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SOME ASPECTS OF THE INTEGRATED APPROACH TO AIR QUALITY MANAGEMENT BASED ON OPTIMIZATION TECHNIQUES

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Abstract: The quantitative evaluation of environmental impact of emission sources is an important step of integrated modeling and the air quality decision support. The problem is especially difficult in the case of a complex, multi-source emission field. The approach discussed in the paper is based on the forecasts of the Eulerian type models of air pollution transport. The aim is to get a quantitative assessment of the contribution of the selected sources, according to the specified, environmental objective function. The approach utilizes the optimal control technique for distributed parameter systems. The adjoint equation, related to the main transport equation of the forecasting model, is applied to calculate the sensitivity of the cost function to the emission intensity of the specified sources. An example implementation of a regional scale, multi-layer dynamic model of SO_2 transport is discussed as the main forecasting tool. The test computations have been performed for a set of the major power plants in a selected industrial region of Poland.

AIR POLLUTION TRANSPORT MODEL

The natural application of air pollution models is forecasting of dispersion of pollutants, analysis of ecological results of some specific meteorological conditions or evaluation of the ecological influence of emission sources. The integrated systems, being recently developed, try to combine a classical environmental model of pollution transport with some economic, technological, social or medical constraints and standards [1, 2, 6, 10]. Such a system, besides the natural scenario analysis, gives the possibility to formulate and solve optimization problems and implement complex air pollution control strategies.

More examples of applications can be found in the cited literature. They relate both to long-term scenario analysis tasks as well as to on-line emission control problems. For example, the long-term strategy of energy sector development or the cost-effective controls of sulfur oxides are discussed [3, 4]. The problem of the regional-scale strategy for emission abatement in a set of the major power plants was also presented in [7], where the solution is searched by the optimal selection of the desulphurization technologies assigned to the modernized emission sources. Another class of air quality management problems which relates to the regional scale is the real-time emission control [8].

In most of deterministic models of air quality, the process of pollution transport is considered as distributed parameter system, governed by the set of advection-diffusion equations, along with the respective boundary and initial conditions. In any optimization procedure, where such model is utilized, the quantitative assessment of the contribution of emission sources to the overall pollution is required. Evaluation of environmental impact of emission sources is more natural in Lagrangian models, where the total pollution is usually calculated as the superposition of individual sources contribution. The task is more challenging in the case of Eulerian models, where the entire emission field (composed of many individual sources) is taken into account in one forecasting run of the model. In the sequel the technique is presented in which the problem is solved basing on the adjoint variable and some optimal control techniques.

Implementation discussed below is sulfur-oriented, but the approach presented can be applied in a more general class of Eulerian forecasting models. Computation of the transport of sulfur pollution is carried out by the multi-layer model [9], which takes into account two basic polluting components: primary SO_2 and secondary – SO_4^{2-}. Transport equations include chemical transformations, dry deposition and scavenging by precipitation. The governing equation, related to one polluting component, averaged over one vertical layer, has the following, general form:

$$\frac{\partial c}{\partial t} + \vec{\upsilon}\nabla c - K_h \Delta c + \gamma c = Q_O + \sum_{i=1}^{N} \chi_i(x,y)\cdot q_i(t), \tag{1}$$

along with the boundary conditions:

$$c = c_b \quad \text{on} \quad S^- = \{\partial\Omega \times (0,T) \,|\, \vec{\upsilon}\cdot\vec{n} \le 0\},$$

$$c = K_h \frac{\partial c}{\partial \vec{n}} \quad \text{on} \quad S^+ = \{\partial\Omega \times (0,T) \,|\, \vec{\upsilon}\cdot\vec{n} > 0\}, \tag{2a}$$

and the initial condition:

$$c(0) = c_0 \quad \text{in} \quad \Omega. \tag{2b}$$

Here we denote:
(0,T) – time interval of the forecast,
Ω – domain considered with the boundary $\partial\Omega = S^+ \cup S^-$,
N – number of the modernized/controlled sources,
c – pollution concentration,
$\vec{\upsilon}$ – wind velocity vector,
$\vec{n}$ – normal outward vector of the domain boundary $\partial\Omega$,
K_h – horizontal diffusion coefficient,
γ – pollution reduction coefficient (due to deposition and chemical transformation),
$q_i(t)$ – emission intensity of the controlled, i-th source,
$\chi_i(x,y)$ – characteristic function of the i-th source location,
$Q_o(x,y,t)$ – background (uncontrolled) emission field.

The transport equation of the form (1–2), which is the base of air quality forecasting model, can also be utilized to assess the environmental impact of individual sources. The base of such evaluation is an environmental cost function – the measure of environmental damage caused by emission sources.

