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A DISPERSION MODEL FOR REGIONAL
AIR POLLUTION PROBLEMS

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A DISPERSION MODEL FOR REGIONAL
AIR POLLUTION PROBLEMS

1 INTRODUCTION

As a part of a study on oxidant formation in Grenland, Norway, a dispersion model for regional air pollution problems has been developed (1). The model has been tested in an area of 16x32 km². The results of this study show that larger scale processes have to be included.

For this purpose a 16x32 grid-points in each of three levels are proposed. Grid distance is 8 km. A telescoping procedure is planned for the local area of Grenland where local emissions are important. The local area of Grenland would then consist of 2x4 gridpoints. In order to separate high and low emissions, three levels are planned. This separation becomes particularly important in periods with low vertical exchange. The model description of local and regional processes follows.

2 GENERAL DESCRIPTION

The dispersion is partly caused by the time variation of the wind field and partly by turbulent exchange. For each of the pollution components the following equation is solved:

$$\frac{\partial c_i}{\partial t} = v_h \cdot \nabla_h c_i - \frac{\partial (w'c_i')}{\partial z} - \nabla_h \cdot (w'c_i') + R_i + Q_i \quad (2.1)$$

Advection	Turbulent exchange	Reactions	Emission
I	III and IV	V	VI

Processes to be included in the model are:

- I : horizontal advection, $\mathbf{V}_h \cdot \nabla c_i$
- II : vertical advection, $w \frac{\partial c_i}{\partial z}$ (assumed to be small and neglected in Eq. (2.1))
- III : turbulent exchange horizontally
- IV : turbulent exchange vertically
- V : chemical reactions (sinks or sources)
- VI : emission from natural and anthropogenic sources

The time derivatives caused by advection, turbulent exchange and by emission (Q_i) are calculated separately. Further new values are calculated using the chemical reaction scheme, the values of the time derivatives and the old concentrations. In this way the time integration follows a method proposed by E. Hesstvedt et.al. (2). The calculation of vertical exchange, follows a method proposed by Pasquill (3).

2.1 Boundary conditions

In the vertical, dry deposition is taken into consideration as a lower boundary condition. At the upper boundary a flux of pollution out of the system is made proportional to the concentration in the upper layer. The factor of proportionality may change with time of day.

In the horizontal, the concentrations along the lateral boundaries are determined by long range transport calculations.

For the horizontal advection upwind finite difference methods are used. The pseudo-spectral method, developed by Christensen and Prahm (4), was found time-consuming although numerical diffusion was reduced. For one or only a few components this method can be used and it is included in the model as an option.

Dry deposition is a sink of pollution at the ground. However, pine forests covering parts of the area are a source of hydrocarbons that may influence the chemical reactions.

3 ADVECTION

In the lowest layer wind measurements close to the ground are used to define a two-dimensional stream function (ψ) along the lateral boundary of the area. A mass-consistent approximation of the horizontal windfield is defined by solving

$$\nabla^2 \psi = 0 \quad (3.1)$$

From a dynamical point of view this windfield will change only as a function of the lateral boundary conditions in the constant flux layer when the vertical exchange of sensible heat and momentum are horizontally homogeneous and quasi-stationary.

The dispersion effect of deviations from this horizontal windfield is taken into account by the description of horizontal turbulent exchange.

4 TURBULENT EXCHANGE

4.1 Vertical exchange

A finite difference approach to estimate vertical exchange, based on K-theory, requires numerical simulation in many atmospheric layers. To avoid the labour and cost of detailed numerical solutions, Pasquill (3) has proposed a "local similarity" treatment of vertical spread from a ground source.

The basic principle is to express the rate of dispersion, $\frac{d\bar{z}}{dt}$, (where \bar{z} is the mean displacement of an ensemble of particles after a given travel time) in terms of basic parameters of the turbulent boundary layer. The assumption is made that the increase in vertical spread, \bar{z} , or alternatively z_m (the extreme vertical displacement), is always determined by two local properties:

- a) σ_w : turbulence intensity, expressed as the standard deviation of vertical wind velocity, and
- b) $\ell(z)$: scale of turbulence prevailing at \bar{z} or z_m .

