

# ***WORKING PAPER***

## **REGIONAL STRATEGIES FOR ATMOSPHERIC PROTECTION USING SIMULATION MODELS**

*M. Ya. Antonovsky  
V.A. Litvin*

April 1989  
WP-89-029

**REGIONAL STRATEGIES FOR  
ATMOSPHERIC PROTECTION USING  
SIMULATION MODELS**

*M. Ya. Antonovsky*  
*V. A. Litvin*

April 1989  
WP-89-029

*Working Papers* are interim reports on work of the International Institute for Applied Systems Analysis and have received only limited review. Views or opinions expressed herein do not necessarily represent those of the Institute or of its National Member Organizations.

INTERNATIONAL INSTITUTE FOR APPLIED SYSTEMS ANALYSIS  
A-2361 Laxenburg, Austria

## **FOREWORD**

The model, MARS, presented in this paper is a complex, ecological-economical model embodied as a multi-goal, automated system designed to assist the development of air quality management strategies for urban and mesoscale regions on the basis of comprehensive monitoring data.

This type of model development could provide an interesting opportunity for beneficial cooperation between our activities related to environmental monitoring and acidification.

B.R. Döös  
Leader, Environment Program

## ABSTRACT

This paper summarizes the results of research on ecological-economic modeling carried out in the Natural Environment and Climate Monitoring Laboratory (GOSKOMGIDROMET) in the period 1979-1987, embodied as a multi-goal, automated system (MARS). The system is designed to assist in developing air quality management strategies for urban and mesoscale regions.

Management decisions on controlling atmospheric pollution are made in practice at several administrative levels, i.e., that of a republic, an economic region, a territorial-production complex, a separate state and so on. Such a territorial scale corresponds to the concept of a mesoscale region. One can consider a city as an elementary territorial administrative unit.

At the present time, management goals for air quality are not simple. In addition, it is impossible to formulate a model capable of estimating realistically the state of the near-earth layer of the atmosphere.

In cities and mesoscale regions, some hundred or even thousand sources of pollutants are situated and the emissions contain various harmful components.

To decrease the pollution of the near-earth layers of atmosphere, some concrete measures (usually from 5 to 15) can be taken at each of the sources. Thus the task of identifying and analyzing the effectiveness of various atmosphere protection strategies is important. The MARS program package solves this complicated task for stationary sources.

A mesoscale region and a city are represented in MARS by a regular grid of 0.5 km to 10 km (usually 1 km for a city and 10 km for a region).

MARS is able to analyze the effectiveness of various control measures. The application of MARS requires a relatively small data bank comprising two parts:

- a) information on natural climatic features of the territory and parameters of emission sources.
- b) information on technology to reduce emission sources.

The first part of the data bank is well worked out and does not cause any difficulties. The second part of the data bank requires a design study of possible technological measures for reducing effluents at the sources. For this it is also necessary to generalize analogues for use in other cities/regions.

Proposed models, algorithms, and program packages are used in the USSR as a basis for strategies of atmosphere protection in cities and regions.

## CONTENTS

1.	<b>Statement of the Problem</b>	1
2.	<b>Structure and Potentials of the Multi-Goal Automated Regional System</b>	2
3.	<b>The Efficiency of the Atmosphere Protective Actions</b>	4
4.	<b>Meso-Scale Models of Transport and Transformation of Sulfur Dioxide in the Atmosphere</b>	8
	<b>Model 1</b>	11
	<b>Model 2</b>	16
5.	<b>Estimation of Maximum Surface Pollutant Concentrations in Cities</b>	25
6.	<b>Choosing Optimal Strategies</b>	30
7.	<b>Information Support</b>	36
8.	<b>Illustrative Examples</b>	43
9.	<b>Experience Gained From the Practical Use of MARS87</b>	58
	<b>References</b>	62

# REGIONAL STRATEGIES FOR FOR ATMOSPHERIC PROTECTION USING SIMULATION MODELS

*M. Ya. Antonovsky and V.A. Litvin\**

## 1. Statement of the Problem

A modeling method for the assessment of the efficiency of emission control strategies for industrial sources has been devised by the Natural Environment and Climate Monitoring Laboratory under the USSR State Committee for Hydrometeorology and Control of the Natural Environment and the USSR Academy of Sciences. This approach is based on the multi-purpose automated dialogue system (MARS) for personal computers using FORTRAN algorithmic language.

Within any given region (which could be chosen from amongst cities, industrial centers, territorial-production complexes, administrative regions, republics), there are, as a rule, several thousand sources each contributing to the pollution of the lower atmosphere. To control pollution, it is necessary to perform various actions which are characterized by different efficiencies:

$$W_m = E_m/R_m, m \in M_i, i \in I \quad (1.1)$$

where

$R_m$  - the cost (e.g. overall investments needed for the realization of the  $m$ -th action);

$M_i$  - the series of actions technically feasible for the  $i$ -th source;

$I$  - the set of air pollution sources in the region.

The effect of the realization of the  $m$ th-action is determined as a difference:

$$E_m = E_m^{(1)} - E_m^{(2)} \quad (1.2)$$

Component  $E_m^{(1)}$  is a basic (before the realization of  $m$ -action) share of a certain source in the lower atmosphere pollution level, and  $E_m^{(2)}$  is a share of the source after the realization of  $m$ -action, which could be defined as the atmosphere protective if  $E_m^{(1)} > E_m^{(2)}$ .

The volume of the atmosphere protective resources is limited:

$$\sum R_m \leq R, m \in M_i, i \in I \quad (1.3)$$

and for every limit  $R^*$  the corresponding optimum program can be found:

$$W = \sum W_m \rightarrow \max, R = R^*, m \in M_i, i \in I \quad (1.4)$$

The reverse setting of a problem reflecting the achievement of a desired state of the atmosphere  $W^*$  is also possible:

$$R = \sum R_m \rightarrow \min, W = W^*, m \in M_i, i \in I \quad (1.5)$$

\* Natural Environment and Climate Monitoring Laboratory GOSKOMGIDROMET and the USSR Academy of Sciences.

Thus, depending upon the setting of a problem, the regional strategy of the atmosphere protection is the realization of (1.4) or (1.5) postulates, i.e., realization of a specific series of the atmosphere protective actions providing the maximum efficiency of  $W$  or the minimum consumption of  $R$  resource.

A succession of the optimum programs with the monotonously increasing  $W$  efficiency values and the all-permissible  $R$  resource consumption determines the function of the efficiency of the atmosphere protective actions in the region. The synthesis of the function is necessary for calculating the amount of the resources used for the protection of the atmosphere as one of the geophysical media.

The optimum function of the atmosphere protective activities efficiency in a region is the final product of calculations done through MARS.

## 2. Structure and Potentials of the Multi-goal Automated Regional System

MARS permits obtaining functions of the atmosphere protective activities efficiency on five types of criteria ( $E_m^{(1)}$  and  $E_m^{(2)}$  calculation methods) including the analysis of the two kinds of expenses (investments and total\*). Each of the criteria could be interpreted depending on the goals of the analysis done. The results of calculation on the criteria chosen represent the solution of the definite practical problem in the field of the atmosphere protection from the pollution.

MARS has two modifications designated for calculations on a level of an industrial center or a city (MARS-1) and on a level of a meso-scale region (MARS-2). Those modifications differ from one another by a composition of initial data base; by model blocks of pollutant dissipation in the atmosphere; and by sets of criteria of the atmosphere protective actions efficiency.

For calculations using MARS there is no need for special knowledge in the field of mathematical modeling or computers. However, at the same time, MARS provides good possibilities for environmental managing based on assessment, monitoring, and control of an air basin pollution level.

An assessment of a pollution level includes the following:

- a) Mapping of pollutants discharge.
- b) Calculation of a structure of economic damage for each of the sources and pollutants.
- c) Mapping of economic damage.
- d) Calculation of fields of pollutant maximum concentrations under normal unfavorable conditions (MARS-1).
- e) Calculation of mean annual sulfur compounds concentrations (MARS-2).
- f) Calculation of mean annual sulfur compounds dry deposition over a region (MARS-2).
- g) Calculation of mean annual sulfur compounds wet deposition over a region (MARS-2).
- h) Calculation of mean annual values of sulfur exportation of a region of eight sectors and of total exportation (MARS-2).
- i) Calculation of indices of potential damage for coniferous forests of a region from sulfur total deposition (MARS-2).
- j) Mapping of sulfur concentrations and deposition and of indices of potential damage for coniferous forests (MARS-2).

---

\* The total expenses could be calculated using one of the known methods of commensuration of diverse economic expenditures directed at the realization of an atmosphere protective action, e.g.,  $P = C + EK$ , where  $C$  - expenses on exploitation for one industrial cycle (1-year),  $K$  - investments realized during several industrial cycles, and  $E$  - norm of the investments efficiency.

The preparation of decision-making towards the monitoring and control of the atmosphere pollution level is provided by:

- a) Analysis of efficiency of initial atmosphere protection efforts.
- b) Analysis of efficiency of all permissible series of the atmosphere protective efforts.
- c) Calculation of an efficiency optimum function.
- d) Plotting of an optimum function.
- e) Establishing of an optimum series of the atmosphere protective actions in accordance with (1.4) or (1.5).
- f) Determination of permissible waste norms for sources in accordance with the optimum series.
- g) Calculation of completing expenses for the optimum series of actions.
- h) Determination of an expedient amount of expenses for the atmosphere protective efforts in a region.
- i) Determination of the effect of a range of regional sources coniferous forests (an index of damage for coniferous forests from sulfur compounds deposition) (MARS-2).

The MARS realized on a personal computer of IBM-PC-AT class analyses the effect of 1,000 enlarged sources and of seven different pollutants on the air basin of a city or a meso-scale region, which are presented by a regular grid 50 x 50 with a step (space) from 0.5km up to 10km, correspondingly.

The MARS structure is given in Figure 2.1. (see p.5).

1. Block of organization, following the development of data bank.
2. Bank of environmental and climatic characteristics.
3. Bank of parameters of stationary atmospheric pollution sources.
4. Block for modeling structure and spatial distribution of economic damage due to the atmosphere pollution.
5. Assessment of economic damage for each of the sources and the pollutants.
6. Spatial distribution of economic damage for each of the pollutants and total.
7. Block for modeling of pollutants dissipation in the atmosphere over a city or an industrial center.
8. Pollutant concentration fields over a city or an industrial center.
9. Block for modeling of sulfur compounds concentrations, dry and wet deposition for a mesoscale region, and of sulfur exportation.
10. SO<sub>2</sub> concentration field.
11. SO<sub>4</sub><sup>2-</sup> concentration field.
12. SO<sub>2</sub> dry deposition field.
13. SO<sub>4</sub><sup>2-</sup> dry deposition field.
14. SO<sub>2</sub> wet deposition field.
15. SO<sub>4</sub><sup>2-</sup> wet deposition field.
16. Sulfur compounds total deposition field.
17. Assessment of sulfur exportation out of a region on eight sectors and of total exportation.
18. Block for modeling index of coniferous forests potential damage in a region due to sulfur compounds total deposition.
19. Spatial distribution of the index of coniferous forests potential damage.
20. Block for modeling parameters of initial atmosphere protective actions.
21. Bank of initial atmosphere protective actions.



22. Block of expenses mode selection.
23. Block of selection criterion of the atmosphere protective efforts efficiency.
24. Block of organization of the bank of actions efficient enough for selected mode of expenses and criterion.
25. Bank of actions efficient for selected mode of expenses and criterion.
26. Block for modeling of permissible technological chains for decreasing wastes from sources and for analysis of their efficiency for selected mode of expenses and criterion.
27. Efficient series of actions for each of the sources (initial information for an optimization model).
28. Block for modeling the optimum strategies of the atmosphere protective efforts.
29. Information on parameters of the optimum strategy.
30. Block of selection (the specific optimum strategy).
31. Block of organization (the series of the atmosphere protective actions corresponding to the optimum strategy selected).
32. The optimum strategy for achieving a predetermined norm of the air basin state.
33. The optimum strategy for expenses distribution on the atmosphere protective actions with a predetermined limit of resource.
34. Block of listing register.

### 3. The Efficiency of the Atmosphere Protective Actions

Apparently, at present, there is no "ideal" index for  $E_m$  effect determination and therefore there is no "ideal" efficiency of  $m$ -action for the atmosphere protection. That is why, depending on an aim of the atmosphere protective strategy, the calculated assessments of effect used in MARS could be divided into five types.

The first type is based on the calculation of the emitted mass of one or several pollutants. Comparison of pollutants included in the effect index could be done by the coefficients of toxicity (reverse value to the maximum allowable concentration). In that case, the efficiency of an action is the reduction of emitted mass per unit of expenses. This index is simple and convenient and there now exists a developed data base for its usage. However, the effect of pollution sources is determined not only by the amount of pollutants entering the lower atmosphere, but also by the peculiarities of pollutant dissipation in the atmosphere and, therefore, by the structure of recipients suffering from adverse waste.

Such moments could be considered while using the index of the second type, namely, of the economic damage from pollution of the lower layer of the atmosphere (*Approximate economic damage estimations ...*, 1986):

$$Y = \gamma \times \sigma \times f \times M \quad (3.1)$$

where

- Y – the economic damage (roubles/year);
- $\gamma$  – the average specific economic damage (roubles/comparison ton) for the USSR is  $\gamma = 2.4$ ;
- $\sigma$  – the dimensionless value characterizing the structure of recipients located in the zone of a source active pollution ( $0.05 \leq \sigma \leq 30$ );
- f – the dimensionless correction for the mode of a pollutant dissipation in the atmosphere to be dependent on an active height of a source, mean annual wind velocity, and rate of admixture disposition ( $1 \leq f \leq 10$ ).

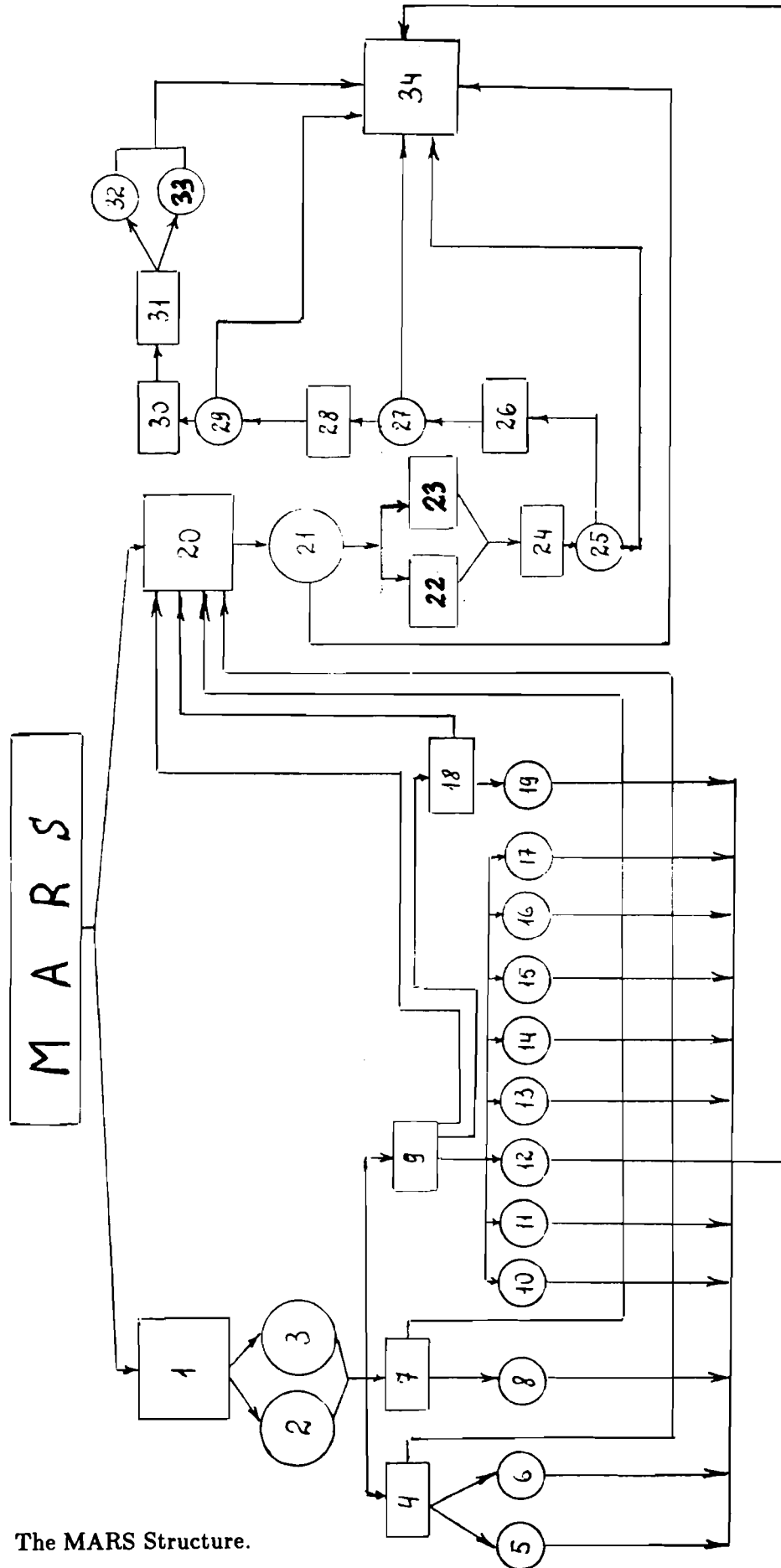


Figure 2.1: The MARS Structure.

For the organized sources (stacks of height  $h < 10\text{m}$ ) the zone of an active pollution is presented by a circle with a center in a point of a source location and with a radius of  $50h$ , but for  $h \geq 10\text{m}$  the zone is a ring formed by radiuses  $R_{inner} = 2\varphi h$ ,  $R_{outer} = 20\varphi h$ , where  $\varphi$  - dimensionless correction for a plume raising

$$\varphi = 1 + \frac{\Delta T}{75} \quad (3.2)$$

where

$\Delta T$  - the drop of temperature (in degrees centigrade) between the mouth of a source and an ambient atmosphere (mean annual temperature): denominator 75 is the temperature in degrees centigrade also.

The given mass of pollutant emission from a source (comparison ton/year):

$$M = \sum_{j=1}^N A_j \times m_j \quad (3.3)$$

where

$m_j$  - the mass of an annual emission of  $j$ -pollutant (ton/year).

Coefficient of relative aggressivity of a pollutant:

$$A_j = a_j \alpha_j \delta_j \lambda_j \beta_j$$

where

$a_j$  - an index of the relative danger of a pollutant presence inhaled by a human being, air;

$\alpha_j$  - the correction for the probability of a pollutant accumulation in environmental compartments, in food chains, and of a pollutant intake into human organism through any means other than inhalation;

$\delta_j$  - the correction for a pollutant effect on various recipients other than humans;

$\lambda_j$  - the correction for the probable secondary discharge of a pollutant into the atmosphere,

$\beta_j$  - the correction for the probable formation of secondary pollutants which are more dangerous than initial pollutants.

$A_j$  values for the most frequently occurring pollutants lie within the limits of 1 to  $12 \times 10^5$ .

While using the index of the second type, the efficiency appears to prevent economic damage per unit of expenses.

The method of economic damage calculation suggested is addressed to particular sources and based on emission accounting and therefore keeps the advantages of the indices of the first type. However the effect on recipients is considered in the nearest vicinity of a source (the zone of the active pollution).

The research results show that pollutants could be transported over long distances, and transformed and deposited on the underlying surface, thus affecting various recipients far beyond the limits of the active pollution zone. Calculation of the atmosphere deposition (indices of the third type) is of special importance when the size of a region is several hundred kilometers. In this case, a decrease in the total deposition per unit of expenses is the criterion of the efficiency.

The fourth type of indice is sulfur exportation out of a region limit (total or for directions). This type of indice is of particular interest for the analysis of the effect of a region under research on bordering regions. It can be also used for producing decisions for implementing the convention on transboundary transport of sulfur compounds and for linking the results obtained through MARS-2 to the models of transboundary transport.

The special meso-scale models of transportation, transformation and deposition of atmospheric pollutants (Section 4) are used for calculating the indices of the third and fourth types.

The fifth type of indice is based on the comparison of the maximum near-the-earth pollutant concentrations, calculated for so-called normal unfavorable meteorological conditions\* to their maximum allowable values; this is most important for urban territories where the major recipient is the population. If there are other recipients sensitive to the pollution of the territory of a city, it is necessary to compare the concentrations to the maximum allowable values for those recipients (secondary norms), but we must bear in mind that such a base of standards is not sufficiently developed nowadays.

The model of an admixture dissipation in the atmosphere (Beryland, 1985) was modified for the purpose of calculating the maximum pollutant concentrations in the near-the-earth layer over urban territories under normal unfavorable conditions. The peculiarity of the modification is a considerable reduction of time needed for calculation; this is most important when using that block in optimization blocks of MARS-1 complex (Section 5). When using indices of the fifth type, the efficiency of actions is evaluated by the decrease of the index of pollutant concentrations per unit of expenses. The corresponding index is decreased per unit of expenses. The corresponding index is determined for those elements of the regular grid where exceeding the calculated concentrations over the maximum allowable ones exists:

$$q_i = \sum_i \sum_k c_j^{(i,k)} / p_j, \text{ for } \forall c_j^{(i,k)} > p_j \quad (3.4)$$

where

- $q_j$  - the index of calculated maximum concentrations of  $j$ -pollutant (the sum of exceeding the maximum occasional of the maximum allowable concentrations in a city);
- $c_j^{(i,k)}$  - the maximum calculated concentration of  $j$ -pollutant in  $(i,k)$  raster element of a regular grid presenting a city;
- $p_j$  - the maximum occasional of the maximum allowable concentration of  $j$ -pollutant in the atmosphere over a settlement.

