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PhD. Darko Kneževic, Associative Professor

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Milivoj Stipanovic

Vid Jovisevic, University of Banja Luka, Bosna and Herzegovina
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INVERSE ESTIMATIONS APPLICATION IN THE FIELD OF DISPERSION MODELING

Andreevski Igor [1], Kanevce Gligor [2], Kanevce Ljubica [3], Stavreva Sevde [4], Popovski Kire [5]

Summary: *Pollutants influence assessment over the environment quality and pollution can be very effectively done using dispersion modeling. There are plenty different types of mathematical dispersion models that are used in the scientific and research community these days. They all have different characteristics and can be distinguish between each other according to the mathematical methods and estimations they used, situations and cases which can be solve and simulate on the best way, accuracy of the predicted situations and concentrations etc. Scientific and researcher all around the world are making large efforts in order to improve dispersion models capabilities and to get more realistic picture of the real ground level pollutant concentrations. Inverse estimations are one of the latest and rarely implemented procedures in the area of dispersion modeling. Present paper takes into consideration some inverse approach methods for improving dispersion models performances.*
Keywords: *Inverse estimations, pollutants dispersion modeling*

1. INTRODUCTION

Although in the past twenty years, the method of inverse approach had been implemented in solving problems in many areas of fundamental science and engineering, however, until a few years ago, it hasn't been used in pollutants dispersion modeling.

Scientific team from Faculty of Technical Sciences in Bitola had made inverse method application as part of research and development activities in the process of analyzing and improving performances of existing computer models which simulate the pollutants dispersion in the atmosphere.

[1] PhD Ass.Prof. I. Andreevski, Bitola, Faculty of Technical Sciences,Macedonia, igor.andreevski@uklo.edu.mk
[2] Academic G. Kanevce, Skopje, Macedonian Academi of Art and Sciences, Macedonia
[3] PhD Full Prof. Lj. Kanevce, Bitola, Faculty of Technical Sciences, Macedonia
[4] MSc Assistant S. Stavreva, Bitola, Faculty of Technical Sciences, Macedonia
[5] PhD Assoc. Prof. K. Popovski, Bitola, Faculty of Technical Sciences, Macedonia

2. MAIN CONDITIONS FOR IMPLEMENTING INVERSE METHODS IN DISPERSION MODELS IMPROVEMENT PROCESS

The main objective of this paper is to present the possibilities and conditions for the inverse approach application in order to improve models that simulate the pollutants dispersion in the atmosphere using the example of dispersion model MADAM algorithm. The process of inverse approach implementation involves fulfillment of a number of conditions, and it takes in several stages, interconnected in-between them as follows:

- Selection and definition of parameters included in dispersion models algorithms that have influence on the estimated ground level pollutants concentration. The inverse method has the task to define new values for some of these parameters.
- The most important condition for realization of researches on possible application of inverse method in dispersion models is to have available appropriate experimental data base with the observed and interdependent data sets, such are: meteorological data, the emission parameters and measured values of pollutants ground level concentration in the pre-defined conditions. The measured pollutants ground level concentrations from the selected experimental data base, for different meteorological-emission-imision scenarios are used in numerical simulations and experiments to determine the feasibility and ways to implement an inverse approach and calculation of new values of the analyzed parameters. Also, it is very important that the data for the all measured values, including ground-level concentrations, are authentic, with a high percentage of accuracy.
- Inverse methods can be applied only if the number of measured data, in the concrete case pollutants ground level concentrations, is greater than the number of unknown parameters whose values are subject to inverse calculation. This means that for the particular analyzed emission hour, for which we know the measured data for meteorological, emission and for the pollutants concentration values, the number of measured concentrations, I_{max}, must be greater than the number of parameters N, which values are subject of inverse analysis, ($I_{max} \geq N$).
- Sensitivity coefficients determine sensitivity of calculated pollutant concentrations by the dispersion model on changes in the value of certain particular variable, parameter or constant, featuring in the model algorithms. Change in the value of certain analyzed parameter revoke a given overall change in calculated pollutant concentration. Determination of ground level concentrations sensitivity coefficients with respect to pre-defined and selected parameters allow us to obtain a general picture of the impact that each parameter has on the concentration values. Concentration sensitivity with respect to analyzed parameters is different in different source distances, X. Knowing pollutants concentrations sensitivity with respect to each analyzed parameter as a function of emission source distance X, defines on which distance rank we should have relevant concentrations measured values so we could apply inverse calculation. In fact, although basic condition, to have measured concentration in a number greater than or equal to the number of parameters whose new values are determine using inverse method, ($I_{max} \geq N$), is satisfied, there is a possibility that we can not implement this inverse calculation or the results would be bad if measured concentrations aren't in the distance ranks X where we have highest or at least higher concentrations sensitivity coefficients values with respect to the analyzed parameters. This means that it must be satisfied the condition $I_{max} \geq N$, but within the distance ranks where there are expressed

sensitivity coefficients values with respect to the concrete influenced parameters. Only parameters with satisfactory values of sensitivity coefficients will be analyzed using the inverse procedure, i.e. the new values for these parameters based on measured pollutants concentrations from the experimental data bases will be calculated.

