Inverse Problems, Design and Optimization Symposium
Miami, Florida,U.S.A., April 16-18, 2007

INVERSE APPROACHES IN IMPROVEMENT OF AIR POLUTION PLUME DISPERSION MODELS FOR REGULATORY APPLICATIONS

Gligor H. Kanevce
Macedonian Academy of Sciences and Arts
Skopje, Macedonia
kanevce@osi.net.mk

Ljubica P. Kanevce
Faculty of Technical Sciences
St. Kliment Ohridski University
Bitola, Macedonia
kanevce@osi.net.mk

Igor B. Andreevski
Faculty of Technical Sciences
St. Kliment Ohridski University
Bitola, Macedonia
igor.andreevski@uklo.edu.mk

George S. Dulikravich
Department of Mechanical and Materials Engineering
Florida International University
Miami, Florida, U.S.A.
dulikrav@fiu.edu

ABSTRACT

This paper deals with the application of inverse concepts for improvement of the Gaussian plume dispersion models. The objective of the paper is an analysis of the possibility of the estimation of parameters appearing in the model on the bases of the available ground level measurements of the concentration, obtained in realized experimental campaigns. Two types of the Gaussian plume models have been analyzed. The Industrial Source Complex Short Term (ISCST3) model has been taken as a representative of the models that describe the boundary layer structure in terms of the Pasquill-Gifford Stability Category and OML model as a representative of the models that describe dispersion processes in terms of basic boundary-layer scaling parameters, such as Monin-Obukhov length, the boundary layer height, friction velocity, and the convective velocity scale. The Levenberg-Marquardt method and a hybrid optimization method of minimization of the least-squares norm were used to solve the present parameter estimation problem.

NOMENCLATURE

a = parameter
A = Pasquill -Gifford stability class
A = constant
b = parameter
B = constant
C = vector of estimated concentrations [μg m^{-3}]
C = constant
C = concentration [μg m^{-3}]
D = Pasquill-Gifford stability class
D = constant
E = constant
E = ordinary least square norm [(μg m^{-3})^2]
h = boundary layer height [m]
H = source height [m]
I = identity matrix
K = scaling coefficient (=10^6)
L = Monin-Obukhov length [m]
M = emission rate [g s^{-1}]
P = vector of unknown parameter
t = time [s]
u^* = friction velocity [m s^{-1}]
U = mean wind velocity [m s^{-1}]
x = downwind distance, [m]
y = crosswind distance, [m]
Y = vector of measured concentrations [μg m^{-3}]
z = height [m]

Greek symbols

σ = standard deviation [m]
ω_* = convective velocity [m s^{-1}]

Subscripts

cnv = convective
ef = effective
in = internal
mch = mechanical
s = stack height

trb = turbulent
y = crosswind
z = height

Superscripts

T = transposed

INTRODUCTION

Air quality simulation models are extensively used in assessing the impacts of combustion plants. A wide variety of dispersion models are available. In assessing the impacts of existing and proposed sources of air pollution on local air quality (up to 20 km from the source), particularly for regulatory applications, the Gaussian-plume models are commonly used [1].

The performances of the atmospheric dispersion models usually are tested against the ground level concentration measurements of some pollutant obtained at the locations around the elevated point source (stack). The experimental campaigns are very expensive and have to be prepared very carefully. Even in the cases when a few hundred receptors are located around the stack, for the particular meteorological conditions only a few receptors will be along the direction of plume travel. So, only a few values will be available for verification of the model for these meteorological conditions.

There are few methods for the validation of the Gaussian-plume models, but the appropriate evaluation method cannot be uniquely defined [2-4]. This paper deals with the application of inverse concepts for improvement of the Gaussian plume dispersion models. The objective of the paper is an analysis of the possibility of the estimation of parameters appearing in the model on the bases of the available ground level measurements of the concentration, obtained in realized experimental campaigns.

Two types of the steady-state Gaussian plume models, the ISCST3 and OML have been analyzed in the paper.