The state of an air basin over a city could be considered satisfactory when:

$$q_j \leq 1 \quad \text{for } \forall j \quad (3.5)$$

The general index of an air basin pollution for several pollutants over a city\*:

$$Q = \sum_j q_j \quad (3.6)$$

At the same time for reaching the satisfactory state of an air basin of a city for several pollutants simultaneously, a more strict condition in comparison to (3.5) should be carried out:

$$Q \leq 1 \quad (3.7)$$

There is a possibility in MARS to produce additional efficiency criteria like (1.1) under different methods of  $E_m$  calculation, if any of the five indices listed above are used. The simplest "dose-effect" model permitting calculation of the index of potential damage

\* The normal unfavorable meteorological conditions presuppose the non-stable stratification of the atmosphere and occur rather frequently during a year. Beryland, (1985) permits the conclusion that a decrease in pollutant maximum concentrations in cities under normal unfavorable conditions to the level of the maximum occasional of the maximum allowable concentrations would provide, as well, values not exceeding the mean daily maximum allowance concentrations. The reverse premise is not considered. That is why the criterion of minimization of "the maximum pollutant concentrations" indices is realized in MARS-1.

\* For a group of pollutants having the property of summarizing their effect.

for coniferous forests of a region from sulfur compounds deposition could serve as an example of such an additional criteria, which illustrates the expediency of the use of MARS in order to protect the atmosphere from pollution.

The method considering the direct effect of sulfur compounds deposition on coniferous forests, devised in the GDR Center for Environmental Formation, is used for the calculation of that index:

$$d = \sum_i \sum_k d_{ik}, \quad (3.8)$$

for

$$d_{ik} = 10 - 10/\exp(v^2/36), \quad (3.9)$$

where

$v$  - the mean annual atmospheric deposition of sulfur compounds on the territory (i,k), a raster element of a regular grid presenting a region (in  $\text{g}/\text{m}^2$ ).

$0 \leq d_{ik} \leq 10$  is an assessment of sulfur atmospheric deposition on coniferous forests in a raster element (i,k).

There is a possibility in MARS-2 of setting the threshold sensitivity of coniferous to sulfur compounds atmospheric deposition. If that threshold value ( $p$ ) is known, then index (3.8) transforms to:

$$d = \sum_i \sum_k d_{ik}, \text{ for } d_{ik} > p \quad (3.10)$$

#### 4. Meso-Scale Models of Transport and Transformation of Sulfur Dioxide in the Atmosphere

Two types of meso-scale models that allow one to compute concentration, dry and wet deposition of atmospheric  $\text{SO}_2$  and  $\text{SO}_4^{2-}$ , as well as sulfur transport out of the region, have been developed, algorithmically presented and tested within MARS to implement the subsystems "Region". The models enable the criteria for minimizing the total deposition and removal of sulfur compounds to develop, as well as to enter, the automated complex of blocks presenting the atmospheric pollutant effects on the regional ecosystems which are constructed according to the "dose-effect" principle.

The models of transport and transformation of sulfur compounds in the atmosphere developed for MARS meet the following requirements:

- The spatial scale of pollutant transport in the atmosphere amounts to several hundred kilometers and corresponds to the size of a territorial administrative unit (meso-scale level);
- The time resolution equals a year (as a rule, the technical and economic parameters of air protection measures which form the basis of the optimization analysis refer to this very period);
- The models have been realized as climatic ones, i.e., pollutant transport is computed for meteorological conditions averaged over a long period (10 years and more) rather than within the fields of real (current) wind and precipitation; this is related to the fact that the efficiency of air protection measures is estimated in prospect;
- The period of calculation using a personal computer is relatively short, since the optimization is carried out in the iterative regime.
- Pollution levels are computed for each of the regional emission sources where air protection measures are carried out.

It should be noted that models which meet all the above requirements are unavailable at present. It is this fact that has stimulated the development of meso-scale transport models based on two approaches:

- Temporal variations of concentrations were calculated within the coordinate system related to the moving mass of the pollutant (Model 1 – Lagrangian approach);
- Pollutant concentration variations are calculated within a spatially fixed coordinate system (Model 2 – Eulerian approach).

The necessity to develop two different types of meso-scale transport models is also caused by the limited possibility of adapting each of them separately using the observational data on atmospheric pollution.

As compared to Model 2, Model 1 requires considerably less time for computer processing, which makes it especially efficient in the block of ecological and economic optimization. In addition, Model 1 allows the calculation of sulfur removal outside the region by sectors. However, the model is highly parameterized (assumptions have been made on the instant and uniform vertical distribution of pollutant concentrations in the mixing layer, uniform horizontal pollutant distribution in a portion, linearity of dry deposition). Comparing the calculations made using both models with observations below the pollution level would allow, on the one hand, to estimate the errors resulting from simplifications adopted in Model 1 and, on the other hand, to adapt each model to the specific regional conditions.

Models 1 and 2 have a number of common peculiarities.

The region is presented as a regular grid whose square rasters usually have dimensions of  $10 \times 10$  km.

A climatic wind rise is introduced for the considered region which presents probabilities of various wind directions and a mean velocity of pollutant transport in the atmosphere.

Transport velocity, recurrence of various wind directions, and the horizontal and vertical coefficients of turbulent exchange are computed as mean ones in the mixing layer. It is assumed that the wind velocity varies exponentially with height; the vertical exchange coefficient linearly increases with height in the mixing layer, remaining constant above it; and the horizontal exchange coefficient varies with height like the wind velocity.

The wind and precipitation field in the region is homogeneous.

Constants of dry and wet sulfur deposition from the atmosphere, chemical transformation of sulfur dioxide into sulfate, turbulent exchange coefficients, the height of the mixing layer, the height of the surface layer, are introduced as mean annual values (averaging period being equal to 10 years) and are constant over the region territory.

Wet deposition of sulfur compounds, chemical transformation of sulfur dioxide into sulfate are described as linear processes.

No consideration is taken of the region relief.

Sulfur dioxide emission shows no variations throughout the year.

Table 4.1. presents designations and dimensions of variables used in model descriptions.

Table 4.1. The use of models 1 and 2 and their dimensions.

Mark of a variable	Variable	Dimensions	
		Model 1	Model 1
1	2	3	4
$\bar{V}$	Mean velocity of pollutant transport in the mixing layer of the atmosphere of a region	km/T	m/sec
$V_0$	Wind velocity near the ground at $Z_0$ height in a region	km/T	m/sec
$\bar{\beta}_m$	Mean wind reiteration of m-direction	dimension-	dimension-

	in the mixing layer in a region	less	less
$\bar{v}_{xm}, \bar{v}_{ym}$	Composite velocities of pollutant transport in the atmosphere in m-direction along OX and OY axes, correspondingly	km/T	-
$\bar{K}_z, \bar{K}_y$	Mean vertical and horizontal coefficients of turbulent exchange in the mixing layer in a region	km <sup>2</sup> /T	m <sup>2</sup> /sec
$K_0$	Vertical coefficient of turbulent exchange near the ground in a region	km <sup>2</sup> /T	m <sup>2</sup> /sec
$T_0$	Air temperature near the ground	-	C°
$P$	Atmosphere stratification parameter in a region (exponent in the exponent law of wind distribution with height)	dimensionless	dimensionless
$H$	Height of the mixing layer in a region	m	m
$h_s$	Height of the surface layer of the atmosphere in a region	m	m
$U$	Precipitation amount in a region	mm/yr	mm/yr
$k_1, k_2$	Coefficient of SO <sub>2</sub> and SO <sub>4</sub> <sup>2-</sup> washout from the atmosphere	1/mm	1/mm
$\tau_{1m}, \tau_{2m}$	SO <sub>2</sub> and SO <sub>4</sub> <sup>2-</sup> residence time relative to wet deposition from the atmosphere, correspondingly	1/mm	1/mm
$\tau_{1d}, \tau_{2d}$	The same, but relative to dry atmosphere	T	-
$\tau_0$	SO <sub>2</sub> residence time in the atmosphere relative to chemical transformation into SO <sub>4</sub> <sup>2-</sup>	T	sec
$L$	Size of a grid raster	km	
$V_1, V_2$	SO <sub>2</sub> and SO <sub>4</sub> <sup>2-</sup> dry deposition rates, correspondingly	km/T	m/sec
$T$	Time interval	min	-
$K$	Interval number after which the tracing of a portion is finished	dimensionless	dimensionless
$\epsilon$	Sulfur mass in a portion, which could not be traced any longer due to a little one	kgS/km <sup>2</sup>	-
$x_{km}, y_{km}$	Coordinates of the center of a portion in k-interval in m-direction	km	-
$X_{km}, Y_{km}$	Size (diameter) of a portion for OX and OY axes in k-interval in m-direction	km	-
$D_{1k}, D_{2k}$	SO <sub>2</sub> and SO <sub>4</sub> <sup>2-</sup> dry deposition from a portion in k-interval	kgS/T	-
$W_{1k}, W_{2k}$	The same, but wet deposition	kgS/T	-
$\Delta M_k$	Chemical transformation of SO <sub>2</sub> into SO <sub>4</sub> <sup>2-</sup> in a portion in k-interval	kgS	-

$M_{1k}, M_{2k}, M_k$	SO <sub>2</sub> , SO <sub>4</sub> <sup>2-</sup> , and SO <sub>2</sub> + SO <sub>4</sub> <sup>2-</sup> mass, correspondingly, remaining in a portion after k-interval	kgS	-
$l=I, \bar{L}_{km}$	Raster numbers in a region "striked" by a portion in k-interval in m-direction	dimensionless	
$D_{1km}^l, D_{2km}^l$ $W_{1km}^l, W_{2km}^l$	SO <sub>2</sub> and SO <sub>4</sub> <sup>2-</sup> dry and wet deposition from a portion over 1-raster "striked" in k-interval in m-direction	kgS/Tkm <sup>2</sup>	-
$D_{1m}^l, D_{2m}^l$ $W_{1m}^l, W_{2m}^l$	SO <sub>2</sub> and SO <sub>4</sub> <sup>2-</sup> dry and wet deposition from a portion over 1-raster in m-direction	kgS/Tkm <sup>2</sup>	-
$D_1^l, D_2^l$ $W_1^l, W_2^l$	SO <sub>2</sub> and SO <sub>4</sub> <sup>2-</sup> mean annual dry and wet deposition over 1-raster of a region	kgS/km <sup>2</sup> yr	-
$C_1^l, C_2^l$	SO <sub>2</sub> and SO <sub>4</sub> <sup>2-</sup> mean annual near the ground concentrations over 1-raster of a region	mcgs/m <sup>3</sup>	-
$\tau$	Duration of a year in T intervals	T/yr	-
$H_e$	Effective height of an emission source	-	m
$H_2$	Source stack geometric height	-	m
$v_b$	Volume of a source emission	-	m <sup>3</sup> c
$D_b$	Diameter of a source (stack) emission	-	m
$T_b$	Temperature of a source emission	-	degrees
$M$	Intensity of SO <sub>2</sub> emission	thou tn SO <sub>2</sub> /yr	thou/tn SO <sub>2</sub> /yr
$C_1(x,y,z),$ $C_2(x,y,z)$	SO <sub>2</sub> and SO <sub>4</sub> <sup>2-</sup> concentration in (x,y,z) (OX axis along the wind)	-	m <sup>3</sup>
$D_1(x,y),$ $D_2(x,y)$ $W_1(x,y),$ $W_2(x,y)$	SO <sub>2</sub> and SO <sub>4</sub> <sup>2-</sup> dry and wet deposition in $t(x,y)$ (OX axis along the wind)	-	thou tn S/km <sup>2</sup> yr
$\alpha_0(x)$	Opening (angle) of a flow, inside of which wind directions effect significantly the pollution in (x,o,o) (OX axis along the wind)	-	degrees
$\Theta(x)$	Mean wind recurrence inside $\alpha_0(x)$ sector in the mixing layer	-	dimensionless

Let us consider each type of meso-scale model in more detail.

### Model 1.

The assessment of mean (for the period of a year and more) atmospheric pollution using trajectory models is usually carried out by successive computations of concentrations and deposition along the observed trajectories and subsequent averaging of the obtained results. Since a 10-year period includes tens of thousands of air trajectories, and the model is to be used in an iterative regime, such an approach to the pollution assessment is unacceptable. Therefore, real trajectories are substituted by a number of straight



ones, each being realized with a certain probability  $\bar{\beta}_m$ . The possibility to consider straight trajectories is related to the meso-scale of pollutant transport in the atmosphere.

The model assumes a one-layer wind. In the mixing layer (at height  $H$ ) pollutants are mixed instantly.

Sulfur emission is presented as a sequence of portions ejected from the source in discrete time intervals  $t=k \cdot T$ ,  $k=0, 1, \dots, K$ , where  $T$  (min) is a time step and  $K$  is the number of the step after which the observation of the portion has ended. The time step is selected so that, first, the distance passed by a portion during the step  $T$  was less than the dimensions of the raster, and second, pollutant portions were superimposed on each other forming a continuous stream.

The sequence of portions emitted by the source forms a stream. The location (coordinates of the center) of the portion and its characteristics (dimensions, dry and wet deposition, chemical transportations) are measured using the model for discrete time period. Successive locations of the portion center in discrete time periods present the trajectory of the portion movement. The stream is stationary during the regional-scale transport. It follows from the condition of stationarity that to calculate the fields of sulfur compound deposition and content, it is sufficient to trace the locations and characteristics of a single portion in the stream. The model considers  $m = \bar{1}, 24$  stationary locations of the stream corresponding to 24 wind directions.

The spatial resolution of the model is presented by the dimensions of the raster. Surface concentrations and deposition (averaged over the raster) are calculated in each raster at each  $m$ -th direction of the stream. Then the results are averaged in all directions to obtain annual assessments.

Dry deposition of  $\text{SO}_2$  and  $\text{SO}_4^{2-}$  is also described as a linear process.

At the initial moment, the portion is uniformly distributed over the raster, its centers coinciding.

The following parameters are calculated at each  $k$ -th step at the  $m$ -th wind direction (stream location).

Coordinates of the portion center:

$$\begin{aligned} x_{km} &= x_{k-1,m} + \bar{v}_{xm}, \\ y_{km} &= y_{k-1,m} + \bar{v}_{ym}, \end{aligned} \quad (4.1)$$

Horizontal widening of the stream is taken into account only if it is directed across the portion movement; horizontal diffusion at each step is shown in Figure 4.1.

$$\begin{aligned} x_{km} &= x_{k-1,m} + 0.2|v_{ym}|, \\ y_{km} &= y_{k-1,m} + 0.2|v_{xm}|. \end{aligned} \quad (4.2)$$

Dry and wet deposition of  $\text{SO}_2$  and  $\text{SO}_4^{2-}$  form the portion. It is assumed that the portion contributes to the deposition at a given raster in cases where its center lies within the portion, i.e., is "covered" by it.

Dry deposition of  $\text{SO}_2$  and  $\text{SO}_4^{2-}$ :

$$D_{1k} = M_{1,k-1} \cdot \frac{1}{r_{1d}}, \quad (4.3)$$

$$D_{2k} = M_{2,k-1} \cdot \frac{1}{r_{2d}}, \quad (4.4)$$

$$D_{1km} = \frac{D_{1k}}{L_{km} \cdot L^2}. \quad (4.5)$$

$$D_{2km} = \frac{D_{2k}}{L_{km} \cdot L^2}. \quad (4.6)$$

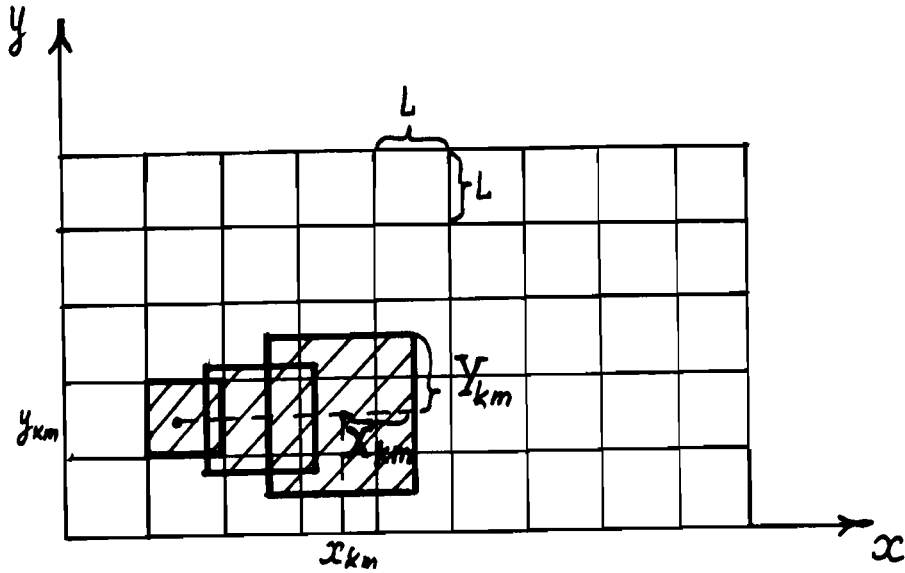


Figure 4.1: The portion movement.

Wet deposition of  $\text{SO}_2$  into  $\text{SO}_4^{2-}$

$$W_{1k} = M_{1,k-1} \cdot \frac{1}{\tau_{1w}}, \quad (4.7)$$

$$W_{2k} = M_{2,k-1} \cdot \frac{1}{\tau_{2w}}, \quad (4.8)$$

$$W_{1km}^l = \frac{W_{1k}}{L_{km} \cdot L^2}, \quad (4.9)$$

$$W_{2km}^l = \frac{W_{2k}}{L_{km} \cdot L^2}. \quad (4.10)$$

Chemical transformation of  $\text{SO}_2$  into  $\text{SO}_4^{2-}$ :

$$\Delta M_k = M_{1,k-1} \cdot \frac{1}{\tau_0} \quad (4.11)$$

Masses of  $\text{SO}_2$ ,  $\text{SO}_4^{2-}$  remaining in the portion:

$$M_{1k} = M_{1,k-1} - \Delta M_k - D_{1k} - W_{1k}, \quad (4.12)$$

$$M_{2k} = M_{2,k-1} - \Delta M_k - D_{2k} - W_{2k}, \quad (4.13)$$

$$M_k = M_{1k} + M_{2k}. \quad (4.14)$$

$\text{SO}_2$  and  $\text{SO}_4^{2-}$  lifetimes in the atmosphere in relation to wet deposition are calculated in the model as:

$$\begin{aligned} \tau_{1w} &= \frac{\tau}{k_1 V}, \\ \tau_{2w} &= \frac{\tau}{k_2 V}, \end{aligned} \quad (4.15)$$

where

$\tau$  – is the duration of the year in the units  $T$  ( $T/\text{year}$ ).

The description of dry deposition as a linear process is adopted according to Izrael (1983), where the analytical solution of the turbulent diffusion equation has resulted in the derivation of the so-called “dry-deposition function” which shows a fraction of pollutant remaining in the atmosphere since the moment of its generation in the absence of other removal processes. The function is shown to be approximated by an exponential relationship. The lifetimes in relation to dry deposition are calculated as:

$$\begin{aligned} \tau_{1d} &= \frac{2\bar{K}_z}{\pi(V_1)^2}, \\ \tau_{2d} &= \frac{2\bar{K}_z}{\pi(V_2)^2}. \end{aligned} \quad (4.16)$$

Testing the conditions for further observation of the portion, the observation ends in cases where:

- The portion has left the region (coordinates of its center do not belong to the region):
- Sulfur content in the portion is below a certain value:

$$\frac{M_k}{L_{km} \cdot L^2} < \epsilon.$$

Since the stream is stationary, the values  $D_{1km}^l$ ,  $D_{2km}^l$ ,  $W_{1km}^l$  and  $W_{2km}^l$  are interpreted as the deposition in the  $l$ -th raster at any moment from the portion of  $k$ -th age at the  $m$ -th location of the stream.

Then the deposition of  $\text{SO}_2$  and  $\text{SO}_4^{2-}$  in the  $l$ -th raster from the portion of all ages at the  $m$ -th location of the stream:

$$D_{1m}^l = \sum_{k=1}^K D_{1km}^l. \quad (4.17)$$

The summation for  $D_{2m}^l$ ,  $W_{2m}^l$ ,  $W_{1m}^l$  is carried out in a similar way.

Mean annual dry and wet deposition of  $\text{SO}_2$  and  $\text{SO}_4^{2-}$  and their concentrations at the  $l$ -th raster of the region:

$$D_1^l = \tau \cdot \sum_{m=1}^{24} D_{1m}^l \cdot \bar{\beta}_m, \quad (4.18)$$

Similarly for  $D_{2m}^l$ ,  $W_1^l$ ,  $W_2^l$ .

Mean annual surface concentrations of  $\text{SO}_2$  and  $\text{SO}_4^{2-}$  :

$$\begin{aligned} C_1^l &= \frac{D_1^l}{V_1 \cdot \tau}, \\ C_2^l &= \frac{D_2^l}{V_2 \cdot \tau}. \end{aligned} \quad (4.19)$$

#### *The assessment of meteorological elements and model parameters.*

While assessing numerical values of  $\bar{V}$ ,  $P$ ,  $H$ ,  $\bar{\beta}_m$ ,  $U$ ,  $\bar{K}_z$ ,  $\bar{K}_y$ , in a specific region, aerological data from the stations located in its territory are used, and data from adjacent regional stations are applied while assessing the boundary values of the variation range of these values used to estimate the sensitivity of the model. Table 4.3 (see p. 8) presents an

example of meteorological element and model parameter calculation performed at one of the north-western regions of the European USSR.

*Transport velocity.*

Wind velocity varies with height  $z$  by an exponential law (*Air Pollution*, 1982):

$$V = V_0 \left( \frac{z}{z_0} \right)^P \quad (4.20)$$

Then mean transport velocity in the mixing layer (at a height  $H$ ) is equal to:

$$\bar{V} = \frac{1}{H} \int_0^H V_0 \left( \frac{z}{z_0} \right)^P dz = \frac{V_0}{P+1} \cdot \left( \frac{H}{z_0} \right)^P, \quad (4.21)$$

and OX and OY axis components of the transport velocity are equal to:

$$\begin{aligned} \bar{v}_{xm} &= \bar{V} \cos \alpha_m, \\ \bar{v}_{ym} &= \bar{V} \sin \alpha_m, \end{aligned} \quad (4.22)$$

respectively, where  $\alpha_m$  is the angle between the OX axis and the  $m$ -th wind direction in the coordinate system selected for the region.