If we analyze concrete example of calculated sensitivity coefficients values of ground level concentrations with respect to several parameters in dispersion model MADAM algorithm, obtained through a numerical simulation and application of Levenberg-Marquardt's method inverse method, in highly unstable weather conditions, represented in Figures 1 to 4, we can draw the following conclusions:

- Figure 1 represents sensitivity coefficients of ground level concentrations with respect to vertical and horizontal dispersion coefficient, σ_y and σ_z, in two alternative MADAM model solutions v.1 and v.3, for unstable weather conditions. On the basis of these results it can be concluded that vertical and horizontal dispersion coefficient has different effect on the concentration values in both model variants, which is primarily due to the different methods of their calculation. Also, it is important to emphasize that their impact is different in different distances *X*, from the emission source to the receptor, for which the concentration is calculated. These tests should be done for more experimental hours and in different weather conditions. The main intention is to cover wider research area with this examination in order to avoid danger to draw the wrong conclusions about the general behavior of the model and its sensitivity in the calculation of pollutant concentrations. These last remarks can be also apply to all subsequent results represented in the graphs in Figures 2, 3 and 4.

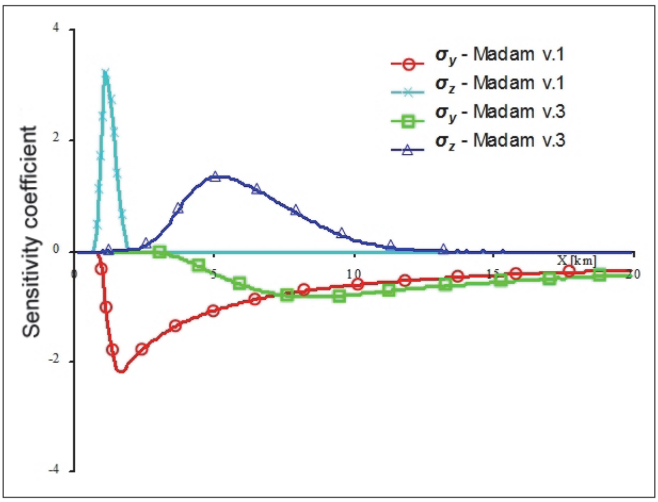

Fig.1 *Ground level concentrations sensitivity coefficients with respect to dispersion coefficients* σ_y *and* σ_z

- Concentration sensitivity coefficients with respect to the mixing layer height in the atmosphere, h_m, and the plume effective height, $h_{s,ef}$, in two model MADAM variants, v.1 and v.3, for unstable weather conditions is shown in

Figure 2. Mixing layer height is meteorological value which is determined through indirect measurements or is calculated using meteorological preprocessor. Therefore, its values are uncertain in some degree, depending on how they are obtained and calculation accuracy. Its role in both model variants algorithms is different, and therefore the degree of its impact on the ground concentration is different. Result from model variant v.3 are showing that mixing layer height has almost no influence on the calculated concentration, while model v.1 results show greatest impact of this parameter in the distance between 2 and 3 [km] from the source, and as we move away from the emission source that influence decreases. However, if we analyze the effective stack height, it can be concluded that in cases of two variants it has an impact on the pollutant concentrations, but in different parts, distances form the source *X*. Thus, in variant 1 its impact is greatest between 1 and 3, and in variant 3 between 5 and 7 [km] from the source.

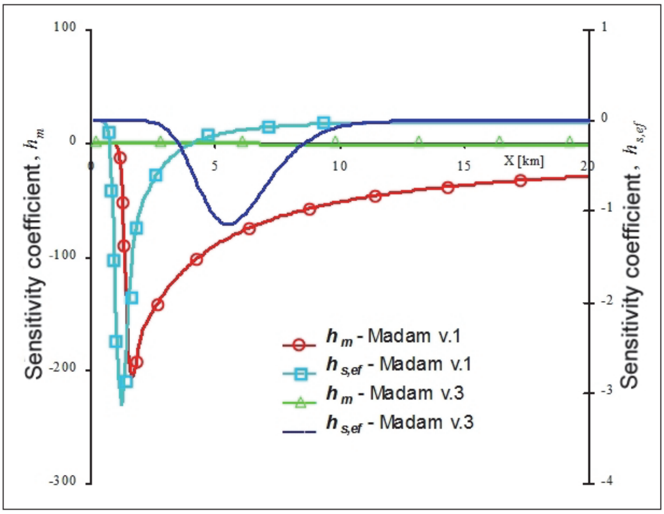

Fig. 2 *Ground level concentrations sensitivity coefficients with respect to mixing layer height h_m, and effective stack height $h_{s,ef}$*

- Analyses made over two previous diagrams are especially interesting in order to establish which of these parameters have the greatest impact on the concentration and on which distance rank X. But, taking in to consideration that dispersion coefficients, mixing layer height and effective stack height are not parameters with constant value, and in fact they are determined by the specific calculation algorithms, they can not be directly be a subject of inverse calculation to determine their new values. However, they are interesting to analyze in order to determined that if some of these parameters have a significant impact on the concentration, then the inverse procedure can be extended by examining the impact and determine new values for some of the empirical constants or parameters featuring in the equations for the parameter specific calculation algorithms.

