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Uncertainty in Integrated Modelling of Air Quality

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1. Introduction

Forecasting models of air quality and the more complex Integrated Assessment Systems (IAM) are recently used for supporting decisions concerning air quality management and emission control policy (ApSimon et al., 2002; Warren & ApSimon, 1999). The natural application of environmental models is predicting dispersion of pollutants, analysis of ecological results of some specific meteorological conditions or evaluation of environmental influence of emission sources. In most of deterministic models of air quality, the process of pollution transport is considered as distributed parameter system and is mathematically described by the set of advection-diffusion equations, along with respective boundary and initial conditions. To quantify possible ecological, economic or health benefits of emission abatement, there is a need to estimate an incremental contribution of the respective group of emission sources to ambient concentrations with a reasonable accuracy. However, due to a very complex, multidisciplinary structure of such systems, there exist many sources of imprecision and uncertainty in the modelling of environmental effects of atmospheric pollution and also in resulting regulatory decisions.

To assess the accuracy of modelling results and a connected decision support process, performance and uncertainty of the model should be evaluated. The straightforward method of such an assessment is usually based on examining a relative agreement between measurements and results of computer simulations. However, the accuracy of such a comparison is usually insufficient because of different spatial scales of these two quantities, where the point measurements are compared with volume-averaged results of simulation. To better characterize the problem, the main sources of variability (temporal, spatial, or inter-individual differences of input data) and uncertainty (imprecise information or lack of information about unknown quantity) should be identified and assessed (Park et al., 2006; Sax & Isakov, 2003). In addition, implementations of operational models of air pollution usually involve some specific simplifications or parameterizations and cannot completely characterize complex physical processes. This is the source of conceptual uncertainty which is also reflected in the final results. In particular, it relates to uncertainty in deriving trajectories in Lagrangian approach or sub-grid effects in Eulerian models. Moreover, due to performance requirements, in operational models some atmospheric processes are parameterized or described in a simplified way. For example, the height of the mixing layer and atmospheric stability are usually evaluated in course of an imprecise heuristic procedure, which is another source of the final uncertainty. However, numerous previous studies have revealed that major uncertainties

(measurement or estimation error) are due to input datasets, e.g. emission inventory and meteorological data, involving more than the model itself (Russel & Dennis, 2000). The uncertainty analysis of emission data is especially significant and challenging in the case of urban or industrial areas. The main problem follows from a high spatial concentration of the large number of emission sources with different technological characteristics, used fuel type and related fuel parameters, composition of polluting compounds, emission intensities, and as a consequence – different range of emission uncertainty.

This chapter addresses the problem of uncertainty in computer modelling of air pollution dispersion, but it also takes into account the impact of this uncertainty on an environment-oriented decision support process. The following sections include an analysis. Section 2 shortly characterizes basic implementations of air pollution transport models, their applications in supporting strategic decisions, and also the general idea of Integrated Assessment Models (IAM). Sections 3 and 4 discuss the main sources of uncertainty (emission intensity, basic meteorological data, model parameters) in air quality modelling and present results of the uncertainty analysis for a regional case study. In Section 5 a regional-scale decision problem is formulated as an emission abatement task, with solution depending on the outcomes of the previous forecasting model. It is mathematically formulated as an integer-type optimization problem. The selected results of the optimization task quantitatively illustrate how uncertainty of air pollution predictions influences decisions generated in the optimization procedure. Section 6 describes general conclusions related to the applicability of air quality forecasting models in environmental decision support systems. Due to the mostly qualitative character of such strategic decisions, the obtained modelling accuracy (including overall uncertainty) is sufficient in the majority of practical applications. Moreover, suggestions concerning the accuracy of optimization algorithms are formulated.

2. Air quality models in decision support systems

In basic applications of air quality models, the processes of air pollution transport are considered as a distributed parameter system, which is governed by the set of transport equations, along with respective boundary and initial conditions. The exact form and structure of a model usually depends on its practical application, type of the polluting compounds considered and the scale of modelling. A model usually takes into account the input data (emission field and meteorological data) as well as the main physical and chemical processes which decide on the transport in the atmosphere and transformations of air pollution components. The mathematical description of these processes within time interval $(0,T)$, related to one polluting compound and a single vertical layer of the atmosphere, usually takes a general form of an advection-diffusion equation

$$\frac{\partial c}{\partial t} + \vec{v} \nabla c - K_h \Delta c + \gamma c = Q \quad (1)$$

along with the respective boundary conditions

$$\begin{aligned} c &= c_b \quad \text{on} \quad S^- = \{ \partial \Omega \times (0,T) \mid \vec{v} \cdot \vec{n} < 0 \}, \\ K_h \frac{\partial c}{\partial \vec{n}} &= 0 \quad \text{on} \quad S^+ = \{ \partial \Omega \times (0,T) \mid \vec{v} \cdot \vec{n} \geq 0 \} \end{aligned} \quad (2)$$

and the initial condition

$$c(0) = c_0 \quad \text{in} \quad \Omega . \tag{3}$$

The following notation is used: Ω - domain with the boundary $\partial\Omega = S^+ \cup S^-$, c - concentration, \vec{v} - wind field vector, K_h - horizontal diffusion coefficient, γ - transformation coefficient, Q - emission field, \vec{n} - outward normal vector. In the case of multi-species or multi-layer models this is the respective set of transport equations which are coupled by the chemical transformation rates and/or by vertical diffusion coefficient. Implementation of the used model relates to the requirements of an application and to the pollutants which are considered. But the basic types of air quality models can differ significantly in approach to the analysis of equations (1)–(3) and also to the scale of modelling. As shown in Fig. 1, spatial and temporal scales of the environmental impact of air pollution are correlated with and, moreover, they directly depend on the *lifetime* of pollutant. This parameter can differ significantly between compounds. Thus, depending on the analysis scale, there are respective categories of modelling: local, regional and global.

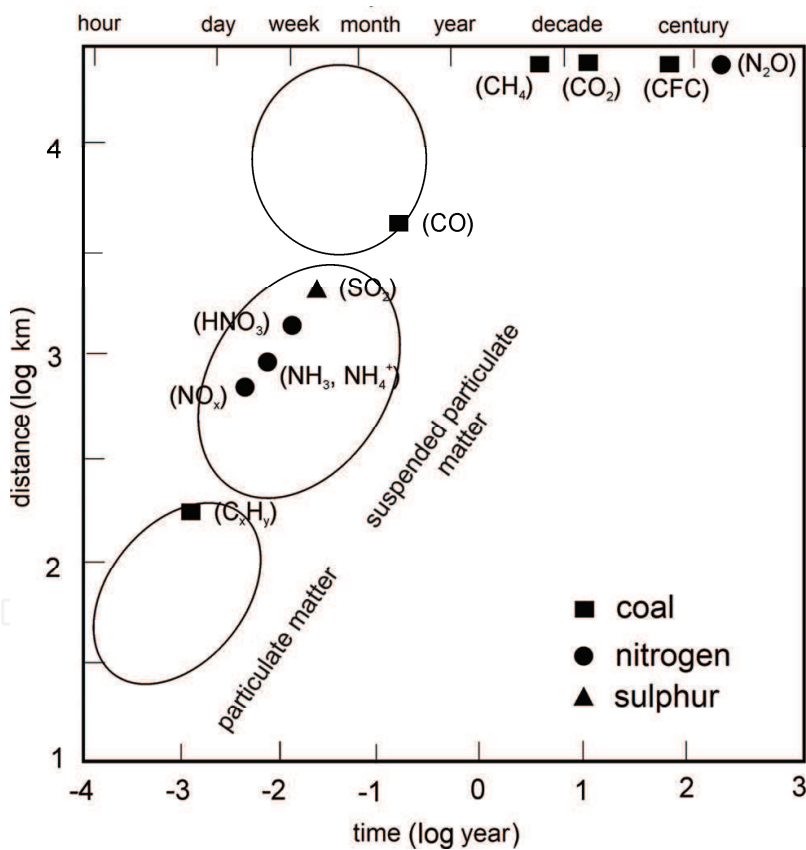


Fig. 1. Correlation of spatial and temporal scale of modelling

Regarding the practical application as well as the scale of modelling, the most common types (implementations) of air pollution models are (Markiewicz, 2004; Sportisse, 2007):

- Gaussian model - based on a simplified, analytical solution of transport equations, originally used mainly for local scale analysis. However, the new generation of

Gaussian models is now available, where variability of main meteorological fields is taken into account, with models also used on regional scale (Scire et al., 2000).