If it is further assumed that ℓ is proportional to the spectral scale, λ_m , dimensional analysis gives:

$$\frac{d\bar{z}}{dt} = \sigma_w f_1 \left(\frac{\lambda_m}{z}\right) \bar{z} \quad (4.1)$$

$$\frac{dz_m}{dt} = \sigma_w f_2 \left(\frac{\lambda_m}{z}\right) z_m \quad (4.2)$$

As a hypothesis, Pasquill (3) proposed the following relations:

$$\frac{d\bar{z}}{dx} = f_3 \left(\frac{K}{u\bar{z}}\right) \bar{z} \quad (4.3)$$

$$\frac{dz_m}{dx} = f_4 \left(\frac{K}{u z_m}\right) z_m \quad (4.4)$$

By using detailed numerical dispersion calculations, these universal functions are estimated as simple power functions that apply from unstable conditions ($L = -7$ m) to moderately stable conditions ($L = 4$ m):

$$\frac{d\bar{z}}{dx} = a \left(\frac{K}{u\bar{z}}\right)^b \quad (4.5)$$

where $a = 0.95$; $b = 1.06$

$$\frac{dz_m}{dx} = c \left(\frac{K}{uz} \right)^d \quad (4.6)$$

where $c = 3.56$; $d = 2.7$.

When $\frac{K}{u}$ is constant with height:

$$\bar{z} = \left(a \left(\frac{K}{u} \right)^b (1 + b)x + z_0^{1+b} \right)^{1/(1+b)} \quad (4.7)$$

where z_0 : initial dispersion.

Three layers are considered in the calculations: one layer for the emission of low level sources, and two upper layers for medium height and high level sources (Figure 4.1).

