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NUMERICAL SIMULATION OF THE SPREADING OF BUOYANT GASES OVER TOPOGRAPHICALLY COMPLEX TERRAIN

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SUMMARY

Numerical analysis has been performed for predicting the dispersion of continuous released neutral gases (i.e. stack gases) from elevated or near-ground sources within regions of complex topography. The three-dimensional non-steady governing transport differential equations are solved by means of the numerical finite volume method, using a collocated variable arrangement. The turbulence effects on the flow property transport 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 employed to predict continuous releases within a fictitious industrial plant. The height of the source, the atmospheric stability class, the topography and the wind speed and primary direction are varied, in order to point out the effect of topography on the pollutant's dispersion.

KEY WORDS Atmospheric dispersion Environmental flow modelling Complex topography Computer simulation Finite volume method

INTRODUCTION

The spreading of neutral or buoyant gases exciting industrial stacks within the atmospheric boundary layer is a phenomenon, that has gained great attention in recent years, owing to the growing concern about environmental pollution. It is mainly influenced by

- meteorological parameters (i.e. wind velocity, atmospheric stability class etc.)
- source data (i.e. mass flux, source height etc.)
- topography of the source's neighbourhood.

In cases where the emitted gases spread over flat terrain or the source is much higher than the surrounding buildings, the resulting concentration distribution can be calculated quite reliably with gaussian-like plume models. When the stack's height is comparable to the height of the surrounding buildings, the distribution patterns are much more complicated, since recirculations, vortices induced by the buildings etc. have a great impact on the flow field and further spreading.

The way the environmental flow field is affected by a given topography depends strongly on the concrete geometrical conditions and it is almost impossible to make any general assumptions and recommendations. Owing to the complexity of the flow it is 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 paper presents a method, which can stimulate the flow and spreading of continuously released hot gases exiting an elevated or near-ground source for a given set of topographical, meteorological and source data. The flow field in the topographically complex terrain is calculated by solving the steady-state Navier–Stokes equations by means of the numerical finite volume method (a standard k–ϵ model

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(Launder and Spalding, 1974) is employed to take turbulence effects on the flow variables transport into account) and the transport of scalar quantities (i.e. enthalpy and mass fraction of pollutant) is calculated by solving the appropriate transport differential equations for these quantities.

THEORETICAL ANALYSIS

Governing equations

The mathematical effort is complicated by considering flows within complex topographies, which demonstrate large recirculation regions and consequent distortion of the primary flow. 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 steady-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. That is, 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

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

The last term on the right-hand side stands for body forces. The specific body forces f_i include only the gravitational vector **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–ϵ-model (Launder and Spalding, 1974) is adopted to complete the closure problem of turbulent flow. From the generalized Boussinesq eddy viscosity concept, by 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

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

The modelled equation for ϵ is

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

Since the flow can be nonisothermal and the fluid is a mixture of air and dispersing stack gas there are two more unknowns, besides the six from the above equations (U, V, W, P, k and ϵ), 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

$$\frac{\partial(\rho U_i T)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\left(\frac{\mu}{Pr} + \frac{\mu_t}{Pr_t}\right)\frac{\partial T}{\partial x_i}\right) + \rho S_T \tag{6}$$

- Mass fraction of a mixture component

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

The values for the model constants are (Launder and Spalding, 1974):

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

Since pressure variations are only small during the spreading, the molecular properties are assumed to be depending only on temperature. For single mixture components the density is being calculated by the ideal gas equation of state, while the remaining relevant properties (i.e. molecular viscosity, specific heat capacity and thermal conductivity) are calculated by a 'power low' assumption $q = q_{ref}(T/T_{ref})^m$, q being an arbitrary property and q_{ref} its reference value at the reference temperature T_{ref}. The exponent m receives different values for different properties according to McEligot *et al.* (1970). The mixture's properties are calculated from formulas provided by Bird *et al.* (1970)

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 (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:

$$U = U_{ref}\left(\frac{z}{z_{ref}}\right)^m \quad T = T_{z=0} + \frac{\partial T}{\partial z} z$$

The exponent m and the temperature gradient $\partial T/\partial z$ are determined by the assumed atmospheric stability class (Pasquill, 1961). The tangential velocities V and W are set to 0. For k a relative turbulence intensity Tu is assumed (typical values $Tu = 1\%\ldots15\%$). For isotropic turbulence Tu is related to k via $k = \frac{3}{2}(TuU)^2$. The distribution of ϵ is deduced from the assumed uniform turbulent transport length scale $k^{1.5}/\epsilon$, which is assigned as $0{\cdot}01 L_{char}$. L_{char} is a characteristic length scale of the flow domain.