- Lagrangian model – where the related trajectory of an air polluting parcel is observed and analyzed, according to the wind field and other meteorological parameters. Mathematical description takes a form of the respective set of ordinary differential equations (source-oriented approach). The advantage of this method is a natural ability to assess individually the environmental impact of selected emission sources via *transfer matrices*. This approach is utilized in the analysis of emission abatement strategy (compare, e.g. Cofala et al., 2010; Holnicki, 2010b; Kelly, 2006).
- Eulerian model – mathematically governed by finite-dimensional approximation of equations (1)–(3), where a modelling region is horizontally and vertically discretized into the respective number of cells. Parameters of numerical scheme (temporal and spatial discretization steps) must be accordingly set, to satisfy stability and monotonicity conditions (Jacobson, 2005). Implementations usually include evolution of pollutant concentrations, including advection, diffusion, chemistry, sedimentation and deposition. This category of models, characterized by high computing requirements, is utilized in the most complex regional and multi-scale implementations (receptor-oriented approach).

Models of air pollution dispersion are recently used in numerous projects regarding air quality analysis and management. Such a model, based on the input dataset (emission inventory and meteorological forecast), can quantitatively evaluate environmental quality and suggest the ways of improvement. For example, the models can be directly used for:

- forecasting of air pollution distribution in the domain,
- assessment of air quality standard violation (critical levels for concentrations or critical loads for depositions),
- assessment of environmental impact of some specified sources,
- selection of optimal locations for new investments,
- simulation and analysis of emission abatement strategies.

Apart from such a direct use of air pollution models, many countries have recently been trying to develop so called *Integrated Assessment Models* (IAM) (ApSimon et al., 2002) which are designed for complex analysis of environmental quality and are to be used for supporting decisions in environmental quality management. The integrated assessment models (compare Fig. 2, according to (Russel & Dennis, 2000)), recently developed, aim to combine a classical pollution transport model with some economic, technological and other constraints and standards. Such a system, aside from the natural scenario analysis, gives also the possibility to formulate and solve optimization problems, which take into consideration certain specified environmental standards. Some general optimization methods give the possibility of implementation of complex air quality control strategies.

A traditional air pollution transport model is one of the components of such an integrated system. Complementary modules allow us to take into consideration some additional relations and constraints, for example technological, economic, demographic, ecological, and others. This system is a tool for a complex analysis of environment-oriented development strategies as well as for solving the respective optimization problems (compare Holnicki, 2006, 2010a). However, irrespective of how complex such a system is, its main component is usually an air pollution dispersion model, with other modules including respective constraints and limits. An important stage of this complex analysis consists in the

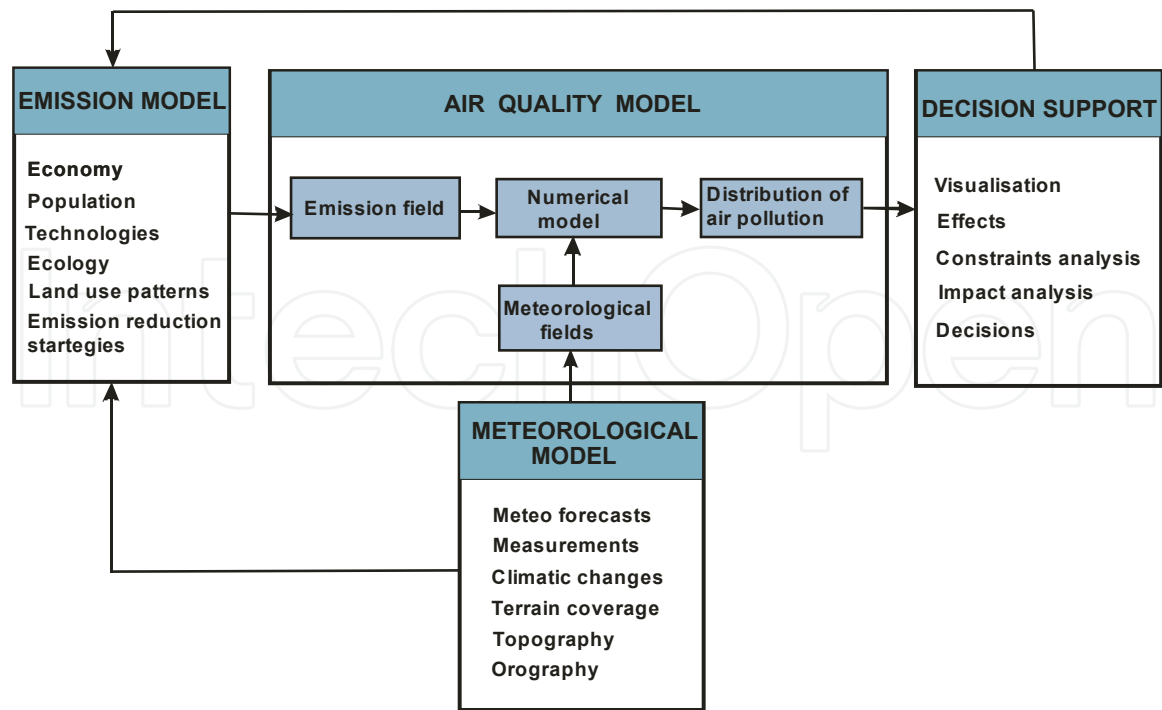


Fig. 2. Exemplary block-diagram of Integrated Assessment Model

assessment of environmental impact of individual emission sources. Such an evaluation is more natural by use of 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. A possible approach in this case was presented in (Holnicki, 2006).

To implement each strategy of air quality management, an air quality damage (air quality cost) function must be defined. Definition of such an index usually relates to the main polluting factors, such as concentration of pollutants (temporary or long-term averaged), cumulated deposition or exceedance of critical loads (Cofala et al., 2010; Holnicki, 2006; Mill & Schlama, 2010). Another important index that is considered in formulation of the optimal emission reduction strategy is the cost of strategy implementation. Denoting, respectively:

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

$\Phi_2(\vec{u})$ – cost of each emission abatement action,

(\vec{u} is the emission vector of controlled sources) 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

$$\begin{cases} \Phi_1(c(\vec{u})) \rightarrow \min, \\ \Phi_2(\vec{u}) \leq \Phi_{2,MAX}, \end{cases}$$

b. Obtaining the assumed air quality standard at the minimum total cost.

$$\begin{cases} \Phi_2(\vec{u}) \rightarrow \min, \\ \Phi_1(c(\vec{u})) \leq \Phi_{1,MAX}. \end{cases}$$

In (Holnicki, 2010a) an emission control problem is considered, where the objective function is formulated in a more general form as compared to 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) emission sources. This general index is as follows:

$$J(c(\vec{q})) = \alpha_1 \int_0^T \int_{\Omega} \varphi_1(c(\vec{q})) d\Omega dt + \alpha_2 \int_0^T \varphi_2(\vec{q}) dt. \quad (4)$$

The respective regularity of the sub-integral functions φ_1 and φ_2 is assumed. The time interval $(0, T)$ depends on the temporal scale of an analysis, and can vary from several hours (short-term forecasts, emission control) to one year (long-term strategy analysis). In all optimization algorithms, it is necessary to assess sensitivity of the quality index to emission of individual sources. An exemplary implementation, based on adjoint transport equations, is discussed in (Holnicki, 2006, 2010a).

In the sequel (compare Section 5) another implementation of an environment-oriented decision task is considered. The problem consists in optimal selection of emission reduction technologies in controlled emission sources in order to obtain the predefined air quality standard at the minimum cost. In this case the main aim is not to solve the optimization problem itself, but to assess how uncertainty of the input data influences the accuracy of a solution to this final decision problem.

3. Sources of uncertainty in air quality modelling

Depending on the model considered, there are numerous potential sources of imprecision and uncertainty in general forecasts of air pollution. The main sources of such uncertainty can be (compare Hanna et al., 1998; Sax & Isakov, 2003; Sportisse, 2007):

- a. input data (emission inventory, meteorological forecast),
- b. model structure, simplifications and parameterizations,
- c. numerical implementation (temporal and spatial domain discretization, applied numerical approximation scheme),
- d. other specific model parameters.