The Industrial Source Complex Short Term (ISCST3) model has been taken as a representative of the models that describe the boundary layer structure in terms of the Pasquill-Gifford Stability Category. ISCST3 is a US EPA regulatory model and is widely used over the world. Formally, in 2000, AERMOD [5] was proposed by the US EPA as a replacement for ISCST3. However, this status has not yet been achieved. The regulatory default option (EPA US, 1995) of the ISCST3 atmospheric dispersion model has been used in this paper [6].

The OML is a modern Gaussian plume model [7, 8]. It does not use traditional discrete Pasquill stability categories, but instead describes dispersion processes in terms of basic boundary-layer scaling parameters, such as Monin-Obukhov length, the boundary layer height, friction velocity, and the convective velocity scale. Typically, the OML model is applied for regulatory purposes. In particular, it is the recommended model to be used for environmental impact assessments when new industrial sources are planned in Denmark.

The Levenberg-Marquardt method and a hybrid optimization method of minimization of the least-squares norm were used to solve the present parameter estimation problem.

An analysis of the influence of the wind speed, stability classes, boundary layer height, and downwind distance from the source on the model parameter estimation, enables the design of appropriate experiments is conducted as well. In order to realize this analysis, the sensitivity coefficients and the determinant of the information matrix were calculated for the characteristic meteorological conditions.

MATHEMATICAL FORMULATION

The Gaussian-plume formula for calculating the concentration of pollutant at downwind distance, x, crosswind distance, y, and height above ground, z, for a continuous point source of strength, M, in a uniform flow with homogeneous turbulence and mean wind velocity at stack height, U_s, can be expressed as

$$C(x,y,z) = \frac{M}{2\pi\sigma_y\sigma_z U_s}\exp\left(-\frac{y^2}{2\sigma_y^2}\right)\cdot V\cdot K \quad (1)$$

where, σ_y and σ_z are standard deviations of lateral and vertical concentration distribution, or, the Gaussian plume dispersion parameters and K is a scaling coefficient.

The vertical term

$$V = \sum_n \left\{ \exp\left[-\frac{\left(z - H_{s,ef} + 2nh\right)^2}{2\sigma_z^2}\right] + \right.$$

$$+\exp\left[-\frac{\left(z+H_{s,ef}+2nh\right)^2}{2\sigma_z^2}\right]\Bigg\}\; n=0\,,\pm 1,\,\pm 2,\ldots \quad (2)$$

accounts for the vertical distribution of the Gaussian plume. It includes the effects of source elevation, $H_{s,ef}$, receptor elevation, z, and limited mixing in the boundary layer of height, h. The series term in equation (2) accounts for multiple reflections of the plume from the ground and at the top of the boundary layer. In the usual practice the terms up to ±4 are taken into the calculations. The effective source height, $H_{s,ef}$, is the sum of the stack height and plume rise.

INVERSE APPROACH

For the inverse problem of interest here, some of the parameters appearing in the Eq.1 are regarded as unknown.

The estimation methodology used is based on the minimization of the ordinary least square norm

$$E(\mathbf{P}) = [\mathbf{Y} - \mathbf{C}(\mathbf{P})]^{\mathrm{T}} [\mathbf{Y} - \mathbf{C}(\mathbf{P})]\,. \qquad (3)$$

Here, $\mathbf{Y}^{\mathrm{T}} = [Y_1, Y_2, \ldots, Y_{\mathrm{imax}}]$ is the vector of measured ground level concentrations of pollutant, $\mathbf{C}^{\mathrm{T}} = [C_1(\mathbf{P}), C_2(\mathbf{P}), \ldots C_{\mathrm{imax}}(\mathbf{P})]$ is the vector of estimated ground level concentrations of pollutant at distances x_{i} (i = 1, 2, …, imax) from the stack, $\mathbf{P}^{\mathrm{T}} = [P_1, P_2, \ldots P_{\mathrm{N}}]$ is the vector of unknown parameters, imax is the total number of measurements, and N is the total number of unknown parameters (imax ≥ N).