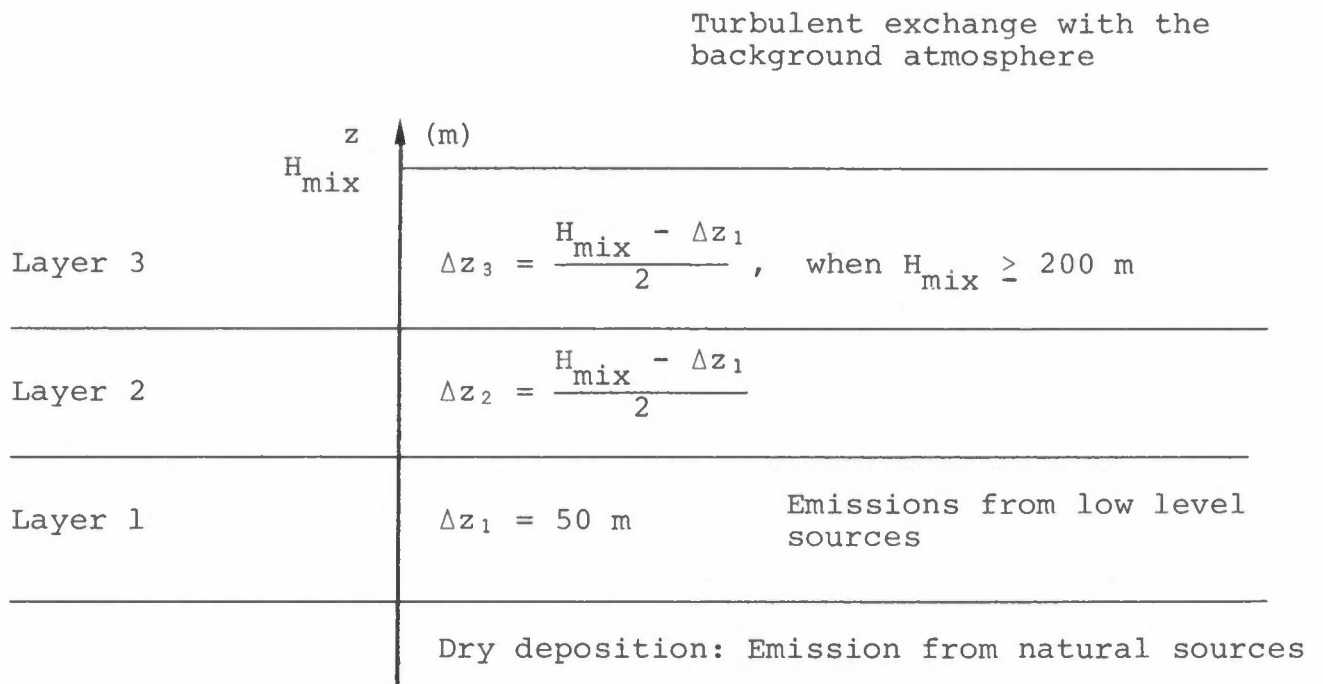


Figure 4.1: The vertical structure of the three-level model.
 When mixing height (H_{mix}) is larger than 200 m, this height is used as the upper limit of Layer 3.

Measurements of temperature stratification with height have been used to determine the mixing height H_{mix} .

It is assumed that the air layer between the first and second level grows according to Equations 4.5 and 4.6, causing an exchange of pollution. The exchange will be proportional to the difference in concentration between the levels. The third layer also exchange pollution with the background air above the mixing height.

The following fluxes are calculated:

F_o : Dry deposition to the ground

F_{1-2} : $(\frac{d\bar{z}}{dt})_{1-2} \cdot (C_2 - C_1)$ - from Layer 1 to Layer 2

F_{2-3} : $(\frac{d\bar{z}}{dt})_{2-3} \cdot (C_3 - C_2)$ - from Layer 2 to Layer 3

F_{3-b} : $(\frac{d\bar{z}}{dt})_{3-b} \cdot (C_b - C_3)$ - from Layer 3 to the background atmosphere.

4.2 Horizontal exchange

Measurements of horizontal wind fluctuations are used to estimate horizontal mixing. The standard deviation of these fluctuations (σ_θ) as used with the wind speed and the grid distance to define a horizontal turbulent exchange coefficient, D , describing the dispersion effect of turbulence element smaller than the grid distance, Δx . The following formula as used:

$$\frac{\partial}{\partial x}(u'C'_i) + \frac{\partial}{\partial y}(v'C'_i) = D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) \quad (4.8)$$

D : horizontal turbulent exchange coefficient

where $D = \sigma_\theta^2 u(z) \Delta x$

Near point sources the dispersion is described by following the movements of particles. The horizontal dimension of the puff increases according to the formula:

$$\sigma_y(t+\Delta t) = \sigma_y(t) + \Delta t \cdot u \cdot \sigma_\theta \cdot B \quad (4.9)$$

$$B = 1.0, \text{ when } \sigma_y < 100 \text{ m}$$

$$B = 0.5, \text{ when } \sigma_y \geq 100 \text{ m}$$

The particles or puffs are growing until their horizontal, σ_y , or vertical, σ_z , standard deviation is equal to half the grid distance. The mass of pollution that follows the puff is then mixed in the area where the particle is. The area is characterized by the gridpoint.

5 SIMPLIFIED SET OF EQUATIONS DESCRIBING WIND, TEMPERATURE AND TURBULENCE IN THE FLUX LAYER

The following nomenclature is used:

z : vertical coordinate, meters

z_0 : roughness-parameter, meters

L : Monin-Obukhov length

c_p : specific heat of air at constant pressure

ρ : density of the air

T_0 : air temperature at the ground

u_*^2 : $-\overline{u'w'}$, vertical flux of momentum

$u_*\theta_*$: $\frac{\overline{w'\theta'}}{c_p\rho} = \frac{H_0}{c_p\rho}$, vertical flux of sensible heat

κ : von Karman's constant

ϕ_m : normalized wind gradient ($\kappa z/u_*$) $(\frac{du}{dz})$

ϕ_h : normalized temperature gradient ($(\kappa z/\theta_*) \frac{d\theta}{dz}$)

To determine the mean air flow close to the ground, the following "parameter" are important:

