Raport Badawczy

Research Report

RB/02/2001

Regional-scale air pollution dispersion model REGFOR1

P. Holnicki, A. Żochowski,

A. Warchałowski

Instytut Badań Systemowych
Polska Akademia Nauk

Systems Research Institute
Polish Academy of Sciences

POLSKA AKADEMIA NAUK

Instytut Badań Systemowych

ul. Newelska 6

01-447 Warszawa

tel.: (+48) (22) 8373578

fax: (+48) (22) 8372772

Pracę zgłosił: dr inż. Piotr Holnicki

Warszawa 2001

Regional-scale air pollution dispersion model REGFOR1

*Piotr Holnicki, Antoni Żochowski *) and Aleksander Warchałowski **)*

*) *Systems Research Institute*
Polish Academy of Sciences
Warsaw

**) *Warsaw University of Technology*
Institute of Environmental Engineering
Systems, Warsaw

Keywords: environment protection, air pollution, mathematical modeling

Abstract: In the paper an implementation of a single-layer dynamic model for SOx air pollution forecasting on regional scale is presented. The computation method simulates the transport of the primary and secondary pollutants following the wind trajectories. The model equations take into account transport, deposition (dry and wet) and chemical transformation processes.

The model is designed for evaluation of the environmental impact of the major emission sources and, eventually, for emission control. The main output consists of the set of unit concentration maps for selected, individual sources, corresponding to the unit emission intensity. The assumed linearity of the dispersion process allows us to treat each source individually, and then compute the total concentration map as a superposition of the individual contributions. The test computations have been performed for the set of major power plants in Poland.

1 The transport model formulation

The model presented in the paper is aimed at computing short-term forecasts of air pollution related to specified emission sources, evaluating contribution of each source in the resulting pollution field and, ultimately, utilizing those data in air quality control. The basic output of the model has a form of 24-hour forecasts of the total SO_2 concentration in the domain or the form of individual maps representing contribution of each emission source. Such a map characterize environmental impact of a specified source.

Calculation of the transport of sulfur pollution is carried out by Lagrangian-type, single layer trajectory model. It calculates concentrations averaged over the mixing layer. The mass balance for pollutants is calculated for air parcels following the wind trajectories. The model is source-oriented, and the trajectory that starts at the specific emission source is observed until the mass of the parcel drops below 1% of its initial value or the parcel leaves the computational area. The technique is in turn applied to all the individual sources, giving the unit *transfer matrices* as a result. Multiplying these matrices by real

emissions and summing over the set of all the sources under consideration, gives the total concentration map.

The model takes into account two basic polluting components, SO_2 and $SO_4^=$. The uniform space discretization step, $h = \Delta x = \Delta y$=10 km is applied in the computational algorithm. Points along the trajectory are determined at discrete time moments, based on the interval τ = 15 min. The main output constitutes the concentrations of SO_2, averaged over the discretization element and the mixing layer height. Due to the total mass of the "packet" of the pollutant emitted over the interval τ the initial concentrations are calculated according to the formulae

$$q_1 = \frac{(1-\beta)E\tau}{HM \cdot h^2}, \qquad (1)$$

$$q_2 = \frac{\beta E\tau}{HM \cdot h^2}, \qquad (2)$$

where q_1, q_2 denote concentrations of SO_2 and $SO_4^=$ [μg/m^3], E [μg/s] is total sulfur emission , β – fraction emitted directly as $SO_4^=$, HM [m] – the mixing layer height.

The continuity equations for both components reflect spatial and temporal transformation of this initial value. They include transport, chemical transformations $SO_2 \Longrightarrow SO_4^=$, dry deposition and scavenging by precipitation and have a form

$$\frac{\partial q_1}{\partial t} + \vec{w}\,\nabla q_1 + (k_{d_1} + k_{w_1})\,q_1 + k_t\,q_1 = 0, \qquad (3)$$

$$\frac{\partial q_2}{\partial t} + \vec{w}\,\nabla q_2 + (k_{d_2} + k_{w_2})\,q_2 = k_t\,q_1, \qquad (4)$$

where

k_{d_i} – dry deposition coefficient [1/s], k_{w_i} – coefficient of wet deposition due to scavenging by precipitation [1/s], k_t – coefficient of chemical transformation $SO_2 \Longrightarrow SO_4^=$ [1/s], $\vec{w} = [u, v]$ – wind velocity vector [m/s]. The emission term does not appear on the right-hand side of (3) and (4), since the model simulates dispersion and environmental impact (spatial and temporal) of the initial concentrations (1) and (2), related to a source.