In the case of model input uncertainty, for instance, meteorological data or emissions are uncertain themselves due to measurement errors, estimation errors and inherent variability. Model conceptual uncertainty appears because a single model parameter or mathematical description can never precisely characterize the considered process. Another conceptual uncertainty occurs because a discrete representation of numerical code is used to represent continuous physical processes and their natural variability.

In the case of emission sources, uncertainty is mainly related to the source category, namely emission intensity, composition of polluting compounds, technological characteristics, etc. For example, relatively low uncertainty characterizes high point sources (representing the energy sector, power plants and heating plants), mainly due to well defined and stable combustion processes and known fuel parameters. Uncertainty is more significant in the case of small and intermediate industrial point sources, where all the combustion parameters are less precise and can change in time. On the other hand, high uncertainty must be assigned to area sources (residential sector of urban agglomerations, distributed industrial sources) and to linear sources (usually representing the transportation system).

Meteorological forecast consists of a set of input data which are the result of a multi-step process of data assimilation (Jacobson, 2005). The consecutive steps of this procedure encompass: measurements, numerical weather prediction (by the specialized meteorological model) and analysis, in order to merge the results and generate the final meteorological dataset for a given time interval. Each of these steps generates certain error which contributes to the final accuracy of the forecast. An additional source of uncertainty is connected with the fact that air pollution models usually apply different space discretization grids than meteorological predictor, and data must be additionally interpolated.

Model induced uncertainty relates directly to the type of the mathematical structure. As an example, one can observe that errors generated by relatively simple Lagrangian models are related to uncertainty in deriving wind trajectories, especially in multi-layer implementations. Moreover, some additional errors are due to neglecting a turbulent diffusion process in most of simplified trajectory approaches. Due to these problems and less precise mathematical representation of the Lagrangian approach, Eulerian models are becoming the dominating forecasting tools in air quality analysis. On the other hand, solving the finite-dimensional approximation of transport equations in this category of models leads to the known numerical problems, such as numerical diffusion effect, spurious oscillations and shape modifications. Some special shape-preserving numerical schemes must be applied to eliminate or reduce these negative effects (compare e.g. Holnicki, 2006; Jacobson, 2005).

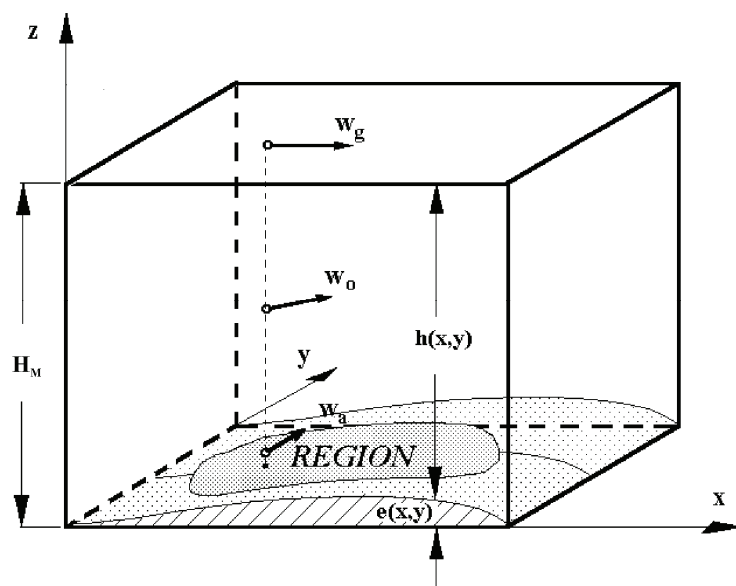


Fig. 3. Mixing height, H_m and vertical wind profile

Commonly used operational models (applied for decision support) of air pollution, to improve performance utilize a simplified mathematical representation which requires some additional meteorological data, usually not included in the standard dataset of weather prediction. These can include, for example, *mixing height* or *atmospheric stability* parameters, which are evaluated in a rather imprecise (heuristic) process, based on some standard meteorological data (Markiewicz, 2004). Mixing height is a key parameter, particularly in models with a rough vertical resolution or in single-layer implementations, where the air pollution concentration is calculated as averaged over the mixing layer (compare Fig. 3).

Approximation of a vertical wind profile is another important feature which characterizes the model accuracy. Wind velocity and direction change vs. elevation, as shown in Fig. 3, due to a wind shear effect. Geostrophic wind vector, $\vec{w}_g = [u_g, v_g]$, at the upper bound of the mixing layer results from the pressure distribution over the domain. The shear of this vector in lower layers is the result of the Coriolis force and the friction between air masses and the Earth surface. In some implementations, the vertical wind profile is assessed based on geostrophic and anemometric wind vectors: \vec{w}_g , \vec{w}_a (Holnicki, 2006; Markiewicz, 2004).

This procedure also contributes to the final uncertainty of model predictions. Atmospheric stability is another key meteorological parameter which strongly contributes to the overall uncertainty. It depends on the vertical gradient of temperature in the mixing layer and has a significant impact on air pollution transport. The reference here is a so called *adiabatic gradient* – when temperature decreases about 10 °C for each 1000 m of height (Jacobson, 2005). This situation refers to neutral conditions of atmospheric stability. If the gradient is greater than adiabatic (temperature decreases more rapidly), there are unstable conditions and it means an intensive mixing process of air pollution. On the other hand, for stable conditions when temperature gradient is less than adiabatic (or reversed), the air pollution mixing process is minimal and pollution plume is narrow. In many practical applications of an operational model, the Pasquill classification of atmospheric stability is applied, as shown in Table 1.

Category	Atmospheric stability class
A	strongly unstable
B	unstable
C	slightly unstable
D	neutral
E	slightly stable
F	stable

Table 1. Atmospheric stability classes

The above mentioned and other model parameters depend on the implementation which is applied. In the next section air pollution model uncertainty is determined based on some specific Eulerian model implementation on regional scale. Emission field is composed of power plants located in the region. To evaluate uncertainty of the model prediction, uncertainty of the main input data as well as the key conceptual model parameters are taken into consideration in a Monte Carlo analysis. Results of the model uncertainty assessment are then used in Section 5 in an analysis of the impact on decision process.

4. Uncertainty analysis – regional case study

The uncertainty analysis has been performed for a regional-scale 3-layer Eulerian model REGFOR3 (Holnicki, 2006, 2010a) applied for Upper Silesia rectangle region shown in Figure 4. Dispersion of SO₂ pollution emitted by 20 dominating power plants has been considered. Space discretization step applied in a numerical process is h=2 km. Resulting concentration values were recorded in 5 fictitious receptor points. Location of receptors and emission sources are shown in Fig. 4.

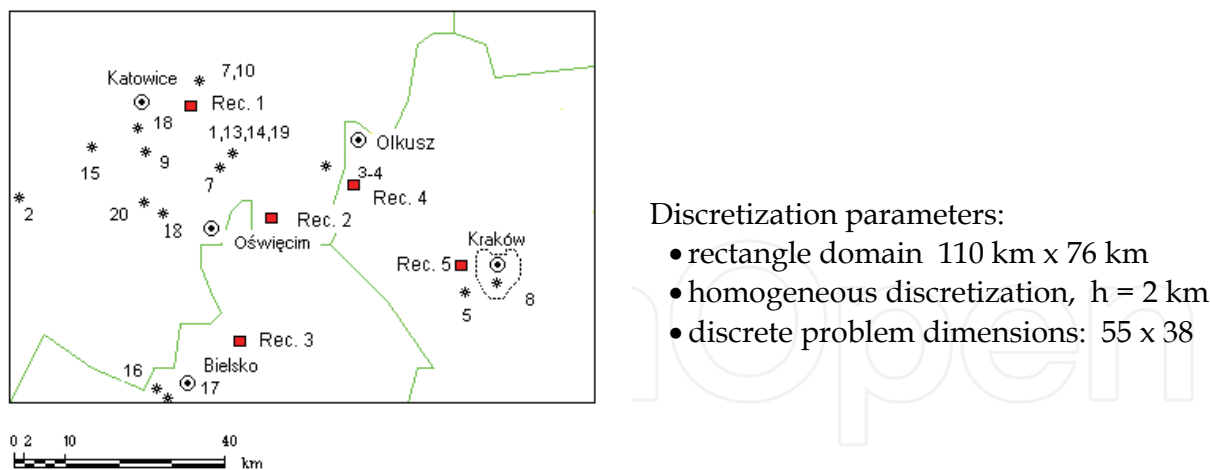


Fig. 4. Computational domain and location of emission sources

The Monte-Carlo algorithm (Hanna et al., 1998; Moore & Londergan, 2001) was applied to carry out the calculations concerning the level of forecast uncertainty. The calculations were performed for the winter season 2005 (meteorological data and emission inventory). The nominal emission intensities within the specified period are shown in Table 2. A numerical experiment consists of three consecutive steps, whose aim is to evaluate the impact of: a) uncertainty of the source emission intensity, b) uncertainty due to the technological

