# Prediction of concentration fluctuations in short-distance gas dispersion

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## 1 Introduction

Concentration fluctuations in gas dispersion is an important factor in many hazard problems, e.g. response to toxic gas, risk of gas ignition, and perception of malodour. Most applied dispersion models do, however, ignore the fluctuations and predict only the mean concentration field. This simplistic approach does not produce adequate input for every response model, e.g. toxic load models based on the time integral of the concentration raised to a substance-specific power, $\int c(t)^p\,dt$ (Griffith, 1991). Furthermore, the use of a steady concentration field raises difficult discussions on the choice of model averaging time, which both should match the time-scale relevant for the risk analysis and enable model validation by field experiments of sometime individual release duration (Wilson 1995). For these reasons it seems appropriate to model gas dispersion as a stochastic process rather than an average field. The reason why this approach is not already supported in regulatory guidelines is probably the complexity of existing models for concentration fluctuations. The objective of the project *Concentration Fluctuations in Gas Releases by Industrial Accidents* (COFIN, 1998-2001, EU ENV4-CT97-0629) was to study existing data and develop new models.

## 2 Data analysis

The experiments were made in several field campaigns prior to this project applying continuous point sources, which usually were positioned near the ground. The data were obtained by a remote-sensing LIDAR system, which detects smoke concentration along a laser beam, usually oriented horizontally across the plume a few hundred meters downstream of the source. The typical release duration was one hour, and the LIDAR response time was practically instantaneous with a spatial resolution of about one metre. From these data we calculate cross-plume profiles of the mean and higher-order statistical moments $\mathrm{E}\{c^n\}$. The instantaneous profiles are very irregular; even with a time averaging of one hour, a perfect Gaussian profile is seldom obtained. Average profiles become much more predictable when calculated in a moving frame of reference following the time-dependent plume centreline, $y_0$. The central part of the moving-frame profiles is approximately Gaussian, as expected, whereas the tails are exponential. We explain the exponential tails by occasional plume breaking caused by large turbulent eddies. A relatively simple function, which reproduces the observed shape of $\mathrm{E}\{c^n|\Delta y\}$ near centreline and tails, is given by:

$$\mathrm{f}(\Delta y) = \exp\left[-\alpha^2\left(\sqrt{1+(\Delta y)^2/(\alpha s)^2}-1\right)\right] \to \begin{cases} \exp\left[-(\Delta y)^2/(2s^2)\right] & \text{for } \Delta y \to 0 \\ \exp\left[-\alpha|\Delta y|/s^2\right] & \text{for } |\Delta y| \to \infty \end{cases}, \quad \Delta y = y - y_0 \qquad (1)$$

We have observed that the shapes of $\mathrm{E}\{c^n|\Delta y\}$ is approximately the same for all *n*. Two-point statistics of the concentration field is remarkably well described by an exponential distance-neighbour function.

$$D(\delta y) \equiv \int \overline{c(\xi+\delta y)\cdot c(y)}\,dy \approx 1/\sigma_1 \exp\left[-|\delta y|/\sigma_1\right] \qquad (2)$$