- The most interesting for analyses, from the aspect of inverse approach application, are concentration sensitivity coefficients with respect to the parameters presented in Figures 3 and 4.

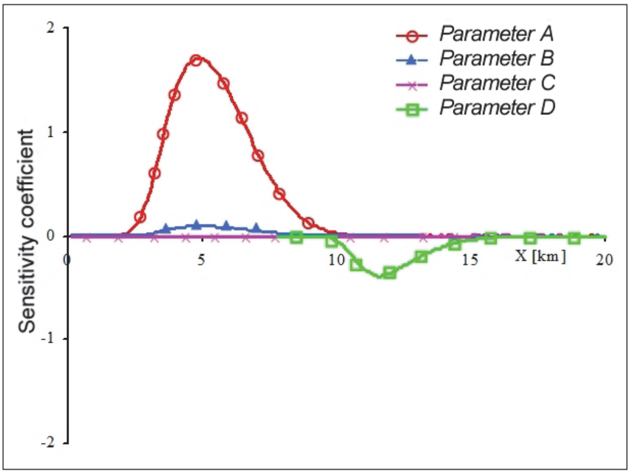

Fig. 3 *Ground level concentration sensitivity coefficient with respect to the parameters A, B, C and D*

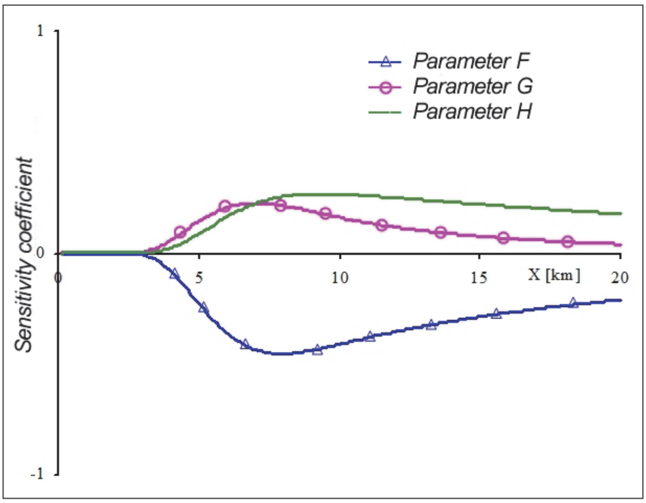

Fig. 4 *Ground level concentration sensitivity coefficient with respect to the parameters F, G and H*

These analyses include determining the impact of some of the constants or the value of certain empirical parameters on the pollutants concentrations in a model MADAM variant. Figure 3 shows that the greatest impact on ground-level concentrations has parameter A, and in the distance interval from 3 up to 9 km. This means that if we want to determine its new value, then we should have the relevant values of measured concentrations for that particular hour, in this distance interval, and in a number greater than the number of parameters which new values we wound like to determine. As in this example, only one parameter, A, is subject of inverse method calculation, then we must have at least two measured concentrations. However as much as measured concentrations we have calculations will be more precise.

- Figure 4 represents concentration sensitivity coefficients with respect to the other three empirical parameters that are also included in the equations for the calculations done in one variant solution of model MADAM. In this case, it is interesting to emphasize that we can come into a situation where we have extreme values of sensitivity coefficients, as is the case for the parameters G and H, on one hand, and the parameter F, on the other hand, while still, keeping in mind that they are almost linearly dependent it is very difficult, almost impossible to simultaneously determine the new values for all of them.

Besides these, there are also other conditions which should be satisfied so we could apply inverse procedure in some dispersion model algorithm. They depend primarily on the specific application of the model, its individual characteristics and parameters derived from its algorithm and which are subject of inverse calculation.

3. CONCLUSION

Paper defines certain terms and conditions that must be followed and fulfilled in order to successfully implement inverse calculations to improve the dispersion models performances.It is important to note once again that it is crucial to choose high-quality experimental data that will be used for realization of numerical simulations, and which would cover most of the potential meteorological-emission-imission scenarios.

Pollutant concentrations measured data should be in that distance interval from the emission sources X where concentration sensitivity coefficients in respect to the analyzed parameters have corresponding distinct values.

As a final, logical step, raises the evaluation and verification of the model results obtained using the inverse calculation. This can be done through several available and widely used procedure for the verification of the results of dispersion models (BOOT, ASTM, etc.), But also the process of validating model new performance can be derived through comparison with data obtained by other verifications of well known and recognized models in the world ranking, which will give more successful general picture of the possibilities, innovations and successes that offers inverse application procedure in the area of computer dispersion models.

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