Journal Offprint Paper

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Numerical simulation of heavy gas cloud dispersion within topographically complex terrain

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Received 26 July 1993

Numerical analysis has been performed for predicting the dispersion of heavy gas clouds released without initial momentum (i.e. dense gas puffs) within regions of complex topography. The three-dimensional non-steady differential equations governing transport are solved by means of the numerical finite volume method, using a collocated variable arrangement with a fully implicit integration over time. The turbulence effects on the flow properties are simulated by the two-equation k–ϵ turbulence model. Comparisons between calculated and measured data are presented, showing good agreement between them. The method is also used to predict a chlorine release within a fictitious industrial plant. The location of the release site, the atmospheric stability class and the wind direction are varied, in order to show the effect of topography on the cloud dispersion.

Keywords: heavy gas dispersion; complex topography; computer simulation

A typical accident scenario for industrial plants is the sudden release of a certain amount of hazardous gas, which is either stored or being transported. The released gas (usually colder, i.e. denser, than the ambient air) forms a dispersing cloud due to advection by wind and diffusional as well as turbulence effects. Exact knowledge about such dispersion processes is very important for evaluating safety risks in industrial plants.

In recent years, many so-called box models have been developed[1–3] in order to evaluate the dispersion of heavy gas clouds. They all contain empirical constants whose values have been estimated from experimental data. The heavy gas dispersion is usually described by mass conservation assumptions and restrictions. However, none of these models takes into account the topography of the surrounding terrain, a fact that makes them irrelevant for practical situations – a release is much more likely to occur within a terrain of highly complex topography (industrial plants, ship terminals etc.) than over a flat area.

The exact evaluation of heavy gas cloud dispersions over non-flat terrain requires exact knowledge about the environmental flow field within that region and over and around the discrete obstacles (buildings etc.) that are situated there. However, the complexity of the flow makes it necessary to treat the problem by solving the governing Navier–Stokes equations and equations for the scalar transport, while applying suitable models for the evaluation of further phenomena (i.e. turbulence modelling).

This article presents a solution procedure for heavy gas dispersion phenomena, that takes into account the topography of the terrain around the release site. In the assumed release scenario, a certain mass of heavy gas is released at time $t = 0$ at a certain location within the calculation domain. The release may be continuous or sudden and the source may be elevated or near the ground. In the case of a sudden release, no initial momentum is assumed for the released heavy gas; i.e. from the calculation's point of view, the mass fraction of the heavy gas at the time of the release is set to 1.0 and the temperature is set equal to that of the heavy gas within the source, but no changes are made to the velocities or turbulent quantities of the flow field. Due to wind advection, diffusion and turbulent effects, the heavy gas disperses within the calculation domain, and flows preferably around and in some cases over the buildings and obstacles situated in it (low obstacles). The method predicts the temporal development of the dispersion and estimates the flow field quantities and concentration distribution at any given time for all discrete points of the calculation domain.

Theoretical analysis

Governing equations

Since the obstacles (buildings) have limited extensions, and recirculations are expected in all three space directions, the problem's solution should consist of the numerical treatment of the fully elliptic non-steady-

0950-4230/94/050391–06

state Navier–Stokes equations. Furthermore, in order to include the highly turbulent nature of the phenomena, a Reynolds average process is imposed on all instantaneous governing equations. The instantaneous value of any turbulent flow property Φ is represented by the sum of a time-average component $\bar{\Phi}$ and a fluctuating component ϕ (i.e. $\Phi = \bar{\Phi} + \phi$). Therefore, the governing equations can be expressed in the tensor notation as follows.

