

A New Insight into the Risk of Gaseous Release Assessment Based on a *Minimax* Approach*

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Received 1 April 2005

An alternative method of the risk assessment for pollutant gas release based on artificial intelligence approach is presented. In principle the method is a pattern recognition developed as a linear discriminative classification problem related as a *Minimax* approach. This procedure has the ability to estimate both the dispersion of pollutant emission and the probabilistic certainty of these values.

A simplified numerical experiment, prediction of the sulphur dioxide concentration from a smokestack, was carried out either using the proposed algorithm implemented in MATLAB package, or a specialized software package SLAB View. Both analyses produced reasonably accurate results. However, the proposed method was able to estimate both dispersion of the pollutant emission and a probabilistic certainty of this value.

Industrial activity can negatively impact the environment quality and human health due to emissions polluting air, soil, and water. Evaluation of environmental and safety hazard is commonly based on the risk assessment. Questions as "what is a substantial risk" or "how safe is safe enough" are problems that trouble the public, industrial community, and regulators. Obviously, the risk assessment is a stage preceding the risk management. The basic key features of the risk assessment are hazard identification and quantification of the likelihood of occurrence (named hazard assessment) and the impact (exposure assessment) associated with each hazard event. Deterministic and probabilistic methods for the risk assessment are now well-established tools for most types of planned and existing industrial, chemical, and hazardous materials installations. Basically, the risk assessment relates to a future event, thus it is an estimate and is therefore uncertain. A number of definitions of risk may be found in the literature. The most usually accepted definitions for "risk" are: the combination of the likelihood and the consequences of a future event; the probability of failure for a number of different hazards; or the product between the probability of occurrence and the quantified consequence of the hazard [1–3].

The risk assessment can be direct, using various analytical or numerical procedures, or indirect, *e.g.* based on an indicator method. Any possible strategy, both direct and indirect, should be focused on the problems of complexity, variability, and uncertainty. Operation of any technological installation is always affected by variations and uncertainties as: fluctuations and variations in operating conditions or service loads, scatters in material properties, uncertainties regarding the analytical models, chemical degradation, data collection, experimental measurements, *etc.* This paper focuses only on air pollution caused by the pollutant complex emissions from a thermopower station stack. Basic knowledge exists and many papers are available in the literature related to air pollution and dispersion estimates [4–7]. Moreover, there are available numerous specialized software packages [8, 9] enabling to compute various dispersion scenarios. Because, basically, these are deterministic simulation approaches, few of these offer the flexibility necessary to integrate the full variability and uncertainty or probabilistic assessments.

Recent achievements in the field of artificial intelligence [10–14] as artificial neural network, genetic algorithms, or pattern recognition/classification, pro-

*Presented at the 32nd International Conference of the Slovak Society of Chemical Engineering, Tatranské Matliare, 23–27 May 2005.

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voked repercussion also in engineering and scientific disciplines. These methods have been developed for universal function approximation, chaos expansion, and problems of genetics and natural selection process. Based on these achievements, new computational techniques were designed for solving air, soil, or water pollution problems involving intricate structural systems. This paper introduces a new insight into the risk assessment of gaseous pollutant release from a continuous source, such as from a smokestack. Using a pattern recognition/classification approach the classical risk assessment was transformed into an approach involving a classification task. For simplicity, only linear discrimination is presented and used in a simplified comparative numerical example.

The method not tied to its original field may be used to estimate the risk arising from a pollutant gaseous release, where risk is defined as the probability that at a given location in the vicinity of an installation, a hazard index (*e.g.* concentration) exceeds a critical limit value. The main goals of this paper are to summarize the pattern recognition methods used for classification and to introduce the algorithm for the risk assessment of the dispersion of pollutant release built on the principle of binary classification task.

Finally we present a simplified numerical example of the algorithm implemented in the MATLAB package and compare the results with those obtained by a specialized software package SLAB View which is based on Ermak's mathematical model that simulates the dispersion of denser-than-air releases [8, 9]. The model approaches are based on a Gaussian model for pollutant gaseous release. Transport and dispersion are calculated by solving the conservation equations of mass, momentum, energy, species, and the cloud half-width. The cloud is modeled depending on the release duration. In the steady-state plume mode, the cross-wind averaged conservation equations are solved on the downwind distance. The time-averaged concentration at a given location is calculated in SLAB View using the instantaneous ensemble averaged concentration, the concentration averaging time, and the assumed cloud lateral and vertical profiles, accounting for effects such as meandering and along-wind dispersion.