A hybrid optimization algorithm OPTRAN [9] and the Levenberg-Marquardt method [10, 11] have been utilized for the minimization of $E(\mathbf{P})$ representing the solution of the present parameter estimation problem.

The Levenberg-Marquardt method is a quite stable, powerful, and straightforward gradient search minimization algorithm that has been applied to a variety of inverse problems. It belongs to a general class of damped least square methods.

An alternative to the Levenberg-Marquardt algorithm, especially when searching for a global optimum of a function with possible multiple minima, is the hybrid optimization program OPTRAN. OPTRAN incorporates six of the most popular optimization algorithms: the Davidon-Fletcher-Powell gradient search, sequential quadratic programming algorithm, Pshenichny-Danilin quasi-Newtonian algorithm, a modified Nelder-Mead simplex algorithm, a genetic algorithm, and a differential evolution algorithm. Each algorithm provides a unique approach to optimization with varying degrees of convergence, reliability and robustness at different stages during the iterative optimization procedure. The hybrid optimizer OPTRAN includes a set of rules and switching criteria to automatically switch back and forth among the different algorithms as the iterative process proceeds in order to avoid local minima and accelerate convergence towards a global minimum.

RESULTS AND DISCUSSION

The standard deviation of vertical concentration distribution, σ_z, is one of the most influental parameters appearing in the model. There are a lot of different expressions for σ_z. The US EPA regulatory model ISCST3 used the Pasquill-Gifford expression [6, 12]

$$\sigma_z = a\,x^b \qquad (4)$$

where, x is the downwind distance of the receptor from the stack. For certain meteorological conditions and distances the parameters a and b have constant values. For example, for unstable conditions, the Pasquill-Gifford stability class A, and for x > 0.5 km, a = 453.85 and b = 2.11660.

Figure 1 illustrates the ground level concentrations (normalized by emission, $C/M\cdot 10^9$) along the plume centerline as a function of downwind distance from the source calculated with ISCST3.

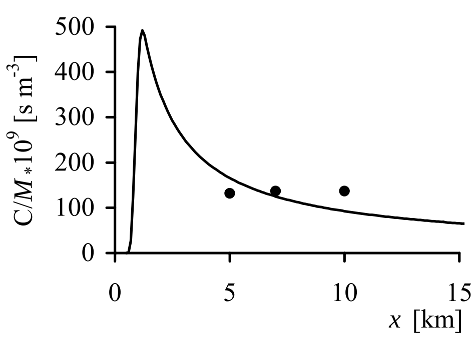

Fig. 1. The ground level concentrations along the plume centerline

The example is for stability class A, wind speed of 2.8 m/s, 187 m high stack and the boundary layer height of 689 m that correspond to one of the conditions in the well known Kincaid experimental campaign [13].

Figure 2 shows the relative sensitivity coefficients $P_j \partial C_i / \partial P_j$, i = 1, 2, for the ground level concentration along the plume centerline with respect to the parameters *a* and *b* in Eq. 4, for the meteorological condition maintained above. It can be seen that they are greater than zero only in the locations from 0.5 to 2 km from the source. Figure 3 presents variations of the determinant of the information matrix if the parameters *a* and *b* are simultaneously considered as unknowns. The maximum determinant value corresponds to the distance of 1.5 km.

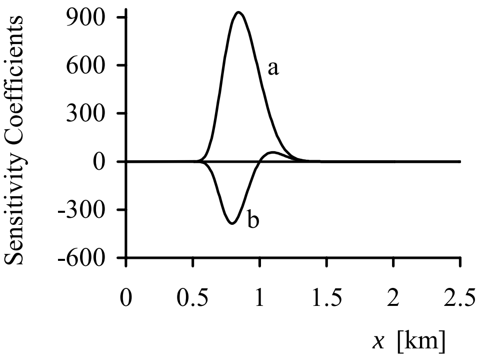

Fig. 2. The relative sensitivity coefficients with respect to the parameters *a* and *b* for the stability class A, wind speed of 2.8 m/s, and the boundary layer height of 689 m