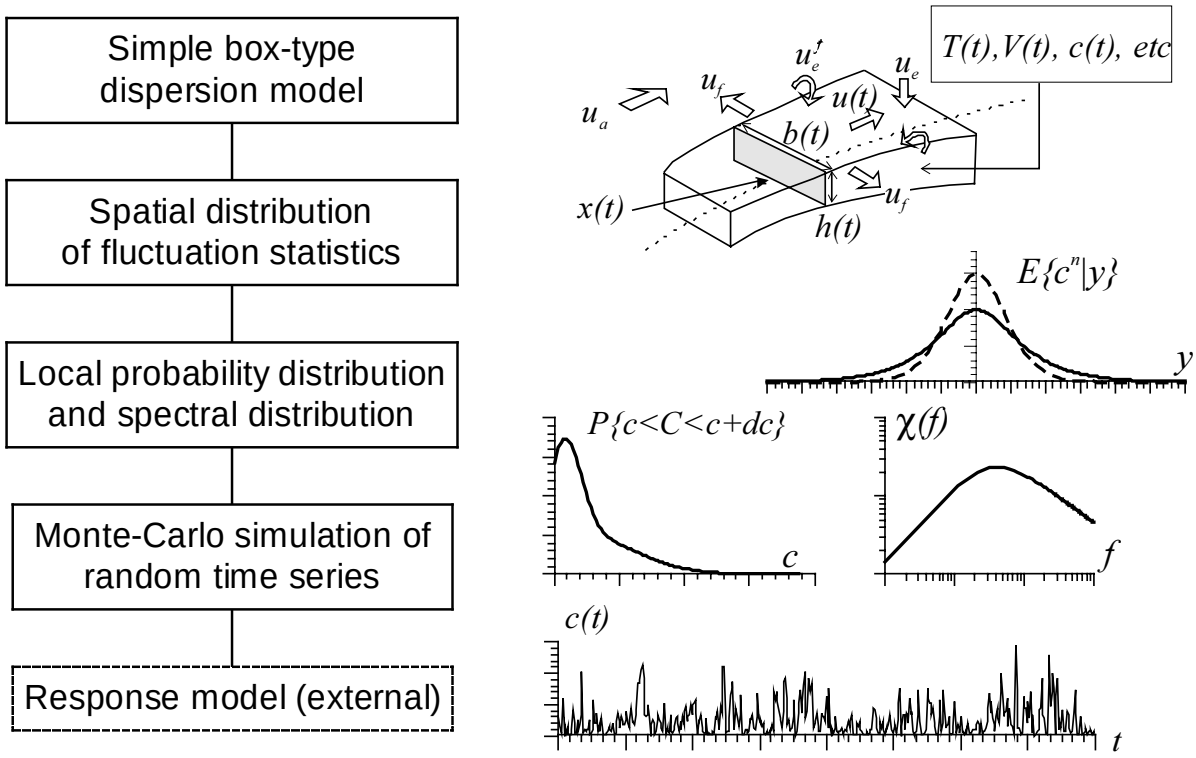


**Figure 1** Model Organisation.

## Model description

*3.1 Dispersion*

The boxes shown on the left-hand side in Figure 1 illustrate modules of the proposed model. For the dispersion calculations we chose a heavy-gas box model with smooth transition to a Gaussian plume of neutral buoyancy. This model type has been implemented in many public available PC programs, e.g. HEGADAS (Witlox, 1994), DEGADIS (Spicer and Havens, 1986), SLAM (Ermak, 1990), and DRIFT (Webber *et al.*, 1992) and it a popular choice for practical risk assessment. The control volume is a vertical cross section in which the spatial distribution of all cloud properties, e.g. concentration and temperature, are considered uniform. The control volume moves downwind while plume dimensions, distance form the source and cloud properties are described by a set of ordinary differential equations. Interchangeable source models for leaking tanks, evaporating pools, etc. provide the boundary conditions.

*3.2 Spatial distribution of concentration statistics*

The top-hat concentration profile consistent with the internal heavy-gas dispersion model is usually hidden from the model user, and instead the concentration field is presented as a smooth cross-plume concentration profile. These profiles are and in accordance with field experiments and analytical solutions based on power-law formulations of the velocity and eddy-diffusivity profiles (e.g. Sutton 1953). In the limit of neutral cloud buoyancy, a surface plume has a Gaussian distribution in lateral distribution whereas the vertical distribution will be somewhere between Gaussian and exponential, depending on aerodynamic surface roughness and atmospheric stability. To allow for the effects of gravitational spreading and area sources, heavy-gas models often operates with a combination of Gaussian edges and a core region of uniform horizontal distribution. Experimental evidence (Britter and Snyder 1988, Nielsen *et al.* 1997) suggests that internal cloud stability brings the vertical profile closer than usual to an exponential shape.