Walls: The normal and tangential velocities are set to 0. For the other variables so-called wall functions (Peric and Scheuerer, 1989) are employed, 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 (Patankar, 1980) 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 chequerboard pattern oscillations, when solving the pressure correction equation, which are likely to occur when using this variable storage scheme (Patankar, 1980), a special interpolation procedure for the calculation of the velocities at the cell faces is adopted (Hsu, 1981; Rhie, 1981, 1983).

The values of convective and diffusive fluxes through the cell faces are calculated by 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 (Khosla and Rubin, 1987). The general structure of the final finite volume equation for a general variable Φ is:

$$A_P \Phi_P = \sum_N A_N \Phi_N + S^U + S^P \Phi_P \tag{8}$$

A_P, A_N are the finite volume coefficients for the point P and its six neighbours, S^U and S^P are the integrated source terms, S^P being the linearized part. Equation (8) is solved with the iterative SIP* method (Stone, 1968). The equation set, consisting of equation (8) written down for each unknown (U, V, W, P, T, C, k and ϵ) is solved with the SIMPLE† algorithm (Patankar and Spalding, 1972).

COMPUTATIONAL RESULTS AND DISCUSSION

The computations are validated by comparison with experimental data (from Slawson and Casnady (1967, 1971)) for a steady-state gas release out of a high stack over flat terrain. Figure 1 compares, on a centre plane through the stack, the computed iso-concentration lines with the measured plume trajectory (marked with •). The calculation domain has 82 grid points in the x-direction (parallel to the main spreading direction), 36 grid points in the y-direction (perpendicular to the x-axis and parallel to the ground) and 56 grid points in the z-direction (negative z-axis in direction of the gravitational vector g). The numerical grid has a non-uniform spacing, being finer around the stack's exit and becoming coarser with increasing distance from the exit. About 2000 iterations are necessary to obtain a convergent steady-state solution. The agreement between computed and measured data appears to be good.

The following computational results show the effect of the atmospheric stability class (atmospheric stratification) on the dispersion of gaseous emissions. The calculation of Figure 1 (atmospheric stability class C, i.e. neutral stratified environment) was repeated under variation of the stability class. One run was performed for an unstably stratified environment (Pasquill class A) and another for a stably stratified environment (Pasquill class F). Figure 2 shows the extensions of the same iso-concentration line (4000 ppm) for the three different stability classes. The iso-line reaches its largest downstream extension for the stably stratified environment (lowest turbulence intensity, i.e. lowest mixing tendency with the surrounding air) and has the smallest extension for the unstable class, owing to the enhanced mixing with the air in this latter case. The numerical result is also consistent with gaussian plume model predictions for dispersion over flat terrains.

* Strongly implicit procedure.

†Semi-implicit method for pressure linked equations.

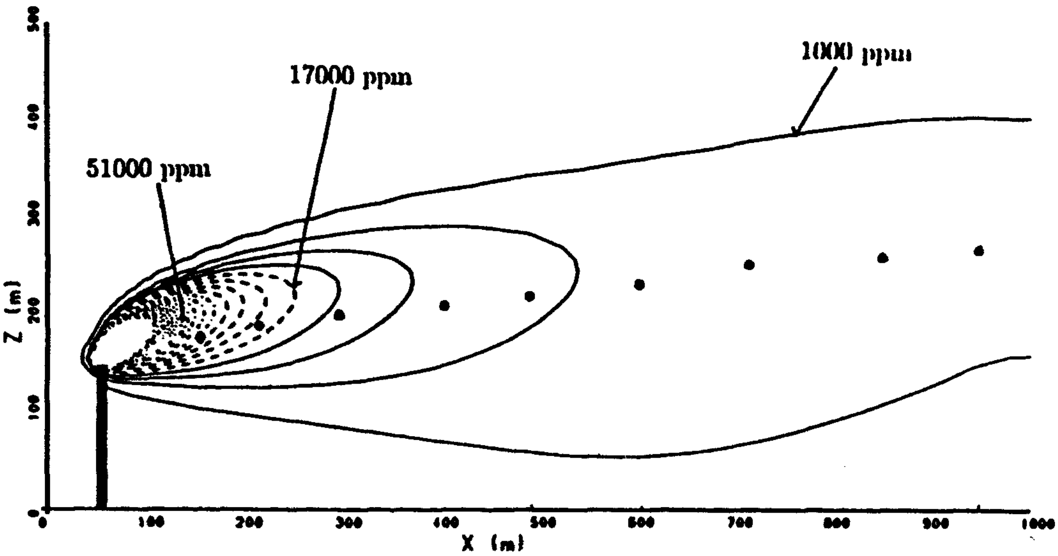

Figure 1. Computed iso concentration contours on a centre place. Simulation with the present method of a measurement performed in Stone (1968) and Patankar and Spalding (1972). Comparison with the measured (•) plume trajectory