*Atmospheric stratification parameter.*

Mean annual values of the stratification parameter are calculated using aerological data on mean monthly wind velocities (for 10 years) obtained at various heights of the mixing layer (see Table 4.2).

*Mixing layer height.*

The mixing layer height is presented in the model as a height where the vertical temperature gradient becomes less than the dry adiabatic one. Mean annual values of  $H$  can be found, e.g., in *Climatic characteristics ...* (1983). Relatively low values of  $H$  are related to the experimental region being situated in the coastal zone.

*Recurrence of various wind directions.*

Recurrence of various wind direction  $\beta_m$  varies with height. Mean recurrence of wind directions in the mixing layer,  $\bar{\beta}_m$ ,  $m=1,12$  was obtained using radio sounding data from a regional station (*New airclimatic reference book ...* 1987) with due regard to the number of wind observations at each level (see Table 4.2). The 12-bearing wind rise was transformed into a 24-bearing one (used in the model) on the assumption that any wind direction within each of the twelve 30-degree sectors can occur with equal probability.

*Precipitation.*

The value  $U$  is taken in the model as the mean annual precipitation (over a period of 75 years) with due corrections to regional station rain gauge measurements. The minimum and maximum mean annual precipitation levels over the region are taken as threshold values.

Table 4.3: Mean annual meteorological parameters used in models 1 and 2.

Station	Atmosphere Stratification parameter	Wind velocity near ground	Height of mixing layer	Height of surface layer	Vertical coefficient of turbulent exchange near ground	Mean vertical coefficient of turbulent exchange in mixing layer	Mean horizontal coefficient of turbulent exchange in mixing layer
	$P$	$V_0$	$H$	$h_s$	$K_0$	$\bar{K}_z$	$\bar{K}_y$
	dimension-less	m/sec	m	m	m <sup>2</sup> /sec	m <sup>2</sup> /sec	m <sup>2</sup> /sec
Regional	0.09	5.1	680	60	0.12	6.9	8.2
In the territory of a neighboring region	0.17	3.2	800	35	0.07	2.4	3.6
In the territory of a neighboring region	0.16	3.5	730	35	0.07	2.4	3.4
Remark	calculation using data from **	data from **	data from *	calculation using formula (4.26)	data from *	calculation using formula (4.25)	calculation using formulae (4.72), (4.73)

\* *Climatic characteristics ...* (1983)

\*\* *New airclimatic ...* (1987)

*Parameters of dry and wet deposition and chemical transformation.*

The values  $\tau_0$ ,  $V_1$ ,  $V_2$  are obtained from generalized literature data.  $\text{SO}_2$  and  $\text{SO}_4^{2-}$  residence times relative to wet deposition can be calculated by the following formula:

$$\tau_w = I^n \Phi \Lambda, \quad (4.23)$$

where  $I^n$  is the precipitation intensity (mm/h), and  $0.7 \leq n \leq 1$ ;  $\Phi$  is the precipitation duration over a year, fractions of a unity;  $\Lambda$  is the Langmuir coefficient dependent on precipitation type, season, etc.

Assuming that in (4.23):  $n = 1.0$ ;  $\Phi = 0.1$ ;  $\Lambda = 3 \cdot 10^{-4} \cdot (10^{-4} \text{ divide } 10^{-3}) \text{ s}^{-1}$  for  $\text{SO}_2$  and  $10^{-3} \cdot (10^{-4} \text{ divide } 3 \cdot 10^{-3}) \text{ s}^{-1}$  for  $\text{SO}_4^{2-}$ , washout coefficients  $k_1$ ,  $k_2$  included in calculation formulae (4.15) were obtained.  $\Phi$  was calculated based on *New airclimatic reference book ... (1987)*.  $\Lambda$  was obtained from generalized literature data.

$\tau_{1d}$ ,  $\tau_{2d}$  were estimated by formula (4.16) taking into account  $V_1$ ,  $V_2$  selected in the model and  $\bar{K}_z$  (mean vertical coefficient of turbulent exchange in the mixing layer) calculated by (4.25), (4.26).  $\bar{K}_z$  was evaluated in the following way. As established by Beryland (1985), the law of  $K_z$  variation with height ( $z$ ) is often described as:

$$K_z(z) = \begin{cases} K_0 \frac{z}{z_0} & z \leq h_s \\ K_0 \frac{h_s}{z_0}, & z > h_s \end{cases} \quad (4.24)$$

where  $K_0$  is the vertical turbulent exchange coefficient near the surface at height  $z_0$ ;  $h_s$  is the height of the atmospheric surface layer.

Then

$$\bar{K}_z = \frac{1}{H} \int_0^H K_z(z) dz = \frac{K_0 h_s}{H z_0} \left( H - \frac{h_s}{2} \right). \quad (4.25)$$

The height of the atmospheric surface layer  $h_s$  can be assessed as (*New airclimatic reference book ... 1987*):

$$h_s = 0.025 \frac{K_0}{z_0 \omega_0}, \quad (4.26)$$

where  $\omega_0$  is the vertical component of the Earth's angular rotation velocity. Table 4.3 presents  $h_s$  and  $\bar{K}_z$  calculated by formulae (4.25) and (4.26) for the aerologic stations of the experimental region.  $K_0$  for the same stations are taken from *Climatic characteristics ... (1983)*.

*Model input data.*

Model 1 for the experimental region includes the following input data required to calculate annual deposition and concentrations of sulfur compounds:

- L - raster size: 10km;
- T - time interval: 10 min.
- x,y - {emission source coordinates, km};
- M -  $\text{SO}_2$  emission from the sources, thousand t  $\text{SO}_2/\text{yr}$ .
- $V_0$  - mean annual wind speed near the surface in the region: 5.1 m/s;
- U - mean annual precipitation in the region; 687 (596-806) mm/yr.

Table 4.2 Mean annual average wind recurrence of various directions in the mixing layer  $\bar{\beta}_m, m = 1, \dots, 12$

m	1	2	3	4	5	6	7	8	9	10	11	12
$\beta_m, \%$	9.0	12.1	13.8	12.2	9.6	7.6	5.9	5.3	6.5	5.3	5.2	7.4

Note: Calculations based on *New airclimatic reference book ...* (1987) data,  $m=1$  – is the south wind, further in 30° clockwise.

$\bar{\beta}_m$  – mean annual, average for the mixing layer recurrence of various wind directions in the region, dimensionless;  $\bar{\beta}_m$  is defined in Table 4.2;

$\tau_{1d}$  – SO<sub>2</sub> residence time relative to dry deposition: 13 (3-25), h;

$\tau_{2d}$  – same for SO<sub>4</sub><sup>2-</sup>: 200(50-800), h;

$\tau_0$  – SO<sub>2</sub> residence time relative to its transformation to SO<sub>4</sub><sup>2-</sup>: 40(30-120), h;

$k_1$  – SO<sub>2</sub> washout coefficient with due regards for precipitation duration over a year: 0.11 (0.036-0.36), 1/mm;

$k_2$  – same for SO<sub>4</sub><sup>2-</sup>: 0.36(0.11-1.08), 1/mm;

$V_1$  – SO<sub>2</sub> dry deposition rate: (0.002(0.001-0.003), m/s;

$V_2$  – same for SO<sub>4</sub><sup>2-</sup>: 0.002(0.001-0.003), m/s;

$\epsilon$  – sulfur mass in an air parcel which cannot be traced further due to its small size: 0.0005 kg S/km<sup>2</sup>;

$P$  – mean annual parameter of the atmosphere stratification: 0.09(0.07-0.17), dimensionless;

$H$  – mean annual mixing layer height for the region: 680(680-940), m.

## Model 2.

The Eulerian approach is based on the analytical or numerical integration of the atmosphere diffusion equation. The application of numerical methods (*Air pollution ...* 1982; Van Egmont and Kessenboom, 1983; Renner et al, 1985) to evaluate the pollution level from each emission source (the number of sources in a region can be as large as a few hundred) would drastically increase the computer time, making the models of this type inapplicable as regards the assessment of the effectiveness of many atmosphere protection activities carried out in the region.

The model proposed hereafter is the realization of the analytical solution of the combined equations of the atmosphere diffusion describing the transport and transformation of SO<sub>2</sub> and chemical transformation products, SO<sub>4</sub><sup>2-</sup>, in the atmosphere.

### *Model peculiarities.*

The vertical component of the wind speed is zero.

Pollutant diffusion is taken into account both in the horizontal and vertical direction. Diffusion along the transport direction is negligible as compared to the advection transport.

The gravitational speed of aerosol deposition in the atmosphere is zero.

The calculated fields of sulfur compound concentrations and deposition are given for the centers of the rasters.

Pollutant transport is stationary in any given direction within the region.

In such conditions with the axis OX directed along the wind and axis OZ along the vertical, the atmosphere diffusion equation for SO<sub>2</sub> is as follows:

$$\bar{V} \frac{\partial C_1}{\partial x} = \bar{K}_y \frac{\partial^2 C_1}{\partial y^2} + \bar{K}_z \frac{\partial^2 C_1}{\partial z^2} - \frac{C_1}{\tau_1} \quad (4.27)$$

with boundary conditions:

$$\begin{aligned} M &= C_1(o, y, z) \delta(y) \delta(z - H_e) \bar{V}, \\ C_1(x, \pm \infty, z) &= 0, \\ C_1(x, y, \infty) &= 0, \\ \bar{K}_z \frac{\partial C_1}{\partial z} \Big|_{z=0} &= V_1 C_1 \Big|_{z=0}. \end{aligned} \quad (3.28)$$

The corresponding equation for the products of SO<sub>2</sub> transformation, SO<sub>4</sub><sup>2-</sup>, is:

$$\bar{V} \frac{\partial C_2}{\partial x} = \bar{K}_y \frac{\partial^2 C_2}{\partial y^2} + \bar{K}_z \frac{\partial^2 C_2}{\partial z^2} - \frac{C_2}{\tau_{2m}} + \frac{C_1}{\tau_0} \quad (4.29)$$

with boundary conditions:

$$\begin{aligned} C_2(0, y, z) &= 0, \\ C_2(x, \pm \infty, z) &= 0, \\ C_2(x, y, \infty) &= 0, \\ \bar{K}_z \frac{\partial C_2}{\partial z} \Big|_{z=0} &= V_2 C_2 \Big|_{z=0}, \end{aligned} \quad (4.30)$$

where C<sub>1</sub> and C<sub>2</sub> – SO<sub>2</sub> and SO<sub>4</sub><sup>2-</sup> atmospheric concentrations, respectively;

M – SO<sub>2</sub> atmospheric emission intensity;

δ – delta-function;

τ<sub>1</sub> – SO<sub>2</sub> residence time relative to wet deposition and chemical transformation to SO<sub>4</sub><sup>2-</sup>;

$$\frac{1}{\tau_1} = \frac{1}{\tau_0} + \frac{1}{\tau_{1m}}$$

H<sub>e</sub> – effective emission height for SO<sub>2</sub>.

Equations (4.27)–(4.30) were analytically solved in Lee (1985), using the Laplace transformations.

$$\begin{aligned} C_1(x, y, z) = \beta_1 \frac{a}{x} e^{-\frac{my^2}{x} - cz} &\left\{ e^{-\frac{s(z-H_e)^2}{x}} + e^{-\frac{s(z+H_e)^2}{x}} \right. \\ &\left. - f\sqrt{x} e^{gz+t(z+H_e)} \operatorname{erfc}\left(\sqrt{\frac{s}{x}}(z+H_e) + \sqrt{gx}\right) \right\}; \end{aligned} \quad (4.31)$$



$$\begin{aligned}
 C_2(x,y,z) = & \beta_1 \frac{B}{x} e^{-\frac{my^2}{z}} \left\{ \left[ e^{-\frac{s(z-H_e)^2}{z}} + e^{-\frac{s(z+H_e^2)}{z}} \right] [e^{-cz} - e^{-FX}] \right. \\
 & - e^{-cz} f\sqrt{x} e^{gz+t(z+H_e)} \operatorname{erfc} \left[ \sqrt{\frac{s}{x}}(z+H_e) + \sqrt{gx} \right] \\
 & \left. + e^{-Fz} [r\sqrt{x} e^{bz+k(z+H_e)} \operatorname{erfc} \left[ \sqrt{\frac{s}{x}}(z+H_e) \right] + \sqrt{bx} - D\sqrt{x} F_0] \right\} \quad (4.32)
 \end{aligned}$$

where

$$\begin{aligned}
 F_0 = & \int_0^{pz} \left\{ \left[ \frac{1}{\sqrt{\pi u}} e^{-\frac{1+Nu^2}{4u}} - \alpha e^{nu+\alpha} \operatorname{erfc} \left( \frac{1}{2\sqrt{u}} + \alpha\sqrt{u} \right) \right] \right. \\
 & \left. \left[ \frac{1}{\sqrt{\pi(pz-u)}} e^{-\frac{z^2}{4H_e(pz-u)}} - \gamma e^{\gamma^2(pz-u)+kz} \operatorname{erfc} \left( \frac{z}{2H_e\sqrt{pz-u}} + \gamma\sqrt{pz-u} \right) \right] \right\} du. \quad (4.33)
 \end{aligned}$$

$$a = \frac{M}{4\pi\sqrt{\bar{K}_y\bar{K}_z}}, \quad (4.34)$$

$$m = \frac{\bar{V}}{4\bar{K}_y} \quad (4.35)$$

$$c = \frac{1}{\tau_1\bar{V}} \quad (4.36)$$

$$s = \frac{\bar{V}}{4\bar{K}_z} \quad (4.37)$$

$$f = \sqrt{4\pi q} \quad (4.38)$$

$$g = \frac{(V_1)^2}{\bar{V}\bar{K}_z} \quad (4.39)$$

$$t = \frac{V_1}{\bar{K}_z} \quad (4.40)$$

$$B = \frac{a\tau_1\tau_2m}{\tau_0(\tau_1-\tau_2m)} \quad (4.41)$$

$$F = \frac{1}{\tau_2m\cdot\bar{V}} \quad (4.42)$$

$$k = \frac{V_2}{\bar{K}_z} \quad (4.43)$$

$$D = r-f \quad (4.44)$$

$$p = \frac{\bar{K}_z}{\bar{V}H_e^2} \quad (4.45)$$

$$N = \frac{4H_e^2(\tau_2m-\tau_1)}{\bar{K}_z\cdot\tau_1\cdot\tau_2m} \quad (4.46)$$

$$\alpha = tH_e \quad (4.47)$$

$$\gamma = kH_e \quad (4.48)$$

$$n = \alpha^2 - \frac{N}{4} \quad (4.49)$$

$$r = \sqrt{4\pi b} \quad (4.50)$$

$$h = \frac{\bar{V}H_e^2}{4\bar{K}_z} \quad (4.51)$$

$$b = \frac{(V_2)^2}{\bar{V}K_z} \quad (4.52)$$

Then according to (4.31)-(4.33) the surface concentration of SO<sub>2</sub> and SO<sub>4</sub><sup>2-</sup> is:

$$C_1(x,y,o) = \beta_1 \frac{a}{x} e^{-\frac{my^2}{x} - cx} \left\{ 2e^{-\frac{h}{x} - f\sqrt{x}} e^{gx+\alpha} \operatorname{erfc} \left[ \sqrt{\frac{h}{x}} + \sqrt{\frac{g}{x}} \right] \right\} \quad (4.53)$$

$$C_2(x,y,o) = \beta_1 \frac{B}{x} e^{-\frac{my^2}{x}} \left\{ 2e^{-\frac{h}{x}} (e^{-cx} - e^{-Fx}) - e^{-cx} f\sqrt{x} e^{gx+\alpha} \operatorname{erfc} \left[ \sqrt{\frac{h}{x}} + \sqrt{\frac{g}{x}} \right] \right. \\ \left. + e^{-Fx} \left[ r\sqrt{x} e^{bz+\gamma} \operatorname{erfc} \left[ \sqrt{\frac{h}{x}} + \sqrt{\frac{b}{x}} \right] - D\sqrt{x} M_0 \right] \right\}, \quad (4.54)$$

where

$$M_0 = F_0(z=0) = \int_0^{px} \left\{ \frac{1}{\sqrt{\pi u}} e^{-\frac{1+Nu^2}{4u}} - \alpha e^{nu+\alpha} \operatorname{erfc} \left[ \frac{1}{2\sqrt{u}} + \alpha\sqrt{u} \right] \right\} \\ \left[ \frac{1}{\sqrt{\pi(px-u)}} - \gamma e^{\gamma^2(px-u)} \operatorname{erfc}(\gamma\sqrt{px-u}) \right] du. \quad (4.55)$$

The coefficients included in (4.53)-(4.55) are determined by (4.34)-(4.52).

Then dry atmospheric deposition of SO<sub>2</sub> and SO<sub>4</sub><sup>2-</sup> can be calculated as:

$$D_1(x,y) = C_1(x,y,o) V_1 \beta_2, \quad (4.56)$$

$$D_2(x,y) = C_2(x,y,o) V_2 \beta_2, \quad (4.57)$$

and wet deposition as:

$$W_1(x,y) = \frac{\int_0^{\infty} C_1(x,y,z) dz}{\tau_{1m}}, \quad (4.58)$$

$$W_2(x,y) = \frac{\int_0^{\infty} C_2(x,y,z) dz}{\tau_{2m}} \quad (4.59)$$

Let us present the obtained calculation formulae omitting all the numerous computations of integrals (4.58), (4.59):

$$W_1(x,y) = \beta_3 \frac{\Delta}{\tau_{1m}\sqrt{x}} e^{-\frac{my^2}{x}-cx} \left[ 1 + e^{gx+\alpha} \operatorname{erfc} \left( \sqrt{\frac{h}{x}} + \sqrt{gx} \right) - \operatorname{erfc} \left( \sqrt{\frac{h}{x}} \right) \right]; \quad (4.60)$$

$$W_2(x,y) = \beta_3 \frac{A}{x} e^{-\frac{my_2}{x}} \left\{ e^{-cx} - e^{-Fx} - e^{-cx} \left[ \operatorname{erfc} \left( \sqrt{\frac{h}{x}} \right) - e^{gx+\alpha} \operatorname{erfc} \left( \sqrt{\frac{h}{x}} + \sqrt{gx} \right) \right] \right. \\ \left. + e^{-Fx} \left[ \operatorname{erfc} \left( \sqrt{\frac{h}{x}} \right) - e^{bx+\gamma} \operatorname{erfc} \left( \sqrt{\frac{h}{x}} + \sqrt{bx} \right) - (\gamma-\alpha)N_0 \right] \right\} \quad (4.61)$$

where

$$N_0 = \int_0^{px} e^{\gamma^2(px-u)} \operatorname{erfc}(\gamma\sqrt{px-u}) \left[ \frac{1}{\sqrt{\pi u}} e^{-\frac{1+Nu^2}{4u}} - \alpha e^{nu\alpha} \operatorname{erfc} \left( \frac{1}{2\sqrt{u}} + \alpha\sqrt{u} \right) \right] du, \quad (4.62)$$

where

$$A = \frac{\Delta\tau_1}{\tau_0(\tau_1-\tau_{2m})}, \quad (4.63)$$

$$\Delta = \frac{M}{4\pi\bar{V}\bar{K}_y} \quad (4.64)$$

The rest of the coefficients included in (4.60)-(4.62) are determined by (4.34)-(4.52).

Coefficients  $\beta_1 = 15.85 \cdot 10^6$ ,  $\beta_2 = 31.536$ ,  $\beta_3 = 5 \cdot 10^8$  serve to reduce  $D_1(x,y)$ ,  $D_2(x,y)$ ,  $W_1(x,y)$ ,  $W_2(x,y)$  to respective dimensions (Table 4.1). Integral  $M_0$  was taken numerically. Since the integrand in (4.55)  $\rightarrow \infty$  at  $u \rightarrow px$ ,  $M_0$  was assessed in the following way: it was taken numerically within the integration range  $[0, 0.95px]$  using the Simpson method; and analytically within the range  $[0.95px, px]$ . At  $u \rightarrow px$  expression  $\gamma e^{\gamma\alpha(px-u)} \operatorname{erfc}(\gamma\sqrt{px-u}) \rightarrow \gamma$ . Therefore, the "analytical addition" can be presented as:

$$M_0|_{0.95}^{px} = \int_{0.95px}^{px} A_0 \left( \frac{1}{\sqrt{\pi(px-u)}} - \gamma \right) du = A_0 \left( \frac{\sqrt{0.2px}}{\pi} - 0.05px\gamma \right), \quad (4.65)$$

where  $A_0 = \frac{A_1+A_2}{2}$ ;  $A_1$  and  $A_2$  - values of expression

$$\frac{1}{\sqrt{\pi u}} e^{-\frac{1+Nu^2}{4u}} - \alpha e^{nu+\alpha} \operatorname{erfc} \left( \frac{1}{2\sqrt{u}} + \alpha\sqrt{u} \right)$$

at points  $u = 0.95px$  and  $u = px$ , respectively.

Integral  $N_0$  was solved numerically using the Simpson method.

Formulae (4.53)–(4.55), (4.56), (4.57), (4.60)–(4.62) are used to calculate mean annual concentrations and deposition of sulfur compounds within the region.

According to (4.53)–(4.55), (4.60)–(4.62) pollutant concentrations and deposition rapidly decrease in the direction perpendicular to the plume axis, as  $\exp(-\frac{my^2}{x})$ . Therefore, the angular spread of the plume (angle  $\alpha_0$ ) in Figure 4.2, within which wind directions (between OB and OB') affect the pollution level in the raster center (p.A), is very small. For instance, at  $1000\text{m} \leq x \leq 400\ 000\ \text{m}$ ,  $0.25^\circ \leq \alpha_0 \leq 0.006^\circ$  if  $\epsilon_0 = 100$  ( $\epsilon_0$  means that the concentration at the plume boundary at p.B is  $\epsilon_0$  times lower than at its axis at p.A).