If all the coefficients in (3), (4) are assumed constant over the interval [t,t+τ], the solutions can be expressed [2] in the following form

$$q_1(t+\tau) = q_1(t)\exp(-(k_{d_1} + k_{w_1} + k_t))\tau, \qquad (5)$$

$$q_2(t+\tau) = \frac{k_t\,q_1(t)}{k_{d_2} + k_{w_2}}\,[1 - \exp(-(k_{d_2} + k_{w_2})\tau] + q_2(t)\exp(-(k_{d_2} + k_{w_2}))\tau. \qquad (6)$$

The coefficients, which represent the decline due to dry deposition in (3)–(6) are defined as follows:

$$k_{d_i} = \frac{v_{d_i}}{HM}, \qquad (i = 1, 2), \qquad (7)$$

where dry deposition velocity for SO_2 – v_{d_1} [m/s] is preprocessed by a specialized algorithm developed at RIVM (the Netherlands) [4,5,6] and modified by the Institute of

Environmental Engineering Systems (Warsaw Institute of Technology). Land-use characteristics utilized in this model are based on [7]. Moreover, basing on the approach presented in [2], the dry deposition velocity for $SO_4^=$ is assumed $v_{d_2} = 0.2 v_{d_1}$.

Wet deposition depends on precipitation intensity and is expressed, in general, as

$$k_{w_1} = \frac{\Lambda_i P}{HM}, \qquad (i = 1, 2). \tag{8}$$

Here P denotes the precipitation height in [mm], accumulated over the time interval. Basing on [2], the scavenging factor for SO_2 reflects the seasonal fluctuations of the air temperature, and is parameterized as follows

$$\Lambda_1 = 3 \cdot 10^5 + 1 \cdot 10^5 \sin[2\pi(T - T_0)/T_a]. \tag{9}$$

T is the current day of the year, $T_0 = 80$ days, and $T_a = 365$ days. For simplicity, the scavenging factor for $SO_4^=$ is assumed constant (compare [2]),

$$\Lambda_2 = 1 \cdot 10^6. \tag{10}$$

In a analogous way, the chemical transformation coefficient in (3)–(6) can be defined according to the formula

$$k_t = a_t + b_t \sin[2\pi(T - T_0)/T_a]. \tag{11}$$

where the parameters a_t, b_t are constant,

$$a_t = 3 \cdot 10^{-6} \ \ [1/s], \qquad b_t = 2 \cdot 10^{-6} \ \ [1/s],$$

while T, T_0 and T_a are defined as in (9).

The main output generated by the model is a set of the unit *transfer matrices* for all the considered emission sources. The respective output matrix relates the respective SO_2 and $SO_4^=$ concentration forecasts to the unit emission intensity of the source. Assuming linearity of the dispersion process, we can compute the total concentration map as a superposition of the individual sources contribution.

The pollution forecast calculated by the model relates to the 24-hours time interval. However, the current concentration of a pollutant at any receptor site also depends on the previous releases from other sources, which are transported and transformed depending on the wind-field and the other meteorological conditions. Ultimately, they form the background concentration field for the forecast.

In order to take the previous pollution into account, it is assumed here that the influence of the released pollutants may be after 3 days neglected. Thus, the model calculates dispersion and transformations of pollutants over the computational area, starting from the time 48 hours before the beginning of the forecast period. The contribution of these pollutants is then taken into account only over that period (the last 24h). The sum of the contributions of all the sources, taken with their real emission in the past two days, constitutes the background concentration of the forecast.

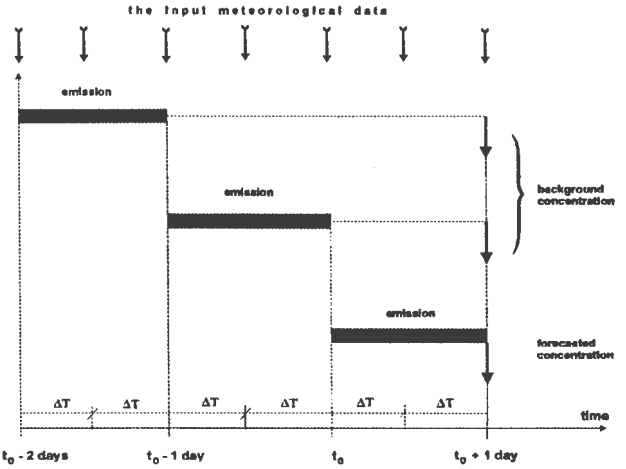

Figure 1: The diagram of the forecast and background concentration computing

Figure 1 explains the algorithm of calculation of the basic forecast and background concentration maps. Let us denote by t_0 the initial time of the current 24-hour forecast, and assume that the basic time interval for the input data is $\Delta T = 12$ h. Then, the sequence of the input data for the interval $\langle t_0, t_0 + 2\Delta T \rangle$ is used for generating the forecat of the concentration map at $t_0 + 2\Delta T$. In the same way, the respective sequence of the input data from two previous two intervals, namely $\langle t_0 - 4\Delta T, t_0 - 2\Delta T \rangle$ and $\langle t_0 - 2\Delta T, t_0 \rangle$ is utilized for generating the background map for the same time moment.

The algorithm of generating the unit pollution maps consists of several steps and is repeated for all the sources under consideration. It consists of the following steps:

- reading the set of the input data,
- interpolating meteorological data in space and time,
- generating the wind trajectory for the period of the forecast,
- calculating the transport of the package along the trajectory,
- calculating the physical and chemical transformations,
- calculating the resulting concentration field.