1. The horizontal stress, $\frac{\partial \tau}{\partial z}$, has to be known for the horizontal equation of motion:

$$\tau = u_*^2 / \rho$$

2. The buoyancy force influences the vertical motion. This force is proportional to the Vaisälä-Brundt frequency for small perturbations:

$$v_s^2 = \frac{g}{T} \left(\frac{dT}{dz} + \frac{g}{c_p} \right)$$

3. For the thermodynamic energy equation, the vertical flux of heat has to be known:

$$\overline{w'\theta'} = u_* \theta_*$$

In Monin-Obukhov similarity theory it is assumed that the vertical fluxes of heat and momentum are the important parameters, together with the height z , and the Vaisälä-Brundt frequency, v_s .

The length parameter, L , and a temperature parameter, θ_* , are here defined as:

$$L \equiv - \frac{u_*^3 T}{\kappa g \overline{u_* \theta_*}}, \quad \theta_* \equiv \frac{\overline{w'\theta'}}{u_*}$$

Two non-dimensional products may be defined, and the π theorem used to describe the vertical gradients in wind speed, $\frac{\partial u}{\partial z}$, and potential temperature, $\frac{\partial \theta}{\partial z}$:

$$\frac{\kappa z}{u_*} \frac{du}{dz} = \phi_m \left(\frac{z}{L} \right)$$

$$\frac{\kappa z}{\theta_*} \frac{d\theta}{dz} = \phi_h \left(\frac{z}{L} \right)$$

It has been proposed (5) to use Businger's empirically determined universal functions (6). When these equations are integrated, with $\zeta = (z + z_0) \cdot L^{-1}$, the following results may then be written:

When $\zeta < 0$:

$$\frac{u}{u_*} = \frac{1}{\kappa} \left(\ln \frac{z}{z_0} - \Psi_1 \right) \quad (5.1)$$

where $\Psi_1 = 2 \ln \left(\frac{1+x}{2} \right) + \ln \left(\frac{1+x^2}{2} \right) - 2 \tan^{-1} (x + \pi/2)$

and $x = (1 - 15 \zeta)^{1/4} = \phi_m^{-1}$

$$\frac{\bar{\theta} - \theta_0}{\theta_*} = 0.74 \left(\ln \frac{z}{z_0} - \Psi_2 \right) \quad (5.2)$$

where $\Psi_2 = \ln \left(\frac{1+y}{2} \right)$

and $y = (1 - 9\zeta)^{1/2} = 0.74 \phi_m^{-1}$

When $\zeta > 0$:

$$\frac{u}{u_*} = \frac{1}{\kappa} \left(\ln \frac{z}{z_0} + 4.7 \zeta \right) \quad (5.3)$$

$$\frac{\bar{\theta} - \theta_0}{\theta_*} = 0.74 \ln \frac{z}{z_0} + 4.7 \zeta \quad (5.4)$$

where $\phi_m = 1 + 4.7 \zeta$

and $\phi_h = 0.74 + 4.7 \zeta$

With measurements of wind and temperature at two levels as input, Equations 5.1 and 5.2, or 5.3 and 5.4, may be solved by iteration to find u_* , θ_* , and L . Only a few iteration steps are necessary.

The turbulent exchange of pollution, K_z , is estimated by using the turbulent exchange of heat, K_h , and the following formula is used:

$$K_z = K_h = 0.35 u_* z / \phi_h (z/L) \quad (5.5)$$

6 DRY DEPOSITION

The deposition of a gas to the ground, and in similar way the evaporation of a gas from the ground, are often discussed in terms of the resistance of the boundary layer to diffuse pollution transport. The resistance, r , is the inverse of the velocity of deposition V_g :

$$r = V_g^{-1} = \frac{\text{concentration difference}}{\text{flux}}$$

The total resistance is further divided into three parts:

$$r = r_a + r_b + r_s \quad (6.1)$$

r_a : aerodynamic resistance in free air

r_b : boundary layer resistance

r_s : surface resistance

The Monin-Obukhov similarity theory may be used to clarify the aerodynamic resistance. The surface resistance is dependent on the chemical affinity between the ground and the gas. The boundary resistance is dependent on diffusion processes close to the ground, where the atmospheric surface layer theory does not apply.