No.	Source	Coordinates	He [m]	Emission SO ₂ [t/d] (Winter)	Emission SO ₂ [t/d] (Summer)
1	Jaworzno III	(21,24)	250	303.2	227.2
2	Rybnik	(1,20)	200	225.2	167.6
3	Siersza A	(30,23)	150	104.0	88.0
4	Siersza B	(30,23)	260	91.8	68.0
5	Skawina	(43,11)	120	90.1	58.6
6	Łaziska I	(8,20)	200	78.0	55.6
7	Będzin B	(18,31)	200	65.0	15.2
8	Łęg	(46,12)	250	52.0	37.2
9	Katowice	(13,25)	250	52.0	37.2
10	Będzin A	(18,31)	160	45.1	30.2
11	Łaziska II	(8,20)	160	34.7	23.1
12	Łaziska III	(8,20)	100	33.8	23.5
13	Jaworzno IIA	(21,24)	120	29.9	19.2
14	Jaworzno IIB	(21,24)	100	25.1	17.7
15	Halemba	(8,25)	110	26.0	17.3
16	Bielsko-Biała	(14,2)	140	18.7	11.2
17	Bielsko-Kom.	(15,1)	250	16.9	7.5
18	Chorzów	(12,27)	100	15.1	7.5
19	Jaworzno I	(20,23)	152	12.3	6.8
20	Tychy	(13,19)	120	11.6	8.6

Table 2. Characteristics of emission sources

parameters of the source, c) uncertainty of the basic meteorological data. The final results represent the total uncertainty regarding these factors.

Table 3 presents the range of uncertainty of the input data, i.e. the emission of sulphur dioxide and technological parameters for 20 analysed sources and the basic meteorological parameters. 1000 sets of test parameters were randomly generated for the specified range of input data uncertainty and the assumed distribution. In order to avoid creating unrealistic meteorological episodes, a correlation between geostrophic and anemometric wind vectors was assumed. Preliminary calculations were carried out for the normal (N) and log-normal distribution (L-N), respectively, for all analysed variables. In the majority of publications (ApSimon et.al., 2002; Hanna et al., 1998), the analysis of uncertainty deals with log-normal distribution. Since, however, the differences in results obtained for both schedules were immaterial (decisive was the width of the uncertainty range), the essential calculations and the results presented in the sequel refer to the normal distribution. The resulting distribution of mean SO₂ concentration is shown in Fig. 5.

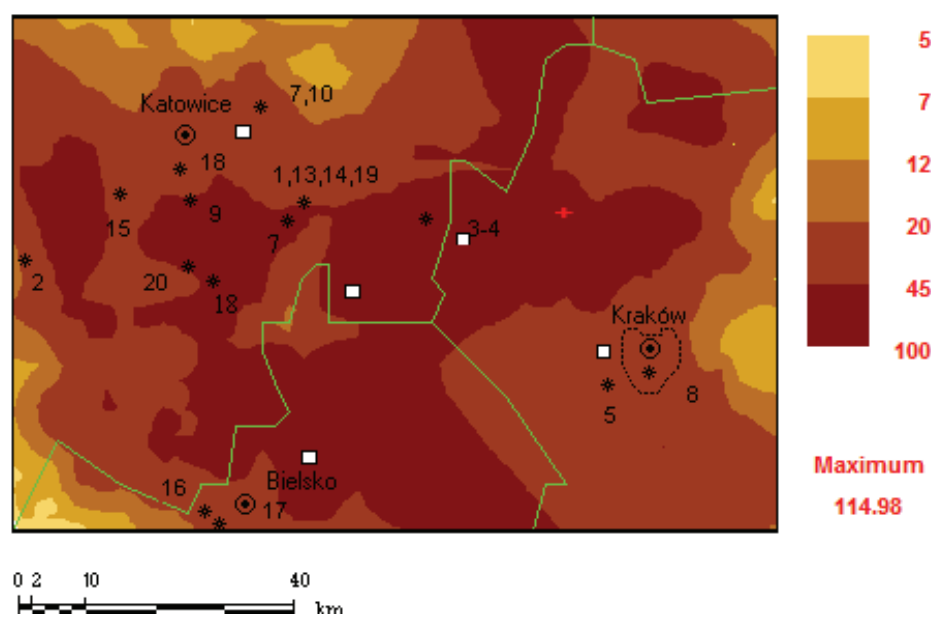


Fig. 5. Mean seasonal SO₂ concentration [μg/m³] in the domain (nominal emission)

Parameter	Uncertainty range (for 95% of data)	Distribution
Emission [g/s]	± 20%	N / L-N
Velocity of outlet gasses [m/s]	± 15%	N / L-N
Temperature of outlet gasses [°K]	± 15%	N / L-N
Mixing height [m]	± 25%	N / L-N
Geostrophic wind components [m/s]	± 25%	N / L-N
Anemometric wind components [m/s]	± 25%	N / L-N
Temperature [°C]	± 25%	N / L-N
Precipitation intensity [mm/h]	± 25%	N / L-N
Atmospheric stability class [-]	± 1	Discrete

