Journal of Hazardous Materials, 17 (1987) 61–80
Elsevier Science Publishers B.V., Amsterdam — Printed in The Netherlands

NUMERICAL ASPECTS OF A LAGRANGIAN PARTICLE MODEL FOR ATMOSPHERIC DISPERSION OF HEAVY GASES

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(Received December 20, 1985; accepted in revised form December 11, 1986)

Summary

The objective of the paper is to develop and analyze a numerical procedure, based on a Lagrangian particle model, for heavy gas dispersion. The paper discusses the numerical solution of the advection diffusion equation, with particular application to atmospheric dispersion of heavy gases. The discretization requirements to control numerical errors are examined for typical applications. The model is demonstrated to alleviate numerical diffusion errors which result from application of low-order finite difference methods, while allowing affordable discretization for heavy gas dispersion predictions of practical interest.

Introduction

The use of transport phenomena models for heavy gas dispersion simulation entails several difficulties. They can be divided in two categories: (1) those related to the adequate description of the relevant turbulent transport processes; and (2) numerical complications.

This paper deals with the second category. It uses a Lagrangian particle method to solve the convection diffusion equations governing atmospheric dispersion of heavy gases. This means that the proposed algorithm uses discrete fluid particles to represent the contaminant with a continuous representation of the atmospheric flow. The physical model used is described in detail elsewhere [1]. Among the numerical problems numerical diffusion is one of the major ones. Its consequences are discussed. A suitable Langrangian technique is then developed and is subsequently investigated by applying it to realistic dispersion scenarios.

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0304-3894/87/$03.50

Physical model

The physical model belongs to the generic category of primitive equation models, since it attempts to solve the dynamical equations for the wind field and the temperature and contaminant field. It describes the transient dispersion of an accidentally released contaminant in the near field, and takes into account the primary heavy gas effects. The model also makes it possible to incorporate the effect of obstacles in the ambient flow field. A detailed discussion is given in Ref. [1].

Under the assumptions of turbulent and incompressible flow, Boussinesq approximation and gradient transfer hypothesis, the basic set of equations may be written as:

$$\nabla \cdot \vec{u} = 0 \tag{1.a}$$

$$\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} = \frac{1}{\rho} \nabla P + \nabla \cdot (\bar{\eta}_m \cdot \nabla \vec{u}) - \frac{\Delta \rho}{\rho} \vec{g} \tag{1.b}$$

$$\frac{\partial c}{\partial t} + \vec{u} \cdot \nabla c = \nabla \cdot (\bar{\eta}_M \cdot \nabla c) + S \tag{1.c}$$

$$\frac{\partial T}{\partial t} + \vec{u} \cdot \nabla T = \nabla \cdot (\bar{\eta}_T \cdot \nabla T) \tag{1.d}$$

In order to solve the above equations, the turbulent exchange coefficients $\bar{\eta}_m$, $\bar{\eta}_M$, and $\bar{\eta}_T$ must be determined at each point by means of a turbulence model.

The present simulation specifies the vertical turbulent viscosities $\eta_{m,z}$ by means of a one-equation "turbulent kinetic energy"-type closure model with an ad hoc prescription for the length scale, i.e. the Nee–Kovasznay model [2]. An additional term has been added to include buoyancy effects.

The vertical mass transfer coefficients are determined from the ratio of the turbulent viscosities and the turbulent Schmidt number

$$\eta_{M,z} = \eta_{m,z} / Sc_t \tag{2}$$

The turbulent Schmidt number is modeled as a function of the local gradient Richardson number based on the local density gradient and the shear of the horizontal wind speed:

$$Sc_t = f_1(Ri)$$

where

$$Ri = \left(\frac{g}{\rho} \frac{\partial \rho}{\partial z} \right) \Big/ \left(\frac{\partial u}{\partial z} \right)^2 \tag{3}$$

The functional relationship is derived from an analysis of stratified flow experiments. The model does not assume the Reynolds analogy between momentum and concentration or temperature transfer. The effective horizontal turbulent mass transfer coefficient is specified as a function of the horizontal wind direction variance, initial source size and time, following the statistical diffusion theory by Smith and Hay [3]: $\eta_{M,y}=f_2(S_o, v'^2, t)$

A Gaussian distribution is assumed for the particle distribution. This is in principle only valid for homogeneous and isotropic turbulence. For height-dependent diffusivities the distribution is only applied locally. This approach is extended here from a linear to a nonlinear dependency, lacking further refinement in the underlying physical turbulence model.

The model will now be used as a vehicle for the discussion of the numerical requirements for heavy gas dispersion simulations. Of course, most of the discussion below will remain relevant beyond the specifics of this particular model.

Motivation for a particle model

In convection-turbulent diffusion problems, the objective is to predict the distribution of a scalar quantity in a fluid flow. The scalar quantity is simultaneously convected with the mean flow and diffused by the turbulence. In the case of a heavy gas release into the atmosphere, the flow may be affected or even dominated by the presence of the contaminant. Most distributed parameter models of such transfer processes have used finite-difference methods for approximating the model (partial differential) equations [4,5], and the central difference (CD) approximation is commonly used for the diffusion terms. However, when the CD approximation is used for the convection terms, numerical instabilities may occur when the convective flux dominates the diffusive flux [6–8]. The relative importance of convection and diffusion is indicated by the grid Peclet number:

$$Pe_i=\frac{u_i \Delta x_i}{\eta_i} \tag{4}$$

where η_i is the diffussivity in the i-direction.