As a novel feature we generalise the profile description to higher-order *statistical* moments, $\mathrm{E}\{c^n|x,y,z\}$. The preliminary length scale $s$ in Equation 1 is eliminated by calculation of the

second-order *spatial* moment of the profile $\sigma_n$, which is used in a new parameterisation. In the case of first-order statistics, $\sigma_1$ is the half plume width easily related to box-model output. Horizontal moving-frame profiles for the general statistical order *n* are:

$$\mathrm{E}_{\mathrm{mov}}\left\{c^n|\Delta y\right\} = \mathrm{M}_{\mathrm{n}} \exp\left[-\alpha_n^2\left(\sqrt{1+\mathrm{K}_2\left(\alpha_n^2\right)\left(\alpha_n^2\,\mathrm{K}_1\left(\alpha_n^2\right)\right)^{-1}\left(\Delta y/\sigma_n\right)^2}-1\right)\right] \tag{3}$$

where $\mathrm{K}_i(x)$ is the modified Bessel function of order *i*. The statistical moment at the moving-frame centreline $\mathrm{M_n}$, the shape parameter $\alpha_n$, and the length scale $\sigma_n$ all depend on the order of the statistics *n*. Data analysis suggests that length scales for the profiles of moments of various order are related by $\left(\sigma_1/\sigma_n\right)^q = n + r(1-n)$, where the parameters are $q$ ≈0.8, $r$ ≈0.8. The ratio $\sigma_1/\sigma_n$ does not seem to relate to meteorological conditions.

Furthermore, it is useful to parameterise the spatial distribution of the fluctuation intermittency defined as the probability of concentrations above a near-zero threshold level $\gamma_{\mathrm{mov}}(\Delta y) = P\left\{C \geq \varepsilon|\Delta y\right\}$.

Having determined the moving-frame profiles we obtain fixed-frame profiles by $\mathrm{E}_{\mathrm{fix}}\left\{c^n|y\right\} = \int \mathrm{E}_{\mathrm{mov}}\left\{c^n|y-y_0\right\}p(y_0)dy_0$ and $\gamma_{\mathrm{fix}}(y) = \int \gamma_{\mathrm{mov}}(y-y_0)p(y_0)dy_0$, where $p(y_0)$ is the probability of a given centre-line position $y_0$. Plume meander is close to a random walk process, so the probability distribution of the centre-line position $p(y_0)$ is expected to be Gaussian.

*3.3 Local probability distribution*

The local probability density function is modelled by a versatile analytical distribution, with local calibration by the statistical moment $\mathrm{E}\left\{c^n\right\}$ and intermittency factor ($0 \leq \gamma \leq 1$). One candidate model is the beta distribution, which has the following probability density function:

$$\mathrm{p}(c) = (1-\gamma)\cdot\delta(c) + \gamma/\mathrm{Be}(a,b)\left(c/c_{\max}\right)^{a-1}\left(1-c/c_{\max}\right)^{b-1} \text{ with } \mathrm{Be}(a,b) = \int_0^1 t^{a-1}(1-t)^{b-1}dt \tag{4}$$

Here, $c_{\max}$ is a local maximum concentration and *a* and *b* are shape parameters ($a>0, b>0$). The moments of this distribution are given by the formula:

$$E\left\{c^n\right\} = \gamma c_{\max}^n \frac{\Pi_{i=0}^{n-1}(a+i)}{\Pi_{i=0}^{n-1}(a+b+i)}, \text{ e.g. } E\{c\} = \gamma c_{\max}\frac{a}{(a+b)} \text{ and } E\left\{c^2\right\} = \gamma c_{\max}^2\frac{a(a+1)}{(a+b)(a+b+1)} \tag{5}$$

which determines the model parameters $(a, b, c_{\max})$. Alternative probability distributions results in moment expressions very similar to Equation 5.