The forecasted contribution of a source in the resulting concentration field is calculated by the multiplication of the respective unit concentration map by the predicted (or the actual) emission quantity of this source. The resulting concentration map is then obtained as the superposition of the individual contributions.

In a similar way the background pollution map is computed according to the diagram shown in Figure 1, but the total emission field represents in this case the real emission intensities of the sources in the previous time intervals, i.e. $\langle t_0 - 4\Delta T, t_0 - 2\Delta T \rangle$ and $\langle t_0 - 2\Delta T, t_0 \rangle$.

2 The wind field submodel

One of the basic meteorological inputs of the pollution transport model is the wind field prediction within the time interval of the forecast. Due to the structure of the transport model, the wind field should be a single-layer approximation of the three-dimensional field, averaged over the mixing layer HM. The implementation has been worked out for the rectangle area 900 km × 750 km shown in Figure 2 in EMEP coordinates. The uniform space discretization step, $h = \Delta x = \Delta y = 10$ km was applied for computational algorithm.

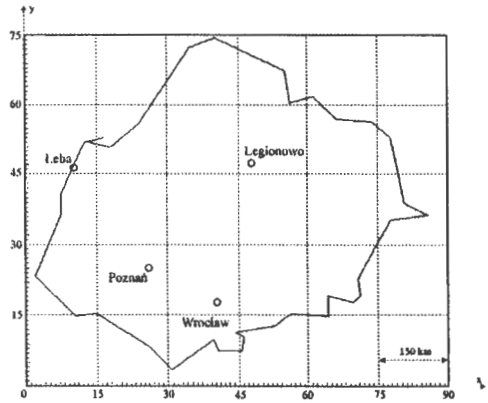

Figure 2: Region in EMEP coordinates and aerological measurement stations

The wind trajectories for the region discussed here are preprocessed basing on the data from four aerological stations shown in Figure 2. The trajectory generation procedure uses the following input data: (i) a complete set of wind field measurements in selected field stations, (ii) the coordinates of emission sources location. The approach applied is based on the spatial and temporal interpolation of the sequence of meteorological data obtained from selected measurement stations. Each station records the set of data twice a day; the respective time interval is ΔT=12 h. The set of measurement data contains the following wind characteristics

- components of the anemometric wind u_A, v_A,

- components of the geostrophic wind (850 hPa) u_G, v_G .

The above data have to be spatially and temporarily interpolated over the computational domain. The resulting wind field, averaged over the mixing layer, should also reflect some additional constraints. One of them, imposed due to the general model of atmospheric circulation, is the continuity condition of the following form:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 . \tag{12}$$

The field is preprocessed by the spatial interpolation of the measured input data, and time interpolation of the consecutive episodes. The approach applied in the interpolation algorithm is based on the assumption, that the movement of the atmosphere has the rotational character – it rotates around certain centers located in regions of high or low pressure. The wind components in such a field satisfy the following relation:

$$[u(x,y), v(x,y)] = k \cdot [-(y - y_0), (x - x_0)] , \tag{13}$$

where point (x_0, y_0) denotes the center of the vortex.

The trajectory is evaluated for an individual package of pollutant, emitted by a source. Denoting by (x_p, y_p) the coordinates of the current position of a pollutant package, the equations of its trajectory have the form

$$\frac{dx_p}{dt} = u(x_p, y_p, t) , \quad x_p(0) = x_0 ; \qquad \frac{dy_p}{dt} = v(x_p, y_p, t) , \quad y_p(0) = y_0 , \tag{14}$$

where (x_0, y_0) is the initial position of the package.

The solution algorithm is based on the simple difference approximation. For the time discretization step τ , one obtains

$$\begin{aligned} x_p((k+1)\tau) &= x_p(k\tau) + \tau u(x_p(k\tau), y_p(k\tau), k\tau) , \\ y_p((k+1)\tau) &= y_p(k\tau) + \tau v(x_p(k\tau), y_p(k\tau), k\tau) . \end{aligned} \tag{15}$$

Since the values of the wind velocity components u and v are measured only every 12 hours, the time interval ΔT has to be additionally discretized due to computational purposes. Therefore, two time scales are applied

- the division of the forecast horizon (e.g. one year) into N 12-hour intervals ΔT ,
- the division of each interval ΔT into m time-steps of the length τ, i.e. $\Delta T = m\tau$.

Thus, the total time period of the forecast is $T_N = m \cdot N \cdot \tau$. At the end of each time interval $(i\Delta T, (i+1)\Delta T)$ we know the wind measurements in meteorological stations. For the moment $t_{i,j} = i\Delta T + j\tau$, $(j < m)$, we must perform the interpolation of the wind vector $\vec{w} = [u, v]$ between two consecutive values: $\vec{w}(i\Delta T)$ and $\vec{w}((i+1)\Delta T)$.

Given the values of the wind vector at every time moment at the measuring stations, the wind components at any selected point of the computational domain are calculated