Table 3. Uncertainty range of the input parameters

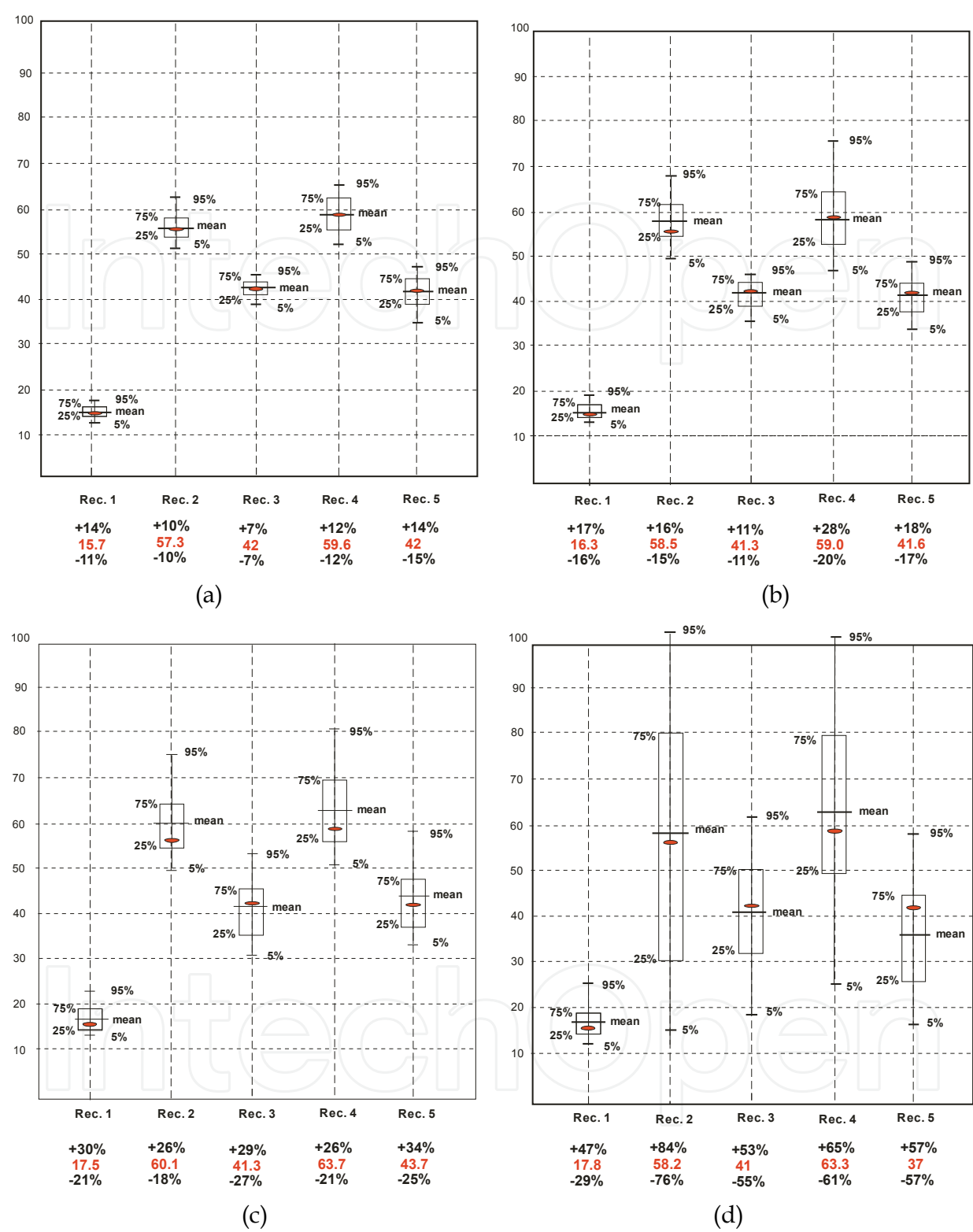


Fig. 6. Impact of input data categories on the resulting forecast uncertainty:
a) uncertainty of the sources' emission intensity,
b) + uncertainty of technological stack parameters,
c) + uncertainty of meteorological forecast (except for atmospheric stability),
d) + impact of atmospheric stability.

The results of calculation were recorded as mean values of SO_2 concentration at receptor points (compare Fig. 4 and Fig. 5 for receptor location), averaged over the simulation period (winter season of the year 2005). Contributions of assumed parameters to the resulting uncertainty of the model forecast are presented in Fig. 6 as standard “box plots”. The presented figures concern 50 and 90 percentile uncertainty ranges of the input dataset, respectively. Full results containing empirical distribution functions and regarding the sample values can be found in (Holnicki, 2010b).

Fig. 6a-b demonstrates that the impact of emission intensity and technological parameters of the source cause uncertainty up to $\pm 20\%$ (for 90% confidence interval). Basic meteorological data (see Fig. 6c), in turn, cause an increase of uncertainty range up to approximately $\pm 30\%$. What is more, the ranges of uncertainty logged in all receptors are broadly similar. A considerable increase in uncertainty occurs after the impact of atmospheric stability is included. In this case, also the substantial variability of results depends on the receptor location. The largest recorded uncertainty of results is connected with receptors No. 2 and 4 (about $\pm 80\%$ and $\pm 63\%$, respectively), with the smallest uncertainty regarding receptor No. 1 (approximately $\pm 30\text{--}45\%$).

There are several reasons of visible and, at the same time, diversified impact of atmospheric stability that must be taken into account. Emission sources considered in the framework of this analysis belong to the category of LCP (Large Combustion Plants – high sources of very large emission intensity). In this category of sources, technological parameters exert a significant impact on the pollution plume dispersion. In conjunction with the fluctuations in atmosphere stability, this gives a very large difference in the spatial scale of a given source impact. On the other hand, very important factors which influence the concentrations recorded at receptor sites are: locations of dominating emission sources, location of the receptors and the dominating wind directions in the specified time interval. The analysis should also take into account the impact of atmospheric balance parameterization, used in the pollution transport model. Moreover, high sensitivity of the model to atmospheric stability may result from the applied parameterization. This, however, requires a more thorough and detailed discussion.

5. Uncertainty in decision support problem

The aim of this section is to illustrate and assess how uncertainties in modelling air pollution transport influence results of the more complex decision support process, where a pollution dispersion model is one of the key components. The decision problem considered in the sequel consists in optimal (at minimum costs) selection of emission reduction technologies within a set of power plants. A regional scale pollution transport model is used as the main forecasting tool, whose uncertainty contributes to the overall uncertainty of the final decision.

5.1 Optimization problem statement

A regional scale decision problem presented in this section constitutes an exemplary implementation of the integrated decision support structure, discussed more generally in Section 2. The task defined in the sequel is sulphur-oriented and addresses the optimal strategy of emission control. It concentrates on the selection of emission reduction

technologies (desulphurization) within a given set of power plants. We assume that there is a set of controlled emission sources (power plants) located in the region under question. Moreover, a set of emission abatement technologies is available. Each desulphurization technology is characterized by certain effectiveness of emission reduction and the unit cost (both for investment and operational costs). Based on these data, optimization problems concerning environmental quality can be formulated (see e.g. Holnicki, 2006, 2010a). One of the possible questions can deal with the optimal allocation of desulphurization technologies to emission sources. The task presented below is aimed at obtaining the required threshold of environmental quality index at minimal costs.

To formally state the optimization problem, the necessary notation must be introduced. Assume that in domain Ω there are N controlled emission sources and we have M desulphurization technologies available. Moreover, we denote:

$\bar{u} = [u_1, u_2, \dots, u_N]$ – emission vector of controlled sources,

$\bar{e} = [e_1, e_2, \dots, e_M]$ – effectiveness vector of desulphurization technologies,

$F = \{f_{ij}\}, (1 \leq i \leq N, 1 \leq j \leq M)$ – matrix of technology abatement cost per unit emission,

$X = \{x_{ij}\}, (1 \leq i \leq N, 1 \leq j \leq M)$ – "0-1" matrix of abatement technology assignment to the controlled sources (decision variable matrix).

The environmental quality index (used in the formulation of required environmental constraints) depends on SO_2 concentration which is the model output. We use a global environmental cost function of the following form:

$$J(c) = \frac{\alpha}{2} \int_{\Omega} w(x,y) \cdot \max^2(0, c(x,y) - c_{ad}) d\Omega, \quad (5)$$

where: $w(x,y)$ – area sensitivity function, c_{ad} – admissible level of SO_2 concentration. Due to the scaling factor α , index J is considered in the sequel as a dimensionless quantity. The concentration forecast, considered as the solution to (1)–(3), is calculated as:

$$c(x,y) = c_0(x,y) + \sum_{i=1}^N A_i(x,y) \cdot u_i, \quad (x,y) \in \Omega, \quad (6)$$

where: $c_0(x,y)$ – background concentration (impact of uncontrolled sources), $A_i(x,y)$ – the unit transfer matrix (relation emission \rightarrow concentration) of the i -th source, u_i – current emission of i -th source.

The unit *transfer matrices*, A_i for the controlled sources are pre-processed off-line by the respective forecasting model. A similar way is used to compute the background pollution field for uncontrolled emissions, including the inflow from the neighbouring regions. The current emission intensity of the i -th source depends on the initial emission level – u_i^0 and the efficiency of the applied abatement technology, according to the formula:

$$u_i = u_i^0 \sum_{j=1}^M (1 - e_j) \cdot x_{ij}, \quad \sum_{j=1}^M x_{ij} = 1, \quad x_{ij} \in \{0,1\}, \quad 1 \leq i \leq N. \quad (7)$$

Cost of emission reduction in each source consists of two components: investment cost and operational cost. Both components depend on the specific abatement technology and on parameters of an energy installation where this technology is to be applied. In this work a simplified approach is utilized. The investment cost of the j -th abatement technology installed in the i -th emission source is calculated as an annual cost, averaged over the entire amortization period. Thus, the total emission abatement cost per year, considered as a sum of desulfurization costs in the respective plants, is considered in the following form

$$C_T = \sum_{i=1}^N u_i^0 \sum_{j=1}^M f_{ij} \cdot x_{ij} = \sum_{i=1}^N u_i^0 \sum_{j=1}^M (f_{ij}^1 + f_{ij}^2) \cdot x_{ij}, \quad (8)$$

where the coefficients: $f_{ij}, f_{ij}^1, f_{ij}^2$ denote the unit, annual investment and operational cost, respectively, of the j -th technology applied to the i -th emission source. Finally, we can state the following:

ALLOCATION TASK (AT): For a given set of admissible solutions, X_{ad}

$$X_{ad} = \{x_{ij} \in \{0,1\}: \sum_{j=1}^M x_{ij} = 1, \quad 1 \leq i \leq N, \quad 1 \leq j \leq M\}$$

assign abatement technologies to emission sources to minimize the total cost

$$C_T = \sum_{i=1}^N u_i^0 \sum_{j=1}^M f_{ij} \cdot x_{ij} \Rightarrow \min$$

and obtain the assumed air quality index $J(c^*) \leq J_0$.