- *Continuity*

$$\frac{\partial(\rho U_i)}{\partial x_i} = 0 \tag{1}$$

- *Momentum*

$$\frac{\partial(\rho U_j)}{\partial t} + \frac{\partial(\rho U_i U_j)}{\partial x_i} = -\frac{\partial P}{\partial x_j} + \frac{\partial}{\partial x_i}\left(\mu_l\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) - \rho\overline{u_i u_j}\right) + \rho f_j \tag{2}$$

The last term on the right-hand side stands for body forces. The specific body forces f_j include only the gravitational vector $\vec{g}$. This buoyancy term, when modelled using the Boussinesq approximation, can be written as:

$$\rho f_j = \rho_0 \cdot \left\{[1-\beta(T-T_0)] + \left[1 + \sum_{k=1}^{N} \alpha_k (C_k - C_{k,0})\right]\right\} \cdot g_j$$

where N is the number of the mixture components, i.e. buoyancy effects due to both temperature and mass fraction gradients are being considered during the solution procedure. The turbulence correlation $\overline{u_i u_j}$ is the time average of $u_i u_j$ and represents the Reynolds stresses, which have to be modelled to close the above set of equations.

In the present analysis, the $k-\epsilon$ model[4] is adopted to complete the closure problem of turbulent flow. From the generalized Boussinesq eddy viscosity concept, in analogy with the laminar flow, the Reynolds stresses can be expressed as:

$$-\rho\overline{u_i u_j} = \mu_t\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\rho k \tag{3}$$

where δ_{ij} is the Kronecker delta function and μ_t is the turbulent viscosity:

$$\mu_t = \rho C_\mu \frac{k^2}{\epsilon}$$

The differential governing equation for k can be expressed as:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho U_j k)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\left(\mu_l + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right) - \rho\overline{u_i u_j}\frac{\partial U_i}{\partial x_j} - C_\mu \rho^2 \frac{k^2}{\mu_t} \tag{4}$$

The modelled equation for ϵ is:

$$\frac{\partial(\rho\epsilon)}{\partial t} + \frac{\partial(\rho U_j \epsilon)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\left(\mu_l + \frac{\mu_t}{\sigma_\epsilon}\right)\frac{\partial \epsilon}{\partial x_j}\right) - C_1 \frac{k}{\epsilon}\rho\overline{u_i u_j}\frac{\partial U_i}{\partial x_j} - C_2 \rho \frac{\epsilon^2}{k} \tag{5}$$

Since the flow can be non-isothermal and the fluid is a mixture of air and dispersing heavy gases, there are two more unknowns, besides the six from the above equations (i.e. the three components of the velocity vector U_i (= U, V, W), the pressure P (implicitly introduced by Equation (1) via the dependency of the gas density ρ on P), k and ϵ), which are necessary in order to complete the problem's closure, i.e the enthalpy h (or equivalently the temperature T) and the mass fraction C of the dispersing heavy gas. The equations for the conservation of these two scalar quantities can be written as follows.

- *Temperature*

$$\frac{\partial(\rho T)}{\partial t} + \frac{\partial(\rho U_i T)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\left(\frac{\mu}{\mathrm{Pr}} + \frac{\mu_t}{\mathrm{Pr}_t}\right)\frac{\partial T}{\partial x_i}\right) + \rho S_T$$

- *Mass fraction of a mixture component*

$$\frac{\partial(\rho C)}{\partial t} + \frac{\partial(\rho U_i C)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\left(\frac{\mu}{\mathrm{Sc}} + \frac{\mu_t}{\mathrm{Sc}_t}\right)\frac{\partial C}{\partial x_i}\right) + \rho S_C \tag{7}$$

The values for the model constants[4] are shown in *Table 1*.

Boundary conditions

The set of elliptic partial differential equations mentioned above can be solved with the following boundary conditions.