THEORETICAL

Pattern recognition methods are procedures commonly used for classification, *i.e.* to establish rules for sorting observations according to different categories or classes. Among the four well-established pattern recognition approaches, *i.e.* template matching, statistical recognition and classification, syntactic or structural matching, and neural networks, the second one was chosen for the purpose of this study.

In statistical pattern recognition, a pattern is represented by a set of d features, viewed as a d -

dimensional feature vector. Given a set of patterns from each class, the objective is to establish decision boundaries, which separate patterns belonging to different classes. The decision-making process or the classifier design establishes such boundaries. Classifier used for supervised methods requires two sets of data, a training data set and a test one. Correspondingly, the recognition system is operated in two modes: training (learning) and classification (testing). The classifier is built (learning) on the training set and is used (testing) on the test set. For the sake of brevity, reader interested in the course of dimensionality and peaking phenomenon, the pitfall of over-trained system, errors estimation, or the classifier stability, is encouraged to read some related studies [10–14].

Generally, in pattern recognition and binary classification problems are given two sets of data in R^n (or in other space): $\{x_1, x_2, \dots, x_N\}$ and $\{y_1, y_2, \dots, y_M\}$. The demanding problem is to find a function $f: R^n \rightarrow R$, which is positive on the first set and negative on the second one, as $f(x_i) > 0$, $i = 1, \dots, N$ and $f(y_i) < 0$, $i = 1, \dots, M$. If these inequalities are fulfilled, function f or its 0-level set $\{x/f(x) = 0\}$, separates, classifies or discriminates the two sets of data. This function f is often named as classifier, and sometimes as decision function.

In linear discrimination, an affine function $f(x) = w^T \cdot x - b$ classifying the points is sought, *i.e.*

$$\begin{aligned} w^T \cdot x_i - b &> 0, & i = 1, \dots, N \text{ and} \\ w^T \cdot y_i - b &< 0, & i = 1, \dots, M \end{aligned} \quad (1)$$

Immediately below the equation all variable symbols should be explained in the text.

From the geometrical point of view, this function corresponds to hyperplane, which separates the two sets of points. Since the strict inequalities in eqn (1) are homogeneous in w and b , they are feasible if and only if the set of nonstrict linear inequalities is feasible

$$\begin{aligned} w^T \cdot x_i - b &\geq 0, & i = 1, \dots, N \text{ and} \\ w^T \cdot y_i - b &\leq 0, & i = 1, \dots, M \end{aligned} \quad (2)$$

w being the set defining the normal vector to the hyperplane and b the offset.

Then, the two sets of points can be linearly discriminated if and only if their corresponding convex hulls, $\{x_1, x_2, \dots, x_N\}$ and $\{y_1, y_2, \dots, y_M\}$, do not intersect. When the two sets of points cannot be perfectly linearly separated, it is possible to seek an affine function, which approximately classifies the points, *e.g.* one that minimizes the number of points misclassified. A heuristic one approximating linear discrimination is based on support vector classifiers, which is a statistical classification method. According to these statements the problem of separating the set of m training vectors belonging to two separate classes was consid-

ered

$$\{(z_i, y_i) | z_i \in R^n, y_i \in \{-1 + 1\}, i = 1, \dots, m\} \quad (3)$$

with a hyperplane, $w^T \cdot z - b = 0$, where y_i ($y_i \approx \text{sign}(w^T \cdot z_i - b)$) is the associated “truth” given by a trusted source. The underlying problem of interest is to establish a decision function $f : R^n \rightarrow \{\pm 1\}$ using input-output training labeled data from eqn (3). In principle, decision function, $f(z)$, is a function the sign of which represents the class assigned to the data points z . If the points are linearly separable, then there exists a vector w and a scalar b

$$\begin{aligned} w \cdot z_i - b &\geq +1 \text{ if } y_i = 1 \text{ and } i \in \text{Class C1} \\ w \cdot z_i - b &\leq -1 \text{ if } y_i = -1 \text{ and } i \in \text{Class C2} \end{aligned} \quad (4)$$