Due to the character of decision variable, the allocation task (AT) is an example of an integer-type optimization. Its numerical analysis requires special algorithms (e.g. heuristic or evolutionary algorithms). In one of the approaches presented in (Holnicki, 2006) the problem is solved by means of a gradient optimization method. For this purpose, the original, integer-type problem is formulated and solved as continuous one. This formulation means that decision variable is continuous, thus the set of admissible solutions is modified as follows:

$$X_{ad} = \{x_{ij} \geq 0: \sum_{j=1}^M x_{ij} = 1, \quad 1 \leq i \leq N, \quad 1 \leq j \leq M\}. \quad (9)$$

Although technologically less realistic (admits technology mixing), the formulation is quite satisfactory from a practical perspective of the decision support and allows application of standard optimization algorithms.

Calculations of the quality index $J(c)$ are based on unit transfer matrices for all of the controlled sources which have been computed off-line by the regional air pollution transport model REGFOR3, presented in more detail in (Holnicki, 2006). The same approach is currently used in uncertainty analysis based on the Monte Carlo procedure. The implementation discussed below is to illustrate how uncertainty of the forecasting model contributes to the accuracy of the decision task.

5.2 Uncertainty in decision support – case study results

Imprecision and uncertainties of the input dataset as well as technological parameters in the combustion process imply uncertainty of air pollution forecasts. Uncertain quantities of concentration are next used as input information in an optimization algorithm, whose aim is to support decisions and to select the best strategy of emission control. The main goal of computations, whose selected results are presented in this section, was to evaluate how uncertainty of air pollution forecasts influences the solution of the optimization problem formulated in Section 5.1 and how it contributes to uncertainty of the final decision.

In the example discussed below we consider 20 controlled sources, as shown in Table 2. Moreover, 8 desulphurization technologies are taken into account (5 basic technologies and 3 combined). The technologies and the respective emission reduction efficiencies are as follows:

1. "do nothing" technology ($e_1 = 0$),
2. low-sulfur fuel ($e_2 \cong 0.30$),
3. dry desulphurization method ($e_3 \cong 0.35$),
4. low-sulfur fuel + dry desulphurization ($e_4 \cong 0.55$),
5. half-dry desulphurization method ($e_5 \cong 0.75$),
6. low-sulfur fuel + half-dry desulphurization ($e_6 \cong 0.83$),
7. wet desulphurization method ($e_7 \cong 0.86$),
8. low-sulfur fuel + wet desulphurization ($e_8 \cong 0.91$).

Given initial emissions of the controlled sources (and the initial value of environmental index J_i), the main task is to obtain an assumed final value, J_o at the minimum cost by the optimal assignment of respective technology to each source. The optimization algorithm used to solve (AT) is based on transfer matrices and it does not need on-line solution of air pollution transport. The Monte Carlo statistical algorithm was utilized to evaluate uncertainty of the optimization task (AT). Thus, 1000 randomly generated sets of emission data for controlled sources were preprocessed and used as the input for the optimization algorithm. Distribution and range of uncertainty of the input emission data should reflect the final uncertainty related to forecasts of air pollution concentrations. To this end, based on the final results presented in Section 4, uncertainty range applied to emission sources used in the optimization process was assumed as the average of 5 resulting receptor values (compare Fig. 6 for forecast uncertainty). Such an approach allows encompassing the impact of all key elements (input emission and meteorological datasets, technological parameters).

Due to editorial limitations, only selected findings of computational tests are shown below (more complete outcomes can be found in the report (Holnicki, 2010b)). They present results of the optimization process (including the impact of uncertainty) for two sets of initial emission intensities: (a) nominal emissions of all sources, as given in Table 2 (initial quality index, $J_i = 3.24 \cdot 10^7$), and (b) emissions increased by 10% (initial quality index, $J_i = 3.92 \cdot 10^7$). Each set of initial input data contains 1000 randomly generated emission episodes for the controlled sources. The normal distribution is assumed with uncertainty range reflecting results of Section 4 (approximately $\pm 50\%$ uncertainty range for 90%

confidence interval). The target (optimal) value of the air quality index in both cases was assumed as $J_o = 1.90 \cdot 10^6$.

src	abatement technologies								emit.
	1	2	3	4	5	6	7	8	
1	.0	.0	.0	.0	.0	.0	1	.0	45.6
2	.4	.0	.6	.0	.0	.0	.0	.0	175.1
3	.0	.0	.0	.7	.0	.0	.3	.0	38.0
4	.0	.0	.0	.0	.0	.0	1	.0	14.3
5	.0	.0	.0	.0	.0	.0	.0	1	9.5
6	.0	.0	.0	1	.0	.0	.0	.0	35.8
7	.0	.6	.0	.4	.0	.0	.0	.0	38.4
8	.0	1	.0	.0	.0	.0	.0	.0	35.9
9	.0	.4	.0	.6	.0	.0	.0	.0	29.2
10	.1	.0	.9	.0	.0	.0	.0	.0	31.3
11	.0	.1	.0	.9	.0	.0	.0	.0	16.9
12	.0	.0	.0	.0	.0	.0	.1	.9	3.7
13	.0	.0	.0	.0	.0	.0	.0	1	3.1
14	.0	.0	.0	.0	.0	.0	.0	1	2.6
15	.0	.0	.0	.3	.0	.5	.0	.2	6.5
16	.0	.0	.0	.5	.3	.2	.0	.0	6.2
17	.0	.0	.5	.5	.0	.0	.0	.0	9.5
18	.0	.0	.0	.0	.0	.2	.0	.8	1.8
19	.0	.0	.0	1	.0	.0	.0	.0	5.6
20	.0	.0	.0	.8	.0	.2	.0	.0	4.4

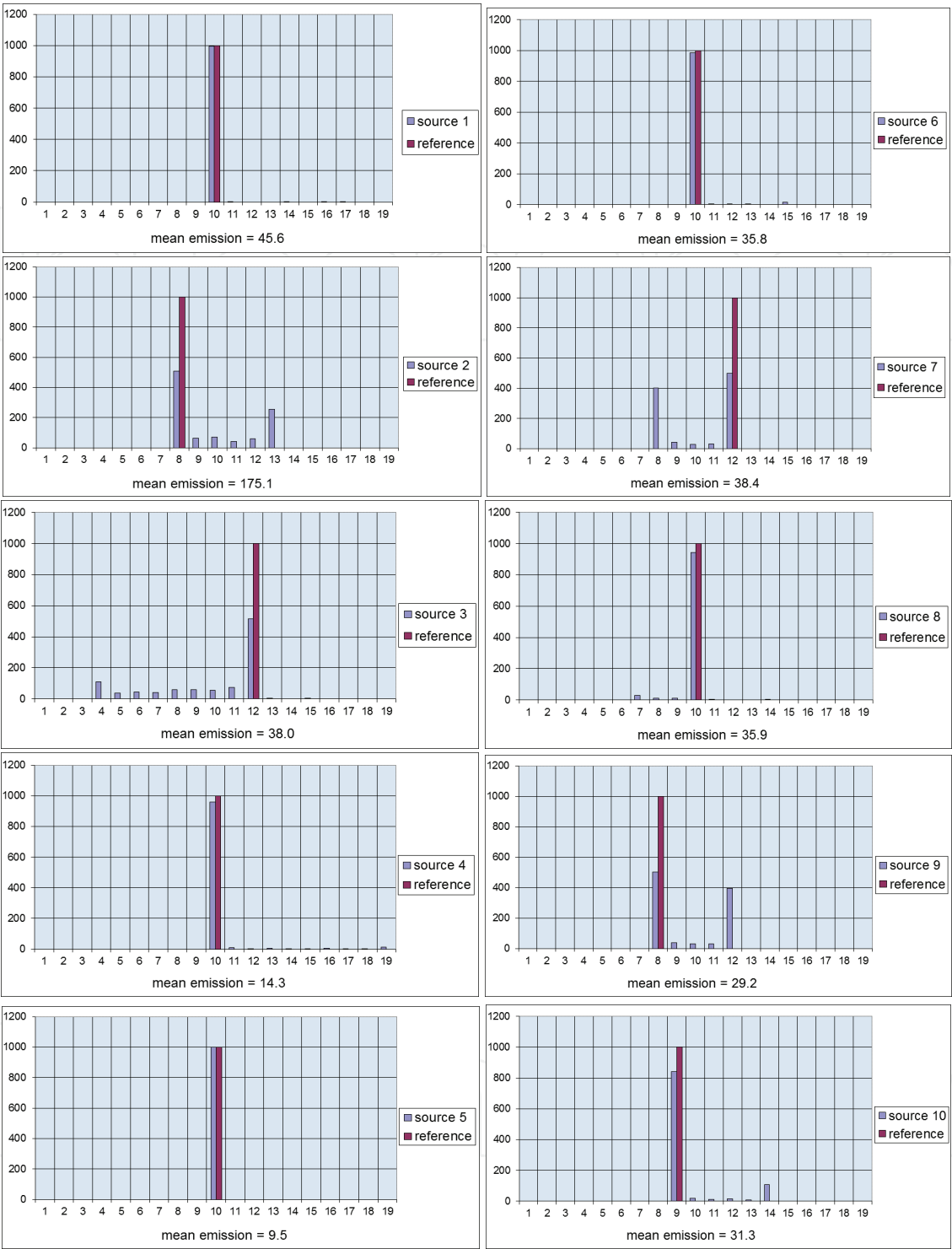
abatement technologies								emit.
1	2	3	4	5	6	7	8	
.0	.0	.0	.0	.0	.0	1	.0	45.5
.0	.0	1	.0	.0	.0	.0	.0	146.3
.0	.0	.0	1	.0	.0	.0	.0	47.3
.0	.0	.0	.0	.0	.0	1	.0	13.7
.0	.0	.0	.0	.0	.0	.0	1	9.5
.0	.0	.0	1	.0	.0	.0	.0	35.5
.0	1	.0	.0	.0	.0	.0	.0	45.5
.0	1	.0	.0	.0	.0	.0	.0	36.4
.0	.1	.0	.9	.0	.0	.0	.0	24.2
.0	.0	1	.0	.0	.0	.0	.0	29.3
.0	.0	.0	1	.0	.0	.0	.0	15.8
.0	.0	.0	.0	.0	.0	.0	1	3.5
.0	.0	.0	.0	.0	.0	.0	1	3.1
.0	.0	.0	.0	.0	.0	.0	1	2.6
.0	.0	.0	.2	.0	.8	.0	.0	5.7
.0	.0	.0	.4	.6	.0	.0	.0	6.2
.0	.0	.6	.4	.0	.0	.0	.0	9.7
.0	.0	.0	.0	.0	.0	.0	1	1.6
.0	.0	.0	1	.0	.0	.0	.0	5.6
.0	.0	.0	1	.0	.0	.0	.0	5.3