- *Symmetry planes:* All gradients normal to the plane and the normal velocity itself are set to 0.
- *Outlet planes:* The gradients of all variables normal to an outlet plane are set to 0. The location of an outlet plane should be far enough downstream from recirculation regions so that the flow is directed outwards from the calculation domain over the entire plane (the flow must have one-way dominated behaviour).
- *Inlet planes:* All variables receive prescribed values at an inlet plane. The profiles for the normal velocity U (wind) and temperature T at the inlet plane are prescribed as functions of the height z above the ground:

$$U = U_{\mathrm{ref}}\left(\frac{z}{z_{\mathrm{ref}}}\right)^m$$

$$T = T_{z=0} + z\frac{\partial T}{\partial z}$$

Table 1 Model constants

C_1	C_2	C_μ	σ_ϵ	σ_k	Pr_t	Sc_t
1.43	1.92	0.09	1.225	1.0	0.9	0.9

The exponent m and the temperature gradient $\partial T/\partial z$ are determined by the assumed atmospheric stability class[5]. The tangential velocities V and W are set to 0. For k, a relative turbulence intensity Tu is assumed (typical values Tu = 1–15%). For isotropic turbulence, Tu is related to k via $k = 3/2(Tu\ U)^2$. The distribution of ϵ is deduced from the assumed uniform turbulent transport length scale $k^{1.5}/\epsilon$, which is assigned as 0.01 L_{char}, where L_{char} is a characteristic length scale of the flow domain.

- *Walls:* The normal and tangential velocities are set to 0. So-called wall functions[6] are employed for the other variables, in order to calculate their profiles normal to the wall.

Numerical method

The whole set of partial differential equations for continuity, momentum, scalars and turbulence model quantities with their initial and boundary conditions are first reduced to algebraic difference equations using the finite-volume method[7] by integrating them over small discrete control volumes formed in the arranged numerical grid. A collocated grid arrangement is used, i.e. all variables are stored in the centre of the control volume.

In order to avoid checkerboard pattern oscillations when solving the pressure correction equation, which are likely to occur when using this variable storage scheme[7], a special interpolation procedure for calculation of the velocities at the cell faces is adopted[8–10].

The values of convective and diffusive fluxes through the cell faces are calculated using upwind and central differences, respectively, and weighing their contributions to the coefficients of the resulting algebraic equation for each point P by means of the deferred correction scheme[11]. The general structure of the final finite volume equation for a general variable Φ is:

$$A_P\Phi_P = \sum_N A_N\Phi_N + S^U + S^P\Phi_P \qquad (8)$$

where A_P, A_N are the finite volume coefficients for the point P and its six neighbours, and S^U and S^P are the integrated source terms, S^P being the linearized part. Equation (8) is solved with the iterative strongly implicit procedure (SIP method)[12]. The equation set, consisting of Equation (8) written down for each unknown (U, V, W, P, T, C, k and ϵ), is solved using the semi-implicit method for pressure-linked equations (SIMPLE) algorithm[13].

Results and discussion

Figure 1 shows a comparison between the calculated results and experimental data[14] for a steady-state heavy gas dispersion (Freon R12) out of a very short stack and around a surface-mounted obstacle. The figure shows measured and calculated heavy gas concentration values on the side walls of the obstacle, located 24 cm downstream of the heavy gas source. The calculation domain had 62 grid points in the x-direction (parallel to the main spreading direction), 52 grid points in the y-direction (perpendicular to the x-axis and parallel to the ground) and 17 grid points in the z-direction (the negative z-axis is in the direction of the gravitational vector $\vec{g}$). The numerical grid is equi-distant, with a uniform spacing of 12 mm in all space directions. About 2500 iterations are necessary to obtain a convergent steady-state solution. The obstacle is shown unfolded on a z-plane parallel to the ground. The main direction of the flow is from left to right. All computed as well as measured values are very small (less than 2 vol%, a limiting value that can also be obtained from the theoretical model in Reference 15). The agreement appears to be good, and the computed values are symmetric along a centre plane through the calculation domain, while the measured values are slightly inconsistent with the symmetrical character of the test case.