The set of vectors given by eqn (3) is considered optimally separated by the hyperplane if it is separated without error and the distance between the closest vectors to the hyperplane $w^T \cdot z = b$ is maximal. Geometrically this is equivalent to maximization of the separation margin or distance between the two parallel hyperplanes $w^T \cdot z = b + 1$ and $w^T \cdot z = b - 1$. The classifier is called a support vector machine because the solution depends only on the points (support vectors) located on the two supporting hyperplanes $w^T \cdot z = b + 1$ and $w^T \cdot z = b - 1$. In a separable problem these support vectors are the closest to the boundaries (the two parallel hyperplanes) in the sense of some optimal criteria. Generally, minimization of the probabilities that data vectors fall on the wrong side of the boundary may do classifier design or the problem of choosing a linear discrimination. A possible way is to attempt to control the misclassification probabilities in a worse case setting as minimizing the worst case – maximum probability of misclassification of future data points. This is in fact a *Minimax* approach which is an alternative for discriminative classification approach. The *Minimax* problem [13, 14] can be interpreted geometrically as minimizing the maximum of the Mahalanobis distances to the two classes.

Thus *Minimax* probabilistic classification is similar to maximum margin classification with respect to the mean of the classes, where a factor depending on the covariance matrices of each of the classes pushes the threshold towards the class with lower covariance. Unlike support vector classification, for which the closest points to the decision boundary are the most important, *Minimax* approach looks at the margin between the means of both classes. The main advantage of the *Minimax* approach is that it can obtain an explicit upper bound of the misclassification probability of future data without making Gaussian or other specific distributional assumptions.

Using the *Minimax* approach one considers a binary classification problem, with z_1 and z_2 denoted random vectors data from each of the two classes, with

means and covariance matrices given by $(\bar{z}_1, \Sigma_{z_1})$ and $(\bar{z}_2, \Sigma_{z_2})$, with $z_1, \bar{z}_1, z_2, \bar{z}_2 \in R^n$ and $\Sigma_{z_1}, \Sigma_{z_2} \in R^{n \times n}$ both symmetric and positive definite or semi-definite. Assuming $z_1 \in \text{Class C1}$ and $z_2 \in \text{Class C2}$, a hyperplane that separates the two classes of points

$$H(w, b) = \{z | w^T \cdot z = b\},$$

$$\text{where } w \in R^n \setminus \{0\} \text{ and } b \in R \quad (5)$$

is sought, with maximum probability with respect to all distributions having mentioned means and covariance matrices

$$\max_{\alpha, w \neq 0, b} \alpha \text{ s.t. } \begin{cases} \inf_{z_1(\bar{z}_1, \Sigma_{z_1})} \text{Prob}\{w^T \cdot z_1 \geq b\} \geq \alpha \\ \inf_{z_2(\bar{z}_2, \Sigma_{z_2})} \text{Prob}\{w^T \cdot z_2 \leq b\} \geq \alpha \end{cases} \quad (6)$$

In the light of a *Minimax* approach the classifier should minimize the misclassification probability using an optimum separating hyperplane, named a *Minimax probabilistic decision hyperplane*, which exists and can be determined solving a convex optimization problem based on the *Minimax probability machine* [13, 14].

Basic concept for the risk quantification of gaseous pollutant emission from a continuous source and the general framework of the algorithm built on the principle of the binary classification task solved using the *Minimax* approach is presented. This algorithm is based on the *most probable point* (MPP) concept developed within the field of structural reliability [15–19], and extended to calculate the risk arising from a gaseous release. Detailed algorithm description was given elsewhere [14–16], thus only some basic aspects of these methods, better known by their acronyms *FORM/SORM*, are discussed.

The starting point is to establish a performance or a system response function, which gives the relation between the model variable inputs (dimensional, operating conditions, physical parameters, etc.) and the chosen performance. In this paper, gaseous pollutant concentration, $C(x_i)$, at different locations along the downwind direction was chosen as the performance function. It depends on a set of governing input parameters represented by the vector of random variables, $x = (x_1, x_2, \dots, x_d) \in R^d$. Such random variables may represent inherent randomness, parameter uncertainty, or a combination of both. The level of pollution from a release source may be evaluated according to a critical concentration, C_R , representing the value of “dangerous or failure concentration” of particular interest. The use of the term “failure” is only customary, because only the likelihood of a particular system state may be of interest. The *limit state function* (LSF) is the locus of points of the performance functions defined as