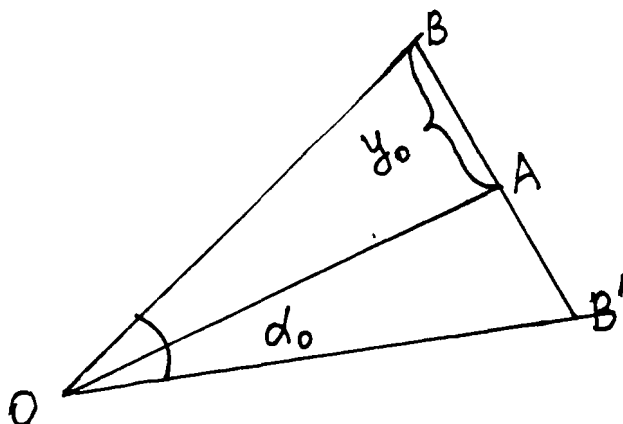


Figure 4.2: Emission source is located at p.O, raster center is at p.A, OA - the plume axis.

Therefore, in this case, a standard assessment of annual pollution levels using the sequential concentration calculation for each wind direction of the  $R$ -point wind rise and their further averaging is unacceptable. (The wind rise should be exceptionally fine in this case, with a time interval of no more than a few minutes). Mean annual pollution fields are calculated in the following way.

For each raster center depending on distance  $X$  from the center to the emission source we determined angular plume spread  $\alpha_0$  within which wind directions affected pollution in the raster center. Assuming that  $\exp(-\frac{my^2}{x}) = \frac{1}{\epsilon_0}$ , the angle is

$$\alpha_0(x) = 2 \arctg \left[ \frac{\ln \epsilon_0}{mx} \right]^{1/2}. \quad (4.66)$$

Distance OA does not differ practically from OB in Figure 4.2 (even at the lowest  $X$  values the difference does not exceed  $10^{-5}$  times). Therefore, differences in pollution levels with the wind blowing along OB (and all intermediate directions between OB and OA) and along OA are determined only by factor  $\exp(-\frac{my^2}{x})$ . Then, integrating  $C_1(x,y,0)$ ,  $C_2(x,y,0)$ ,  $W_1(x,y)$ ,  $W_2(x,y)$  over the plume cross-section, i.e., replacing factor  $\exp(-\frac{my^2}{x})$  by the factor given below, we would take into account pollution contribution in the raster center from all wind directions within the angular plume spread:

$$\frac{1}{2y_0} \int_{-y_0}^{+y_0} \exp(-\frac{my^2}{x}) dy = \sqrt{\frac{\pi}{4 \ln \epsilon_0}} \operatorname{erf}(y_0), \quad (4.67)$$

where

$$y_0 = \left[ \frac{\ln \epsilon_0}{m} \right]^{1/2} x = AB, \text{ Figure 4.2.}$$

Assuming that any wind direction is equally probable within angular plume spread  $\alpha_0$ , we would obtain a mean annual probability of wind direction realization within sector  $\alpha_0$  for each raster center, with a given mean annual  $R$ -point wind rose for the region  $\bar{\beta}_m, m=\bar{1}, R$ :

$$\Theta(x) = \frac{\alpha_0(x)R}{360^\circ} \bar{\beta}_m \quad (4.68)$$

where  $m'$  - point number of the  $R$ -point wind rose comprising sector  $\alpha_0$  (sector axis).

Mean annual concentrations, dry and wet deposition of  $\text{SO}_2$  and  $\text{SO}_4^{2-}$  from a given emission source in the raster centers are calculated by formulae (4.52)-(4.54), (4.60), (4.60)-(4.62) multiplying them by respective recurrences  $\Theta(x)$  estimated from (4.68). Factor  $\exp(-\frac{my^2}{x})$  in the calculation formulae is replaced by (4.67), and  $x$  - distance from the emission source to the raster center.

*Assessments of meteorological elements and model parameters.*

$\bar{\beta}_m, H, V, \bar{K}_z, V_0, h_s, k_1, k_2, V_1, V_2, \tau_0, P, \bar{V}, \tau_{1m}, \tau_{2m}$  were estimated similar to model 1 and have similar numerical values.

The effective emission height for the source is calculated as

$$H_e = H_2 + \Delta H$$

where

$H_2$  - geometric height of the emission source (stack height);

$\Delta H$  - plume rise calculated in the model based on recommendations (Beryland, 1985):

$$\Delta H = \frac{2,39\sqrt{v_b}}{D_b V_0} \left[ 1 + \frac{6,57 D_b (T_b - T_0)}{273^\circ + T_0} V_0 \right], \quad (4.69)$$

where

$v_b, D_b, T_b$  - source emission volume, diameter and temperature;

$T_0, V_0$  - mean annual surface air temperature and wind speed.

To calculate horizontal diffusion coefficient  $\bar{K}_y$  we used the following relation obtained in Beryland (1985):

$$K_y(z) = Gv(z), \quad (4.70)$$

where

$G$  - a certain numerical coefficient.

It can be assessed (as in Beryland, 1985) proceeding from the condition above the surface layer  $K_y K_z$ . Taking  $h_s$  at the surface layer boundary as

$$Gv(z=h_s) = k_z(z=h_s) \quad (4.71)$$

and taking into account (4.20), (4.24), we would obtain:

$$G = \frac{K_0}{V_0} \left[ \frac{h_s}{z_0} \right]^{1-p} \quad (4.72)$$

Then, with due regard for (4.20) and (4.72),  $\bar{K}_y$  is:

$$\bar{K}_y = \frac{1}{H} \int_0^H K_y(z) dz = G \frac{V_0}{p+1} \left[ \frac{H_0}{z_0} \right]^p \quad (4.73)$$

$\bar{K}_y$  was calculated by (4.73) using data from Table 4.3.

*Model input data.*

Model 2 included the following input data:

$H_2, D_b$  – height and diameter of emission stacks in the region, m;

$v_{bi}$  – volume of emission from sources,  $m^3/s$ ;

$T_b$  – emission temperature, degr.C;

$T_0$  – mean annual surface air temperature in the region, degr.C;

$\bar{K}_z$  – mean annual, average for the mixing layer vertical turbulent exchange coefficient in the region:  $6.9 (2.4 \div 6.9), m^2/s$ ;

$\bar{K}_y$  – mean annual average for the mixing layer horizontal turbulent exchange coefficient in the region:  $8.2(3.4 \div 8.2), m^2/s$ ;

as well as  $L, x, y, M, V_0, \bar{\beta}_m, P, V, H, V_1, V_2, \tau_0, k_1, k_2$  defined as model 1 input data which have similar numerical values.

## 5. Estimation of Maximum Surface Pollutant Concentrations in Cities

Surface concentrations from an emission source at any urban site are estimated on the basis of the analytical solution of the atmosphere diffusion equation (Beryland, 1985) under the following conditions:

- atmospheric pollutant dispersion over a period comparable to the time of transport from the source to the given point in a stationary process (Marchuk, 1982);
- the underlying surface totally reflects the pollutant, i.e., it does not interact with the soil, does not accumulate, and turbulent air flows return it to the atmosphere;
- the vertical component of the wind speed is zero (in the case of a light pollutant possessing no transport speed of its own); in the case of a heavy pollutant the gravitational deposition rate is taken into account;
- effective emission source height is used (corrected for the thermal plume rise).

Surface concentrations averaged at 20–30 minutes are determined for the so-called normal unfavorable weather conditions occurring during an unbalanced (unstable) stratification of the atmosphere, i.e., during an intensive vertical mixing throughout the boundary layer (about 1 km.) which differs essentially from the zero temperature gradient. In this case it is assumed that the vertical turbulent exchange coefficient in the surface layer increases linearly with height (exchange model) (*New airclimatic reference book ...*, 1987), the wind speed varies with height according to the power law, and the horizontal turbulent exchange coefficient is proportional to the wind speed.

Thus the parameters governing pollutant dispersion conditions are the functions of the wind speed and for each emission source a “dangerous” speed  $U_{iM}$  can be calculated at which the surface concentration along the plume axis (i.e., when the wind is directed from the source to the calculated point) has the maximum value.

In cases where the surface concentration is estimated for a group of sources each of which has its own dangerous speed and direction of wind (with the plume axis direction being determined by the source and calculated point coordinates), assumptions on these conditions common to all emittants should be taken.

In dispersion block MARS-1, the directions of the wind blowing from the source are selected with a certain fixed angular step (usually  $5^\circ$  or  $10^\circ$ , which corresponds to 72 or 36 directions providing the required accuracy of maximum concentration assessment). The common dangerous wind speed for  $N$  emittants of the  $k$ -th pollutant is estimated as a mean weighted value (the modified dangerous wind speed):

$$U^{(k)} = \frac{\sum_{i=1}^N C_{iM}^{(k)} U_{iM}}{\sum_{i=1}^N C_{iM}^{(k)}} \quad (5.1)$$

where

$C_{iM}^{(k)}$  - maximum concentration of the  $k$ -th pollutant from the  $i$ -th source along the plume axis, achieved at dangerous wind speed  $U_{iM}$ .

Then the maximum concentration of the  $k$ -th pollutant emitted from  $N$  sources under normal unfavorable weather conditions at a calculated point with coordinated  $(x, y)$  is

$$C^{(k)}(x, y) = \max_{\varphi, U^{(k)}} \sum_{i=1}^N C_i^{(k)}(x, y, \varphi, U^{(k)}), \quad (5.2)$$

where

$C_i^{(k)}$  - surface concentration produced by the  $i$ -th source at wind direction  $\varphi$  and dangerous wind speed  $U^{(k)}$ .

The accuracy of  $C^{(k)}(x, y)$  estimates depend on the adequacy of the selection of the wind speed and the direction at which the total surface concentration is calculated by formula (5.2). Therefore, MARS-1 envisages the possibility of varying the modified dangerous wind speed within  $0.5 \text{ m/s} - 4 \cdot U^{(k)}$  (since dangerous speeds for the major urban emittants vary within this particular range) with the following averaging of the relevant calculated  $C_{iM}^{(k)}$ .

Normal unfavorable weather conditions are relatively frequent during the year (unlike anomalous unfavorable weather conditions, e.g., inversions with calms, fogs, etc.). As is shown in Beryland (1985), mean diurnal concentrations do not exceed mean daily MPCs if surface concentrations calculated for normal unfavorable weather conditions do not exceed single maximum permissible sanitary standards averaged over 20 minutes (the opposite statement is not true). Therefore, MARS-1 uses maximum permissible pollutant concentrations under normal unfavorable conditions as a criterion for the respective assessment.

In Beryland (1985), where the calculation model of maximum concentrations under normal unfavorable conditions is summarized on the basis of numerical methods, correlations are obtained for the determination of the "dangerous" wind speed (at a windcock level - usually 10m above the ground) for the  $i$ -th emission source  $\text{m/s}$  depending on parameters  $v_M$ .\*

$$U_M = \begin{cases} 0,5, & \text{if } v_M \leq 0,5, \\ v_M, & \text{if } 0,5 < v_M \leq 2, \\ v_M(1+0,12\sqrt{f}), & \text{if } v_M > 2, \end{cases} \quad (5.3)$$

where

$$f = 1621,14 \frac{V^2}{H^2 D^3 \Delta T}, \Delta T > 0, f < 100, \quad (5.4)$$

and

$$v_M = 0,65 \frac{(V \Delta T)^{1/3}}{H}. \quad (5.5)$$

\* To simplify the formulae, the  $i$ -th source index will be omitted whenever possible.

In formulae (5.4) and (5.5)

- V - volume of the gas/air mixture (m<sup>3</sup>/s);
- H - emission source height (m);
- D - source outlet diameter (m);
- $\Delta T$  - temperature difference between the emitted gas/air mixture and ambient air (degr.C),

If  $\Delta T > 0$  and  $F < 100$ , the source emission is considered warm (or otherwise cold) and  $U_M$  is determined using the following formulae:

$$U_M = \begin{cases} 0,5, & \text{if } v_M \leq 0.5 \\ v_M, & \text{if } 0.5 < v_M \leq 2, \\ 2,2 v_M, & \text{if } v_M > 2 \end{cases} \quad (5.6)$$

where

$$v_M = 1,655 \frac{V}{DH} \quad (5.7)$$

The maximum concentration (mg/m<sup>3</sup>) is reached at "dangerous" wind speed  $u_M$  at distance  $X_M$  from the source along the plume axis:

For warm emission:

$$C_M = \frac{A \cdot M \cdot F \cdot m \cdot n}{H^2 (V \Delta T)^{1/3}} \quad (5.8)$$

For cold emissions:

$$C_M = 0,125 \frac{A \cdot M \cdot F \cdot D \cdot n}{V^4 \sqrt{H^3}} \quad (5.9)$$

where

- A - coefficient depending on the temperature stratification of the atmosphere and governing the conditions for the vertical and horizontal atmospheric dispersion of noxious materials ( $s^{2/3} \cdot mg \cdot degr.^{1/3} / g$ );
- M - pollutant mass emitted into the atmosphere per unit time (g/s);
- F - a dimensionless coefficient taking into account the vertical component of the pollutant transport speed (deposition rate) in the atmosphere;
- m, n - dimensionless coefficients taking into account the conditions for gas/air mixture release from the source outlet:

$$m = \frac{1}{0,67 + 0,1\sqrt{f} + 0,34^3\sqrt{f}}, \quad (5.10)$$

$$n = \begin{cases} 3 & \text{if } v_M \leq 0,3, \\ 3 - \sqrt{(v_M - 0,3)(4,36 - v_M)}, & \text{if } 0,3 < v_M \leq 2, \\ 1, & \text{if } v_M > 2. \end{cases} \quad (5.11)$$

Coefficient A, which also depends on the surface layer height and underlying surface roughness, is calculated for open, flat terrains in various geographical regions of the USSR and, accounting for relief correction, varies within 100-260. For other countries, A can be taken based on the similarity of the climatic characteristics of the turbulent regime.



Parameter  $F$  differs for gases, light aerosols, and dust. It is dependent on the particle size distribution which is related to the performance of dust collecting facilities in cases where they are installed at the source. For gases and aerosols (with the settling rate below 5 m/s  $F = 1$  , for dust which is transported as a heavy pollutant,  $F$  equals 2, 2.5 and 3 if the performances of dust collecting facilities are over 90%, 90–75% and below 75%, respectively.

The maximum surface pollutant concentration  $C_M$  along the plume axis (in the direction of an average wind) is achieved at distance  $X_M$  from the emission source (m):

$$X_M = \begin{cases} dH & \text{if } F = 1 \\ \frac{5-F}{4} dH, & \text{if } F \geq 2. \end{cases} \quad (5.12)$$

Parameter  $d$  is calculated as a function of  $v_M$  determined for warm and cold emissions by formulae (5.5) and (5.7) respectively.

For warm emissions:

$$d = \begin{cases} 4,95 v_M (1 + 0,28^3 \sqrt{f}), & \text{if } v_M \leq 2, \\ 7 \sqrt{v_M} (1 + 0,28^3 \sqrt{f}), & \text{if } v_M > 2. \end{cases} \quad (5.13)$$

For cold emissions:

$$d = \begin{cases} 11,4 v_M & \text{if } v_M \leq 2, \\ 16,1 \sqrt{v_M}, & \text{if } v_M > 2. \end{cases} \quad (5.14)$$

If the dangerous wind speed is taken as the modified value (5.2), deviation  $U_M$  from  $U^{(k)}$  is possible for each  $i$ -th emission source. In this case the maximum surface concentration is

$$C_{MU} = r \cdot C_M \quad (5.15)$$

where

$r$  - dimensionless quantity determined depending on the relation  $q = U^{(k)}/U_M$ :

$$r = \begin{cases} 0,67q + 1,67q^2 - 1,34q^3, & \text{if } q \leq 1, \\ \frac{3q}{2q^2 - q + 2}, & \text{if } q > 1. \end{cases} \quad (5.16)$$

Surface pollutant concentrations in the atmosphere along the plume axis at distance  $x$  from the source are calculated by the following formulae:

$$C_x = s_1 \cdot C_{MU}, \quad (5.17)$$

where

$s_1$  - dimensionless quantity, which depending on relation

$$z = \frac{x}{X_M} \quad (5.18)$$

satisfies the following conditions:

$$s_1 = \begin{cases} 3z^4 - 8z^3 + 6z^2, & \text{if } z \leq 1, \\ 1,13/(0,13z^2 + 1), & \text{if } 1 < z \leq 8, \\ z/(3,58z^2 - 35,2z + 120), & \text{if } z > 8 \text{ and } F=1, \\ 1/(0,1z^2 + 2,47z - 17,8), & \text{if } z > 8 \text{ and } F \geq 2. \end{cases} \quad (5.19)$$

When the calculated point is shifted perpendicular to the plume axis at distance  $y$ , the surface pollutant concentration in the atmosphere is

$$C_y = s_2 \cdot C_x, \quad (5.20)$$

where

$s_2$  - dimensionless quantity given for wind speed  $U_{subM}$  and relation  $g=y/x$ :

$$s_2 = \frac{1}{(1+8,4U_M g^2)(1+28,2U_M^2 g^4)} \quad (5.21)$$

Thus, the surface pollutant concentration at a point with coordinates  $(x,y)$  from the  $i$ -th emission source, dangerous wind speed  $U^{(k)}$  and a fixed transport direction  $\varphi$  (along the plume axis  $x$ ) is

$$C_{iU}(x,y) = r \cdot s_1 \cdot s_2 \cdot C_M. \quad (5.22)$$

Distance  $X_{MU}$  where the surface concentration  $C_{MU}$  is achieved is

$$X_{MU} = p \cdot X_M, \quad (5.23)$$

where

$$p = \begin{cases} 3 & \text{if } q \leq 0,25, \\ 8,43(1-q)^5 + 1, & \text{if } 0,25 < q \leq 1, \\ 0,32q + 0,68, & \text{if } q > 1. \end{cases} \quad (5.24)$$

To determine the maximum surface concentration fields for several pollutants in a city whose territory is represented by a regular grid, one usually has to calculate about 1000 matrices each of which contains over 1000 elements. Such calculations, associated with the exhaustive search of wind directions and speeds, require much computer time. Therefore, MARS-1 employs a number of methods reducing the calculation time based on prescribing an "expediency constant"  $\epsilon^{(k)}$ . The constant is taken equal to 0.05  $P^{(k)}$  where  $P^{(k)}$  - maximum permissible atmospheric concentration of the  $k$ -th pollutant (sanitary standard).

When calculating surface concentrations at every algorithm step, various means for adjusting the components of formula (5.24) are used to fulfill the following condition:

$$C_{iU}^{(k)} > \epsilon^{(k)}. \quad (5.25)$$

If condition (5.25) cannot be fulfilled, calculations for the  $i$ -th source at a given algorithm step are interrupted.

A. Maximum concentration  $C_{subiM}^{(k)}$  (5.8) or (5.9) is tested. If for the  $i$ -th source

$$C_{iM}^{(k)} < \epsilon^{(k)}, \quad (5.26)$$

the source is not considered for the  $k$ -th pollutant.

Thus,  $U^{(k)}$  (5.1) is determined taking into account only emittants for which relation (5.26) is fulfilled, so parameter  $N$  (number of sources included in calculations for the  $k$ -th pollutant) can differ from the total number of emission sources considered in the model

B.  $C_{iMu}^{(k)}$  is tested (5.15). If for the  $i$ -th source

$$C_{iMU}^{(k)} < \epsilon^{(k)}, \quad (5.27)$$

the source is also omitted from further calculations for the  $k$ -th pollutant.

- C. Based on (5.19), the radius of the pollution zone  $R_{iz}^{(k)}$  is established for each  $i$ -th source at

$$s_1 = 0,05P^{(k)}/C_{iMU}^{(k)}, \quad (5.28)$$

which is found from (5.17).

$R_{iz}^{(k)}$  determines the coordinates of calculated points of the urban regular grid, at which concentrations are to be calculated. The application of pollution zone radii allows a drastic reduction in the number of calculated points due to the peculiarities of elevated and low emissions.

- D. According to (5.21), the flux dispersion angle perpendicular to the plume axis is established at

$$s_2 = 0,05P^{(k)}/C_x, \quad (5.29)$$

$g = tg\alpha$  is determined where  $\alpha$  - the angle required.

Thus, the  $i$ -th source pollution zone is a sector with angle  $\alpha$  of a circle with radius  $R_{iz}^{(k)}$  (in the upwind direction (at  $x < 0$ ) pollutant concentrations are 0).

Test runs of MARS-1 indicated that the calculation time of a dispersion model for 200 emission sources and 7 pollutants based on a result grid of  $30 \times 34$  does not exceed 15 minutes for personal computers. The result is quite satisfactory when using the model considered in the optimization block.

## 6. Choosing Optimal Strategies

Several hundred or even thousand pollutant emission sources are disposed in the territory of a real city/region. 5-15 air protection measures can be implemented at each of them, some activities may be united in various sets. Thus, a great number of variants of air basin protection from the pollution arises whose comparative analysis requires the use of special optimization algorithms.

Within MARS, optimal strategies are being selected on the basis of an algorithm including three stages.

### A. Forming the bank of initial measures.

Constructing the bank includes an analysis of each action on pollutant emission decrease which is technically available for the considered source. Such measures are noted by great variety, carried out for a single or several emitters and, in general cases, can change any parameter characterizing the conditions of pollutant emission into the atmosphere of the city/region. Therefore, MARS provides the possibility to analyze a wide range of innovations aimed at air basin protection, making it possible to:

- change any combination of parameters characterizing a single emitter;
- change any combination of parameters characterizing several emitters;
- eliminate the emitter;
- eliminate the emitter with partial or complete transfer of its functions to other emission sources located or newly disposed at the territory of the city/region;
- remove the emitter or several emitters to another city/region;
- select the least dangerous dislocation of single or several emitters in the city/region.

The considered optimization algorithm suggest splitting the bank of initial measures into groups uniting pollution sources with similar technological processes (any air protection measure is definitely related to an emitter). MARS specifies no strict requirements on the composition of the group, however, the bank division according to a certain principle (e.g., industrial) expedites the interpretation of results obtained at subsequent algorithm stages.

Let  $L$  be the number of groups in the initial action bank,  $l = 1, \overline{L}$ . The number of measures in each group  $M_l$ ,  $m = \overline{1, M_l}$ .

