE is another measure of the size of the error produced by the model.

Systematic and unsystematic RMSE:

$$RMSE_{s} = \left(\frac{1}{T}\sum_{t=1}^{T} \left(O_{t} - \hat{P}\right)^{2}\right)^{0.5}$$
 (A.7)

$$RMSE_{u} = \left(\frac{1}{T}\sum_{t=1}^{T} (\hat{P} - P_{t})^{2}\right)^{0.5}$$
(A.8)

where

$$\hat{P}_t = a + bO_t \tag{A.9}$$

with a and b being the intercept and slope of the regression line:

$$a = \overline{P} - b\,\overline{O} \tag{A.10}$$

$$b = \left[\sum_{t=1}^{T} \left(O_t - \overline{O}\right) \left(P_t - \overline{P}\right)\right] / \left[\sum_{t=1}^{T} \left(O_t - \overline{O}\right)^2\right]$$
(A.11)

Here  $RMSE^2 = RMSE_s^2 + RMSE_u^2$ .

Willmott (1982) argues that systematic and unsystematic root mean square error gives valuable information on the possibility of model improvement.

For a good model the unsystematic portion of the RMSE is much larger that the systematic, while a large systematic RMSE indicates a poor model. For a more thourough discussion, see Willmott (1982).

Correlation coefficient:

$$r = \frac{1}{T} \sum_{t=1}^{T} \left( O_t - \overline{O} \right) \left( P_t - \overline{P} \right) / \left( \sigma_o \cdot \sigma_P \right)$$
(A.12)

This is the ordinary product-moment correlation coefficient.

Index of agreement:

$$IA = 1 - \sum_{t=1}^{T} \left( P_t' - O_t' \right)^2 \right) / \sum_{t=1}^{T} \left( |P_t'| + |O_t'| \right)^2$$
(A.13)

where

$$P_t' = P_t - \overline{O} \quad and \quad O_t' = O_t - \overline{O}$$
 (A.14)

The index of agreement has been recommended by Willmott (1982), as a better parameter to describe the "agreement" between the two time series  $O_t$  and  $P_t$ .

The index IA is a number between 0 and 1, with 0 indicating worst agreement, and 1 indicating best agreement.

When impact of new sources is considered, concentration has to be predicted. To evaluate the accuracy of the peak concentration prediction, the following parameters are considered:

$$R_m = P_m / \theta_m \tag{A.15}$$

$$\Delta = \Delta t_m \tag{A.16}$$

where

 $\Delta t_m$  = Difference of timing of occurrence of situation peak.

The ratio of predicted and observed concentrations should also be calculated for some percentiles to characterize the models behaviour for different pollution situations.



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REPORT SERIES	REPORT NO. OR 57/2000	ISBN 82-425-1225-6						
SCIENTIFIC REPORT		ISSN 0807-7207						
DATE	SIGN.	NO. OF PAGES 40	PRICE NOK 60,-					
TITLE	PROJECT LEADER							
Evaluation of urban scale time-dep elements in Oslo, Norway	Knut Erik Grønskei							
	NILU PROJECT NO.							
	E-91029D							
AUTHOR(S)	CLASSIFICATION *							
Knut Erik Grønskei, Frederick Gra	Α							
	CONTRACT REF.							
Norwegtan Institute for Air Research P.O. Box 100 2027 Kjeller, Norway ABSTRACT Hourly data on emission, wind and dispersion conditions are used to calculate hourly NO <sub>x</sub> -concentrations in a 1 km grid system based on a time dependent finite difference dispersion model in three levels. The pollution contribution from roads and point sources are accounted for by a subgrid model based on Gaussian line source and point source models. Results of concentration calculations are evaluated by using data from eight stations for three winter months (1.11.91-29.2.92) and from the three main stations for two summer months (1.530.6.92). The relative importance of the prosesses affecting the NO <sub>2</sub> -concentrations in an urban area as a function of advection time from a line source are discussed. A balance between NO, NO <sub>2</sub> and O <sub>3</sub> is found when the advection time is larger than 600-1000 s. The high NO <sub>2</sub> -concentrations occur when the O <sub>3</sub> -concentrations are very low.								
NOKWEGIAN IIILE Evaluering av en tidsavnengig spredningsmodell								
KEYWORDS								
Dispersion	Oslo	Nitrogen oxides						
ABSTRACT (in Norwegian) Timevise data for utslipp, vind og spredningsbetingelser brukes for å beregne timevise NO <sub>x</sub> -konsentrasjoner i et km-gridsystem basert på en tidsavhengig, endelig differensmodell i tre lag. Forurensningsbidrag fra veier og fra punktkilder tas hensyn til ved Gaussiske subgridmodeller for linje- og punktkilder. Beregningsresultatene er kontrollert ved data fra åtte stasjoner i tre vintermåneder og fra tre stasjoner i to sommermåneder. Betydning av prosesser som påvirker NO <sub>2</sub> -konsentrasjonen er drøftet. En balanse mellom NO, NO <sub>2</sub> og O <sub>3</sub> foreligger når adveksjonstiden er større enn 600-1000 s. Høye NO <sub>2</sub> -konsentrasjoner opptrer samtidig med lave ozon- konsentrasjoner. * Classification A Unclassified (can be ordered from NILU)								
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