THE OBJECTIVE FUNCTION AND THE ADJOINT VARIABLE

To implement any strategy of air quality management, the air quality damage (air quality cost) function must be defined. Definition of such an index usually takes into account the main polluting factors, such as concentration of pollutants (temporary or long-term averaged), cumulated deposition or exceedance of the critical loads [4, 10]. Another important index that is considered in formulation of the optimal emission reduction strategy is the cost of implementation of such strategy. Denoting, respectively,

$\Phi_1(c(\vec{q})$ – environmental damage index related to air pollution, and

$\Phi_2(\vec{q})$ – cost of any emission abatement action,

the following two basic formulations of the optimization problems related to air quality control can be considered:

a) minimization of the environmental damage subject to the total cost constraint:

$$\begin{cases} \Phi_1(c(\vec{q}) \to \min, \\ \Phi_2(\vec{q}) \le \Phi_{2,MAX}. \end{cases}$$

b) obtaining the assumed air quality standard at the minimum total cost:

$$\begin{cases} \Phi_2(\vec{q}) \to \min, \\ \Phi_1(c(\vec{q}) \le \Phi_{1,MAX}. \end{cases}$$

In the sequel, the objective function is considered in a more general form, as the weighted sum of two components, representing environmental damage (related to the concentration of polluting factor) and emission reduction cost in the controlled (or modernized) sources, respectively. This general index is as follows:

$$J(c(\vec{q})) = \alpha_1 \int_0^T \int_\Omega \varphi_1(c(\vec{q}))\, d\Omega\, dt + \alpha_2 \int_0^T \varphi_2(\vec{q})\, dt. \tag{3}$$

The sufficient regularity of subintegral functions, φ_1 and φ_2 is assumed. The time interval $(0.T)$ depends on the temporal scale of analysis, and can vary from 6 hrs (short-term forecasts, emission control) to one year (long-term strategy analysis).

In any optimization algorithm it is necessary to assess sensitivity of this index to emission of individual sources. The direct method of calculation uses the consecutive reduction of emission level of the sources under question – the impact is then represented by the related change of environmental index (3). In this approach, however, the main transport equation must be consecutively solved many times, for all the sources considered. This means that, e.g. in the case of emission control, the most time-consuming step of analysis has to be repeatedly performed.

Another approach is presented below. The first component of the functional (3) indirectly depends on the emission intensity of the controlled sources, and is related to emission via the transport equation (1). This fact can be formally expressed by the gradient of this index. The gradient components of functional (3), with respect to emission intensities, are as follows:

$$\frac{\partial J}{\partial q_i}(\vec{q}) = \alpha_1 \int_0^T \int_\Omega \frac{\partial \varphi_1}{\partial c} \cdot \frac{\partial c}{\partial q_i}(\vec{q})\, d\Omega\, dt + \alpha_2 \int_0^T \frac{\partial \varphi_2}{\partial q_i}(\vec{q})\, dt \qquad (i = 1, \ldots, N). \tag{4}$$

To compute the above gradient components, the derivatives $\partial c/\partial q_i$ are required, which can not be directly calculated. The applied procedure, based on the optimal control theory, allows us to calculate functions (4) in one simulation run of the transport equation. It is known [12, 13] that the components of expression (4) can be uniquely characterized by the solution (c) of the state equation (1), and the solution (p^*) of the following adjoint equation:

$$-\frac{\partial p^*}{\partial t} - \vec{\upsilon}\nabla p^* - K_h \Delta p^* + \gamma\, p^* = \frac{\partial \varphi_1}{\partial c}(c) \quad \text{in} \quad (0,T), \tag{5}$$

along with the boundary conditions:

$$p^* = 0 \quad \text{on} \quad S^-, \text{ and } K_h \frac{\partial p^*}{\partial \vec{n}} + (\vec{\upsilon}\cdot\vec{n})p^* = 0 \quad \text{on} \quad S^+, \tag{5a}$$

and the final condition (for the end of the time interval):

$$p^*(T) = 0 \quad \text{in} \quad \Omega. \tag{5b}$$

The parabolic equation (5) is solved for the negative time and the reversed direction of wind. It can be shown (compare [9, 11, 12]) that – due to the specific form of the boundary conditions in (1) and (5) – the solution of the adjoint equation allows us to calculate effectively the components of the gradient (4). They have the following form:

$$\frac{\partial J}{\partial q_i}(\vec{q}) = \alpha_1 \int_0^T\!\!\int_\Omega \chi_i(x,y)\, p^*(x,y,t)\cdot\frac{\partial \varphi_1}{\partial c}\, d\Omega\, dt + \alpha_2 \int_0^T \frac{\partial \varphi_2}{\partial q_i}(\vec{q})dt, \quad (i = 1,\ldots,N). \tag{6}$$

Thus, functions (6) can be utilized in assessment of the contribution of emission sources to environment deterioration, which is measured in the sense of the objective function (3). To calculate the impact of the specified emission sources, one must:

- solve the state equation,
- solve the adjoint equation,
- calculate gradient components (6).

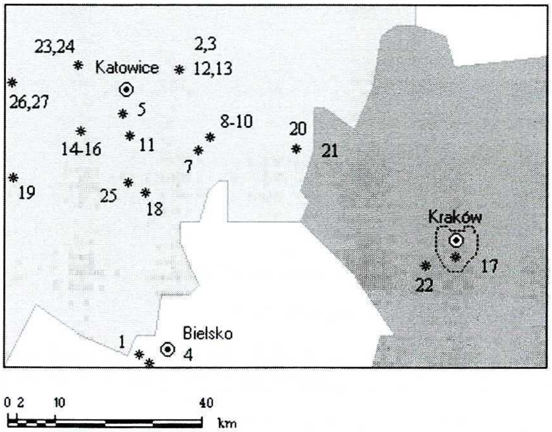
The transport and the adjoint equations must be solved only once in one step of the optimization algorithm. The method presented has been applied for the real-data case study concerning the industrial region of Upper Silesia.