Figures 2 and *3* show the simulated temporal development (10 s, 70 s, 130 s, 180 s) of a suddenly released heavy gas cloud (chlorine) on a z-plane parallel and about 2.5 m above the ground within a fictitious industrial plant with 25 discrete buildings. (*Figure 4* shows a top view of the topography of the investigated fictitious plant.) The iso-concentration lines correspond to the limit of lethality for chlorine (40 ppm)[16]. The release of 50 m^3 of chlorine occurred at different locations for the two test runs (marked as • in *Figure 4*) and the wind direction (from left to right in both figures) changed from south in *Figure 2* to west in *Figure 3*. Although the calculation domain is much shorter in the latter case, one can see that it takes almost the same time in both cases until the 40 ppm iso-concentration line disappears from the calculation domain. This is due to the main orientation of the buildings, i.e. located with their shorter or longer sides perpendicular to the wind direction (*Figures 2* and *3*, respectively). When the longer sides are perpendicular to the wind direction, there is a greater resistance to the cloud dispersion. *Figure 2* shows how streets with a main axis parallel to the main wind direction allow the gas cloud to form a leading current and make its dispersion easier.

The test run with the wind blowing from the south was repeated with variation of the atmospheric stability class. The first run was performed for an unstably stratified environment (Pasquill class A), the second for a neutral environment (Pasquill class C) and the third for a stably stratified environment (Pasquill class F). *Figure 5* shows the time plot of the chlorine concentration at a fixed location (marked as X on *Figure 4*) for the three test runs. All three time plots are almost identical. This implies that the turbulence enhancement caused by the buildings lies orders of magnitude above the natural turbulence of the environmental flow (expressed by the stability classes), so that the latter has almost no influence on the dispersion of the cloud over topographically

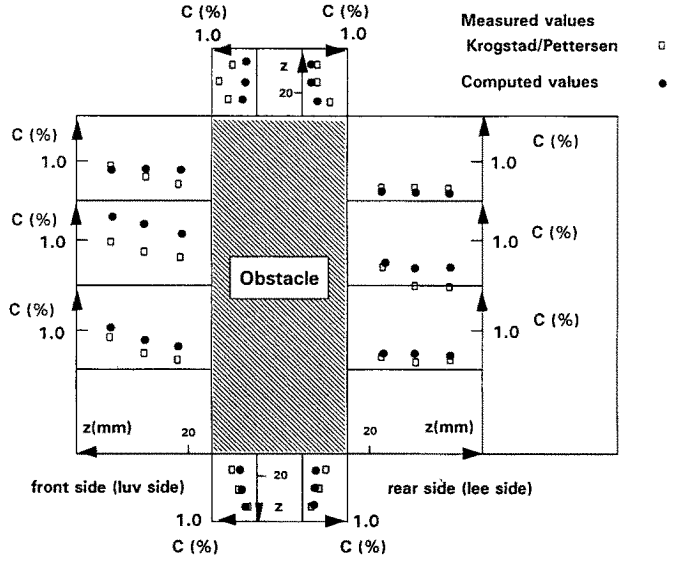

Figure 1 Comparison between computed (•) and measured (□) values for the Freon R12 concentration on an obstacle's side walls (continuous R12 release; experimental data from Reference 14, computations using the present method)