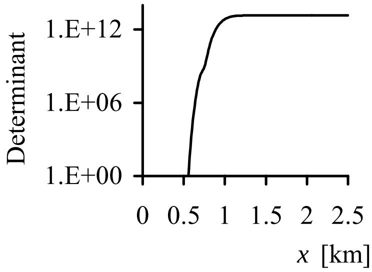

Fig. 3. Determinant of the information matrix if the parameters a and b are simultaneously considered as unknowns

From the previous analysis it can be concluded that at least two errorless concentration measurements are needed for the estimation of the unknown parameters *a* and *b* in the range of 0.5 to 2.0 km. In the Kincaid experimental campaign the receptors were located at 2, 3, 5, 7, and 10 km. For the analyzed case there were only three reliable measured concentrations, at 5, 7 and 10 km (Fig. 1). Consequently, the unknown parameters *a* and *b* can not be estimated for this case.

The other very influental parameter appearing in the Gaussian plume models is the boundary layer height, *h*. Figure 4 shows the relative sensitivity coefficients for the ground level concentration along the plume centerline with respect to the boundary layer height *h*, for the analyzed meteorological condition.

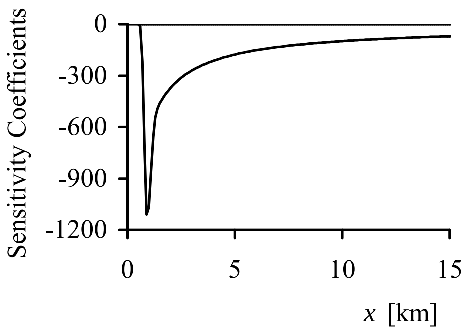

Fig. 4. The relative sensitivity coefficients with respect to the boundary layer height

Figure 5 presents transient variations of the determinant of the information matrix if the boundary layer height is considered as unknown parameter.

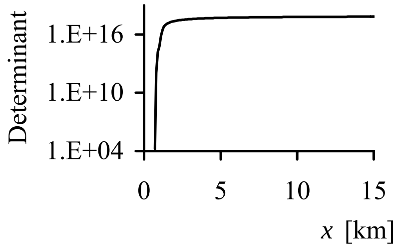

Fig. 5. Determinant of the information matrix if the boundary layer height is considered as unknown parameter

For the analyzed example (stability class A, wind speed of 2.8 m/s), in the report [13] two different values for the boundary layer height are presented. The measured value for *h* was 226 m and the calculated 689. The measured value is unreal, because is much smaller then the effective plume height which is 688 m in this case. So the ground level concentrations should be zero in this case.

The boundary layer height can be estimated from the available ground level concentration from the experimental campaign, by using an inverse approach. On the bases of the ground level measurements of the normalized concentration of 132, 137, and 136.8 at 5, 7 and 10 km respectively, we obtained a value of 809 m for the boundary layer height. It corresponds well with the boundary layer height of 689 reported in [13] having in mind that the methods for calculating the boundary layer height are not of high accuracy.

Similar analyses can be conducted for all other available data for different meteorological conditions.

For neutral conditions, the Pasquill-Gifford stability class D, we have several ranges of data for coefficients *a* and *b*, depending on the value of distance *x*. For example, for $3 < x \leq 10$ km, a = 33.504 and b = 0.60486 and for $10 < x \leq 30$ km, a = 36.650 and b = 0.56589.

In Fig. 6 the ground level concentrations along the plume centerline calculated with ISCST3 are compared with the measurements for an example of the Kincaid experimental campaign [13] with stability class D and wind speed of 10.6 m/s.