TEST COMPUTATIONS – EVALUATION OF THE METHOD ACCURACY

The test calculations have been performed for the set of 27 major power plants in the region of Upper Silesia and Krakow in Poland (Fig. 1). The aim of the experiment was:

- to evaluate and compare the environmental impact of each controlled source by the adjoint variable method, discussed above,
- to examine accuracy of this technique, by comparing computational results with some reference data.

The main parameters of the analyzed emission sources are presented below in Table 1.



Discretization parameters

- rectangle domain 110 km x 76 km,
- homogeneous discretization, h = 2 km,
- discrete problem dimensions: 55 x 38.

Fig. 1. Computational domain and location of the emission sources

Table 1. Emission parameters of the controlled sources

No	Source	Coordinates	Stack [m]	SO_2 emission [kg/h]	
				Winter	Summer
1	Bielsko Biała	(14,2)	160	426.91	256.15
2	Będzin A	(18,31)	95	94.89	63.25
3	Będzin B	(18,31)	135	132.82	31.63
4	Bielsko-Kom.	(15,1)	250	426.9	189.74
5	Chorzów	(12,27)	100	363.66	180.25
6	Halemba	(8,25)	110	569.24	379.48
7	Jaworzno I	(20,23)	152	284.61	158.12
8	Jaworzno II A	(21,24)	100	573.60	379.48
9	Jaworzno II B	(21,24)	120	664.08	426.91
10	Jaworzno III	(15,1)	300	6324.60	4743.45
11	Katowice	(18,31)	95	1106.81	790.58
12	Łagisza A	(18,31)	160	948.69	695.71
13	Łagisza B	(18,31)	200	1359.79	1011.94
14	Łaziska I	(8,20)	200	1660.21	1185.86
15	Łaziska II	(8,20)	160	758.95	505.97
16	Łaziska III	(8,20)	100	727.95	505.97
17	Łęg	(46,12)	260	1106.81	790.58
18	Miechowice	(14,17)	68	161.28	117.01
19	Rybnik	(1,20)	300	4711.83	3510.15
20	Siersza A	(30,23)	150	1929.00	1423.04
21	Siersza B	(30,23)	260	2055.49	1739.27
22	Skawina	(43,11)	120	1992.25	1296.55
23	Szombierki A	(9,31)	110	164.44	113.84
24	Szombierki B	(9,31)	120	170.76	110.68
25	Tychy	(13,19)	120	110.68	177.09
26	Zabrze A	(2,29)	60	205.55	158.12
27	Zabrze B	(2,29)	120	221.36	145.47

The cost functional used in the test is defined as a special case of (3), for $\alpha_1 = 1/2$ and $\alpha_2 = 0$, in the following form:

$$J(c(\vec{q})) = \frac{1}{2}\int_0^T\int_\Omega w\,[\max(0, c(\vec{q}) - c_{ad}]^2\, d\Omega\, dt, \tag{7}$$

where c_{ad} is a constant, admissible level of SO_2 concentration.

To get the final results more illustrative and easier for natural interpretation, the area sensitivity function $w(x, y)$ introduced in relation (7) was defined as the following weight function:

$$w(x,y) = \begin{cases} 1 & (x,y) \in \text{Kraków area}, \\ 0 & \text{outside Kraków}. \end{cases} \tag{8}$$

Thus, the environmental impact of emission sources under consideration was computed in the sense of deterioration of this protected domain.

For the objective function (7), the components of the gradient function are as follows:

$$\frac{\partial J}{\partial q_i}(\vec{q}) = \int_0^T\int_\Omega \chi_i(x,y)\, p^*(x,y,t)\, d\Omega\, dt \quad \text{for}, (i = 1,\ldots,N) \tag{9}$$

and, according to (5), the right-hand of the adjoint equation has the form: $w \cdot \max[0, c(\vec{q}) - c_{ad}]$.

As far as the emission and meteorological data is concerned, the test computations were accomplished for the selected, representative year (1996). The meteorological conditions are characterized by the respective sequence of the input data sets (entered in 12-hr steps). The one-year interval was split down into four 3-month periods, and calculations were performed for 4 quarters, respectively. The multilayer, regional scale model [7, 9] was applied in the forecasting part of computations. The finite-dimensional approximation of equations (1) and (5) is based on the computationally efficient semi-Lagrangian scheme, which is a combination of the linear finite element method and the method of characteristics. The details related to numerical algorithm can be found in [9].

The direct calculation approach was used to evaluate the accuracy of the discussed method (based on the application of the adjoint equation (5)). For the consecutive 3-month periods of the selected year, the following quantities were calculated:

- averaged distribution of SO_2 concentration for the nominal emissions, according to the set (1),
- nominal value of the index J^0 according to (7),
- averaged distribution of SO_2 concentration for emission reduced by 50% for the controlled sources ($i = 1,\ldots,N$),
- reduced value of the index, J^i – related to a given source,
- relative contribution of the controlled sources (reference value), according to the formula:

$$R_i = \frac{J^o - J^i}{J^o} \quad (i = 1,\ldots,N). \tag{10}$$

Table 2 presents selected numerical results of this evaluation. They show the relative contribution of the considered emission sources in the sense of the air quality index (7), compared with the direct assessment of such an impact, calculated due to (10).