For the constant flux layer of the atmosphere, the following equation may be written:

$$c_* u_* = K_z \frac{\partial c}{\partial z} \quad (6.2)$$

c : pollution concentration
 c_* : flux of pollution divided by the friction velocity.

Together with Equations 5.4 and 5.5, Equation 6.2 may be used to calculate the variation of concentration with height in a stable atmosphere:

$$c(z) - c_0 = c_* \left(2.1 \ln \frac{z}{z_0} + 13.4 \left(\frac{z - z_0}{L} + \frac{z_0}{L} \ln \frac{z}{z_0} \right) \right) \quad (6.3)$$

where: $c_* = (c - c_0) / f(z, z_0, L)$

when $f(z, z_0, L) = \left(2.1 \ln \frac{z}{z_0} + 13.4 \left(\frac{z - z_0}{L} + \frac{z_0}{L} \ln \frac{z}{z_0} \right) \right)$

In correspondance with Equation 6.2:

$$c_* u_* = (c - c_0) u_* / f(z, z_0, L) \quad (6.4)$$

where: $r_a = f(z, z_0, L) / u_*$

Further:

$$\frac{c_0}{r_b + r_s} = u_* c_* = (c - c_0) u_* / f(z, z_0, L) \quad (6.5)$$

Similar equations may be written for an unstable atmosphere. In this case vertical exchanges in the atmosphere are most effective, and the boundary layer and surface resistance often limit dry deposition ($r_b + r_s \gg r_a$). When the deposition velocity is of the order of 1 cm/s, the effect becomes important when the model keeps track of the pollution during several hours.

In mesoscale modelling dry deposition is considered for SO₂, NO, NO₂, O₃, and aerosols. The deposition velocities are determined by measurements. To consider emissions of hydrocarbons from forest areas, Equation (6.5) may also be used. To determine the emissions from a homogeneous area, it is necessary to measure concentrations at two levels, as well as parameters determining the aerodynamic resistance.

The following empirically determined values for dry deposition (8) are used as maximum values for Level 1 in the model:

$$V_{\max} = \frac{1}{r_b + r_s} \quad (6.6)$$

For O₃ : V_{max} = 0.6 cm/s
For NO : V_{max} = 0.1 "
For NO₂ : V_{max} = 0.2 "
For PAN : V_{max} = 0.2 "

When $r_a \gg r_b + r_s$, it is the turbulent flux in the surface layer that determines dry deposition.

Before comparing calculated concentrations for the surface layer (25 m level) with observed values 2 m above the ground, corrections have to be made for the concentration gradient close to the ground.

7 NUMERICAL METHODS FOR CALCULATING HORIZONTAL ADVECTION AND DIFFUSION

7.1 Finite difference methods

To describe the numerical methods that are used the following simplified equation is considered:

$$\frac{\partial c}{\partial t} = - u \frac{\partial c}{\partial x} \quad (7.1)$$

For the local time derivative the Euler forward scheme is used:

$$\left[\frac{\partial c}{\partial t} \right]_{(j)}^{(n)} \approx \frac{c_{(j)}^{(n+1)} - c_{(j)}^{(n)}}{\Delta t} = - \left(u \frac{\partial c}{\partial x} \right)_{(j)}^{(n)} \quad \text{Euler Forward scheme}$$

The Adam-Bashforth scheme is more accurate:

$$\frac{c_{(j)}^{(n+1)} - c_{(j)}^{(n)}}{\Delta t} = + \frac{3}{2} \left(u \frac{\partial c}{\partial x} \right)_{(j)}^{(n)} - \frac{1}{2} \left(u \frac{\partial c}{\partial x} \right)_{(j)}^{(n-1)} \quad \text{Adam-Bashforth scheme}$$

$$f_{(j)}^{(n)} = f(j\Delta x, n\Delta t)$$

The subscripts denote the value of the function in the grid-point $x = j\Delta x$, at the time $t = n\Delta t$.