As was shown above, to analyze and control the atmospheric pollution in the city/region, MARS applies various criteria formalized using a complex of models aimed at calculating the economic damage, assessing the potential danger to coniferous forests and sulfur compound transport, evaluating the maximum surface concentrations of pollutants. Let us assume that  $Q$  types of criteria used ( $q = 1, Q$ ) allows an integrated assessment of the air basin pollution level in the city/region.

Then, at stage A, a matrix is calculated for each group

$$E_l = (E_m^q) \quad (6.1)$$

which consists of  $M$  lines and  $Q$  columns, where  $E_m^q$  is the effect of implementing the  $m$ -th action according to the  $q$ -th criterion. Then each line of the matrix  $E_l$  presents the "criterion vector" and the action  $M$  is effective in cases of at least a single element

$$E_m^Q > 0. \quad (6.2)$$

The total number of efficient actions comprising the bank:

$$M = \sum_{l=1}^L M_l \quad (6.3)$$

#### B. Forming the permissible sets of measures.

According to the possibilities of the initial bank "permissible sets of measures" can be formed for each  $l$ -th emitter group which present various types of air protection activity in the city/region. The set is considered permissible if it includes no "alternative pair" of measures. Two measures are called alternative if they cannot be simultaneously implemented to reduce pollutant emissions either for technical reasons or due to the inexpediency of such a combination. The situation frequently occurs, e.g., while using two types of dust collectors with equal efficiency at a single source or simultaneous transfer of a boiler house to gaseous fuel and the installation of sulfur refining equipment. Combined implementation of activities depends on a number of specific conditions and, in general, one fails to formalize the search for alternative pairs in a large set of air protection measures. Therefore, while formalizing the bank of initial actions, the table of alternatives is assumed for each group in the form of square logic matrices having the dimension  $M_l$ .

Taking account of alternative pairs while establishing permissible sets is necessary to provide practical efficiency of the analytical results.

Let us fix criterion  $q^* = q, q = \overline{1, Q}$  (a corresponding column of the matrix  $E_l$ ,  $l = \overline{1, L}$  and select the type of costs (capital or total).

Let us distinguish the measures within the  $l$ -th group for which

$$E_m^{q^*} > 0, m = \overline{1, M_l} \quad (6.4)$$

Then all permissible sets of measures could be made up for the  $l$ -th group whose number, in case of the absence of alternative pairs, is equal to:

$$S = \sum_{p=1}^{M_l^*} C_{M_l^*}^p = 2^{M_l^*} \quad (6.5)$$

where  $C$  is the number of combination of  $M_l^*$  - the number of measures that satisfy the requirements (6.4) for the group  $l$ . When  $p=1$  the analysis includes the initial measures of the  $l$ -th bank group.

Considerable values of  $M_l^*$  and a small number of alternative pairs  $S$  can become quite large, however, not all permissible sets are efficient. Therefore, each set successfully formed according to formula (6.5) is compared to the earlier compiled ones. One of the

two sets is considered efficient if:

- at lower costs it provides equal or larger effect;
- at equal costs it provides larger effect;
- at larger costs it provides larger effect;
- at smaller costs it provides smaller effect.

The set having the above characteristics is memorized and used in further analysis, and the one which at larger or equal costs provides smaller effect is excluded from subsequent analysis.

Thus, for each group  $l$ , a monotonic sequence of combined air protection measures is formed which provides increased effect at raised costs.

To describe these sequences let us introduce the functions:

$$Z_l = g_l(X), \quad l=\overline{1, L} \quad (6.6)$$

where  $X$  denotes the costs of a relevant efficient set of measures;  $Z_l$  is the effect achieved at given costs in the group  $l$ .

The costs of air protection measures are of a discrete nature, i.e., a specific action requires a certain fixed amount of costs and, depending on the allocated funds, the activity is either implemented completely or not carried out at all. At the same time the effect of measures is nonlinearly related to the costs. Therefore, the "cost-effect" functions (6.6) for the group  $l$  are discrete, nonlinear, assigned in the form of tables and, in general, it is impossible to evaluate their mathematic parameters. Besides, the number of cost levels  $N_l$  for the measures of the  $l$ -th group (the domain of  $X$ ) corresponding to the number of efficient permissible sets can be rather considerable, their sum amounting to several thousand variants. Thus, further analysis of  $N = \sum_{l=1}^L N_l$  permissible effective sets requires the use of specific optimization models.

### C. Optimizing the distribution of costs of air protection measures.

A special distribution model is meant to evaluate optimal sets of air protection measures in the city/region depending on the type of costs and criteria selected at stage B (the set of permissible effective variants is used as initial information). The obtained permissible effective sets are characterized by their alternative nature within each group  $l=\overline{1, L}$ . Therefore, at stage C, optimal sets are compiled by combining the measures referring to different groups.

Optimal sets determine optimal cost-effect functions for the city/region in general, which is the main result of MARS.

Completely alternative nature  $N_l$  of effective sets within group  $l$  allows to present cost distribution as a sequence of dynamic programming steps. While enabling to solve discrete problems, such an approach specifies no strict requirements to mathematical properties of the functions (6.6).

The optimization model has the following form:

$$\sum_{l=1}^L Z_l = R(X_1, X_2, \dots, X_L) \rightarrow \max. \quad (6.7)$$

$$Z_l = g_l(X_l), \quad l=\overline{1, L}; \quad (6.8)$$

$$\sum_{l=1}^L X_l \leq K; \quad (6.9)$$

$$X_l \geq 0, \quad l=\overline{1, L}, \quad (6.10)$$

where  $X_1, X_2, \dots, X_L$  are the costs of air protection measures carried out at the sources of the 1, 2,  $\dots$ ,  $L$  groups, respectively.

Model (6.7)–(6.10) maximizes the total effect of air protection measures within the allocated costs  $K$ . While realizing model (6.7)–(6.10), dynamic programming allows to obtain a family of solutions (optimal sets), each corresponding to a certain level of costs not exceeding  $K$ . Thus, relationship (6.9) serves as the upper limit.

Since the multitude of permissible effective combinations (stage B) is discrete and finite ( $N$ ), a complete optimal set can be compiled in which the costs  $K_m$  are maximum in respect to the possibilities of initial measure bank. Substitution into the right-hand part of inequality (6.5)  $K=K_m$  would yield a complete optimal cost-effect function for the city/region obtained for the whole multitude of efficient variants. Complete optimal cost-effect function characterizes the achieved technological progress in the protection of an air basin, the condition of which is described by a relevant criterion  $q^*$ .

The main principle of constructing a multi-step procedure to solve model (6.7)–(6.10) using dynamic programming consists of the following.

Assuming that at stage B discrete values of costs are obtained within each group  $l$  for permissible effective sets:

$$V^{(l)} = V_n^{(l)}, n=1, N_l \quad (6.11)$$

Let us introduce the sequence of steps  $t=1, L-1$  and determine the functions:

$$f_1(y_1) = \max[g_1(X_1) + g_2(X_2)], y_1 \in U^{(1)}, y_1 \leq K; \quad (6.12)$$

$$X_1 \in V^{(1)}$$

$$X_2 \in V^{(2)}$$

$$X_1 + X_2 \leq K$$

$$f_2(y_2) = \max[f_1(y_1) + g_3(X_3)], y_2 \in U^{(2)}; \quad (6.13)$$

$$y_1 \in U^{(1)}$$

$$X_3 \in V^{(3)}$$

$$y_1 + X_3 \leq K$$

$$f_t(y_t) = \max[f_{t-1}(y_{t-1}) + g_t(X_t)], y_t \in U^{(t)}; \quad (6.14)$$

$$y_{t-1} \in U^{(t-1)}$$

$$X_t \in V^{(t)}$$

$$y_{t-1} + X_t \leq K$$

where  $U^{(t)}$  is the definition domain of argument  $y_t$  representing the sub-multitude  $\bigcup_{i=1}^t V^{(i)}$ .

$f_t(y_t)$  characterizes the maximum effect obtained from the distribution of costs  $K$  by  $t+1$  groups and presents the optimal cost-effect function for these groups.

Recurrent correlation (6.14) is the operator of transition from step  $t-1$  to step  $t$ .

Thus the multi-step procedure presents the solution of model (6.7)–(6.10) as a pairwise combination of permissible effective sets referring to different group  $l = \overline{1, L}$  (Bursh-tein, 1968).

The described process can be illustrated by the scheme (Figure 6.1).

Let us consider the multi-step computer procedure of solving model (6.7)–(6.10).

I.  $t=1$  (the first step). Calculation of total estimates

$$\left. \begin{aligned} v_{ij} &= v_i^{(1)} + v_j^{(2)} \\ z_{ij} &= z_i^{(1)} + z_j^{(2)} \end{aligned} \right\} \quad i=1, N_1, j=1, N_2 \quad (6.15)$$

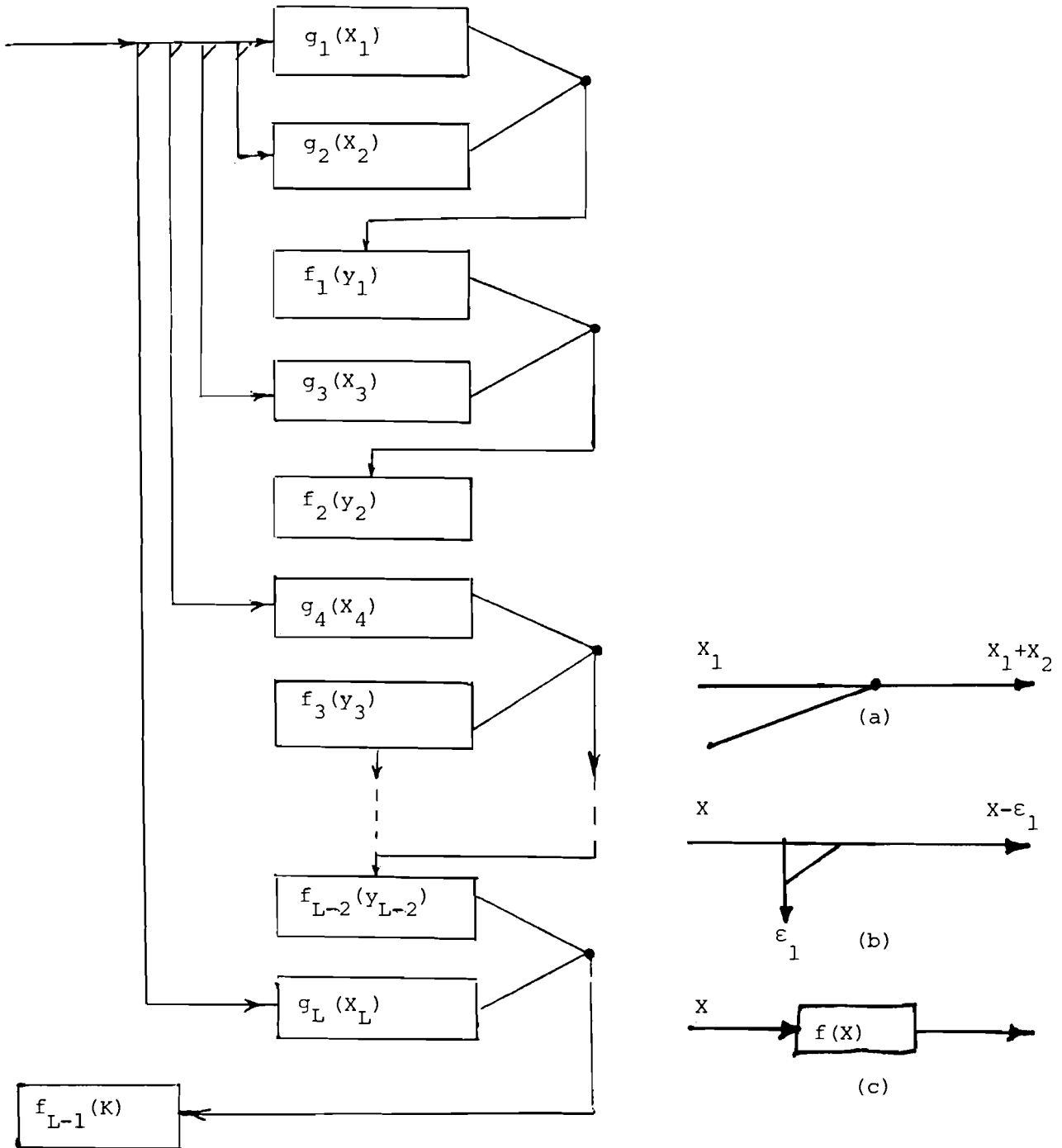


Figure 6.1: Functional scheme of cost distribution.

- (a) addition of variables;
- (b) distribution unit;
- (c) function generator.

for discrete values of costs and relevant effects (groups 1 and 2):

$$\begin{aligned} & v^{(1)}, v_2^{(1)}, \dots, v_{N_1}^{(1)}; v_1^{(2)}, \dots, v_{N_2}^{(2)} \\ & Z_1^{(1)}, Z_2^{(1)}, \dots, Z_{N_1}^{(1)}; Z_1^{(2)}, Z_2^{(2)}, \dots, Z_{N_2}^{(2)} \end{aligned} \quad (6.16)$$

and construction of vectors

$$\left. \begin{aligned} v &= (v_i^{(1)}, v_j^{(2)}, v_{ij}) = (v_r) \\ Z &= (Z_i^{(1)}, Z_j^{(2)}, Z_{ij}) = (Z_r) \end{aligned} \right\} r = \overline{1, N^*}, N^* = N_1 + N_2 + N_1 \cdot N_2 \quad (6.17)$$

II. Arranging components of vector  $v$  according to the rising of costs.

III. Exclusion of inefficient estimates. If

$$r_2 > r_1 \wedge Z_{r_2} - Z_{r_1} \leq \epsilon, r_1 = \overline{1, N^*}, r_2 = \overline{1, N^*}, \quad (6.18)$$

variant  $r_2$  is considered inefficient as compared to  $r_1$ , and  $r_2$ -th elements of vectors  $v$  and  $Z$  are excluded. The constant  $\epsilon$  determines the accuracy of model solution (the number of optimal cost-effect function components). Thus,  $\epsilon$  helps to rarefy (decrease dimensionability) of vectors  $v$  and  $Z$  at each step.

IV. Testing the limitations of (6.9). If

$$v_r > K, r = \overline{1, N^*}, \quad (6.19)$$

the elements of vectors  $v$  and  $Z$  under number  $r, r+1, \dots, N^*$  are excluded from further analysis.

V. Test:  $t=L-1$ . If the condition is fulfilled, we transfer to item VIII, otherwise to item VI.

VI. Step  $t+1$ . At the  $t$ -th step we obtain resultant cost vectors and relevant effects

$$\left. \begin{aligned} y_t &= (y_i^{(t)}) \\ w_t &= f_t(y_t) = (w_i^{(t)}) \end{aligned} \right\} i = \overline{1, N_t^*} \quad (6.20)$$

Calculation of total estimates

$$\left. \begin{aligned} v_{ij} &= y_i^{(t)} + v_j^{(t+1)} \\ Z_{ij} &= w_i^{(t)} + Z_j^{(t+1)} \end{aligned} \right\} i = \overline{1, N_t^*}, j = \overline{1, N_{t+1}^*} \quad (6.21)$$

where  $v_j^{(t+1)}$  are components of vector  $v_{t+1}$ ;  $Z_j^{(t+1)} = g_{t+1}(v_j^{(t+1)})$ , and make up

$$\left. \begin{aligned} v &= (y_t^{(t)}, v_j^{(t+1)}, v_{ij}) = (v_r) \\ Z &= (w_t^{(t)}, Z_j^{(t+1)}, Z_{ij}) = (Z_r) \end{aligned} \right\} r = \overline{1, N^*}, N^* = (N_t^* + N_{t+1}^* + N_t^* N_{t+1}^*) \quad (6.22)$$

VII. Transition to item II.

VIII. Completed calculations. An optimal cost-effect function for the city/region is obtained.

The above process of constructing the optimal cost-effect function allows to memorize the ordinal number of each action included in the optimal set in a corresponding group of the initial bank formed according to the criterion  $g^*$  and selected type of costs. Therefore, the algorithm being realized, any optimal strategy can be finalized in a certificate presenting the plan of air protection measures in the city/region, depending on the allowed funds or according to the given standard value of the criterion.



The considered algorithm is characterized by fast response and allows to carry out imitation calculations.

## 7. Information Support

MARS-based calculations employing various performance criteria require the following initial data.

Table 7.1. Initial data for calculations employing various performance criteria.

Initial data	Types of criteria
<b>Emission source parameters (individual for each source)</b>	
Height, m	2, 3*, 4, 5, 6
Diameters, m	3*, 4, 5, 6
Emission rate, m <sup>3</sup> /s	3*, 4, 5, 6
Emission temperature, degr.C	2, 3*, 4, 5, 6
Dust removal coefficient, %	2, 5
Source coordinates, km	2, 3, 4, 5, 6
Mean annual emission of pollutants (individual for each pollutant), thousand t/yr	1, 2, 3, 4, 6
Maximum pollutant emission (individual for each pollutant), g/s	5
<b>Technological and economic characteristics of atmosphere protection activities (individual for each type of activity)</b>	
Capital outlays required to implement the activity, thousand rbl.	1, 2, 3, 4, 5, 6
Total expenses required to implement the activity, thousand rbl.***	1, 2, 3, 4, 5, 6
Changes in pollutant emission after the implementation of the activity at each relevant source (percent of the initial emission from the source)	1, 2, 3, 4, 5, 6
<b>Characteristics of a raster grid representing a city/region</b>	
Region size (number of raster elements from west to east and from south to north)	1, 2, 3, 4, 5, 6
Grid spacing (raster element size), km	1, 2, 3, 4, 5, 6
Relative danger coefficients $\sigma$ for each raster element	2
<b>Meteorological characteristics</b>	
Mean annual precipitation, mm/yr	2, 3, 4, 6
Mean annual surface wind speed within 8-speed wind rose, m/s	2, 3, 4, 6
Mean annual surface wind recurrence within 8-point wind rose	2, 3, 4, 5, 6
Mean annual wind recurrence in the mixing	

layer within 12-point wind rose	3, 4, 6
Mean annual surface air temperature, degr.C	2, 3**, 4, 6
Surface air temperature in July/January at 1 p.m., degr. C	5
Mean annual parameter of atmosphere stratification (exponent in the power law of wind speed change with height)	3, 4, 6
Mean annual height of the mixing layer, m	3, 4, 6
Mean annual height of the mixing layer, m	3, 4, 6
Vertical and horizontal turbulent exchange coefficients average for the mixing layer, sq.m/s	3*, 4, 6
<b>Physiochemical parameters</b>	
Sulfur dioxide dry deposition rate, m/s	3, 4, 6
Sulfate dry deposition rate, m/s	3, 4, 6
Sulfur dioxide residence time in the atmosphere relative to its chemical transformation to sulfate, hr	3, 4, 6
Coefficient of sulfur dioxide washout from the atmosphere with precipitation, 1/mm	3, 4, 6
Coefficient of sulfate washout from the atmosphere with precipitation, 1/mm	3, 4, 6
Sulfur dioxide residence time in the atmosphere relative to dry deposition, hr	3**, 4, 6
Sulfate residence time in the atmosphere relative to dry deposition, hr	3**, 4, 6

\* When model 1 is used to calculate the parameters of sulfur dioxide atmospheric transport and transformation.

\*\* When model 2 is used to calculate the parameters of sulfur dioxide atmospheric transport and transformation.

\*\*\* In case the performance of atmosphere protection activities is evaluated by total expenses.

The figures in Table 7.1 stand for the following types of criteria:

1. maximum reduction of pollutant emission mass;
2. maximum prevention of the economic damage;
3. maximum reduction of total atmospheric deposition of sulfur compounds within the region;
4. maximum reduction of sulfur transport outside the region;
5. maximum reduction of the surface concentration index in the city;
6. maximum reduction of the index of potential threat to coniferous forests in the region caused by sulfur compound deposition.

*Emission source parameters.*

Such information can be obtained from atmospheric pollution source inventories or state statistical reports. Respective urban/regional services dispose of this type of information nowadays.

Since the number of atmosphere pollution sources in a city/region usually equals several hundred or even thousand and exceeds the permissible dimensions of respective models, it is necessary to select the largest ones combining together the smaller sources. The latter can be combined, for instance, by method (*Recommendations on source ... 1983*) for emittants whose parameters differ within the following limits:

- not more than 10 m in height;
- not more than by the factor of 2 in outlet diameters and air/gas mixture volume;
- not more than by the factor of 1.5 in air/gas mixture overheat.

The size of the area over which sources are combined should satisfy the following condition

$$L = 0,5 l \sqrt{\frac{\delta}{1-\delta}} \quad (7.1)$$

where

- L – maximum distance between the source combined, m;
- l – minimum distance from the source combined to the calculation grid points;
- δ – allowable error related to the reduction of the coordinates of the sources combined to the coordinates of an equivalent source (usually  $\delta \leq 25\%$ ).

Parameters of the equivalent source are calculated as:

$$H_0 = \frac{H_{\min} + H_{\max}}{2} ; \quad (7.2)$$

$$D_0 = \frac{D_{\min} + D_{\max}}{2} ; \quad (7.3)$$

$$V_0 = \frac{V_{\min} + V_{\max}}{2} ; \quad (7.4)$$

$$T_0 = \frac{T_{\min} T_{\max}}{2} \quad (7.5)$$

$$X_0 = \frac{X_{\min} + X_{\max}}{2} \quad (7.6)$$

$$Y_0 = \frac{Y_{\min} + Y_{\max}}{2} ; \quad (7.7)$$

$$F_0 = \frac{F_{\min} + F_{\max}}{2} \quad (7.8)$$

$$M_0 = \sum_{i=1}^N M_i , \quad (7.9)$$

where

- $H_0$  – stack height;
- $D_0$  – stack outlet diameter;
- $V_0$  – emission volume;
- $T_0$  – air/gas mixture temperatures;
- $X_i, Y_0$  – coordinates;

$F_0$  - dust removal coefficient;

$M_0$  - equivalent source emission mass.

MARS can be used to calculate air basin pollution by seven different pollutants from 800-1000 sources in a city/region based on personal computers.