Table 2. Assessment of relative contribution of emission sources

No.	Term 1		Term 2		Term 3		Term 4	
	calc.	refer.	calc.	refer.	calc.	refer.	calc.	refer.
1	1.22	0.13	0.20	0.35	0.43	0.50	0.53	0.11
2	0.08	0.16	0.05	0.26	0.07	0.12	0.19	0.23
3	0.11	0.20	0.03	0.14	0.04	0.08	0.28	0.21
4	2.07	0.01	0.43	0.10	0.40	0.05	1.62	0.02
5	0.30	0.22	0.24	0.63	0.22	0.44	0.21	0.28
6	0.54	0.26	0.48	1.06	0.37	0.33	0.26	0.32
7	0.54	0.48	0.43	0.49	0.22	0.77	0.75	0.24
8	0.81	1.00	1.04	0.31	0.61	0.80	0.83	1.10
9	1.16	0.44	1.36	0.48	1.13	0.80	1.07	0.88
10	31.65	9.59	10.71	6.44	33.82	13.20	23.26	4.44
11	2.39	0.78	1.14	1.50	4.01	1.26	1.57	0.50
12	0.63	0.89	0.55	1.94	1.32	1.13	1.79	1.17
13	3.17	1.33	0.77	2.42	2.64	0.81	2.33	1.59
14	1.79	0.17	1.21	2.06	0.89	0.25	1.15	0.31
15	0.81	0.11	1.09	0.87	0.47	0.14	0.47	0.16
16	0.77	0.24	0.71	1.27	0.43	0.40	0.46	0.31
17	7.67	0.08	9.46	1.08	12.08	0.62	0.05	0.02
18	0.20	0.05	0.23	0.28	0.11	0.05	0.14	0.06
19	3.87	0.50	6.04	3.50	1.39	1.05	2.21	1.03
20	34.41	6.41	12.70	16.23	20.28	13.72	22.08	5.96
21	40.44	4.14	18.80	15.08	21.00	11.43	25.09	4.43
22	204.49	59.95	77.31	67.59	156.53	72.17	230.75	62.49
23	0.08	0.05	0.12	0.24	0.12	0.12	0.10	0.06
24	0.09	0.04	0.10	0.23	0.09	0.09	0.11	0.06
25	0.29	0.05	0.33	0.44	0.18	0.18	0.18	0.08
26	0.15	0.04	0.12	0.25	0.11	0.11	0.06	0.06
27	0.16	0.04	0.12	0.24	0.08	0.08	0.06	0.07

For the selected quarter, the neighboring columns of the table compare the relative impact of emission sources (left column) with the reference value (right column). Both sets of results show the dominating impact of the source No. 22 (Skawina power plant) and the intermediate contribution of sources No. 10, 20, 21. On the other hand, there is a group of power plants with minor or negligible influence, in the sense of the assumed criterion function.

The results confirm good agreement of two sets of results, the calculated and the reference data. Relatively low contribution of source No. 17 (Łęg power plant) to the protected area results from very high stack of this plant, so the source affects rather distant receptors. The correlation coefficient of calculated and reference data is high, and for four quarters considered is over 0.95. This confirms correctness of the computational method discussed in the previous section. It can be useful in future applications concerning integrated environmental systems, decision support problems as well as the real-time emission control.

It must be noticed that the adjoint variable p^* in (5) has no unique physical dimension, because it always depends on the form of the objective function (3). Thus, the calculated and the reference data presented in the related columns of Table 2 have the different physical meaning (and units) and they cannot be directly compared. On the other hand, the results are sufficient to assess the relative influence of the discussed sources. To facilitate a direct comparison of the results, the calculated values of the gradient components can be normalized, e.g. with respect to the maximum value for a given term. In any case, the correlation of the related series can be calculated (the value is above 0.95), and it shows the good compatibility of two sets of results.

Figure 2 presents two maps, averaged for the winter season: distribution of SO_2 concentration and the respective adjoint variable. The maps illustrate the meaning of the adjoint variable in evaluation of the impact of emission sources. It can be observed that the area of high values of this variable coincides with location of the most contributing emission sources.

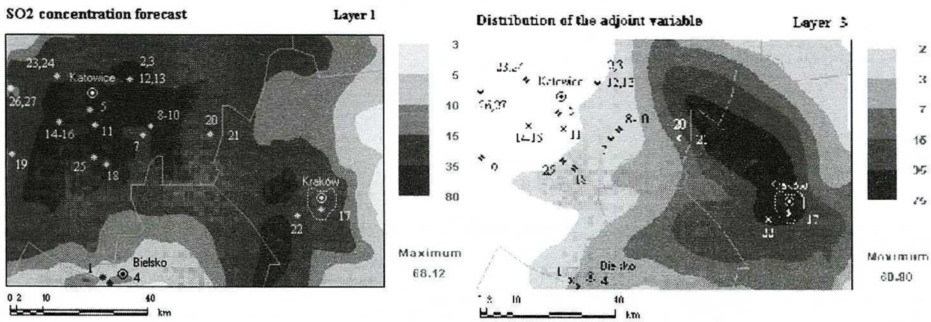


Fig. 2. Concentration of SO_2 [$\mu g/m^3$] (left) and the adjoint variable (right) (Winter 1996)

APPLICATION – THE REAL TIME EMISSION CONTROL

Statement of the emission control problem

Basing on the forecasts of the pollution dispersion model, the real-time emission control problem for the system of sources located in a given area can be formulated. We assume in the sequel that the set of the major power plants located in the region form the controlled emission field. The general idea of control consists in minimizing a predefined environmental cost function, according to the changing meteorological conditions, by modification of the emission intensity (supervised by the regional coordinating center for redistribution of the energy production) within the set of the selected controlled sources. Some substantial economic and technological constraints can also be taken into account.