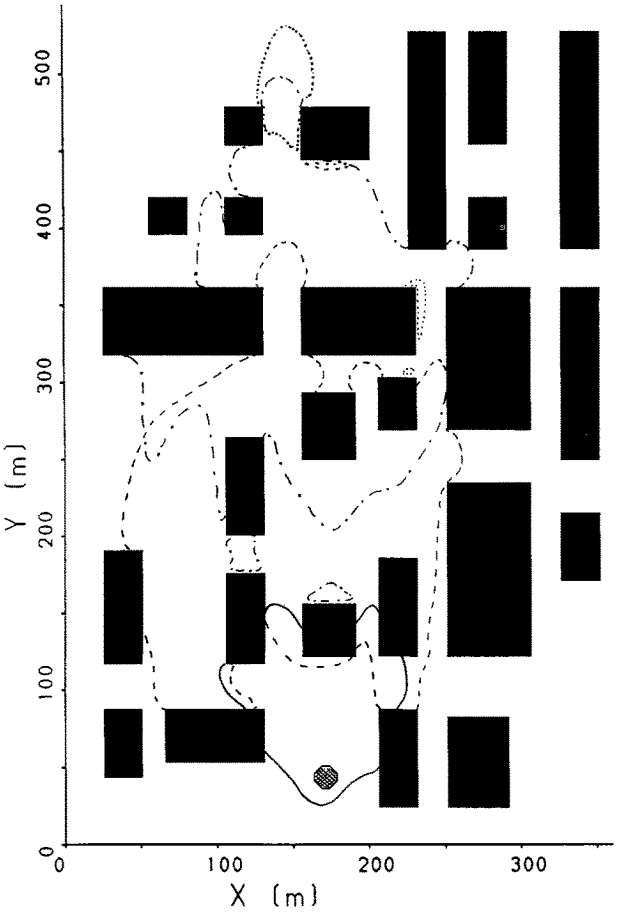

Figure 2 Temporal development of the 40 ppm chlorine iso-concentration line on a *z*-plane at height 2.5 m above ground; wind coming from the south: (—) 10 s; (- - - -) 70 s; (- - -) 130 s; (· · ·) 180 s after release

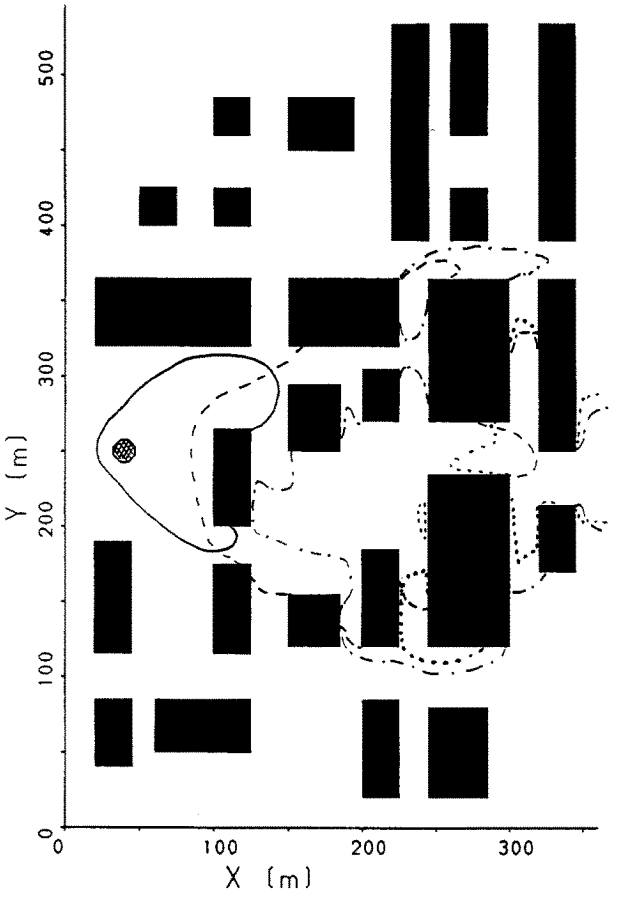

Figure 3 Temporal development of the 40 ppm chlorine iso-concentration line on a *z*-plane at height 2.5 m above ground; wind coming from the west: (—) 10 s; (- - - -) 70 s; (- - -) 130 s; (· · ·) 180 s after release