*Raster grid characteristics.*

MARS presents the territory of a city/region as a rectangle with a superimposed regular grid. The rectangle is described by the three parameters given in Table 7.1. The coordinate system of the city/region starts in the left lower corner of the rectangle. In MARS, all computations are carried out for the vertices of the left lower corners of respective raster elements.

*Technological and economic characteristics of initial atmosphere protection activities.*

An atmosphere protection activity in MARS

- is technologically feasible for a given source;
- reduces pollutant emission;
- contains the economic assessment of expenses.

When preparing information on the technological and economic characteristics of atmosphere protection activities, one should employ the most complete set using data from enterprises whose sources are considered, information from research and design institutions, literature data, domestic and foreign experience. In this case MARS would be able to realize one of its essential advantages - high technological and spatial resolution of model calculations.

Since atmosphere protection activities are characterized by high variability and are closely connected with the specific peculiarities of emittents, at present it is not possible to suggest an unambiguous methodology for composing the initial data bank for a given city/region. However, for each source type a "universal" activity series can be selected, which can usually be employed when developing the initial data bank. Let us give a few examples referring to emittents encountered in any city/region.

*Large-scale power protection facilities:*

- gas treatment (electrostatic precipitators, wet ash collectors, battery cyclones);
- Nitrogen oxide emission reducing processes (  $\alpha$  coefficient - excess air - reduction, stack gas recirculation, two-stage fuel combustion, installation of straight-flow burners, steam supply into boiler furnaces, catalytic reduction of nitrogen oxides);
- processes reducing atmospheric emission of sulfur dioxide (stack gas desulfurization using lime, magnesite and ammonia-digestion technique, fluidized-bed fuel combustion, conversion to fuels with a lower sulfur content).

*Industrial and municipal boilers:*

- elimination owing to power production from other sources;
- conversion to fuels with a lower sulfur content.

*Machine building and metal-processing enterprises:*

- installation of various dust collectors (fibre filters, wet dust collectors, Venturi scrubbers, etc.);
- replacement of heating furnaces by the induction ones;
- replacement of cupolas by induction furnaces;
- installation of core-making machines instead of driers;
- reburning of cupola gases.

*Building material production:*

- installation of various dust collectors (electrostatic precipitators, bag filters);
- stack gas desulfurization using lime (at rotating furnaces of large cement plants).

These examples (far from being complete) can be extended in the process of accumulating experience of MARS application to various cities/regions. In this respect the application of MARS is considered one of the most realistic ways to compose inventories of atmosphere protection activities. In practice, when preparing data on initial activities, it is convenient to use a system of specific indices developed with regard to various atmosphere protection processes and associated with specific sources. This approach can be considered another step towards composing a classification of atmosphere protection activities.

As an illustration, let us give data characterizing the variations of specific cost indices for some technological solutions which are often used: energy production to reduce the emission of ash (Table 7.2); nitrogen oxides (Table 7.3); and sulfur oxides (Table 7.4). Similar grounds to determining the characteristics of various air protection measures can also be developed for other industries.

Table 7.2 Ash emission decreasing characteristics.

Measure name	Emission Decrease %	Capital Costs rub/Km <sup>3</sup> /hour	Operational Costs rub/Mm <sup>3</sup>
Multicyclone	95.0	225	13.5
Recirculation Multicyclone	95.0	250	14.0
Bag-filter	95.0	170	13.5
Wet Venturi	96.0	135	9.0
Wet Scrubber	96.0	105	7.5
Wet Scrubber D	98.0	120	8.0
Electric Precipitator UG-2-3	98.0	690	30.0
Electric Precipitator UG-3-3	99.0	780	26.0
Electric Precipitator UG-2-4	99.0	885	39.0
Electric Precipitator UG-3-4	99.5	900	31.5
Centrifugal Scrubber plus Electric Precipitator UG-2-3	99.5	765	23.0

**Table 7.3** NO<sub>x</sub> emission decreasing characteristics for the set of measures. Gas and liquid fuel.

Measure name	Emission Decrease %	Vapour productiv. of boiler	Capital Costs rub/Km <sup>3</sup> /hour	Operational Costs rub/Mm <sup>3</sup>
Stright flow burners	20.0	220-670	78	0.6-2.0
		950-1750	46	
		2650-3650	27	
Boilers transfer to combustion with low air access	30.0	220-670	156	0.4-4.0
		950-1750	129	
		2650-3650	18	
Transfer to direct injection or installation of aeration for high moisture coal	50.0	220-670	123	5.0-15.0
		950-1750	66	
		2650-3650	36	
Complex of measures	60.0	220-670	280	6.0-20.0
		950-1750	214	
		2650-3650	53	

**Table 7.4** NO<sub>x</sub> emission decreasing characteristics for the set measures. Pulverized coal fuel.

Measure name	Emission Decrease %	Vapour productiv. of boiler	Capital Costs rub/Km <sup>3</sup> /hour	Operational Costs rub/Mm <sup>3</sup>
Two stage combustion	20-25	120-170	120	1.5-2.6
		210-275	110	
		320-500	78	
		640-670	59	
		800-1250	55	
Gas recyculation into combustion core for solid bottom	20-25	120-170	245	2.0-4.0
		210-275	175	
		320-500	120	
		640-670	100	
		800-1250	80	
Transfer to direct injection or installation of aeration mills for high moisture coals	20-25	120-170	600	7.0-18.0
		210-275	500	
		320-500	480	
		640-670	325	
		800-1250	280	
Furnace tranfer from liquid to solid slag removal for high moisture coals	20-25	120-170	1760	27.9-96
		210-275	1050	
		320-500	700	
		640-670	500	
		800-1250		

About 150-250 large air pollution sources are usually considered in real cities with the population of 0.5-1 million people. The initial bank usually includes 100-200 measures on reduction of the most typical pollutant emissions. In meso-scale regions the amount of aggregated sources usually makes up 300-500, the number of initial measures being equal to 150-200, since MARS-2 treats sulfur compounds as "the main" pollutant.

*Calculation of relative danger coefficients.*

The mean values of  $\sigma$  in each raster of the regular grid are evaluated in accordance with *Approximate economic damage ...* (1986):

$$\sigma = \frac{\sigma_i \cdot S_i}{S},$$

where  $S$  is the area of the raster;  $S_i$  the area within the raster covered by the  $i$ -th type of recipients (forests, agricultural lands, populated areas, etc.).  $\sigma_i$  values are tabulated.

To assess the areas occupied by various recipients in each raster one can use the data on the land use structure in the given region. If a city is considered, a single value of  $\sigma$  can be calculated for the whole territory in accordance with the population density.

*Calculation of meteorological parameters.*

To evaluate meteorological parameters, one can use climatic hand-book data for relevant aerologic stations situated in (or adjacent to) the territory of the city/region. Calculation methods are considered in detail in Section 4.

*Physico-chemical parameters.*

These parameters are obtained by generalizing reported data, in particular from reviews (Eliassen, 1980; Air pollution, 1982; Ryaloshapko, 1983; Galperin, 1985; Fisher, 1983; Henry et al., 1984).

The formation and accompaniment of a data base in MARS is carried out by special programs.

### 8. Illustrative Examples

The calculation was done for a hypothetical city and region. The test city is represented by the regular grid 9 × 6 with a space of 1 km. Twelve sources emitting six types of pollutants into the air basin are located on its territory. All the data necessary for calculation using the MARS model blocks are given in Tables 8.1, 8.2, and 8.3. The maximum emissions (in g/sec) are used for calculation of the near ground concentrations under normal unfavorable conditions.

Table 8.1 Data about the city.

Number of sources: 12

Wind directions	South	S-West	West	N-West	Nord	N-East	East	S-East
Reiteration speed(m/s):	0.150 5.9	0.170 6.4	0.130 5.9	0.100 5.6	0.100 4.8	0.100 5.1	0.110 4.6	0.140 5.3

Mean annual speed of the wind near the surface (m/s): 5.5000  
 Mean annual temperature of the air ( C ): 5.0000  
 Temperature in June/July in 13.00 ( C ): 19.0

Regular grid parameters for the city:

The number of cells from the West to the East (X-axes): 9  
 The number of cells from the South to the Nord(Y-axes): 6  
 Grid step (km): 1.0  
 Accuracy of the "SIGMA" calculation: 4

Pollutant number upon which the data have been entered: 1 2 3 4 6 7

"SIGMA matrix"

test (city)

6	1.60	2.40	2.70	0.80	3.40	3.90	3.10	5.20	5.90
5	4.00	4.00	4.00	6.20	7.80	6.30	4.60	4.20	3.40
4	2.30	2.60	2.90	3.60	2.80	1.30	1.40	1.40	2.30
3	1.60	0.50	0.80	3.10	3.60	2.30	2.70	2.80	4.30
2	4.00	4.00	1.50	1.90	5.20	5.10	5.20	6.30	7.00
1	4.00	3.60	1.30	1.80	4.20	4.60	5.00	4.10	3.20
	1	2	3	4	5	6	7	8	9

Table 8.2 Information about the sources of the city.

Number	H m	Diam m	Temp. grad.C	Volume 3 m /s	Coeff SIGMA	% Dust sep.	Total emission of pollutants ktons/year							Source Coordinat., km	
							Dust	SO 2	NO X	NH 3	CH	HF	CO	X	Y
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1.	200.0	8.1	138.0	225.9	3.49	0.0	0.500	25.600	1.150	0.000	0.000	0.000	1.344	2.25	3.50
2.	83.0	7.4	220.0	303.8	3.90	0.0	0.210	9.700	0.540	0.000	0.000	0.000	0.000	7.50	4.90
3.	103.0	4.8	200.0	81.7	3.49	0.0	0.054	1.200	0.100	0.000	0.000	0.000	0.000	5.70	2.10
4.	20.0	0.6	210.0	0.3	4.66	0.0	0.000	0.130	0.020	0.000	0.000	0.000	0.000	4.49	4.92
5.	20.0	0.3	200.0	0.5	2.08	0.0	0.070	0.090	0.010	0.000	0.000	0.000	0.016	2.67	1.83
6.	18.0	0.6	160.0	0.1	3.52	0.0	0.050	0.040	0.000	0.000	0.000	0.000	0.008	8.22	2.43
7.	15.0	0.5	45.0	0.0	2.71	0.0	0.060	0.060	0.000	0.000	0.000	0.000	0.014	6.46	3.81
8.	24.0	0.8	180.0	0.5	4.18	0.0	0.010	0.140	0.010	0.000	0.000	0.000	0.002	3.57	3.30
9.	102.0	2.0	45.0	19.4	3.15	0.0	0.000	9.700	4.300	0.000	0.000	0.000	0.000	1.50	5.16
10.	33.0	0.8	20.0	1.6	4.14	81.1	1.100	0.000	0.000	0.000	0.000	0.220	0.000	4.31	1.66
11.	30.0	0.4	20.0	1.5	4.49	0.0	3.200	0.000	0.000	0.000	0.000	0.000	0.000	5.12	3.87
12.	23.0	0.6	37.0	2.6	2.00	0.0	0.020	0.000	0.000	1.503	0.000	0.008	0.000	1.91	1.72
Total emission of pollutants in region							5.3	46.7	6.1	1.5	0.0	0.2	1.4		



Table 8.3 Max emission data (city).

Source number	MAX emission, g/s						
	Dust	SO <sub>2</sub>	NO <sub>X</sub>	NH <sub>3</sub>	CH	HF	CO
1	17	18	19	20	21	22	23
1.	40.30	990.00	312.00	0.00	0.00	0.00	107.53
2.	40.60	960.10	72.60	0.00	0.00	0.00	0.00
3.	10.10	560.30	18.40	0.00	0.00	0.00	0.00
4.	0.00	8.00	0.70	0.00	0.00	0.00	0.00
5.	3.70	4.90	0.40	0.00	0.00	0.00	0.76
6.	2.70	2.70	0.00	0.00	0.00	0.00	0.48
7.	3.90	3.60	0.00	0.00	0.00	0.00	0.90
8.	1.00	12.00	1.10	0.00	0.00	0.00	0.20
9.	0.00	304.60	132.40	0.00	0.00	0.00	0.00
10.	7.40	0.00	0.00	0.00	0.00	6.90	0.00
11.	62.20	0.00	0.00	0.00	0.00	0.00	0.00
12.	3.50	0.00	0.00	45.97	0.00	0.26	0.00

The structure of the economic damage according to the sources and pollutants is obtained (Table 8.4) after realization of the model of determination.

Table 8.4 Economic damage structure in the city.

Source Number	Full economic damage components Krubles/year							Full economic Damage Krubles/year	Full economic Damage %
	Dust	SO <sub>2</sub>	NO <sub>X</sub>	NH <sub>3</sub>	CH	HF	CO		
1	2	3	4	5	6	7	8	9	10
1.	1883.3	330.4	37.0	0.0	0.0	0.0	1.1	2251.77	10.09
2.	883.8	217.6	30.2	0.0	0.0	0.0	0.0	1131.48	5.07
3.	203.5	21.5	4.5	0.0	0.0	0.0	0.0	229.52	1.03
4.	0.0	8.4	3.2	0.0	0.0	0.0	0.0	11.62	0.05
5.	157.1	2.6	0.7	0.0	0.0	0.0	0.0	160.52	0.72
6.	190.3	2.2	0.0	0.0	0.0	0.0	0.0	192.57	0.86
7.	175.4	3.2	0.0	0.0	0.0	0.0	0.0	178.60	0.80
8.	45.1	7.9	1.4	0.0	0.0	0.0	0.0	54.38	0.24
9.	0.0	288.4	318.4	0.0	0.0	0.0	0.0	606.79	2.72
10.	952.9	0.0	0.0	0.0	0.0	938.3	0.0	1891.26	8.48
11.	15526.5	0.0	0.0	0.0	0.0	0.0	0.0	15526.49	69.59
12.	43.1	0.0	0.0	15.4	0.0	17.3	0.0	75.78	0.34
Total	20061.0	882.2	395.4	15.4	0.0	955.6	1.2	22310.77	
%	89.9	4.0	1.8	0.1	0.0	4.3	0.0		100.00

The results obtained at the A stage of the optimization algorithm are given in Tables 8.5–8.7. Here the bank of initial actions is divided into groups, where each of columns 6–21 characterizes the corresponding action from the point of view of one of the criteria. Expenses on realization of the given action are shown in columns 4 and 5 of the tables. The table of alternatives associated with each of the groups permits composition of permissible series at the stage B of the algorithm.



Table 8.6 Initial measures database for emission decrease in the sources ("+" increase, "-" decrease).

A. group 2

Number meas.	Number Sour.	Invest. K rb/year	Full expend. K rb/year	Pollutants emission variations, Ktons/year							Variation damage K rb/year	
				Dust	SO <sub>2</sub>	NO <sub>x</sub>	NH <sub>3</sub>	CH	HF	CO		
2.	1.	4.	16.8	9.1	0.000	-0.130	-0.014	0.000	0.000	0.000	0.000	-10.7
2.	2.	4.	10.0	-6.6	0.000	-0.020	-0.020	0.000	0.000	0.000	0.000	-227.4
2.	3.	5.	6.0	-7.4	-0.069	0.070	0.020	0.000	0.000	0.000	0.000	-221.1
2.	4.	6.	6.0	-4.6	-0.049	0.030	0.000	0.000	0.000	0.000	0.000	-224.4
2.	5.	7.	9.0	-6.2	-0.059	0.040	0.000	0.000	0.000	0.000	0.000	-223.1

B.

Number group	Number measurment	Source number	Index variations							Total
			Dust	SO <sub>2</sub>	NO <sub>x</sub>	NH <sub>3</sub>	CH	HF	CO	
1	2	3	14	15	16	17	18	19	20	21
2.	1.	4.	0.00	-1.08	-0.25	0.00	0.00	0.00	0.00	-1.32
2.	2.	4.	0.00	-1.08	-0.35	0.00	0.00	0.00	0.00	-1.43
2.	3.	5.	0.00	0.00	-0.11	0.00	0.00	0.00	0.00	-0.11
2.	4.	6.	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2.	5.	7.	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

C. The table of the incompatible measures group 2

	1	2	3	4	5
1	*	*			
2	*	*			
3			*		
4				*	
5					*

Table 8.7 Initial measures database for emission decrease in the sources ("+" increase, "-" decrease).

A. group 1

Number meas.	Number Sour.	Invest. K rb/year	Full expend. K rb/year	Pollutants emission variations, Ktons/year							Variation damage K rub/year	
				Dust	SO <sub>2</sub>	NO <sub>X</sub>	NH <sub>3</sub>	CH	HF	CO		
1	2	3	4	5	6	7	8	9	10	11	12	13
3.	1.	9.	7840.0	1000.0	0.000	-9.700	-4.300	0.000	0.000	0.000	0.000	-606.8
3.	2.	10.	650.0	99.0	-1.093	0.000	0.000	0.000	0.000	0.000	-0.220	-1885.3
3.	3.	11.	60.4	27.0	-3.139	0.000	0.000	0.000	0.000	0.000	0.000	-15513.8
3.	4.	12.	1260.0	178.0	0.000	0.000	0.000	-1.423	0.000	-0.003	0.000	-21.3

B.

Number group	Number measurment	Source number	Index variations							Total	
			Dust	SO <sub>2</sub>	NO <sub>X</sub>	NH <sub>3</sub>	CH	HF	CO		
1	2	3	14	15	16	17	18	19	20	21	
3.	1.	9.	0.00	-8.89	-47.18	0.00	0.00	0.00	0.00	0.00	-56.06
3.	2.	10.	0.00	0.00	0.00	0.00	0.00	-11.61	0.00	0.00	-11.61
3.	3.	11.	-17.30	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-17.30
3.	4.	12.	0.00	0.00	0.00	-36.06	0.00	0.00	0.00	0.00	-36.06

C.

The table of the incompatible measures group 3

	1	2	3	4
1	*			
2		*		
3			*	
4				*

The major results of the MARS-I use for calculations for a hypothetical city are the optimum functions of expense-effect received for various criteria for the investments presented in Figure 8.1.

Curves 1,2,3, are the optimum trajectories of particulate matter, SO<sub>2</sub>, NO<sub>x</sub> annual emission reduction, correspondingly.

Curve 4 characterizes the possibility of the economic damage prevention.

Curves 5,6 are plotted for the index of particle concentrations and for the total index of all six pollutant concentrations participating in calculation.

The example of the optimum series of actions for the A point, corresponding to an expense of 10.8 mln. roubles (the optimum strategy) is given in Table 8.8.

Table 8.8 Optimal strategy ("+" increase, "-" decrease).

Resource 4 Criterion 21 Expenditures limit 10800 KRub.

Number group	Number meas.	Number Sour.	Invest. Krub	Full expend. Krub	Pollutant emission variations, Ktons/year							Variation damage K/rub/year
					Dust	SO <sub>2</sub>	NO <sub>x</sub>	NH <sub>3</sub>	CH	HF	CO	
1	2	3	4	5	6	7	8	9	10	11	12	13
3.	3.	11.	60.4	27.0	-3.139	0.000	0.000	0.000	0.000	0.000	0.000	-15513.8
2.	2.	4.	10.0	-6.6	-0.000	-0.020	-0.020	0.000	0.000	0.000	0.000	-227.4
3.	4.	12.	1260.0	178.0	-0.000	0.000	0.000	-1.423	0.000	-0.003	0.000	-31.3
3.	2.	10.	650.0	99.0	-1.093	0.000	0.000	0.000	0.000	-0.220	0.000	-1885.3
2.	3.	5.	6.0	-7.4	-0.069	0.000	0.020	0.000	0.000	0.000	-0.016	-221.1
3.	1.	9.	7840.0	1000.0	0.000	-9.700	-4.300	0.000	0.000	0.000	0.000	-606.8
1.	3.	1.	70.8	20.5	0.000	0.000	-0.259	0.000	0.000	0.000	0.000	-17.7
1.	6.	2.	87.5	73.3	0.000	0.000	-0.270	0.000	0.000	0.000	0.000	-16.1
1.	1.	1.	700.0	1657.7	-0.500	-25.600	-0.287	0.000	0.000	0.000	-1.344	-2224.2
1.	5.	2.	95.2	27.5	0.000	0.000	-0.162	0.000	0.000	0.000	0.000	-10.1
Total			10779.9	3069.0	-4.801	-35.250	-5.278	-1.423	0.000	-0.223	-1.360	-20743.8
Total (%)					-91.0	-75.5	-86.1	-94.7	0.0	-97.9	-98.3	-93.0

Number group	Number meas.	Number Sour.	Pollutant emission variations, Ktons/year							Full Index	Efficiency
			Dust	SO <sub>2</sub>	NO <sub>x</sub>	NH <sub>3</sub>	CH	HF	CO		
1	2	3	14	15	16	17	18	19	20	21	22
3.	3.	11.	-17.3	0.0	0.000	0.00	0.00	0.00	0.00	-17.30	-0.286
2.	2.	4.	0.0	-1.08	-0.350	0.00	0.00	0.00	0.00	-1.43	-0.143
3.	4.	12.	0.0	0.0	0.000	-36.06	0.00	-0.00	0.00	-36.06	-0.029
3.	2.	10.	0.0	0.0	0.000	0.00	0.00	-11.61	0.00	-11.61	-0.018
2.	3.	5.	0.0	-0.00	-0.110	0.00	0.00	0.00	0.00	-0.11	-0.018
3.	1.	9.	0.0	-8.89	-47.180	0.00	0.00	0.00	0.00	-56.06	-0.007
1.	3.	1.	0.0	0.0	-0.170	0.00	0.00	0.00	0.00	-0.17	-0.002
1.	6.	2.	0.0	0.0	-0.070	0.00	0.00	0.00	0.00	-0.07	0.001
1.	1.	1.	0.0	-0.0	-0.180	0.00	0.00	0.00	0.00	-0.18	-0.000
1.	5.	2.	0.0	0.0	-0.020	0.00	0.00	0.00	0.00	-0.02	-0.000
Total			-17.30	-9.99	-48.08	-36.06	0.00	-11.61	0.00	-123.01	
Total (%)			-79.91	-58.95	-71.45	-76.15	0.00	-60.37	0.00	-71.34	

The regional test is calculated for a territory of 60 km × 50 km ( 6 × 5 with the space of 10 km) and seven sources of five pollutants.