To formally state the optimal control problem, we below define the basic conditions. Let us assume that in a given domain Ω there are N controlled emission sources described by certain spatial and temporal characteristics (location – $\chi_i\ (x, y)$, stack height, etc.) and emission intensity – $q_i\ (t)$, respectively. There is also a set of uncontrolled emission sources Q that form the background pollution field.

State equation – we consider a concentration of the polluting factor $c(x, y, t)$, which satisfies the following transport equation:

$$\frac{\partial c}{\partial t} + \vec{\upsilon}\,\nabla c - K_h \Delta c + \gamma\, c = Q + \sum_{i=1}^{N} q_i \quad \text{in} \quad \Omega \times (0,T) \tag{11}$$

with the boundary and initial conditions (1a–b). Emission characteristics of the controlled sources are represented by the product:

$$q_i(x,y,t) = \chi_i(x,y)\,F_i(u_i(t)) \quad \text{for } i = 1,\ldots,N,$$

where $F_i(u_i(t))$ is the temporal characteristics of emission intensity. Vector function $\vec{u} = [u_1,\ldots,u_N]$ denotes here the control and represents the production level (e.g. energy production of the power plant). Functions F_i, $(i = 1,\ldots, N)$ relate energy production level of the respective plant, to the emission intensity, which is the right side of the state equation.

Cost functional to be minimized consists of two components: environmental cost function (air quality damage) and cost of the control. It is defined as follows:

$$J(\vec{u}) = \frac{\alpha_1}{2}\int_0^T\int_\Omega w[\max(0,\, c(\vec{u}) - c_{ad})]^2 \; d\Omega\, dt \; + \; \frac{\alpha_2}{2}\int_0^T \sum_{i=1}^{N} \beta_i (u_i(t) - u_i^*)^2 . \quad (12)$$

Here the coefficients α_1, α_2, β_i, (i = 1,...., N) are given constants, where $\alpha_1 \geq 0$, $\alpha_2 \geq 0$, $\beta_i > 0$. The area sensitivity function satisfies the inequality $0 \leq w(x, y) \leq 1$ and c_{ad} is a constant, admissible level of concentration. Functions u_i^*, $(i = 1,\ldots, N)$ stand for the nominal production level of the controlled sources.

Constraints imposed on the production level of the controlled emission sources represent some technological and economic requirements, and are as follows:

$$\underline{u}_i \leq u_i(t) \leq \bar{u}_i \qquad \text{for } i = 1,\ldots,N, \quad (13a)$$

$$\sum_{i \in N_j} \delta_{ij} \underline{u}_i(t) \geq d_j \;\; \text{for } i = 1,\ldots,N, \;\; N_j \subset \{1,\ldots,N\}. \quad (13b)$$

Inequalities (13a) define the lower and upper technological limits on the real production level of the plant under consideration. Conditions (13b) represent constraints of total energy demand (for the region under question), which is imposed on the j-th subset of plants, with some coefficients δ_{ij}.

We denote by $U_{ad} \subset H^1(0,T;R^N)$ the set of admissible controls defined by (13). It is known [11, 12] that the state equation (11) has a unique solution $c = c(\vec{u})$ determined for a given $\vec{u} \in H^1(0,T;R^N)$ and for fixed, constant parameters K_h and γ of the state equation, where $K_h > 0$.

Optimal control problem (P) – find the element $\vec{u}^0(t)$ which minimizes the cost functional (12) over the set of admissible controls:

$$J(\vec{u}^0) = \inf_{\vec{u} \in U_{ad}} J(c(\vec{u}))$$

where $c(\vec{u})$ satisfies the state equation (11).

Optimality conditions – it can be shown [11, 12], that the solution of (P) can be uniquely characterized by the following system of the optimality conditions. Find $(\vec{u}^o, c^o, p^o)$, where $\vec{u}^o = [u_1^o,\ldots,u_N^o] \in U_{ad}$, such that the following conditions are satisfied:

a) state equation:

$$\frac{\partial c^o}{\partial t} + \vec{\upsilon}\,\nabla c^o - K_h \Delta c^o + \gamma c^o = Q + \sum_{i=1}^{N} \chi_i F_i(u_i^o) \;\; \text{in } \Omega \times (0,T), \quad (14)$$

$$c^o = c_b^o \;\; \text{on } S^-, \;\; K_h \frac{\partial c^o}{\partial \vec{n}} = 0 \;\; \text{on } S^+, \quad (14a)$$

$$c^o(0) = c_0^o \quad \text{in} \quad \Omega. \tag{14b}$$

b) adjoint equation:

$$-\frac{\partial p^o}{\partial t} - \upsilon \nabla p^o - K_h \Delta p^o + \gamma p^o = \alpha_1 w \cdot \max(0, c^o - c_{ad}) \text{ in } \Omega \times (0,T), \tag{15}$$