Table 4. Optimal fuzzy solution (left) and reference continuous solution (right) for optimization parameters: $J_i = 3.24 \cdot 10^7$; $J_o = 1.90 \cdot 10^6$; $C_T \approx 190$.

src	abatement technologies								emit.
	1	2	3	4	5	6	7	8	
1	.0	.0	.0	.0	.0	.0	1	.0	50.0
2	.2	.0	.8	.0	.0	.0	.0	.0	174.7
3	.0	.0	.0	.3	.0	.0	.7	.0	27.8
4	.0	.0	.0	.0	.0	.0	1	.0	15.2
5	.0	.0	.0	.0	.0	.0	.0	1	10.4
6	.0	.0	.0	1	.0	.0	.0	.0	39.2
7	.0	.3	.0	.7	.0	.0	.0	.0	37.3
8	.0	.8	.0	.2	.0	.0	.0	.0	37.6
9	.0	.2	.0	.8	.0	.0	.0	.0	28.6
10	.0	.0	1	.0	.0	.0	.0	.0	32.8
11	.0	.0	.0	1	.0	.0	.0	.0	17.8
12	.0	.0	.0	.0	.0	.0	.0	1	4.0
13	.0	.0	.0	.0	.0	.0	.0	1	3.5
14	.0	.0	.0	.0	.0	.0	.0	1	2.9
15	.0	.0	.0	.1	.0	.4	.0	.5	5.0
16	.0	.0	.0	.2	.3	.4	.1	.0	5.3
17	.0	.0	.3	.7	.0	.0	.0	.0	9.5
18	.0	.0	.0	.0	.0	.1	.0	.9	1.8
19	.0	.0	.0	1	.0	.0	.0	.0	6.2
20	.0	.0	.0	.5	.0	.4	.0	.1	3.8

abatement technologies								emit.
1	2	3	4	5	6	7	8	
.0	.0	.0	.0	.0	.0	1	.0	50.0
.0	.0	1	.0	.0	.0	.0	.0	161.1
.0	.0	.0	1	.0	.0	.0	.0	28.0
.0	.0	.0	.0	.0	.0	1	.0	15.1
.0	.0	.0	.0	.0	.0	.0	1	10.4
.0	.0	.0	1	.0	.0	.0	.0	39.0
.0	1	.0	.0	.0	.0	.0	.0	32.5
.0	1	.0	.0	.0	.0	.0	.0	40.0
.0	.1	.0	.9	.0	.0	.0	.0	26.0
.0	.0	1	.0	.0	.0	.0	.0	32.2
.0	.0	.0	1	.0	.0	.0	.0	17.3
.0	.0	.0	.0	.0	.0	.0	1	3.9
.0	.0	.0	.0	.0	.0	.0	1	3.5
.0	.0	.0	.0	.0	.0	.0	1	2.9
.0	.0	.0	.2	.0	.8	.0	.0	5.0
.0	.0	.0	.4	.6	.0	.0	.0	5.0
.0	.0	.6	.4	.0	.0	.0	.0	8.7
.0	.0	.0	.0	.0	.0	.0	1	1.7
.0	.0	.0	1	.0	.0	.0	.0	6.2
.0	.0	.0	1	.0	.0	.0	.0	5.8

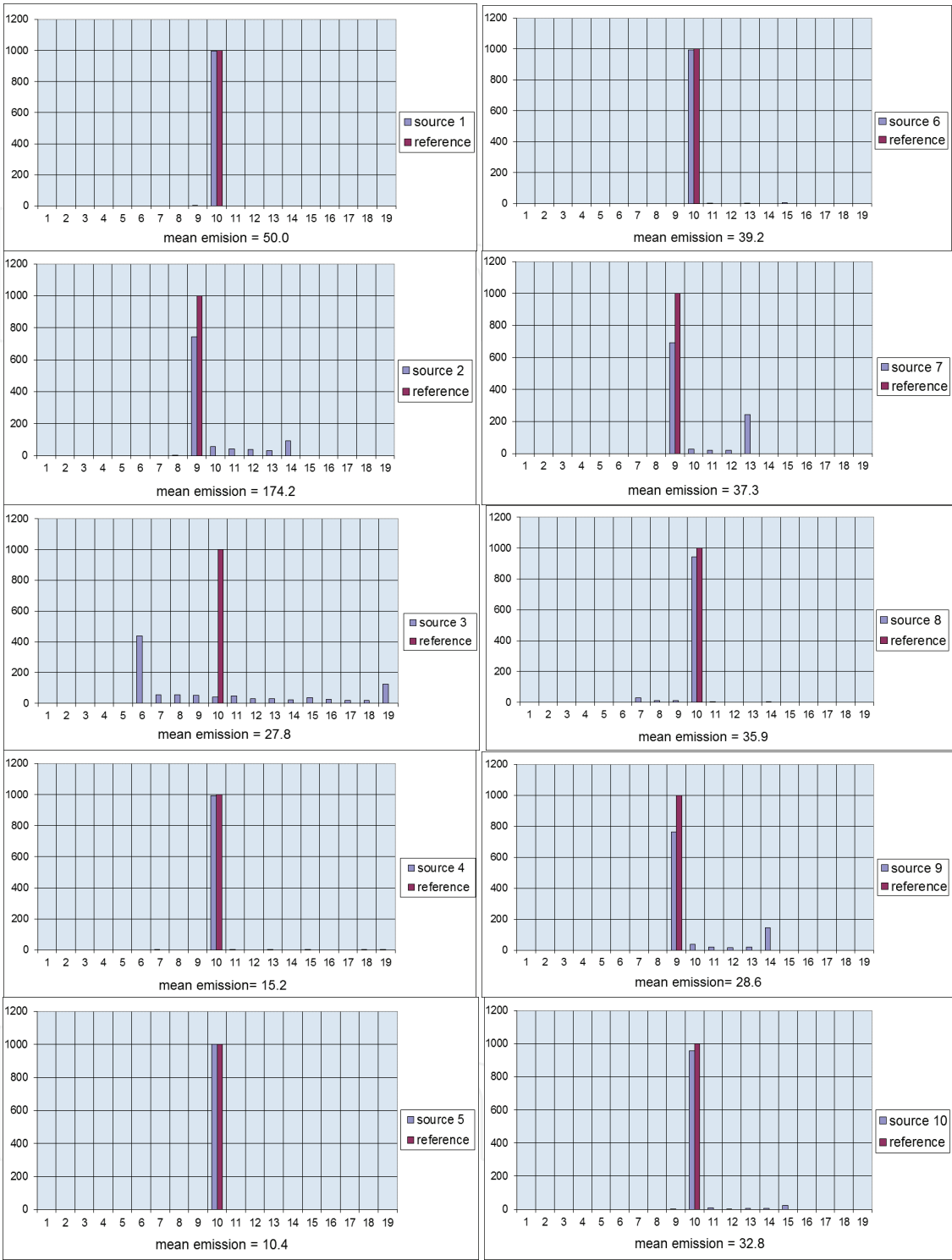
Table 5. Optimal fuzzy solution (left) and reference continuous solution (right) for optimization parameters: $J_i = 3.92 \cdot 10^7$; $J_o = 1.90 \cdot 10^6$; $C_T \approx 208$.