In order to evaluate the influence of a complex near-source topography on the spreading of stack gases, calculations were performed using as a reference case the topography of a fictitious industrial plant with a chimney only slightly higher than the surrounding buildings (28 m v. 15–24 m). Figure 3 illustrates as a paradigm the pollutant's concentration on the ground for the basic topography and Pasquill class C.

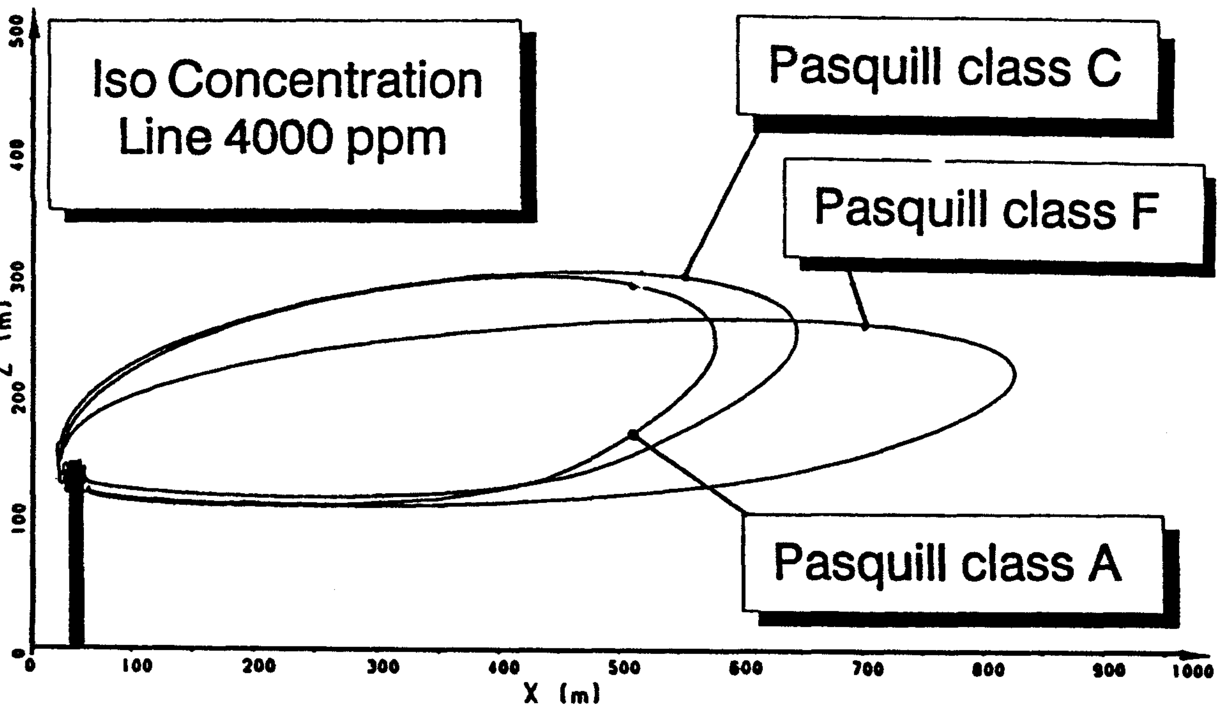

Figure 2. Iso-concentration lines on a centre plane for three different atmospheric stability classes (A: unstable, C: indifferent, F: stable stratification)

The wind velocity 20 m above the ground is 5 m/s, whereas the gases' exit velocity is 4 m/s. The stack's exit is within the wake of the upstream located buildings and is being greatly influenced by the vortices and recirculations induced by those buildings. This leads to a great overall enhancement of the turbulence and the flow's complexity and to a simultaneous reduction of the atmospheric stability class's significance on the dispersion process. This thesis is being emphasized by the numerical results summarized in Table 1. The location of the maximal ground concentration relative to the stack's location ($x = 0$, $y = 0$) and the value of this maximum are shown for three different test runs with the basic topography of Figure 3 and three different atmospheric stability classes (A, C and F). The differences between the values are very small, underlining the reduction of the stability class's significance for the dispersion process.