$$p^o = 0 \quad \text{on } S^-, \quad K_h \frac{\partial p^o}{\partial \vec{n}} + \vec{\upsilon} \cdot \vec{n} p = 0 \quad \text{on } S^+, \tag{15a}$$

$$p^o(T) = c_0^o \quad \text{in} \quad \Omega. \tag{15b}$$

c) minimum of the quality functional:

$$\sum_{i=1}^{N} \left\{ \alpha_1 \int_0^T \int_\Omega \chi_i F_i'(u_i^o) p^o (v_i - u_i^o) \, d\Omega dt + \alpha_2 \int_0^T \beta_i (u_i^o - u_i^*)(v_i - u_i^o) \, dt \right\} \geq 0 \tag{16}$$

$$\forall \vec{v} = [v_1, \ldots, v_N] \in U_{ad}.$$

Optimality conditions (14) – (16) can be utilized as a base for construction of a gradient optimization algorithm, which consists of the following steps:

- solve the state equation (14),
- solve the adjoint equation (15) in the reversed direction of time,
- calculate components of the gradient vector – $J'(\vec{u})$, according to the left side of (16).

Implementation and results of test computations are discussed in the next section.

The real-data case study

The general approach presented in Section 2 has been implemented and tested on a real data case. The test calculations were performed for the selected region of Upper Silesia (Poland) and the set of 27 major power plants, considered as the controlled emission sources. Figure 1 presents the domain considered and the location of the controlled emission sources.

To formally state the optimal control problem which is to be solved, certain simplifications have been introduced to the general formulations discussed above. We assume that the set of admissible controls U_{ad} is given by:

$$U_{ad} = \left\{ \vec{u} \in L^2(0,T;R^N) \,|\, \vec{u}(t) \text{ satisfies (13) for a.a. } t \in (0,T) \right\}, \tag{17}$$

where condition (13b) has a form of the total energy demand constraint:

$$\underline{u}_i \leq u_i(t) \leq \bar{u}_i \text{ for } i = 1, \ldots, N \text{ and } \sum_{i=1}^{N} \delta_i u_i(t) \geq d. \tag{18}$$

Furthermore, we assume for simplicity that function that relates emission to production level in the state equation (11) is identity, i.e. $F_i(u_i) = u_i$ for $i = 1,...N$.

The computational domain shown in Figure 1 was discretized with the homogeneous grid (space discretization step $h = 2$ km). Surroundings of Kraków (indicated by the dashed line) was defined as a region of high sensitivity, with the respective form of the weight function $w(x, y)$, defined by (8).

Computational results shown below represent the real-time emission control for one 12-h time interval and two selected meteorological scenarios: (A) North-West, moderate wind and neutral atmospheric stability conditions, (B) West, weak wind and neutral atmospheric stability conditions. The nominal emissions of the controlled sources refer to the Winter season values, as presented above in Table 1.

Numerical implementation of the optimal control problem (P) discussed in Section 2 is based on the gradient method of linearization [9]. The consecutive iterations of the computational algorithm consist of the following steps:

a) solve the state equation in $(0,T)$,
b) calculate the value of the quality index $J(\bar{u})$,
c) solve the adjoint equation for the reversed wind direction and the reversed time,
d) calculate the components of the gradient $J'(\bar{u})$,
e) perform the consecutive optimization step.

General optimization results related to the quality index and computational efficiency of the algoritm are shown in Table 3. The respective reduction of air quality index is 0.88 for scenario (A) and 0.74 for scenario (B), respectively. The optimal control results, related to modifications of the controlled sources, are also shown in a graphical form in Figures 3–4, for episodes A and B (according to Table 3). The top maps indicate the differences in the distribution of SO_2 concentration for the reference emission (no control) and for the emission control strategy suggested by the optimization procedure. Some differences in concentration field can be observed within the high sensitivity area.

Table 3. General optimization results for two meteorological scenarios

Scenario	No of iteration	Quality index		Reduction factor
		initial	final	
A	4	78.2	71.5	0.88
B	3	6.84	5.07	0.74

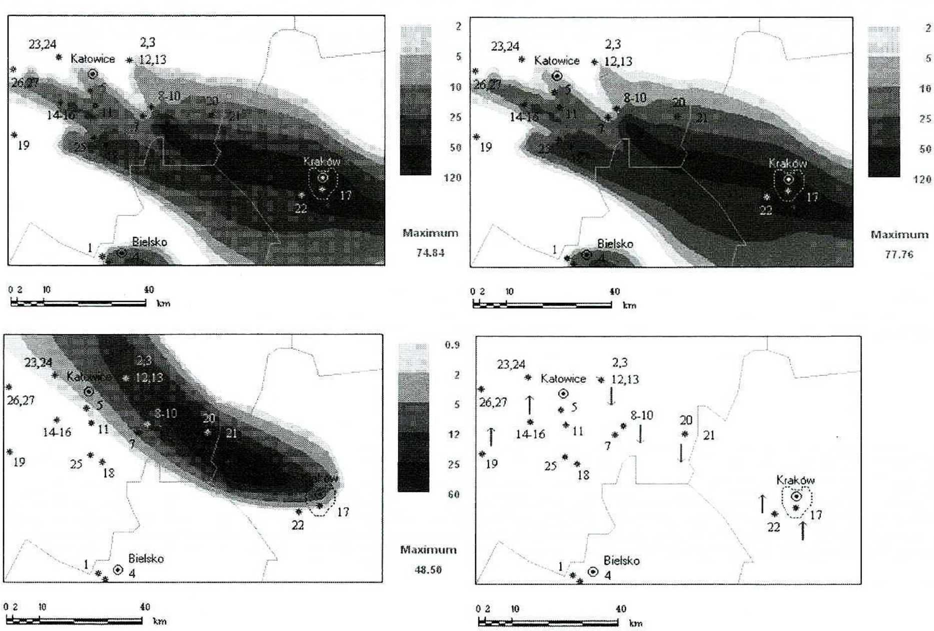


Fig. 3. Computational domain and the emission control (scenario A)