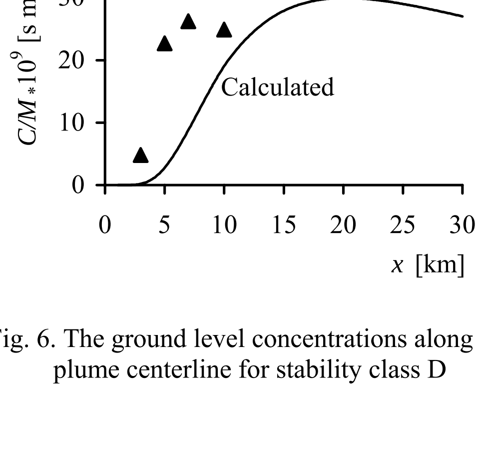

Fig. 6. The ground level concentrations along the plume centerline for stability class D

For this case two different values for the boundary layer height are presented as well. The measured value for *h* was 815 m and the calculated 3156 m. But, from the variations of the relative sensitivity coefficients with respect to the boundary layer height for stability class D and wind speed of 10.6 m/s (Fig. 7) it can be concluded that in this case the model is insensible for $h \geq 800$ m.

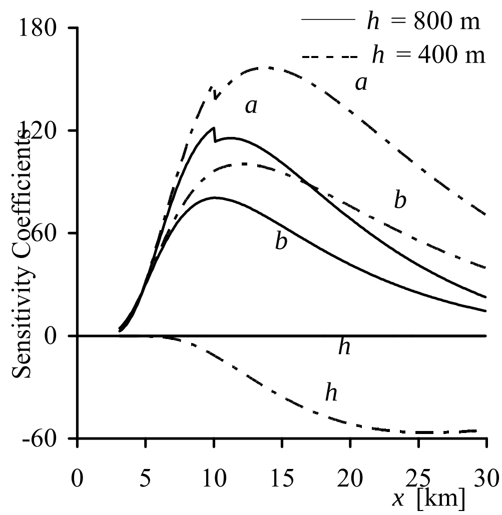

Fig. 7. The relative sensitivity coefficients with respect to the parameters *a*, *b* and *h* for the stability class D, wind speed of 10.6 m/s, and for two different values of boundary layer height

For this case there were six measured ground level concentrations, at 3, 5, 7, 10, 15 and 20 km (Fig. 6). Three of these are in the range of 10 to 30 km from the source. On the bases of these measured concentrations we simultaneously estimated parameters *a* and *b* and boundary layer height, *h*. The obtained values are: a = 39.409, b = 0.56618 and h = 500 m. The relative sensitivity coefficients with respect to the boundary layer height are equal to zero in the range of 3 to 10 km. So the boundary layer height can not be estimated from the measurements in this range. But, by using the value for *h* estimated above (h = 500 m), the parameters *a* and *b* can be estimated from the measured ground level concentrations at 3, 5, 7 and 10 km. The obtained values are: a = 66.357 and b = 0.35523.

In Fig. 8 the measured ground level concentrations along the plume centerline for the analyzed case of the stability class D are compared with the calculated from Eq. 1 with the estimated values for parameters *a* and *b*, and boundary layer height *h*.

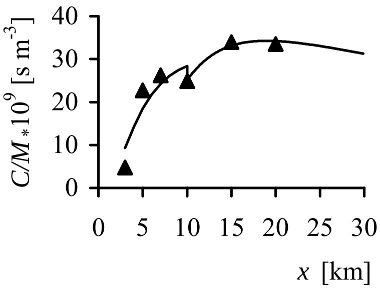

Fig. 8. Comparison of the measured ground level concentrations against those concentrations calculated from Eq.1 with the estimated values of parameters *a*, *b* and *h* for the stability class D