*3.4 Simulation of random time series*

Simulation of random processes is greatly simplified when the target probability functions are Gaussian. The main advantage is that a linear transformation of a vector $y_j$ with Gaussian components will map into another Gaussian vector $x_i = L_{ij}y_j$, where $L_{ij}$ is the transformation matrix. If the input variables $y_j$ are uncorrelated Gaussian deviates, e.g. simulated by the Box-Muller algorithm (Press et. al 1992), the covariance matrix of the transformed process is $K = LL^T$, where $L^T$ is the transposed matrix. Covariance matrices are always non-negative definite and the transformation matrix $L$ may be found by Cholesky, or 'square root', decomposition of the

covariance matrix (Press et. al 1992). Another useful property is that a Fast Fourier Transform (FFT) of a Gausian time series maps onto a Gaussian spectral distribution, and vice versa. Spectral representations $X_i(f)$ and $X_j(f)$ the time series $x_i(t)$ and $x_j(t)$ may be modelled by uncorrelated Gaussian input $X_i(f) = L_{ik}(f)Y_k(f)$ and transformed into time domain by inverse FFT (Press et. al 1992). The starting point for numerical simulation is the cross spectrum matrix, which is decomposed for every frequency, $\chi_{ij}(f) = L(f)L^*(f)$. In general, we must use complex algebra here since cross-correlation functions may be asymmetric in time with corresponding complex cross spectra. The spectral matrix will however be Hermitian $\chi_{ij}(f) = \chi^*_{ij}(f)$, and decomposition by Cholesky's method is possible when complex calculus is allowed.

Several techniques have been proposed for simualtion of non-Gaussian variable, as reviewed by Gurley *et al.* (1997). For the present application we prefer the correlation-distortion method, which is based on a vector translation process, which maps Gaussian time series into non-Gaussian ones $x_i(t) \rightarrow c_i(t)$. The translation of the *i*th time series $x_i(t)$ is a monotonic function $c_i(t) = g_i\left[x_i(t)\right] = F_{C_i}^{-1}\left[\phi_{X_i}\left[x_i(t)\right]\right]$, where $F_{Ci}$ is the marginal distribution of $c_i(t)$ and $\phi_{X_i}$ is a Gaussian distribution. The difficulty of this procedure is that the transformation distorts the spectral distribution. Gioffrè *et al.* (2000) showed that the cross correlation functions of the two processes $\rho_{c_i c_j}(\tau)$ and $\rho_{x_i x_j}(\tau)$ for a given time lag $\tau$ are related to each other by an integral involving the two translation function $g_i\left[X_i(t)\right]$ and $g_j\left[X_j(t)\right]$. The procedure is then to seek correlation functions for the Gaussian processes $\rho_{x_i x_j}(\tau)$, which reproduces the target correlations for the non-Gaussian processes $\rho_{c_i c_j}(\tau)$. Knowing the correct Gaussian correlations functions one obtains the cross-spectra of the Gaussian processes $\chi_{ij}(f)$ by FFT, simulate correlated Gaussian times series as above, and finally translate these into non-Gaussian time series by $c_i(t) = g_i\left[x_i(t)\right]$.

**Discussion**

The presented model is intended to be an add-on to a conventional heavy-gas box model or Gaussian-plume model. Firstly, spatial distributions of the statistical moments of concentration fluctuations are predicted; secondly, local PDFs in accordance with the moments are deduced; and finally correlated time series are simulated at fixed observation points. A similar technique might have been applied with other types of dispersion models. With correct parameterisation of the statistical properties, the simulation technique will produce time series with specified moments up to the third order. Thus, the general shape of the probability distribution will be realistic whereas high-concentration extreme values may be less certain. Spectral and cross-spectral distributions will be of second-order accuracy. Exeedance statistics of the simulated time series are not necessarily reproduced, since accurate modelling of these would have to take the joint probability distribution of concentration and its time derivative into account (Yee 2001). This information is, by the way, difficult to obtain with great experimental precision.

The selected field experiments provided new and reliable knowledge on the horizontal crosswind distribution of fluctuation statistics. There are areas where better data are needed, most importantly regarding vertical and downwind distributions. It should also be said, that signal noise makes the determination of the intermittency factor uncertain. Finally, we need better information on the spatial structure and spectral distribution of the fluctuations. The authors are aware of some new field experiment, which will help to fill these gabs in knowledge and are most interested in learning about other works in this direction.

The proposed model is an extension to the type of dispersion model usually applied in risk assessment. The extended model is capable of predicting local probability distributions and simulating realistic time series. This information should provide a good starting point for detailed physical and toxicological response modelling.

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