Unrealistic results are obtained with CD methods when Pe_i is greater than 2 [4]. Introduction of an artificial diffusivity limits Pe and stabilizes the calculation. Alternative "upwind" or donor cell difference schemes for the convection terms, although stable, introduce false (numerical) diffusion for high Peclet numbers. It can be demonstrated [6] that the upwind scheme results in a false diffusivity of

$$\eta_{a,i}=0.5u_i \Delta x_i=\frac{|Pe|\,\eta_i}{2} \tag{5}$$

which is the same value used to stabilize central difference schemes. The associated "false" diffusion can be the principal source of numerical errors. The problem may not be too serious when streamlines are aligned with the grid lines in a steady state calculation since in this case diffusion occurs only in the direction of the velocity vector and may have little effect if convection is the dominant physical process. However, in more complex flow fields, the streamlines may not be aligned with the numerical grid lines. If there is a significant gradient of the transported quantity in the direction normal to the velocity vector, the associated numerical diffusion error may even obscure the physical diffusion being modeled. This can be demonstrated by simulating the pure advection of a scalar step in a uniform velocity field which is diagonal to the numerical mesh [6–9].

The simulation of the turbulent flows resulting from accidental release of heavy gases in the atmospheric boundary layer is particularly demanding. First, the flow field is usually multidimensional, as in the gravity spread which immediately follows release or in the recirculating flows around obstacles. Second, vertical mixing may be severely damped and require the use of very low physical diffusivities. In contrast to the usual passive pollutant dispersion problems, accidental releases often occur at ground level, where diffusivities are also low. To estimate the magnitude of the problem, two typical scenarios are investigated:

1. Continuous release of a heavy gas from a boiling liquid pool;
2. Instantaneous release of heavy gas as in the Thorney Island series of field experiment [10].

Continuous releases

We assume a vertical exit velocity of 0.1 m/s at the pool surface (characteristic of a boiling cryogenic liquid). The ambient wind profile is neutral with a friction velocity of 0.13 m/s. The turbulence model is described by Schreurs and Mewis [1]. Figure 1 shows the vertical diffusivity versus gradient Richardson number for two heights (respectively 1 m and 10 m above ground level). In Fig. 1 we have also plotted the false vertical diffusivities [4] required to stabilize the central difference scheme for three vertical spatial resolutions ($\Delta z = 1$ m, 0.5 m, 0.1 m). The numerical solution is distorted when the stabilizing diffusivities are comparable with or greater than the physical values. Figure 1 shows that numerical diffusion is more severe close to ground level. With a vertical spatial resolution of 1 m, the false diffusivity near the ground is of the same order of magnitude as the physical diffusivity even without heavy gas stratification effects. It is obviously impractical to use the model to estimate turbulent diffusion with the low diffusivities which characterize dispersion in density-stratified flows.

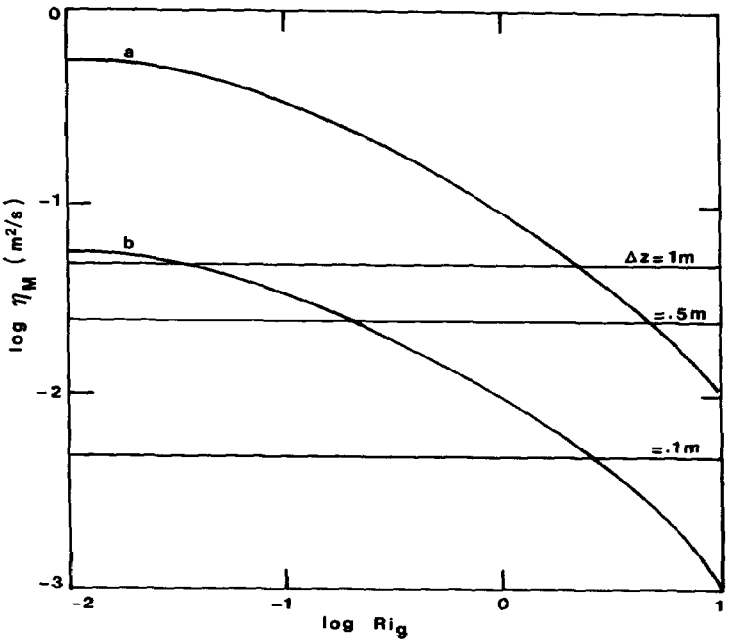

Fig. 1. Comparison between the physical diffusivity and the numerical diffusivity for spatial resolutions of 0.1, 0.5 and 1 m (vertical): a - 10 m above ground level; b - 1 m above ground level.