Tables 8.9 and 8.10 comprise the data on the region and pollutants necessary for calculation using MARS-2 as a region.

Table 8.9 Data about the region.

Number of sources: 7

Wind directions	South	S-West	West	N-West	Nord	N-East	East	S-East
Reiteration	0.400	0.100	0.100	0.050	0.050	0.050	0.050	0.200

Wind directions	Dir. 1	Dir. 2	Dir. 3	Dir. 4	Dir. 5	Dir. 6	Dir. 7	Dir. 8	Dir. 9	Dir.10	Dir.11	Dir.12
Reiteration	0.200	0.200	0.050	0.050	0.050	0.050	0.050	0.050	0.050	0.050	0.100	0.100

Mean annual speed of the wind near the surface (m/s): 5.1000  
 Mean annual temperature of the air ( C ): 5.0000  
 Mean annual height of the layer permeation (m): 680.0000  
 Mean annual precipitation (mm/year): 700.0000  
 Mean annual atm. stratification parameter: 0.0900  
 Mean ann. vertic. diffusion coeff. in layer permeation (m\*\*2/s): 6.9000  
 Mean ann. goriz. diffusion coeff. in layer permeation (m\*\*2/s): 8.2000  
 SO2 time span relative to its transformation into SO4(hour): 67.0000  
 SO2 time span relative to its dry deposition (hour): 13.0000  
 SO4 time span relative to its dry deposition (hour): 300.0000  
 SO2 wash-out coefficient (1/mm): 0.3600  
 SO4 wash-out coefficient (1/mm): 0.3600  
 SO2 dry deposition speed (m/s): 0.0100  
 SO4 dry deposition speed (m/s): 0.0020  
 Time interval (min): 10.0000

Regular grid parameters for the region:

The quantity of cells from the West to the East (X-axes): 6  
 The quantity of cells from the South to the Nord(Y-axes): 5  
 Grid step (km): 10.0  
 Accuracy of the "SIGMA" calculation: 10

Pollutant numbers upon which the data has been entered: 1 2 3 4 6

Agressive pollutants coefficients:

1.Dust 45.0  
 2.SO2 16.5  
 3.NOx 41.1  
 4.NH3 4.6  
 5.CH 1.3  
 6.HF 980.0  
 7.CO 1.0

"SIGMA matrix"  
 TEST REGION

5	2.30	2.80	3.20	3.80	4.60	4.50
4	2.10	2.70	3.80	3.90	5.10	4.00
3	1.00	3.20	3.60	4.40	4.70	4.50
2	1.60	2.70	2.40	3.90	4.90	5.20
1	2.20	2.60	3.70	3.20	3.80	3.80
	1	2	3	4	5	6

Table 8.10 Information about the sources. Listing 1.

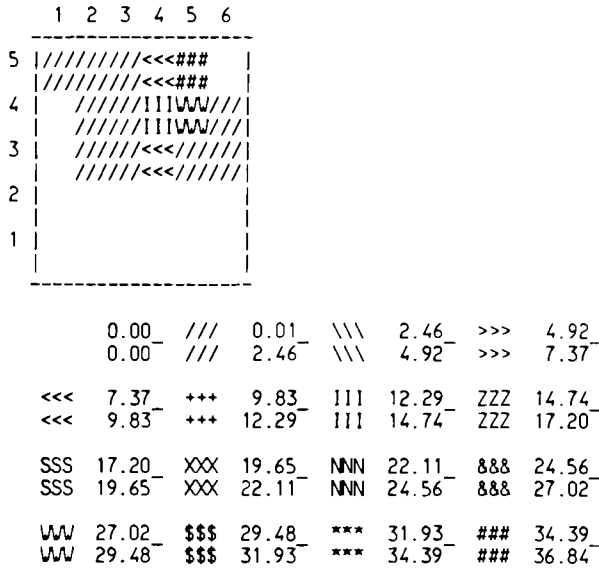
Number	H m	Diam m	Temp. grad.C	Volume 3 m /s	Coeff SIGMA	% Dust sep.	Total emission of pollutants ktons/year							Source Coordinat., km		
							Dust	SO 2	NO X	NH 3	CH	HF	CO	X	Y	
							8	9	10	11	12	13	14	15	16	
1.	100.0	2.0	220.0	97.0	3.62	90.0	0.800	10.00	2.000	0.000	0.000	0.000	0.000	0.000	31.60	35.80
2.	150.0	3.0	230.0	160.0	4.42	70.0	0.500	15.00	2.000	0.000	0.000	0.000	0.000	42.40	28.30	
3.	250.0	4.0	200.0	800.0	3.39	92.0	13.000	55.00	9.000	0.000	0.000	0.000	0.000	24.90	28.20	
4.	80.0	0.8	200.0	103.0	3.15	94.0	1.200	12.00	4.000	0.000	0.000	0.000	0.000	25.10	49.00	
5.	100.0	1.8	150.0	47.0	3.93	0.0	1.000	8.00	0.800	0.000	0.000	0.000	0.000	34.70	28.70	
6.	50.0	0.4	50.0	7.0	5.10	0.0	0.900	0.00	0.000	1.000	0.000	0.100	0.000	41.80	29.30	
7.	80.0	0.6	40.0	4.6	4.41	0.0	1.700	0.00	0.000	2.500	0.000	0.280	0.000	41.20	43.00	
Total emission of pollutants in region							19.1	100.0	17.8	3.5	0.0	0.4	0.0			

The structure of the economic damage according to sources and pollutants and the distribution of the total economic damage along the elements of the regular grid are presented in Table 8.11.

Table 8.11 Economic damage structure in the region.

Source Number	Full economic damage components Krubles/year							Full economic Damage Krubles/year	Full economic Damage %
	Dust	SO <sub>2</sub>	NO <sub>x</sub>	NH <sub>3</sub>	CH <sub>4</sub>	HF	CO		
1	2	3	4	5	6	7	8	9	10
1.	42.1	193.1	96.2	0.0	0.0	0.0	0.0	331.46	1.56
2.	192.8	246.2	81.8	0.0	0.0	0.0	0.0	520.74	2.44
3.	311.7	483.5	197.1	0.0	0.0	0.0	0.0	992.19	4.66
4.	68.9	252.7	209.8	0.0	0.0	0.0	0.0	531.46	2.49
5.	4249.5	207.8	51.8	0.0	0.0	0.0	0.0	4509.10	21.16
6.	4957.2	0.0	0.0	20.7	0.0	437.0	0.0	5414.87	25.41
7.	8100.0	0.0	0.0	37.1	0.0	876.6	0.0	9013.68	42.29
Total	17922.3	1383.3	636.6	57.7	0.0	1313.6	0.0	21313.50	
%	84.1	6.5	3.0	0.3	0.0	6.2	0.0		100.00

Economic damage distribution in the region (%)  
 TEST REGION Pollutant 1  
 1% of the economic damage = 179.223 Krubles/year



The calculation results on the model of transport, transformation and deposition of SO<sub>2</sub> in the atmosphere of the region and the distribution of the potential damage indices for coniferous from sulfur compounds total deposition, as well, are presented in the same table.

Tables 8.12-8.14 are the bank of the initial regional actions.



Table 8.12 Initial measures database for emission decrease in the sources ("+" increase, "-" decrease).

group 1

Number meas.	Number Sour.	Invest. K rb/year	Full expend. K rb/year	Pollutants emission variations, Ktons/year								Variation damage K rub/year
				Dust	SO <sub>2</sub>	NO <sub>x</sub>	NH <sub>3</sub>	CH	HF	CO		
2	3	4	5	6	7	8	9	10	11	12	13	
1.	1.	360.0	170.0	-0.618	-1.000	0.000	0.000	0.000	0.000	0.000	0.000	-51.9
2.	1.	370.0	90.0	-0.654	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-34.5
3.	1.	1860.0	520.0	0.000	-1.000	-0.400	0.000	0.000	0.000	0.000	0.000	-38.6
4.	1.	3000.0	700.0	0.000	-3.000	0.000	0.000	0.000	0.000	0.000	0.000	-57.9
5.	2.	4800.0	500.0	0.000	-4.500	-1.000	0.000	0.000	0.000	0.000	0.000	-114.7
6.	2.	190.0	50.0	-0.470	-1.500	0.000	0.000	0.000	0.000	0.000	0.000	-205.9
7.	2.	5000.0	600.0	0.000	-9.000	0.000	0.000	0.000	0.000	0.000	0.000	-147.7
8.	2.	3500.0	400.0	0.000	-3.750	0.000	0.000	0.000	0.000	0.000	0.000	-61.5

Number meas.	Number sour.	Variation total deposit. Ktons/year	Variation Sulphur transfer out of region, Ktons/year								Variation index danger conifer	
			Total	sector1	sector2	sector3	sector4	sector5	sector6	sector7		sector8
2	3	14	15	16	17	18	19	20	21	22	23	24
1.	1.	-0.04	-0.46	-0.129	-0.095	-0.059	-0.034	-0.033	-0.033	-0.033	-0.043	-0.06
2.	1.	0.00	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.00
3.	1.	-0.04	-0.46	-0.129	-0.095	-0.059	-0.034	-0.033	-0.033	-0.033	-0.043	-0.06
4.	1.	-0.12	-1.38	-0.388	-0.284	-0.178	-0.102	-0.099	-0.099	-0.099	-0.129	-0.16
5.	2.	-0.18	-2.07	-0.599	-0.415	-0.257	-0.145	-0.145	-0.154	-0.155	-0.201	-0.34
6.	2.	-0.06	-0.69	-0.200	-0.138	-0.086	-0.048	-0.048	-0.051	-0.052	-0.067	-0.13
7.	2.	-0.36	-4.14	-1.199	-0.829	-0.515	-0.291	-0.291	-0.308	-0.311	-0.401	-0.56
8.	2.	-0.15	-1.73	-0.499	-0.346	-0.215	-0.121	-0.121	-0.128	-0.129	-0.167	-0.29

The table of the incompatible measures  
group 1

	1	2	3	4	5	6	7	8
1	*	*						
2	*	*						
3			*					
4				*				
5					*			*
6						*		
7							*	
8					*			*

Table 8.13 Initial measures database for emission decrease in the sources ("+" increase, "-" decrease).

group 2

Number meas.	Number Sour.	Invest. K rb/year	Full expend. K rb/year	Pollutants emission variations, Ktons/year								Variation damage K rb/year
				Dust	SO <sub>2</sub>	NO <sub>x</sub>	NH <sub>3</sub>	CH	HF	CO		
2	3	4	5	6	7	8	9	10	11	12	13	
1.	3.	44000.0	5780.0	-0.381	-37.320	-2.700	0.000	0.000	0.000	0.000	-309.1	
2.	3.	1280.0	350.0	0.000	-11.000	-1.800	0.000	0.000	0.000	0.000	-136.1	
3.	3.	2480.0	370.0	-1.950	-5.500	0.000	0.000	0.000	0.000	0.000	-95.1	
4.	4.	700.0	1650.0	-1.200	-12.000	-1.000	0.000	0.000	0.000	0.000	-374.1	
5.	4.	150.0	70.0	-0.960	0.000	0.000	0.000	0.000	0.000	0.000	-55.1	
6.	4.	5640.0	2920.0	-1.200	-12.000	-3.400	0.000	0.000	0.000	0.000	-500.0	
7.	3.	2000.0	300.0	0.000	-11.000	0.000	0.000	0.000	0.000	0.000	-96.7	

Number meas.	Number sour.	Variation total deposit Ktons/yr	Variation Sulphur transfer out of region, Ktons/year										Variation index danger conifer
			Total	sector1	sector2	sector3	sector4	sector5	sector6	sector7	sector8		
2	3	14	15	16	17	18	19	20	21	22	23	24	
1.	3.	-1.86	-16.80	-4.618	-3.394	-2.135	-1.277	-1.277	-1.277	-1.277	-1.548	-9.17	
2.	3.	-0.55	-4.95	-1.361	-1.000	-0.629	-0.376	-0.376	-0.376	-0.376	-0.456	-3.50	
3.	3.	-0.27	-2.48	-0.681	-0.500	-0.315	-0.188	-0.188	-0.188	-0.188	-0.228	-1.83	
4.	4.	-0.35	-5.65	-1.622	-1.182	-0.739	-0.433	-0.411	-0.387	-0.383	-0.495	-0.28	
5.	4.	0.00	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.00	
6.	4.	-0.35	-5.65	-1.622	-1.182	-0.739	-0.433	-0.411	-0.387	-0.383	-0.495	-0.28	
7.	3.	-0.55	-4.95	-1.361	-1.000	-0.629	-0.376	-0.376	-0.376	-0.376	-0.456	-3.50	

The table of the incompatible measures group 2

	1	2	3	4	5	6	7
1	*						
2		*					*
3			*				
4				*	*	*	
5				*	*	*	
6				*	*	*	
7		*					*

Table 8.14 Initial measures database for emission decrease in the sources (“+” increase, “-” decrease).

group 3

Number meas.	Number Sour.	Invest. K rb/year	Full expend. K rb/year	Pollutants emission variations, Ktons/year								Variation damage K rub/year
				Dust	SO <sub>2</sub>	NO <sub>x</sub>	NH <sub>3</sub>	CH	HF	CO		
2	3	4	5	6	7	8	9	10	11	12	13	
1.	5.	1000.0	120.0	-0.280	1.000	1.000	0.000	0.000	0.000	0.000	0.000	-4210.8
2.	6.	650.0	100.0	-2.584	0.000	0.000	0.000	0.000	0.000	-0.380	0.000	-14292.5
3.	6.	1260.0	200.0	0.000	0.000	0.000	-0.947	0.000	0.000	-0.041	0.000	-197.4
4.	7.	700.0	100.0	-1.190	0.000	0.000	-2.110	0.000	0.000	-0.280	0.000	-9013.7
5.	7.	350.0	150.0	-1.054	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-5022.0

Number meas.	Number sour.	Variation total deposit. Ktons/yr	Variation Sulphur transfer out of region, Ktons/year										Variation index danger conifer
			Total	sector1	sector2	sector3	sector4	sector5	sector6	sector7	sector8		
2	3	14	15	16	17	18	19	20	21	22	23	24	
1.	5.	0.00	0.50	0.139	0.124	0.077	0.041	0.031	0.022	0.024	0.043	0.59	
2.	6.	0.00	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.00	
3.	6.	0.00	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.00	
4.	7.	0.00	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.00	
5.	7.	0.00	0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.00	

The table of the incompatible measures group 3

	1	2	3	4	5
1	*				
2		*	*	*	*
3		*	*		
4		*		*	*
5		*		*	*

Figure 8.2 represents the optimum functions of expense-effect calculated for the three types of criteria:

- the maximum decreasing of total sulfur compounds emission;
- the maximum prevention of the economic damage from the atmosphere pollution in the region.

Table 8.15 is the optimum series of actions for B point (Figure 8.2) corresponding to the expense of 63.7 mln. roubles and decreasing of sulfur compounds deposition for 85.8%.

Table 8.15 Optimal strategy ("+" increase, "-" decrease).

Table 8.15: Optimal strategy ("+" increase, "-" decrease)

Resource 4 Criterion 14 Investments 63700.0 Krub.

Number group	Number meas.	Number Sour.	Invest. Krub	Full expend. Krub	Pollutant emission variations, Ktons/year								Variation damage K rub/year
					Dust	SO <sub>2</sub>	NO <sub>x</sub>	NH <sub>3</sub>	CH	HF	CO		
1	2	3	4	5	6	7	8	9	10	11	12	13	
2.	4.	4.	700.0	1650.0	-1.200	-12.000	-1.000	0.000	0.000	0.000	0.000	-374.1	
2.	2.	3.	1280.0	350.0	0.000	-11.000	-1.800	0.000	0.000	0.000	0.000	-136.1	
1.	6.	2.	190.0	50.0	-0.470	-1.500	0.000	0.000	0.000	0.000	0.000	-205.9	
1.	1.	1.	360.0	170.0	-0.618	-1.000	0.000	0.000	0.000	0.000	0.000	-51.9	
2.	3.	3.	2480.0	370.0	-1.950	-5.500	0.000	0.000	0.000	0.000	0.000	-95.1	
1.	7.	2.	5000.0	600.0	0.000	-9.000	0.000	0.000	0.000	0.000	0.000	-147.7	
2.	1.	3.	44000.0	5780.0	-0.381	-37.320	-2.700	0.000	0.000	0.000	0.000	-309.1	
1.	4.	1.	3000.0	700.0	0.000	-3.000	0.000	0.000	0.000	0.000	0.000	-57.9	
1.	5.	2.	4800.0	500.0	0.000	-4.500	-1.000	0.000	0.000	0.000	0.000	-114.7	
1.	3.	1.	1860.0	520.0	0.000	-1.000	-0.400	0.000	0.000	0.000	0.000	-38.6	
Total			63670.0	10690.0	-4.619	-25.500	-6.900	0.000	0.000	0.000	0.000	-1531.0	
Total(%)					-24.2	-25.5	-38.8	0.0	0.0	0.0	0.0	-7.2	

Number group	Number meas.	Number sour. K t/year	Variation total deposit.	Variation Sulphur transfer out of region, Ktons/year								Variation index damage conifer	Efficien. c.14/c. 4	
				Total	sector1	sector2	sector3	sector4	sector5	sector6	sector7			sector8
1	2	3	14	15	16	17	18	19	20	21	22	23	24	26
2.	4.	4.	-0.3	-5.7	-1.622	-1.182	-0.739	-0.433	-0.411	-0.387	-0.383	-0.495	-0.28	0.000
2.	2.	3.	-0.5	-5.0	-1.361	-1.000	-0.629	-0.376	-0.376	-0.376	-0.376	-0.456	-3.50	0.000
1.	6.	2.	-0.1	-0.7	-0.200	-0.138	-0.086	-0.048	-0.048	-0.051	-0.052	-0.067	-0.13	0.000
1.	1.	1.	-0.0	-0.5	-0.129	-0.095	-0.059	-0.034	-0.033	-0.033	-0.033	-0.043	-0.06	0.000
2.	3.	3.	-0.3	-2.5	-0.681	-0.500	-0.315	-0.188	-0.188	-0.188	-0.188	-0.228	-1.83	0.000
1.	7.	2.	-0.4	-4.1	-1.199	-0.829	-0.515	-0.291	-0.291	-0.308	-0.311	-0.401	-0.56	0.000
2.	1.	3.	-1.9	-16.8	-4.618	-3.394	-2.135	-1.277	-1.277	-1.277	-1.277	-1.548	-9.17	0.000
1.	4.	1.	-0.1	-1.4	-0.388	-0.284	-0.178	-0.102	-0.099	-0.099	-0.099	-0.129	-0.16	0.000
1.	5.	2.	-0.2	-2.1	-0.599	-0.415	-0.257	-0.145	-0.145	-0.154	-0.155	-0.201	-0.34	0.000
1.	3.	1.	0.0	-0.5	-0.129	-0.095	-0.059	-0.034	-0.033	-0.033	-0.033	-0.043	-0.06	0.000
Total			-3.82	-39.09	-10.926	-7.931	-4.973	-2.929	-2.901	-2.907	-2.908	-3.611	-16.08	
Total(%)			-85.80	-85.82	-85.732	-85.843	-85.816	-86.062	-86.084	-85.867	-85.847	-85.601	-68.34	

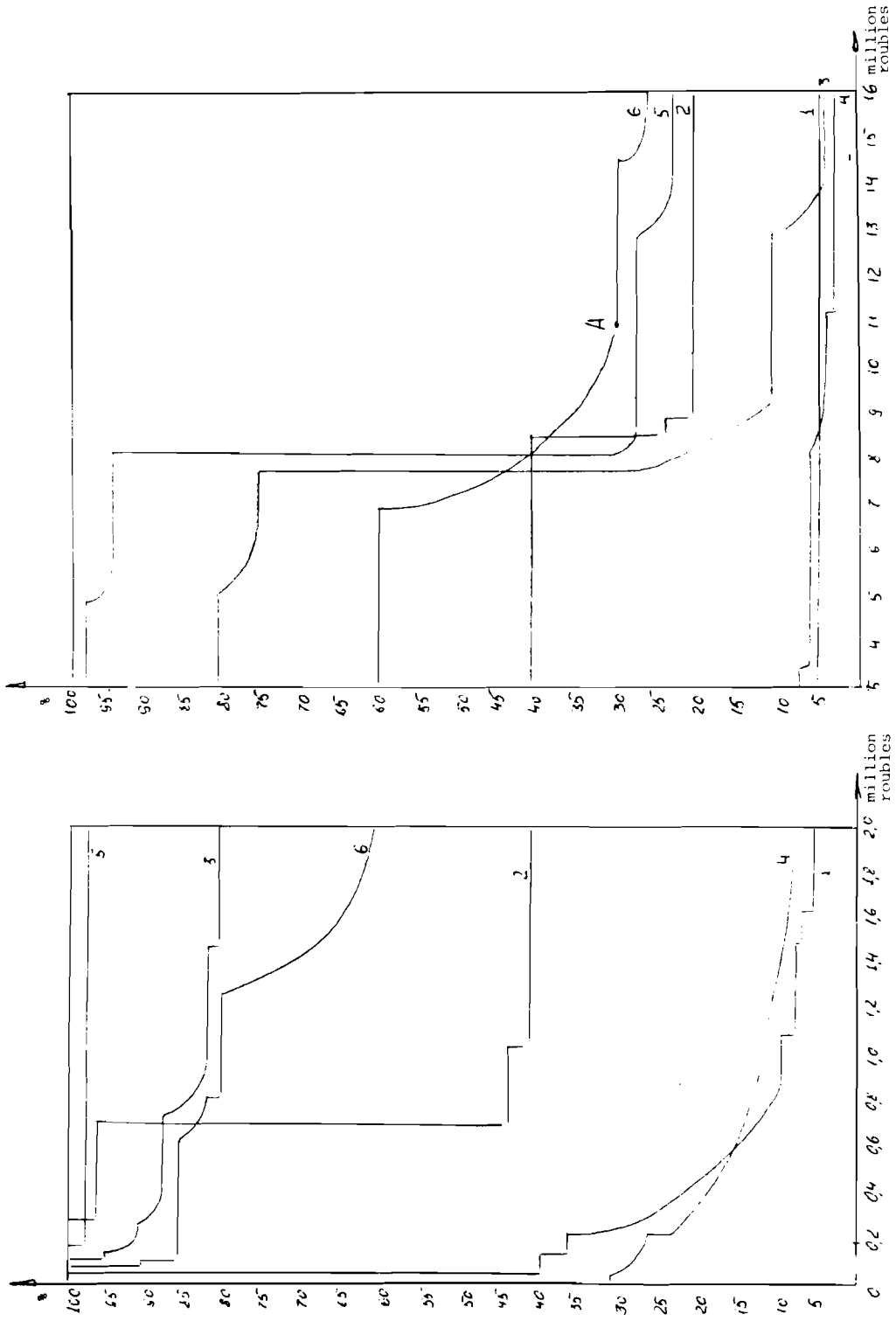


Figure 8.1 Optimum functions of expense-effect (city).