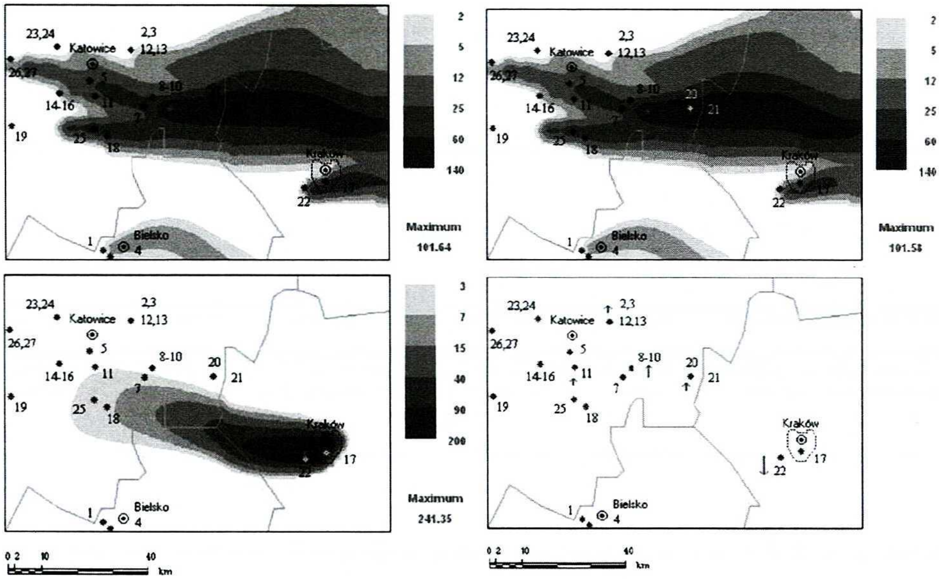


Fig. 4. Computational domain and the emission control (scenario B)

The correlation between the adjoint variable distribution and location of the dominating controlled emission sources can be seen in the bottom part of the figure. The area of high values of the adjoint variable coincides with locations of the sources, which significantly contribute to the overall environmental cost function, for the current meteorological conditions (wind direction). These sources have the emissions respectively reduced, as the result of the optimization algorithm; the respective changes in emission intensities are shown in the right part of the figure. On the other hand, to satisfy the energy demand constraints (18), the production level (and emission level) of certain sources must be risen. These are the sources located outside the area of high influence (compare the left part of the figure), which do not contribute to the quality functional for the scenario considered.

The quantitative results presenting the relative modification of emission levels, as a result of the controlling action, are shown in the last columns of Table 4. The correlation between these precise results and the graphical interpretation (e.g. the spatial distribution of the adjoint variable) of Figures 3–4 can be easily seen. The obtained results show good performance and computational efficiency of the algorithm; the optimum is reached in a few iterations and the resulting accuracy of the optimal solution is satisfactory.

The applications of the technique discussed in the paper concentrate on the problem of the real-time emission control. Presented results show, that some elements of the technique can also be utilized in long-term analysis of regional scale sustainable development. The remark refers to the adjoint variable, which indicates the area which is the most influencing from the environmental perspective. Thus, in long-term analysis, distribution of this variable can be an important factor in supporting decisions of the planned energy sector investments and their location within the region.

The obtained results confirm the possibility of the effective utilizing of air pollution transport models and the discussed above technique in the real-time emission control. The

Table 4. Emission parameters of the controlled sources and the optimal control results

No	Source	Coordinates	Stack [m]	Emission kg/h]	Control (A)	Control (B)
1	Bielsko-Biała	(14,2)	160	426.91	1.00	1.00
2	Będzin A	(18,31)	95	94.89	1.00	1.00
3	Będzin B	(18,31)	135	132.82	1.00	1.00
4	Bielsko-Kom.	(15,1)	250	426.9	1.00	1.00
5	Chorzów	(12,27)	100	363.66	1.00	1.00
6	Halemba	(8,25)	110	569.24	1.00	1.00
7	Jaworzno I	(20,23)	152	284.61	1.00	1.00
8	Jworzno II A	(21,24)	100	573.60	1.00	1.00
9	Jaworzno II B	(21,2)	120	664.08	0.80	1.00
10	Jaworzno III	(15,1)	300	6324.60	0.80	1.04
11	Katowice	(18,31)	95	1106.81	1.10	1.01
12	Łagisza A	(18,31)	160	948.69	1.00	1.01
13	Łagisza B	(18,31)	200	1359.79	0.90	1.01
14	Łaziska I	(8,20)	200	1660.21	1.10	1.00
15	Łaziska II	(8,20)	160	758.95	1.00	1.00
16	Łaziska III	(8,20)	100	727.95	1.00	1.00
17	Łęg	(46,12)	260	1106.81	1.10	1.00
18	Miechowice	(14,17)	68	161.28	1.00	1.00
19	Rybnik	(1,20)	300	4711.83	1.25	1.00
20	Siersza A	(30,23)	150	1929.00	0.80	1.02
21	Siersza B	(30,23)	260	2055.49	0.80	1.02
22	Skawina	(43,11)	120	1992.25	1.10	0.82
23	Szombierki A	(9,31)	110	164.44	1.00	1.00
24	Szombierki B	(9,31)	120	170.76	1.00	1.00
25	Tychy	(13,19)	120	110.68	1.00	1.00
26	Zabrze A	(2,29)	60	205.55	1.00	1.00
27	Zabrze B	(2,29)	120	221.36	1.00	1.00