The concrete topographical facts have a great influence on the spreading. Table 2 summarizes the same quantities as Table 1 for four different test runs with topography variations. Test run (i), a reference case, uses the basic topography from Figure 3. In test run (ii) the building on the stack's luv side (marked as building V in Figure 3) has been omitted, while in test run (iii) the building on the stack's lee side (marked as E in Figure 3) has been left out. Finally in test run (iv) the stack's height has been increased, now being 45 m instead of 28 m, while the rest of the topography remains unchanged. The results imply, that the omission of the building on the stack's luv side allows that emitted gases to spread further and mix better with the surrounding air than in the reference case, since the influence of a downwards directed vortex, close to the stack's exit, is now no more present. Omitting the building on the stack's lee side causes the gases to fall on the ground earlier and with an increased peak concentration value, since an upwards directed vortex, induced by the impact of the primary flow on the front side (luv side) of the building, that lifted and carried the gases further during the reference case, is now missing. Increasing the stack's height moves the source out of the vortex-affected regions of the calculation domain and allows a further spreading and better mixing of the emitted gases with the surrounding air.

Figure 4 shows the pollutant's ground concentration for the basic topography and Pasquill class C, but with the wind coming from another direction (west instead of north in the previous computations). The

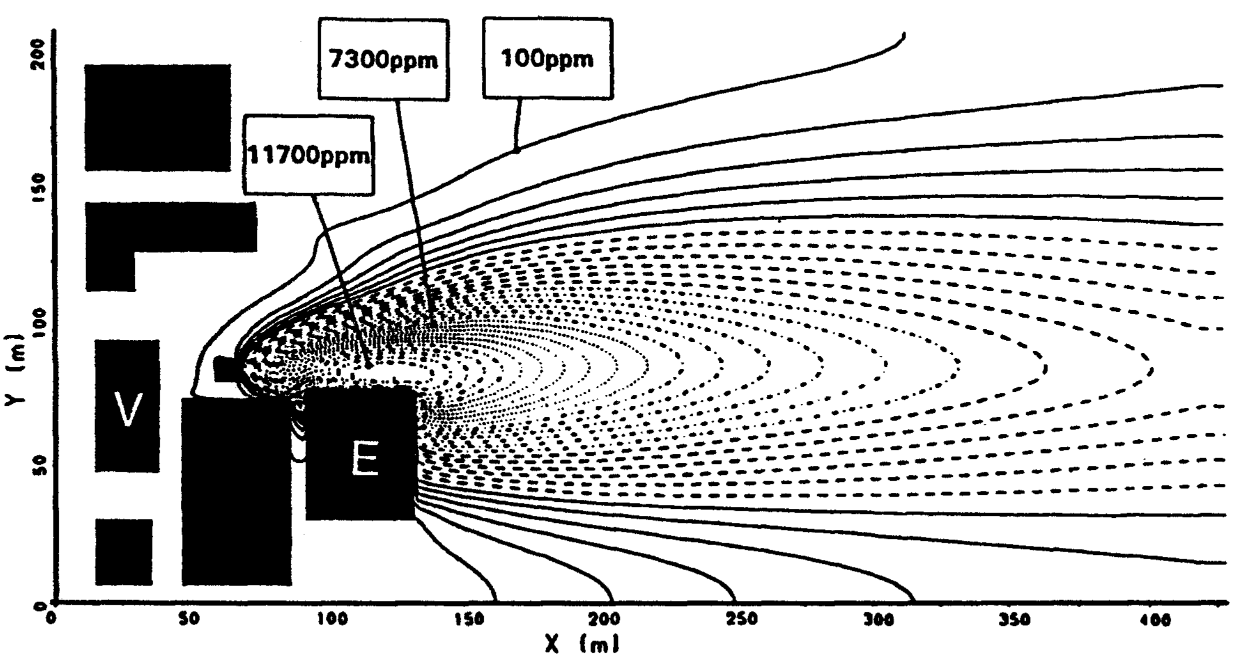

Figure 3. Top view of the terrain of a fictitious industrial plant; iso-concentration lines on the ground for Pasquill class C

Table 1. The value of the maximal ground concentration and its location for different Pasquill classes; basic topography

Pasquill class	C_{max} (ppm)	X_{max} (m)	Y_{max} (m)
A	11 700	45	0
C	11 700	50	0
F	11 500	48	−10

Table 2. The value of the maximal ground concentration and its location for different topographies

Test run	Comments	C_{max} (ppm)	X_{max} (m)	Y_{max} (m)
(i)	basic topography	11 700	45	0
(ii)	luv building omitted	9 100	80	0
(iii)	lee building omitted	12 300	45	−8
(iv)	higher stack	4 400	135	−10

distribution pattern is once again quite different, because of the relative topographical changes (the building on the stack's luv is now higher than in Figure 3 and causes the pollutant to fall down earlier).