$$\text{LSF} = C_R - C(x_i) = 0 \quad (7)$$

The algorithm and all the approximations work in a transformed space U^d of standard normal, independent and uncorrelated variates $\mathbf{u} = (u_1, u_2, \dots, u_d) \in U^d$ obtained from the iso-probabilistic transformations (Rackwitz, Fiessler, Rosenblatt) of the basic random variables $\mathbf{x} = (x_1, x_2, \dots, x_d) \in R^d$. The variates \mathbf{u} is a set of standard parameters with cumulative distribution function d -dimensional Gaussian, that is the mean equal to 0 and identity for the variance. Applying this transformation to eqn (7) one gets

$$\text{LSF}(u) = C_R - C(u_i) = 0 \quad (8)$$

representing the boundary between the safe and failure regions. Such transformed LSF corresponds to a failure limit hypersurface. The failure region F defined by the existence of a limit state function the nonpositive values of which define the nonreliability domain is expressed as

$$F = \{\mathbf{u} \in U^d | \text{LSF}(u) \leq 0\} \quad (9)$$

The safety region S defined by the existence of a limit state function the positive values of which define the reliability domain is expressed as

$$S = \{\mathbf{u} \in U^d | \text{LSF}(u) \geq 0\} \quad (10)$$

Since the probability density in the standard normal space decays exponentially with the distance from the origin, the optimum point on the failure limit hypersurface for approximating the safety index lies closest to the origin $\mathbf{u}^* = (u_1^*, u_2^*, \dots, u_d^*)$. This point is often named as the *most probable point* (MPP). Safety index β is defined as the scalar minimum distance, in the standard normal space, between the origin and the MPP of the limit state function.

Regarding the target of this study, the safety region S could be associated with the downwind distances, at which the current value of concentration does not exceed the critical concentration, C_R . Similarly, the failure region F corresponds to those downwind dis-

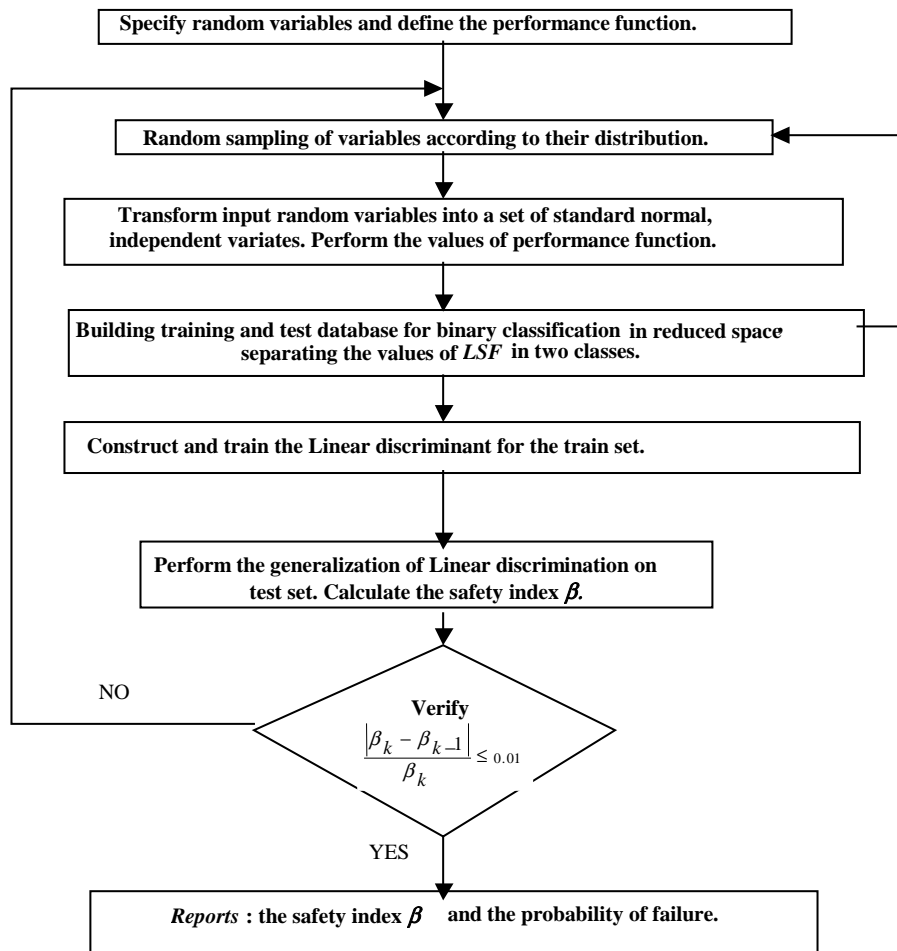


Fig. 1. The basic flowchart of the proposed method.