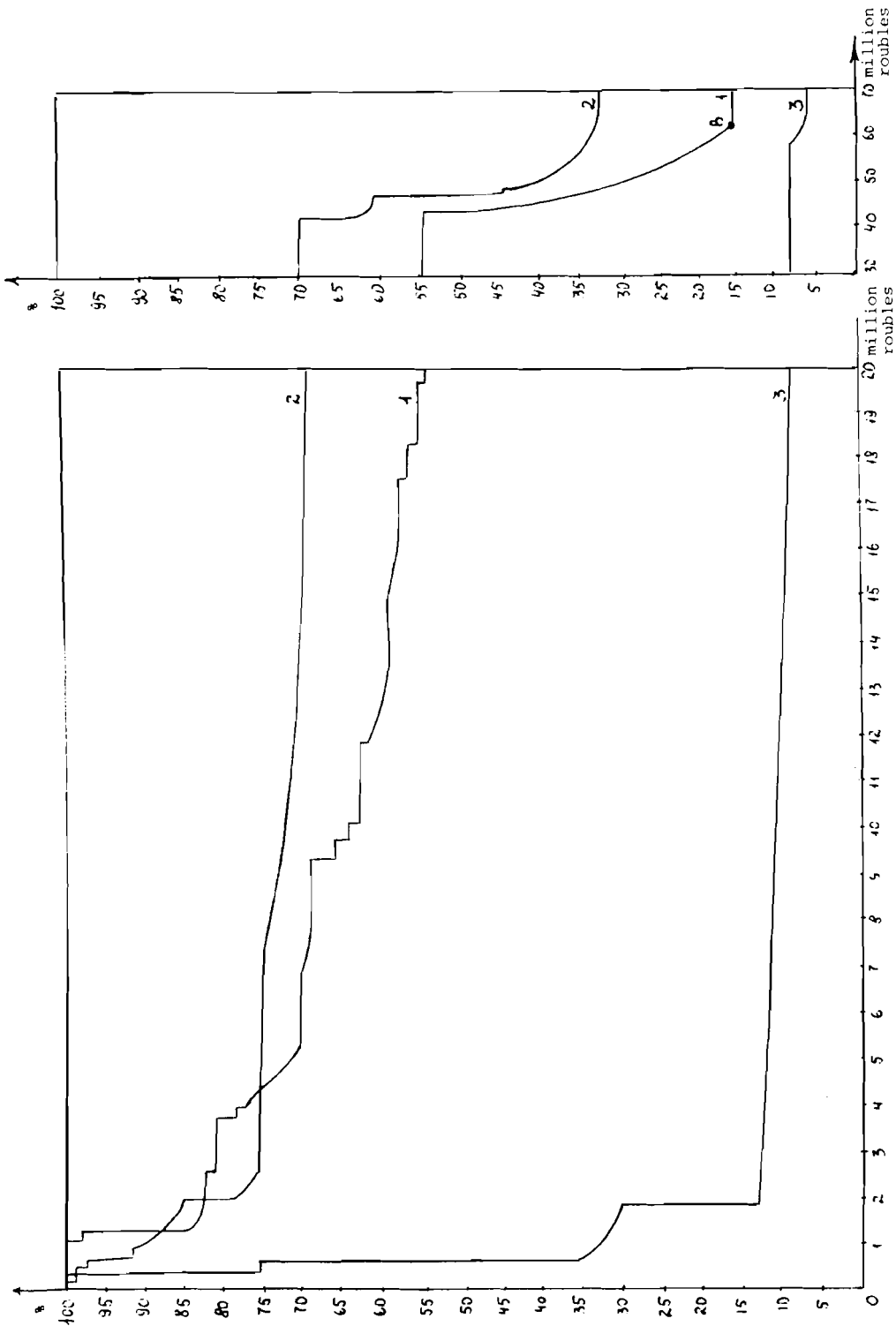


Figure 8.2 The optimum functions of expense effect calculated for the three types of criteria.

### 9. Experience Gained from the MARS Practical Use

The system of models devised was used in the USSR to assess the efficiency of atmosphere protective actions in a particular city and region. The region (Estonian SSR) was presented by a regular grid of  $32 \times 32$  with a cell size of  $10 \text{ km} \times 10 \text{ km}$ . Calculations were done for 298 enlarged sources of atmosphere pollution and 176 initial actions were analyzed.

In the grid of the industrial center of Tallin City of  $30 \times 34$  with a cell of  $1 \text{ km} \times 1 \text{ km}$ , 149 enlarged sources were located.

Calculation results for seven pollutants (particulate matter,  $\text{SO}_2$ ,  $\text{NO}_x$ ,  $\text{NH}_3$ ,  $\text{CH}_4$ ,  $\text{HF}$ , and  $\text{CO}_2$ ) on each of the criteria included in the MARS and in the initial data banks, are nowadays used in practice.

The examples of spatial distributions of emission, economic damage, and the maximum surface concentrations of particulate matter,  $\text{SO}_2$  and  $\text{NO}_x$  for the capital of Estonia, Tallin, are given in Figures 9.1, 9.2, and 9.3. The maximum surface concentrations are calculated in MARS parts for dangerous wind directions indicated in the corresponding positions of the matrix (first direction is the wind from the West to the East, further counterclockwise in 10 degrees).

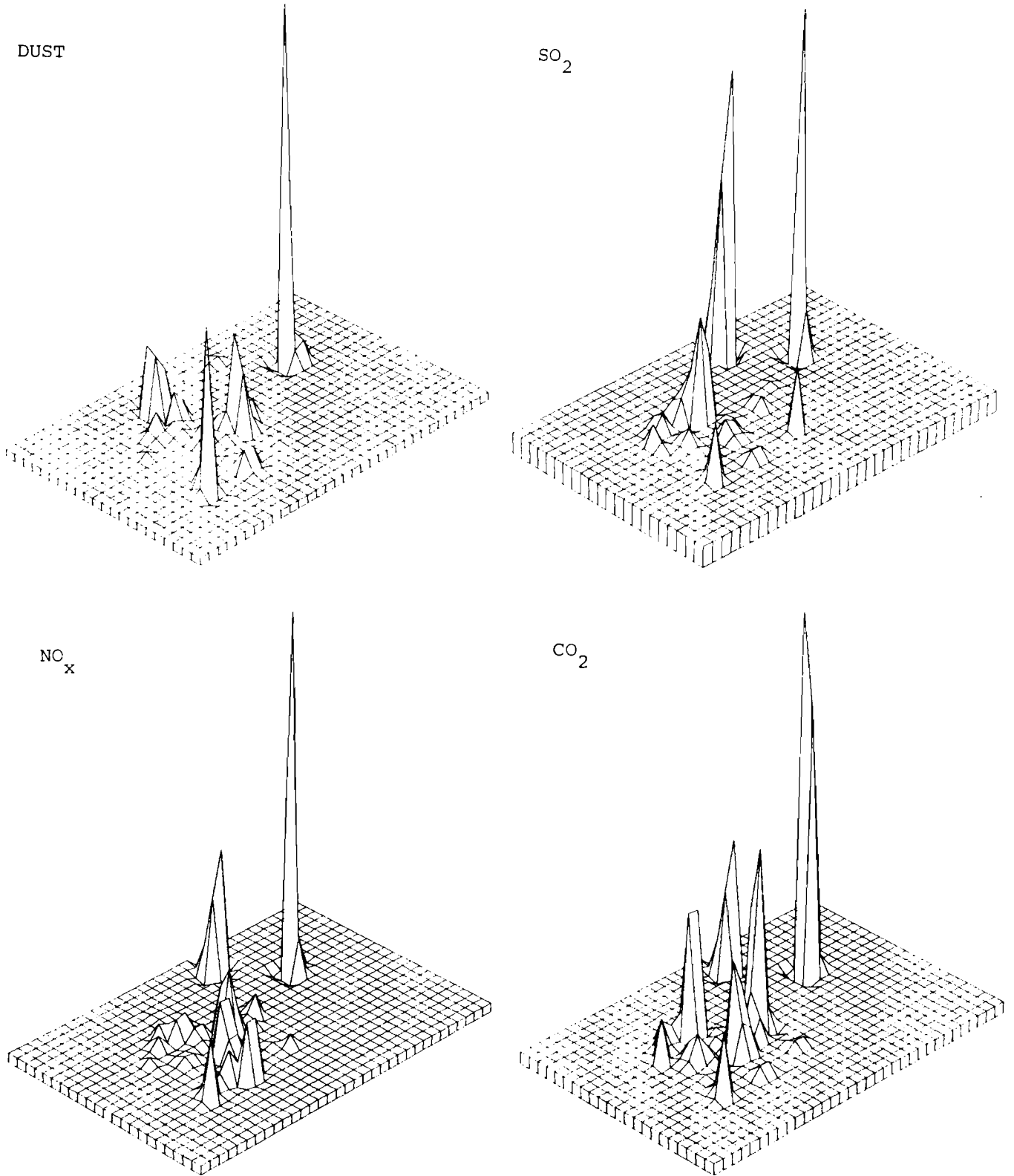


Figure 9.1 Examples of spatial distributions of particulate matter emissions.



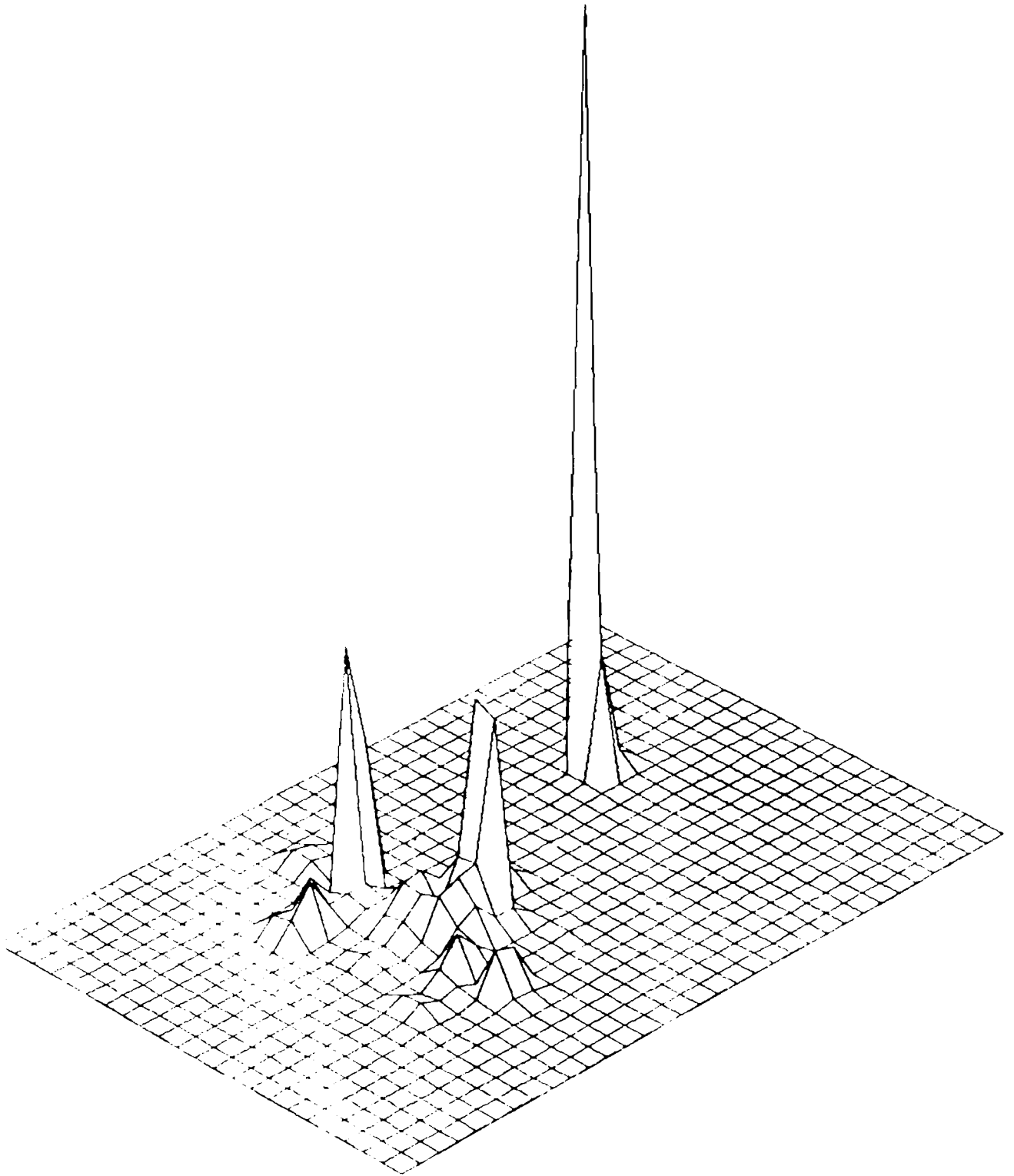
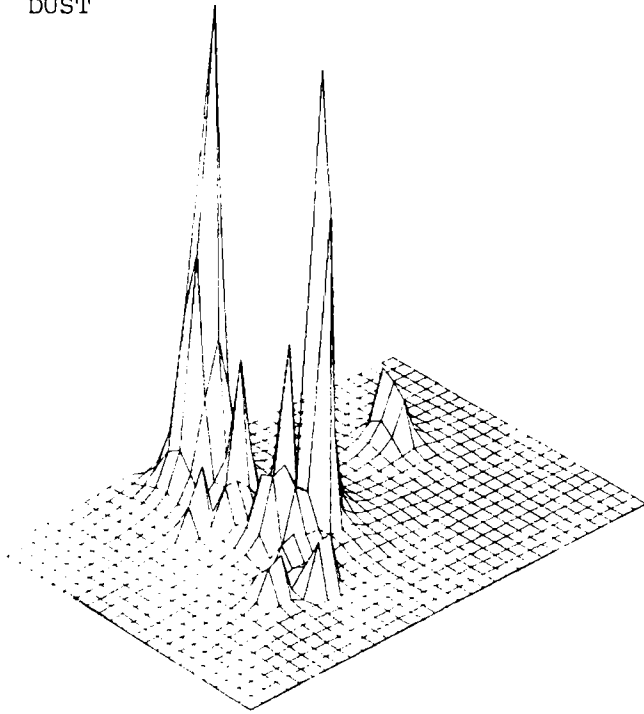
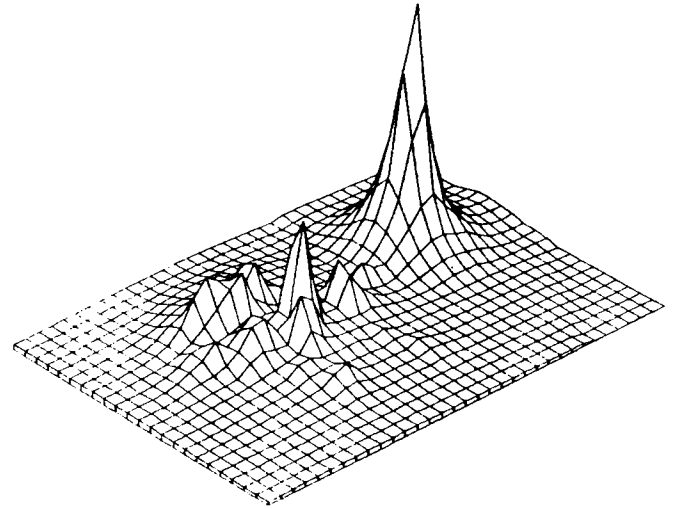


Figure 9.2 Examples of spatial distributions of economic damage in Tallin (Estonia, USSR).

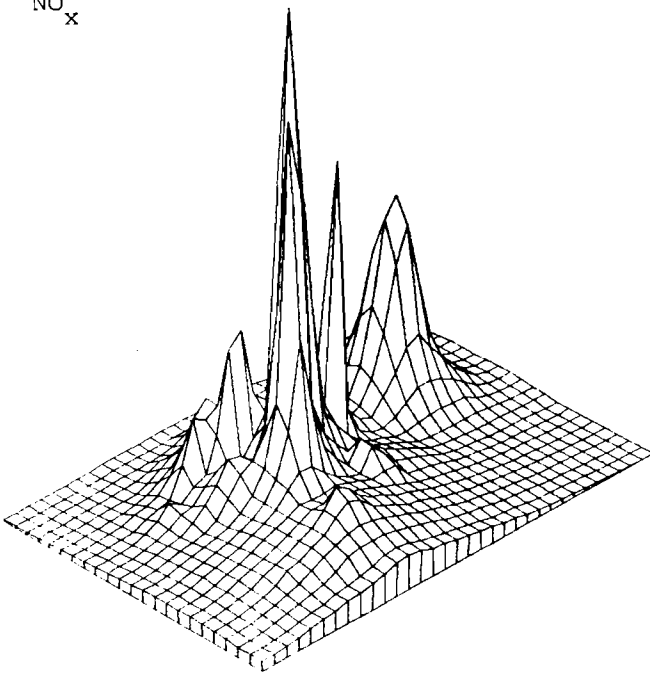
DUST



SO<sub>2</sub>



NO<sub>x</sub>



CO<sub>2</sub>

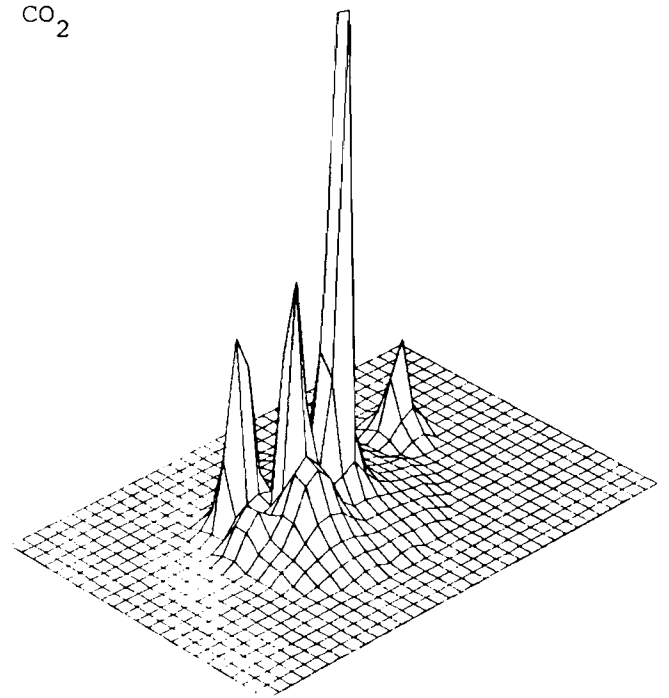


Figure 9.3 Examples of the maximum sulfur concentration of particulate matter in Tallin (Estonia, USSR).

### Acknowledgments

The authors wish to thank Prof. R.E. Munn, Prof. B.R. Döös, and Dr. S. Golovanov for their valuable advice. They would also like to thank M. Weinreich for the editing, organization, and final preparation of this paper.

### References

- Air Pollution: Assessment Methodology and Modeling. 1982. NATO -- Challenges of Modern Society Series: Vol.1. Plenum Press.
- Approximate Economic Damage Estimations of Air Pollution. 1986. Temporary methodology of calculations of environment protection activities' economic effectiveness and of assessment of economic damage caused by environmental pollution. Moscow: Economica. In Russian.
- Beryland, M.E. 1985. Air pollution predicting and control. Leningrad: Hydromet. In Russian.
- Burshtein, I.M. 1968. Dynamical programming in planning. Moscow: Economica. In Russian.
- Climatic Characteristics of Air Pollution Transport in Atmosphere. 1983. Leningrad: Hydromet. In Russian.
- Eliassen, A. 1980. A review of long-range transport modeling. *App.met.* 19:3:231-240.
- Galperin, M.V. 1985. Statistical fluctuation of atmosphere pollutants deposition rates and their influence on transport processes. *Proceedings of Institute of Applied Geophysics* 62. In Russian.
- Fisher, B. 1983. A review of the processes and models of long-range transport of air pollutants. *Atm. Env.* 17:10:1805-1515.
- Henry R. 1984. Review of receptor model fundamentals. *Atm. Env.* 18:11:1507-1515.
- Izrael Yu.A. 1983. Acid rains. Leningrad: Hydromet. In Russian.
- Lee, N. 1985. Three dimensional analytical models. *Atm. Env.* 19:12:1951-1957.
- Marchuk, A.I. 1982. Role of mathematical modeling in environmental problems. Moscow: Nauka. In Russian.
- New Airclimatic Reference Book on Marginal Stratum of Atmosphere over Territory of the USSR. 1987. Leningrad: Hydromet. Nos. 5,8.
- Recommendations on Source Conjunction in Preparation of Data for Computer calculation of Air Pollution. 1983. *Proceedings of State Geophysical Observatory.* In Russian.
- Renner, E., V. Ratzlaff, and W. Rolle. 1985. A Lagrangian multi-level model of transport, transformation and deposition of atmospheric sulfur dioxide and sulfate. *Atm. Env.* 19:11:1351-1359.
- Ryaloshapko, A.G. 1983. Atmospheric cycles of sulfur. Global biochemical cycle of sulfur and human activity. Moscow: Nauka. In Russian.
- Van Egmont D., and H. Kessenboom. 1983. Mesoscale air pollution dispersion models. *Atm. Env.* 17:2:257-274.