Categories:

1) 0.0 - 0.15	6) 0.55 - 0.65	11) 1.05 - 1.15	16) 1.55 - 1.65
2) 0.15 - 0.25	7) 0.65 - 0.75	12) 1.15 - 1.25	17) 1.65 - 1.75
3) 0.25 - 0.35	8) 0.75 - 0.85	13) 1.25 - 1.35	18) 1.75 - 1.85
4) 0.35 - 0.45	9) 0.85 - 0.95	14) 1.35 - 1.45	19) 1.85 - 1.95
5) 0.45 - 0.55	10) 0.95 - 1.05	15) 1.45 - 1.55	

Fig. 7. Histogram of emission [t/d] for optimal solutions (sources 1-10; $J_i = 3.24 \cdot 10^6$)



Categories:

1) 0.0 - 0.15	6) 0.55 - 0.65	11) 1.05 - 1.15	16) 1.55 - 1.65
2) 0.15 - 0.25	7) 0.65 - 0.75	12) 1.15 - 1.25	17) 1.65 - 1.75
3) 0.25 - 0.35	8) 0.75 - 0.85	13) 1.25 - 1.35	18) 1.75 - 1.85
4) 0.35 - 0.45	9) 0.85 - 0.95	14) 1.35 - 1.45	19) 1.85 - 1.95
5) 0.45 - 0.55	10) 0.95 - 1.05	15) 1.45 - 1.55	

Fig 8. Histogram of emission [t/d] for optimal solutions (sources 1-10; $J_i = 3.92 \cdot 10^6$)

The basic, discrete-type solutions of the discussed optimization problems are shown in Table 4 and Table 5, respectively. Each set consists of two tables, with the first one relating to the fuzzy (reflecting uncertainty of data) solution and the second one to the reference, basic solution connected with the nominal values of emission in all sources. The original task is defined as an integer optimization problem, but the reference solution may also show some “fuzziness” due to the continuous approach applied in the optimization algorithm. Effect of the solution uncertainty can be observed by comparing both tables: left – for an uncertain solution and right – for a reference solution. It can be observed that in both cases (Table 4 and Table 5, respectively) there are 8–9 sources with an exact solution, with the remaining sources having more fuzzy (which means uncertain) character.

Other type results of the discussed optimization tasks are presented in Figures 7–8. They show the histograms of emission intensities relating to the optimal solution (only 10 dominating emission sources are presented), which include the impact of the input data uncertainty. The fuzzy emission distribution reflecting resulting uncertainty is once again compared with the basic (reference) solution obtained for the nominal initial emission (no uncertainty). It can be seen that the solutions for about 5-6 sources are exact (coincide with the reference solution) while the others demonstrate the impact of the input data uncertainty. One can also observe the correlation between the histograms and discrete-type solutions presented in Tables 4–5.

6. Summary

The aim of the computational tests presented in the previous section was to assess the uncertainty impact of modelling air pollution dispersion, when a pollution transport model is a part of a more complex decision support system. In the discussed implementation, the decision searched is defined as the result of an environment-oriented optimization problem. The utilized implementation addresses the problem of the optimal (minimum cost) allocation of emission abatement technologies, subject to the assumed (required) air quality standard which must be achieved (AT problem). The air quality is measured by means of the criterion function (5), which directly depends on an air pollution concentration, evaluated by a regional scale forecasting model (REGFOR3 Eulerian model (Holnicki, 2006; 2010a) is used). Uncertainties generated by the forecasting model (discussed in Section 4) manifest themselves in the final solution of the decision problem (results in Section 5).

The Monte Carlo analysis algorithm was applied to assess overall uncertainty of the optimization problem (AT). Selected results presented in Section 5 illustrate optimal solutions for two sets of the input data that relate to the mean emission intensity of the sources: (a) nominal emissions as shown in Table 2 (Winter season is considered), and (b) emissions increased by 10%. Randomly generated set of 1000 initial emissions was prepared for both cases, with the normal distribution of the data and uncertainty range corresponding to the results of Section 3.

Two types of results are presented. The first one has the form of a discrete-type solution that shows which emission reduction technologies should be applied in power plants under consideration to satisfy conditions of the (AT) problem. Some general conclusions can be formulated based on the two initial data case studies. Irrespectively of the initial data, identical or very approximate solutions were found for about 10 sources. These are the

sources No. 1, 4, 5, 6, 10-14, and 19. The fuzzy (uncertain) solution is also identical or very approximate to the reference one. Moreover, it can be observed that in the other sources, where fuzziness of the solution is more significant, the suggested choice of abatement technologies corresponds with the reference solution. Generally, more significant uncertainty characterizes the same sources, irrespectively of the assumed initial emissions. These are, first of all, sources with minor emission intensity or those located near the boundary of the computational region. The second group of results presents the histograms of each source's emissions which refer to the optimal solution to (AT). The fuzzy (uncertain) solution is once again compared with the reference one, obtained for the nominal input emission data. Moreover, in the optimal solution to all sources presented in Fig. 7–8, the dominating emission value of the distributed (with uncertainty) emissions coincides with the reference solution. On the other hand, while comparing the correspondence between the respective sources in Figures 7–8 and Tables 4–5, one can also see the correlation between these two types of results.

General conclusion that follows from the above tests relates to the applicability of operational air pollution transport models for supporting decisions in the field of environment protection policy. Most of decisions related to air quality management have a rather qualitative character. Thus, based on the results of the discussed case study, a more general opinion can be stated that, in spite of forecasting models' uncertainty, the accuracy of air quality predictions is sufficient for most of the applications and such predictions can be useful in decision support processes as well as in a strategic policy formulation regarding air quality management. On the other hand, taking both the needs of applications and uncertainty of the modelling process into consideration, utilization of very precise and time-consuming optimization algorithms seems to be unfounded. In this case, a sufficient, accurate and justified decision can be made upon application of simpler and more computationally efficient heuristic methods.

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Advanced Air Pollution

Edited by Dr. Farhad Nejadkoorki

ISBN 978-953-307-511-2

Hard cover, 584 pages

Publisher InTech

Published online 17, August, 2011

Published in print edition August, 2011

Leading air quality professionals describe different aspects of air pollution. The book presents information on four broad areas of interest in the air pollution field; the air pollution monitoring; air quality modeling; the GIS techniques to manage air quality; the new approaches to manage air quality. This book fulfills the need on the latest concepts of air pollution science and provides comprehensive information on all relevant components relating to air pollution issues in urban areas and industries. The book is suitable for a variety of scientists who wish to follow application of the theory in practice in air pollution. Known for its broad case studies, the book emphasizes an insightful of the connection between sources and control of air pollution, rather than being a simple manual on the subject.

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Piotr Holnicki (2011). Uncertainty in Integrated Modelling of Air Quality, Advanced Air Pollution, Dr. Farhad Nejadkoorki (Ed.), ISBN: 978-953-307-511-2, InTech, Available from:

<http://www.intechopen.com/books/advanced-air-pollution/uncertainty-in-integrated-modelling-of-air-quality>

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