For the spatial derivatives the upwind finite difference method is used:

$$\left[u \frac{\partial c}{\partial x} \right]_{(j)}^{(n)} \approx u_j^n \cdot \frac{c_{(j)}^{(n)} - c_{(j-1)}^{(n)}}{\Delta x}, \quad \text{when } u_{(j)}^{(n)} > 0$$

$$\approx u_j^n \cdot \frac{c_{j+1}^{(n)} - c_j^{(n)}}{\Delta x}, \quad \text{when } u_{(j)}^{(n)} < 0$$

To avoid numerical diffusion, the fact that each Fourier component is a solution of Equation (7.1) is favouring the pseudo-spectral method. The method is described by Christensen and Prahm (4). According to their results, it is an advantage to use the scheme of Adam-Bashford for the time intergration (7). In this work the dispersion of a large number of components had to be considered, and the scheme of Adam-Bashford would introduce computer storage problems.

A periodic function, known in a finite number of gridpoints $2N$, may be written as sum of Fourier components, as shown in Equation (7.2):

$$c_n = \sum_{k=0}^N a_k \cos \pi k \frac{n}{N} + \sum_{k=1}^N b_k \sin \pi k \frac{n}{N} \quad (7.2)$$

$$a_k = \frac{2}{2N} \sum_{n=1}^{2N} c_n \cos \left(k\pi \frac{n}{N} \right)$$

$$a_0 = \frac{1}{2N} \sum_{n=1}^{2N} c_n$$

$$b_k = \frac{2}{2N} \sum_{n=1}^{2N} c_n \sin \left(k\pi \frac{n}{N} \right)$$

The discrete function $c(x_n)$, known in $2N$ points, may be written without error in the form given above. To estimate numerically the derivative of the function $c(x_n)$, the derivative of the corresponding continuous function given below is:

$$c(x) = \sum_{k=0}^N a_k \cos \left(\frac{2\pi}{L_k} x \right) + \sum_{k=1}^N b_k \sin \left(\frac{2\pi}{L_k} x \right) \quad (7.3)$$

$$\frac{dc(x)}{dx} = - \sum_{k=1}^N \frac{2\pi}{L_k} \cdot a_k \sin \left(\frac{2\pi}{L_k} x \right) + \sum_{k=1}^N b_k \cos \left(\frac{2\pi}{L_k} x \right) \quad (7.4)$$

$$\frac{d^2c(x)}{dx^2} = - \sum_{k=1}^N \left(\frac{2\pi}{L_k} \right)^2 a_k \cos \left(\frac{2\pi}{L_k} x \right) - \sum_{k=1}^N \left(\frac{2\pi}{L_k} \right)^2 b_k \sin \left(\frac{2\pi}{L_k} x \right) \quad (7.5)$$

$$L_k = \frac{2N\Delta x}{k}$$

The Equations 7.4 and 7.5 are used to estimate the derivatives in the grid points:

$$\begin{aligned} \left(\frac{dc}{dx} \right)_n = & - \sum_{k=1}^N \left(\frac{2\pi}{L_k} \right) a_k \cdot \sin \left(\frac{2\pi}{L_k} n\Delta x \right) + \\ & \sum_{k=1}^N \left(\frac{2\pi}{L_k} \right) \cdot b_k \cdot \cos \left(\frac{2\pi}{L_k} n\Delta x \right) \end{aligned} \quad (7.6)$$

$$\begin{aligned} \left(\frac{d^2c}{dx^2}\right)_n &= -\sum_{k=1}^N \left(\frac{2\pi}{L_k}\right)^2 \cdot a_k \cos\left(\frac{2\pi}{L_k} n\Delta x\right) \\ -\sum_{k=1}^N \left(\frac{2\pi}{L_k}\right)^2 \cdot b_k \sin\left(\frac{2\pi}{L_k} n\Delta x\right) & \end{aligned} \quad (7.7)$$

7.2 Time integration - numerical stability

To evaluate the numerical stability conditions, the forward time step combined with the pseudo-spectral method are used to solve the equation:

$$\frac{\partial c}{\partial t} = -u \frac{\partial c}{\partial x} + D \frac{\partial^2 c}{\partial x^2} \quad (7.8)$$