Table 1. Main Values of Simulation Parameters

Real variable	Measured values	Statistical distributions
Wind speed, $w/(m\ s^{-1})$	$V1 \in \langle 1.4, 2.8 \rangle$	Weibull with mean $\mu = 2.33\ m\ s^{-1}$ and $\sigma \cong 0.1\mu$
Downwind distance along plume centerline, x/m	$V2 \in \langle 0, 15000 \rangle$	Normal with mean $\mu = 3000; 5000; 8000$ and $\sigma \cong 0.1\mu$
Effective stack height, H/m	$V3 = 35$	Normal with mean $\mu = 35$ and $\sigma \cong 0.1\mu$
SO ₂ Emission rate, $Q/(mg\ m^{-3})$	$V4 = 143 \times 10^3$	Normal with mean $\mu = 143 \times 10^3$ and $\sigma \cong 0.1\mu$
Vertical distance from ground level, z/m	$Z_0 = 2$	Constant values representing the height of the point for estimation
Critical concentration, $C_R/(mg\ m^{-3})$	$C_R = 0.125$	Critical values of polluting emissions for SO ₂ reported to human health according to Romanian O.M.A.P.M - 462/2002

Only open country area and grass terrain with a surface roughness $\mu_{Z_0} = 0.02\ m$.

Table 2. Main Simulation Conditions

Atmospheric stability class	Dispersion parameter	
	Horizontal, σ_y/m	Vertical, σ_z/m
A	$0.22 (1 + 0.0001x)^{-0.5}$	0.20x
B	$0.16 (1 + 0.0001x)^{-0.5}$	0.12x
C	$0.11 (1 + 0.0001x)^{-0.5}$	$0.08 (1 + 0.0002x)^{-0.5}$

Dispersion equation \Rightarrow Current concentration of pollutant emission

$$C(x, 0, z, H) = \frac{Q}{2\pi w \sigma_y \sigma_z} \left[\exp\left(-\frac{1}{2} \left(\frac{z-H}{\sigma_z}\right)^2\right) + \exp\left(-\frac{1}{2} \left(\frac{z+H}{\sigma_z}\right)^2\right) \right]$$

Limit state function

$$LSF = C_R - \frac{Q}{2\pi w \sigma_y \sigma_z} \left[\exp\left(-\frac{1}{2} \left(\frac{z-H}{\sigma_z}\right)^2\right) + \exp\left(-\frac{1}{2} \left(\frac{z+H}{\sigma_z}\right)^2\right) \right]$$

tances, for which the current value of concentration exceeds the critical concentration C_R . From a probabilistic viewpoint, the first-order approximation for the probability of “failure” represents the probability that the current values of concentration will exceed the critical concentration C_R and is given by the following expression [17–19]

$$P_f = \text{Prob} \{ \mathbf{u} \in U^d | LSF(\mathbf{u}) \leq 0 \} = \Phi(-\beta) \quad (11)$$

where $\Phi(-\beta)$ is the standard normal cumulative density function. Proposed algorithm identifies the decision function that represents the hyperplane (eqn (5)) as the locus of points of the performance functions in transformed standard normal space U^d . The algorithm (Fig. 1) estimates the location of the *most probable point* (MPP) and calculates the safety index β . Once the location of the MPP, in the standard normal space has been found and the safety index β was calculated, probability that the current values of concentration at different downwind distances exceeded the critical concentration, C_R , might be evaluated. Informatively in this paper we can associate “patterns” with values of classes for LSF.

EXPERIMENTAL

Proposed algorithm developed in *MATLAB* language predicts centerlines concentration downwind for SO₂ pollutant emission. These values were used to estimate the level of pollution from a gaseous release source, particularly the sulphur dioxide dispersion from a smokestack. The plume dispersion is modeled with the Gaussian plume equation of Pasquill—Gifford, using formulas recommended by Briggs [4, 5]. For simplicity the analysis focuses only on several variables suspected of significantly affecting transport and dispersion of denser-than-air releases: wind speed, atmospheric stability, emission rate of the pollutant, emission source characteristics, and one-terrain roughness class (Table 1).