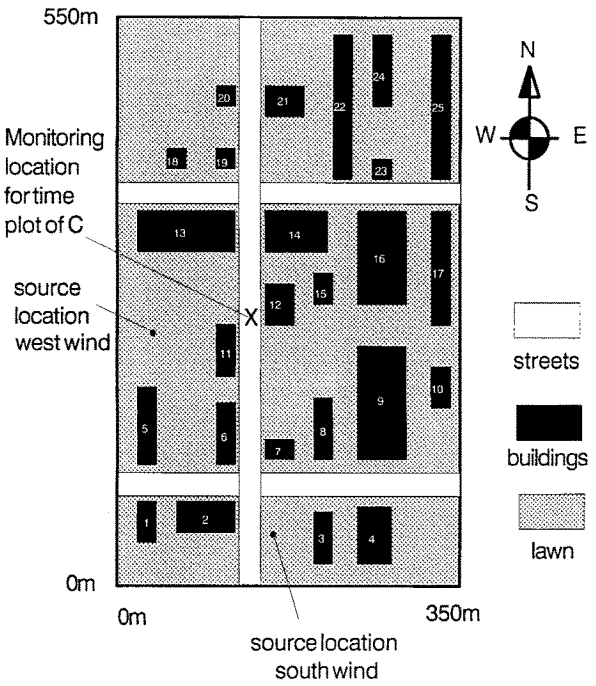

Figure 4 Top view of the topography of the fictitious industrial plant

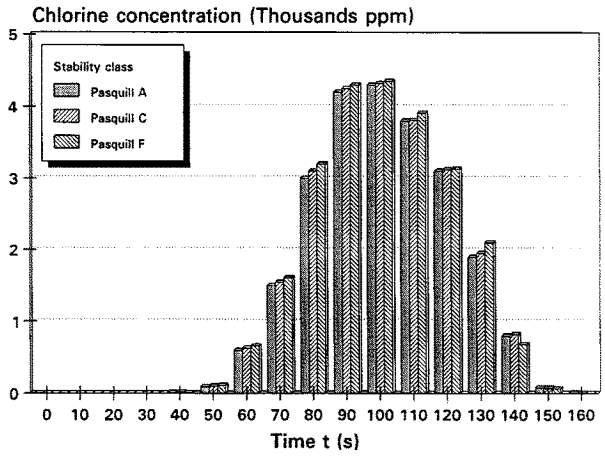

Figure 5 Time plots of the chlorine concentration at the location marked as X (see *Figure 4*) for three different atmospheric stability classes (A: unstable; C: indifferent; F: stable stratification); wind coming from the south

complex terrain. The dispersion is ruled entirely by the flow regime, induced by the specific topography. All these calculations were performed on a Cray Y-MP computer at the Technical University of Munich and required almost four hours of processor time each.

Concluding remarks

A method is presented which is able to calculate the dispersion of heavy gas clouds over topographically complex terrains. The numerical treatment of the non-steady three-dimensional governing equations was performed by means of the finite-volume method. The turbulent nature of the flow was accounted for by the k–ϵ model (with no special empirical adjustment for environmental flows), which is shown to contribute significantly to the accurate calculation of the variations in flow field quantities.

The prediction can be performed for different topographies, meteorological conditions, source data and released gases. During the development of the method, great attention was paid to making the procedure flexible and suitable for many different release scenarios. The calculations require huge computational effort, which makes the method unsuitable for faster-than-real-time predictions during an accidental release. It should be used while planning a new plant, in order to evaluate the safety hazards for different potential accidents and to increase the safety situation.

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Nomenclature

C_k	Mass fraction of mixture component k
f_i	Body force in i-direction
g	Gravitational vector
k	Turbulent kinetic energy
L	Length scale
m	Exponent for wind velocity profile
P	Pressure
Pr	Prandtl number
Pr_t	Turbulent Prandtl number
S_T	Source term in temperature equation
S_C	Source term in mass fraction equation
Sc	Schmidt number
Sc_t	Turbulent Schmidt number
t	Time
T	Temperature
Tu	Turbulence intensity
U, V, W	Velocity in the x-, y- and z-directions

x, y, z	Space coordinates
α_k	Expansion coefficient due to mass fraction differences of component $k \left(= -\frac{1}{\rho}\frac{\partial \rho}{\partial C_k}\right)$
β	Thermal expansion coefficient $\left(= -\frac{1}{\rho}\frac{\partial \rho}{\partial T}\right)$
ϵ	Dissipation rate for turbulent kinetic energy k
μ	Dynamic viscosity
μ_t	Eddy viscosity
ρ	Density
Φ	General transported quantity