The computations were performed on a 100 × 72 × 32 non-uniform numerical grid on the CRAY Y-MP supercomputer system of the Technical University of Munich and each required about 3000 iterations to converge.

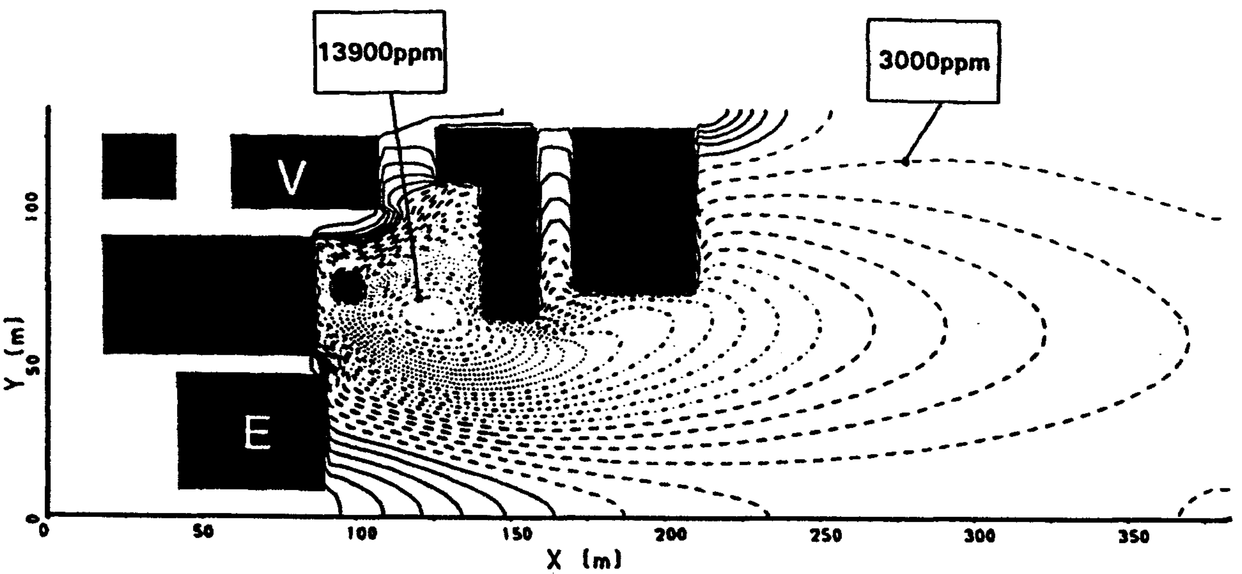

Figure 4. Ground concentration distribution for the basic topography and Pasquill class C. Wind direction changed by 90°.

CONCLUDING REMARKS

A method is presented, capable of calculating the dispersion of neutral or buoyant gases exiting a stack over topographically complex terrains. A finite-volume scheme is used for the numerical treatment of the governing equations. The turbulent nature of the flow is accounted for by a standard $k-\epsilon$ model. Calculations were performed for different topographies and meteorological conditions. They underline the significance of the concrete topography on the spreading in cases where the emitting stack is not much higher than the surrounding buildings. The topography's influence exceeds by far the influence of the natural turbulence in the environmental flow (expressed in terms of an atmospheric stability class) on the spreading. A strong correspondence has been demonstrated between the distortion of the primary flow by the buildings and the pollutant concentration distribution. The presented simulations clearly indicate the complexity of the flow and of the concentration distribution patterns for emissions within topographically complex terrain. They demonstrate the method's feasibility and capability of producing correct results, within the ranges of engineering accuracy requirements.

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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 x-, y- and z-direction
x,y,z	= space co-ordinates
α_k	= expansion coefficient due to mass fraction differences of component $k(= -(1/\rho)(\partial\rho/\partial C_k))$
β	= thermal expansion coefficient $(= -(1/\rho)(\partial\rho/\partial T))$
ϵ	= dissipation rate for turbulent kinetic energy k
μ	= dynamic viscosity
μ_t	= eddy viscosity
ρ	= density
Φ	= general tranported quantity

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