The OML model is chosen as a representative of the models that describe dispersion processes in terms of basic boundary-layer scaling parameters, such as Monin-Obukhov length, *L*, the boundary layer height, *h*, friction velocity, u^*, and the convective velocity scale, ω_*. For the previous example of the Kincaid experimental campaign with stability class D and wind speed of 10.6 m/s, the following values are presented: Monin-Obukhov length, L = - 408.7 m, friction velocity, u^* = 0.98 m/s, measured boundary layer height, h = 815 m, and the calculated boundary layer height, h = 3156 m. For the meteorological conditions with $L < 0$, the following expressions for the standard deviation of vertical concentration distribution, σ_z, are used in the OML model [8]:

$$\sigma_z^2 = \sigma_{z,trb}^2 + \sigma_{z,in}^2 \tag{5}$$

where $\sigma^2_{z,trb}$ is the turbulent contribution and $\sigma^2_{z,in}$ is internal dispersion. The $\sigma^2_{z,trb}$ is calculated as a sum of the mechanical and convective contributions:

$$\sigma_{z,trb}^2 = \sigma_{z,cnv}^2 + \sigma_{z,mch}^2 \tag{6}$$

In this case, when the effective plume height $H_{s,ef} > 0.1h$, the convective contribution to σ^2_z is:

$$\sigma_{z,cnv}^2 = A \cdot \omega_*^2 \cdot t^2 \tag{7}$$

where the time scale is t = x/U$_s$.

The mechanical contribution to σ^2_z is:

$$\sigma_{z,mch}^2 = B \cdot u_*^2 \cdot t^2 \cdot \exp\left(C \cdot \frac{t \cdot u_*}{H_{s,ef}}\right) \tag{8}$$

for $\dfrac{t \cdot u_*}{H_{s,ef}} < 1$,

and,

$$\sigma_{z,mch}^2 = B \cdot u_*^2 \cdot t^2 \cdot \exp C \tag{9}$$

for $\dfrac{t \cdot u_*}{H_{s,ef}} \geq 1$.

The internal dispersion parameter or the contribution due to entrainment of the ambient air into a rising plume is determined from:

$$\sigma_{z,in}^2 = \Delta H \cdot \frac{1}{D} \cdot \exp\left(E \cdot \frac{\omega_{p,pos}}{U_s}\right) \tag{10}$$

where

$$\Delta H = H_{s,ef} - H_s.$$

The constants *A, B, C, D* and *E* in the previous equations have the following values in the OML model: 0.33, 1.2, 0.6, 2.506628, and 0.6, respectively. The possibility of simultaneous estimation of the constants *A* to *E* together with the boundary layer height, *h*, has been analyzed in this paper. In order to perform this analysis, the relative sensitivity coefficients for the ground level concentration along the plume centerline for the meteorological condition of the stability class D, maintained above, were calculated.

The sensitivity coefficients with respect to the parameters *D* and *E* are very small. This indicates that the constants *D* and *E* cannot be estimated in this case. Figure 9 shows the relative sensitivity coefficients with respect to the parameters *A* and *h*, for two different values of *h*.

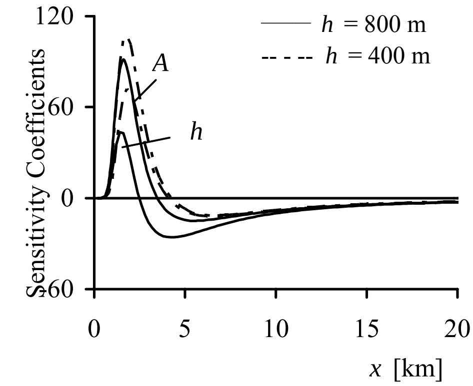

Fig. 9. The relative sensitivity coefficients with respect to the parameters *A* and *h*

The sensitivity coefficients with respect to the parameters *B* and *C* are very similar to them.

For this case there were six measured ground level concentrations, at 3, 5, 7, 10, 15 and 20 km. On the bases of these measured concentrations we simultaneously estimated parameters *A, B, C,* and mixing height, *h* by using the inverse approaches. The obtained values are: $A = 0.24635$, $B = 0.1$, $C = 0.42729$, and $h = 360$ m.

In Fig. 10 the measured ground level concentrations along the plume centerline for the analyzed case are compared with the calculated with the constants *A, B* and *C* used in the OML and measured boundary layer height, $h = 815$ m, reported in [13] and with the calculated with the parameters *A, B, C* and *h* estimated in this paper by using the inverse approaches.