Because of the lack of sufficient experimental data, the numerical experiments were conducted based on averaged experimental measured data or arbitrary probability distributions through simulation. Thus these simulations might substitute real data as inputs to consequence models or simply illustrate the process. Assessments are done based on centerlines concentration. These values should estimate the level or the risk

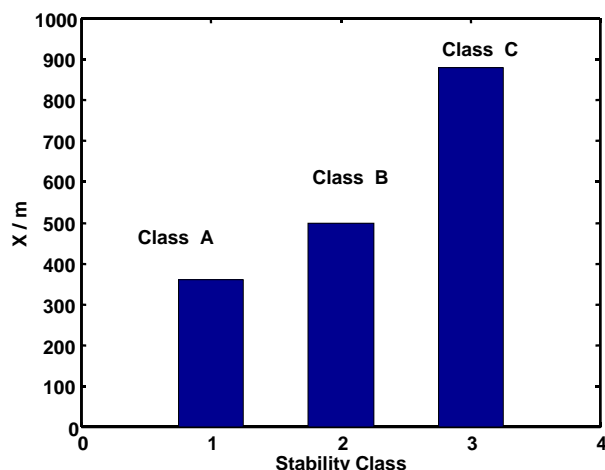


Fig. 2. Deterministic LSF simulations along the downwind direction according to the stability classes.

of pollution from a gaseous release source; particularly they can simulate a centerline dispersion of sulphur dioxide from a smokestack. By the same reasons, dispersion coefficients (horizontal $-\sigma_y$ and vertical $-\sigma_z$) were estimated as a function of the distance, atmospheric stability category, and the surface roughness according to formulas recommended by Briggs. A general description for all simulated conditions is listed in Table 2. In order to solve the above-mentioned problem, several simplifications were adopted, *i.e.* Gaussian Plume model with total reflection, continuous, uniform emission rate of pollutant, and a simplified dispersion model. Moreover, molecular diffusion and longitudinal turbulent diffusion was neglected given the turbulent diffusion and the wind displacement, respectively.

With atmospheric stability omitted as an uncertain variable, it is reasonable to approximate the wind speed frequency from the physics of the process. On the other hand, Weibull probability distribution is quite flexible in representing the distribution of many single-sided random variables. An appropriate approximation for the wind speed frequency is a Weibull analytic distribution [16, 17]. In these simplified conditions we must mention that basically our model becomes closed to one deterministic. The limit state function eqns (7) and (8) were simulated along the downwind direction according to the basic statistical distribution of the parameters of LSF. Based on these probability simulations, the current values of sulphur dioxide centerlines concentration exceeding the critical concentration were calculated. For a better comparability of the results simulations based on SLAB View were conducted in the same simplified conditions and assumptions. Comparative assessments are done based on centerlines concentration related to surfaces of constant concentration (isopleth) in Fig. 3.