- c: pollution concentration
- u: wind speed
- D: turbulent exchange coefficient

A solution of a linear equation can be expressed in the form of a Fourier series where each harmonic component also is a solution. The Equations 7.6 and 7.7 are used in Equation 7.8, and the behaviour of the following numerical solution is studied:

$$c_{(j)}^{(r)} = \omega^r e^{ikx_j} = \omega^r (\cos kx_j + i \sin kx_j)$$

$c_{(j)}^{(r)}$: pollution concentration at a grid point $x_j = j \cdot \Delta x$,
at the time $t_r = r\Delta t$

Δx : grid distance

Δt : time step

ω^r : amplification factor raised to the power of r

$i = \sqrt{-1}$: imaginary unit of a complex number

k : wave number

Using the Euler Forward scheme for time integration (see p.17) the approximation of Equation 7.8 for this numerical solution reads:

$$\frac{(\omega^{r+1} - \omega^r) e^{ikx_j}}{\Delta t} = -u ik \omega^r e^{ikx_j} - Dk^2 \omega^r e^{ikx_j}$$

Δt : time step

$$\frac{\omega - 1}{\Delta t} = -u ik - Dk^2$$

$$\omega = 1 - Dk^2 \Delta t - uik \Delta t \quad (7.9)$$

The condition for a stable scheme is that the amplification factor be less than one. The time step then has to be smaller than a specified value:

$$\Delta t < \frac{2D}{(Dk_m)^2 + u^2} = \frac{2D}{D^2 \left(\frac{\pi}{\Delta x}\right)^2 + u^2} \quad (7.10)$$

$k_m = \left(\frac{\pi}{\Delta x}\right)$ = the maximum wave number that may be resolved in the grid system.

It is seen that the turbulent exchange coefficient has to be larger than zero for the numerical scheme to be stable.

The stability conditions of other finite difference schemes may be evaluated by the same method.

8 CONCLUDING REMARKS

The model has been programmed by defining subroutines for each of the processes described in the previous section (9).

When applying the model in certain areas, a better description is needed for some of the processes. For instance, in complex terrain a better model, based on dynamical principles, is needed to describe inhomogeneous wind and dispersion conditions.

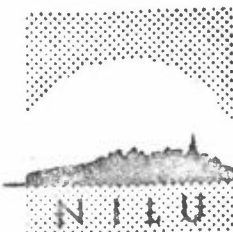
The model has further been developed to include a telescoping procedure using a Lagrangian procedure close to the large sources.

A finite difference approximation is suitable for the mesoscale, and quasi-Lagrangian approach may be used for long range transport calculations.

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TITTEL A dispersion model for regional air pollution problems	PROSJEKTLEDER K.E. Grønskei	NILU PROSJEKT NR 01480
FORFATTER(E) K.E. Grønskei F. Gram	TILGJENGELIGHET ** A	OPPDRAUGSGIVERS REF.
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3 STIKKORD (å maks.20 anslag) Regional	Dispersion	Model
REFERAT (maks. 300 anslag, 5-10 linjer) Tidsvariasjonen i konsentrasjonen i tre nivå beskrives ved numeriske metoder for: a) adveksjon, b) vertikalutveksling, c) horisontaldiffusjon, d) kjemiske reaksjoner, e) utslipp fra naturlige og antropogene bilder. Tørravsetning og utveksling med omgivelsene er innarbeidet som grensebetingelser. På grunnlag av beskrivelsen er det utarbeidet et programsystem hvor hver av prosessene er subrutiner.		
TITLE En regional spredningsmodell		
ABSTRACT (max. 300 characters, 5-10 lines) The time variation in concentration in three levels is considered by describing: a) advection, b) vertical exchange, c) horizontal diffusion, d) chemical reactions, e) emission from natural and antropogenic sources. Dry deposition and exchange with the surroundings are taken into consideration as boundary conditions. Based on the description a program system is developed favouring a telescoping procedure.		

**Kategorier: Åpen - kan bestilles fra NILU A
Må bestilles gjennom oppdragsgiver B
Kan ikke utleveres C