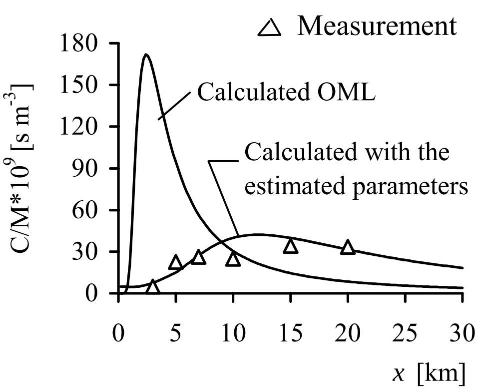

Fig. 10. Comparison of the measured ground level concentrations with the calculated for the stability class D

Very good agreement between the experimental and calculated ground level concentrations has been obtained.

CONCLUSIONS

The inverse problem of simultaneous estimation of the most influental parameters appearing in the Gaussian plume models by using ground level concentrations measurements has been analyzed in this paper. Two types of the steady-state Gaussian plume models the ISCST3 and OML have been analyzed in the paper.

The Levenberg-Marquardt and the hybrid optimization method OPTRAN were applied for evaluation of the unknown parameters.

It can be concluded that by using the experimental campaign data it can be estimate simultaneously some of the most influental parameters appearing in the Gaussian plume models. But the inverse approaches can be most useful if simulated data, obtained from the more sophistical models, are used for validation and improvement of the simple and broadly used for regulatory purposes, the Gaussian plume dispersion models.

REFERENCES

1. P. S. Arya, *Air Pollution Meteorology and Dispersion*, Oxford University Press, 1999

2. R. H. Olesen, *Tools for Model Evaluation, Air Pollution Modeling and Its Application XII*, Sven-Erik Gryning and Nadine Chaumerliac eds., Plenum Press, New York, 1998

3. R. H. Olesen, Model Validation Kit – status and outlook, *5th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purpose*, Rhodes, (1998)

4. R. H. Olesen and J. C. Chang, Consolidating tools for model evaluation, *10th international conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes*, Sissi, Crete, (2005)

5. U.S. Environmental Protection Agency, *Preferred/Recommended Models*, *AERMOD Modeling System*, http://www.epa.gov/scram001/dispersion_prefrec.htm#aermod

6. EPA U.S., *User's guide for the Industrial Source Complex (ISC3) dispersion*, Environmental Protection Agency, EPA-454/B-95-003a, 1995

7. P. Lofstrom and R. H. Olesen, *User's Guide for OML-MULTI – An Air Pollution Model for Multiple Point and Area Sources*, National

Environ. Research Institute, Roskilde, Denmark, 1996

8. R. Berkowicz, R. H. Olesen and U. Torp, *Air Pollution Modeling and Its Application V*, C. De Wispelaere, F. A. Schiermeier and N. V. Gillani eds., Plenum Publishing Corporation, 1986

9. G. S. Dulikravich, T. J. Martin, B. H. Dennis and N. F. Foster, Multidisciplinary hybrid constrained GA optimization, *Evolutionary Algorithms in Engineering and Computer Science: Recent Advances and Industrial Applications (EUROGEN'99)*, K. Miettinen, M. M. Makela, P. Neittaanmaki and J. Periaux eds., John Wiley & Sons, Ltd., Jyvaskyla, Finland, 231-260. (1999)

10. D. W. Marquardt, An algorithm for least squares estimation of nonlinear parameters, *J. Soc. Ind. Appl. Math*., **11**, 431-441. (1963)

11. M. N. Ozisik and H. R. B. Orlande, *Inverse Heat Transfer: Fundamentals and Applications*, Taylor and Francis, New York, 2000

12. A. F. Gifford, Use of Routine Meteorological observations for Estimating Atmospheric Dispersion, *Nuclear Safety*, **2**, 47-51., (1961)

13. N. E. Bowne and R. J. Londergan, *Overview, Results, and Conclusions for the EPRI Plume Model Validation and development Project: Plains Site*, EPRI report EA-074, 1983