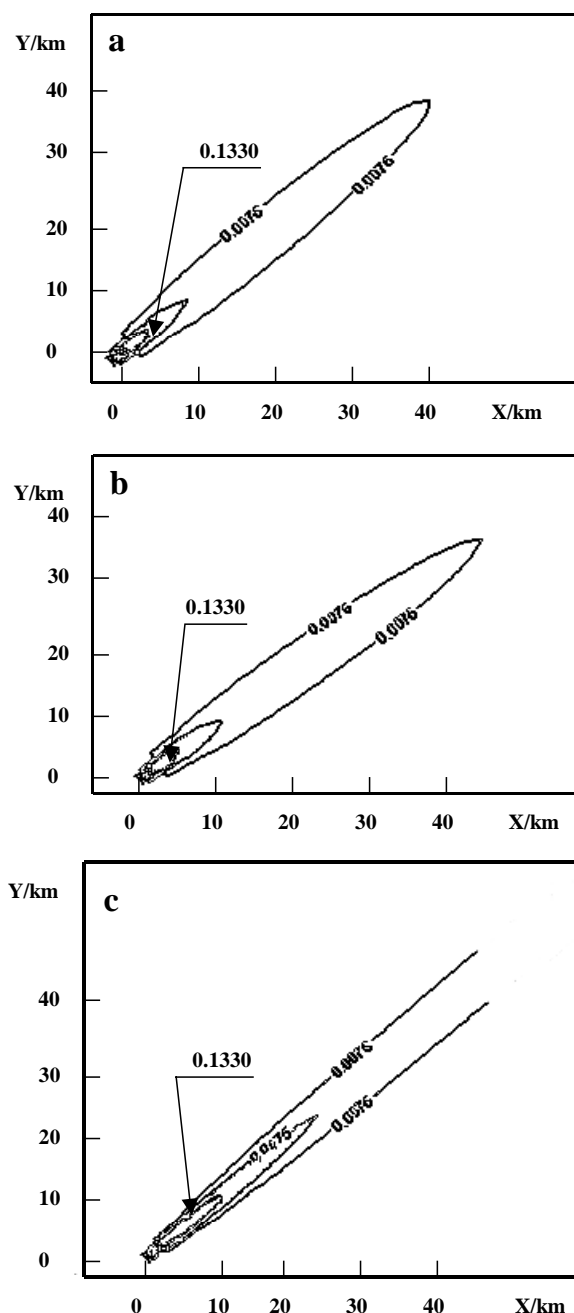


Fig. 3. Simulated dispersion values of SO_2 pollutant concentration (ppm) in SLAB View software package. Simulated values (isopleth) for atmospheric stability class: a) A, b) B, and c) C.

RESULTS AND DISCUSSION

Main drawback of many specialized software packages is the lack of probabilistic outputs and thus a poor measure for the results certainty. Proposed algorithm rectifies this drawback enabling to estimate both dispersion of the pollutant emission and the probabilistic certainty of the pollutant concentration values.

Deterministically simulated estimates of plume length are presented in Figs. 2 and 3. For the open

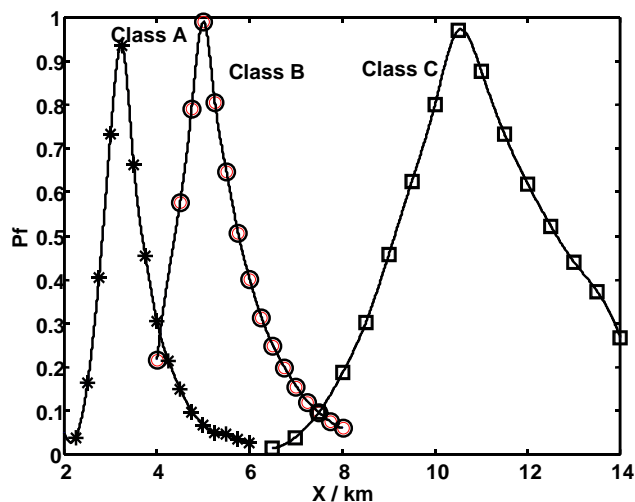


Fig. 4. Probabilistically simulated values for critical plume length of SO₂ pollutant emission.

country terrain the critical centerlines concentration plume length varies from 3000 to 10000 m, depending on the atmospheric stability conditions. The results presented in Figs. 2—4 indicate that the worst case for dispersion of sulphur dioxide from a smokestack results for C category of the atmospheric stability. Such critical centerlines concentration plume length represents the boundary between the “safe” and “failure” regions in the sense of LSF as a difference between the critical pollutant concentration, C_R , and the current values of SO₂ concentration.

The maximum critical plume length of about 10000 m was calculated for atmospheric stability condition of the type C. Certainty of deterministically simulated values was confirmed by the values obtained using *Minimax* simulation. Probabilities of simulated values (Fig. 4) were higher than 95 %, *i.e.* a good confidence value.

In general, a reasonable agreement of the two simulations using either specialized software package SLAB View, or the proposed probabilistic *Minimax* algorithm was observed. Some minor differences occurred only in the case of the deterministic LSF simulation along the downwind direction according to the stability classes, especially for the atmospheric stability class C (Figs. 2, 3c, and 4). A major distinction, given the basic method and the specialized software package, is that the proposed algorithm utilizes the full magnitude of all variables, not only of those of importance, or very sensitive. This increases robustness of the algorithm, as whole random nature of the LSF is employed. More or less cumbersome, this application reveals the complementary nature and the opportunity of assessments based on artificial intelligence approaches for engineers, especially for chemical engineers concerned with risk management.

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