accuracy and performance of the computer implementation of the model is satisfactory from the point of view of the possible future applications of this approach.

CONCLUSIONS

The aim of the paper is to formulate and test the method of the quantitative evaluation of ecological impact of emission sources, based on the predictions of Eulerian-type air pollution forecasting models. This impact is measured in the sense of the predefined environmental damage function. As stated in Section 2, the emission field of the controlled sources and air pollution dispersion processes are considered as a distributed parameter system, which is governed by the respective set of transport equations. Consequently, respective optimization techniques for distributed parameter systems (compare [11, 12]) are utilized in characterization of the ecological impact of emission sources. The paper consists of the following basic parts:

- formulation of the general form of the regional-scale air quality model,
- definition of the environmental objective function,

- formulation of the optimization problem and the computational algorithm, based on the gradient of the objective function and the adjoint variable,
- testing the efficiency and accuracy of the algorithm for the real-data case study.

The key module of the system is the numerical model of air pollution transport. The accuracy of the respective finite-dimensional approximation scheme applied for solving the transport and adjoint equations constitutes the basic problem. Both equations must be solved, at least once, in every iteration of any gradient optimization algorithm. Numerical solution of this type of evolutionary equations is especially sensitive to the properties of the numerical scheme applied. It is known that the crucial role in the final accuracy of the method play monotonicity and positivity of approximation method, as discussed by Holnicki [8, 9]. These properties are particularly important in an optimization process, since the solution of the state equation is entered as an input of the adjoint equation. For this reason, in the applications presented in the paper, an effective, shape preserving scheme, based on a combination of the method of characteristics and the piecewise-quintic spatial interpolation [9], is used for simulation of air pollution transport.

Another important point of implementation relates to the spatial characteristics of emission sources that form the controlled emission field. Since in the application considered in the paper that field is composed of the pointwise sources – the case is especially sensitive to shape-preserving properties of the numerical approximation scheme. The test computations, performed for two selected episodes, confirm good accuracy of the solution to transport equation as well as satisfactory integration of the method with the optimization algorithm. The obtained results also show that the method is computationally effective (the optimum reached in a few iterations – see Table 3) and the resulting accuracy of the optimal solution is sufficient, having in perspective future applications.

The utilization of the techniques discussed in the paper concentrates on the problem of the real-time emission control. Presented results show that some elements of this approach can also be applied in long-term analysis of regional scale environmental tasks, e.g. in sustainable development problems, as discussed by Chang [2] or Haurie *et al.* [6]. The remark refers to the adjoint variable, which indicates the most influencing area from environmental perspective. Thus, in long-term analysis, distribution of this variable can also be an important factor in supporting decisions concerning the planned energy sector investments and their location within the region.

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WYBRANE ASPEKTY ZINTEGROWANEGO ZARZĄDZANIA JAKOŚCIĄ POWIETRZA Z WYKORZYSTANIEM TECHNIK OPTYMALIZACYJNYCH

Jedną z istotnych funkcji zintegrowanego systemu oceny jakości powietrza atmosferycznego jest ilościowe oszacowanie wpływu poszczególnych źródeł emisji na zagrożenie środowiska. Problem ten jest szczególnie trudny w przypadku dużych aglomeracji miejsko-przemysłowych charakteryzujących się bardzo złożonym opisem pola emisji i dużą liczbą źródeł. W podejściu prezentowanym w pracy, jako podstawowe narzędzie prognostyczne wykorzystano eulerowski model rozprzestrzeniania się zanieczyszczeń atmosferycznych w skali regionalnej. Wyniki prognoz modelu wykorzystano do oszacowania ilościowego udziału wybranych (dominujących) źródeł emisji w zagrożeniu środowiska. Udział ten jest określany z punktu widzenia przyjętego wskaźnika jakości powietrza atmosferycznego. Sformułowanie matematyczne ma postać zadania sterowania optymalnego dla systemu o parametrach rozłożonych (opisanego odpowiednim układem równań transportu zanieczyszczeń). Równanie sprzężone wykorzystano do oceny wrażliwości przyjętego wskaźnika jakości ze względu na wielkość emisji poszczególnych źródeł sterowanych. Podejście to wykorzystano do sformułowania i rozwiązania zadania sterowania emisją w czasie rzeczywistym. Przedstawiono przykładowe wyniki dotyczące implementacji zadania dla wybranego regionu przemysłowego.