Instantaneous releases

The complex flow patterns which occur during the gravity spread of a collapsing heavy gas cloud introduce further difficulties. We consider an instantaneous release of 2000 m^3 gas with density twice that of air. From the Thorney Island field experiments [10], we know that the physical diffusion time needed to dilute the cloud maximum concentration to 1% by volume is of order of one minute. A measure of the importance of false diffusion is obtained by determining the false diffusivities from eqn. (5) along the three coordinate directions for the conditions immediately following release (the worst conditions for numerical diffusion). Substitution of these (maximum) false diffusivities in the analytical solution of the diffusion equation [11] gives a time scale needed for the false diffusivities to dilute the cloud maximum concentration to 1 vol%. If this numerical time scale is comparable to the physical time scale, a good numerical solution cannot be produced. Table 1 summarizes the analysis and indicates that numerical diffusion is a serious concern. Table 1 also indicates that overcoming the problem by using very fine computational grids becomes impractical for 3-D problems.

The following remedies for the illustrated problems are being studied:

TABLE 1

Analysis of false diffusion for a Thorney Island-type release

Release characteristics - instantaneous heavy gas spill: volume = 2000 m^3, width = 12 m, length = 12 m, heigth = 14 m, and $\rho_g = 2\,\rho_a$.

Spatial resolution			Number of cells $\times 10^3$		Time scale
Δx(m)	Δy(m)	Δz(m)	N_s	N_F	T_* (s)
3	3	3.5	16	22	12
3	3	2	28	32	14
2	2	2	63	71	19
2	2	1	126	130	23
2	2	0.5	252	249	29
1	1	0.5	1008	970	47

N_s: number of cells required to represent the source under a quarter-symmetry option; N_F: number of cells required to represent a calculation domain of 150 m × 150 m × 20 m (in quarter-symmetry); T_*: time in seconds to dilute the cloud to 1% with false diffusivities

Note: Table 1 assumes no ambient wind conditions. The time scale T_* would, however, not significantly change over an ambient wind speed range of 0–6 m/s because the initial cloud motion remains the overriding effect.

- Reduction of the physical eddy diffusivity to account for the false diffusion inherent in the scheme [12]. This approach is not viable in our application because of the low physical diffusivities involved.
- Second-order difference schemes for scalar advection (such as Crowley's method), followed by filtering of numerical oscillation [13] or "anti-diffusive" corrections [14].
- Higher-order spatial discretization methods [4]. These methods have not yet found widespread application in practice because of their relative complexity, and they have not been tested for application to the present problem.
- Functional methods (finite element, spectral models [9,15,16]).
- Lagrangian particle methods. This technique has been extensively used in other applications [17] including air pollution modeling [18,19].

Conceptual basis for a particle model

In Langrangian particle models, the dispersion is simulated with pseudo-particles (representing the contaminant gas) which can be advected and diffused by the flow field. The prescriptions for particle displacement must be consistent with the governing transport equation. The influence of the contaminant on the flow is accounted for by integrating the influence of individual particles over the Eulerian mesh cells. The Eulerian computational cells are used to convert particle positions to concentrations at times and places of interest. The false diffusion problem is effectively eliminated. The effect of too

large Eulerian cell size relative to the cloud dimension (i.e. near the source) is to reduce information about the spatial position of the particle. This effect does not affect the accuracy with which the cloud development is predicted unless strong gradients are induced by a complex flow pattern. Although we can anticipate improved numerical performance (in this regard) for particle models, systematic computational experiments are necessary to examine the following aspects of the approach:

- consistency of the solution procedure with the governing physical model,
- sensitivity of concentration predictions to particle number and spatial resolution.

Consider the component mass balance (advection–diffusion) equation:

$$\frac{\partial c}{\partial t}+u_i\frac{\partial c}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\eta_{M,i}\frac{\partial c}{\partial x_i}\right)+S \tag{6}$$

We incorporate the turbulence closure method suggested for accidental releases of heavy gases by Schreurs and Mewis [1].

Rewriting the diffusion equation in the following form:

$$\frac{\partial c}{\partial t}+\frac{\partial}{\partial x_i}\left[\left(u_i-\frac{\eta_{M,i}}{c}\frac{\partial c}{\partial x_i}\right)c\right]=S$$

we consider a convection process with velocity

$$u_i'=u_i-\frac{\eta_{M,i}}{c}\frac{\partial c}{\partial x_i} \tag{7}$$

This approach has been suggested by Sklarew [20] to simulate air pollution. Particles are placed in the fluid region with the number of particles in a cell proportional to the concentration. When these particles are advected with the velocity u_i', the resulting particle distribution approximates the solution of the diffusion equation, eqn. (6). The second term in eqn. (7) represents the average speed with which particles diffuse relative to the main flow. The computed diffusion depends on computed values of concentration gradients and therefore requires sufficient cells to give proper resolution of the concentration gradients. Consequently, the technique is only a partial improvement over conventional Eulerian grid schemes. A particle treatment that would not require such fine resolution is desirable.

An alternative procedure to simulate the diffusion process has been proposed by Hotchkiss and Hirt [21] and Sicilian and Hirt [22]. The technique has been applied for hydrogen mixing in reactor containment buildings [23]. The turbulent diffusion is modeled as a stochastic process, using a randomized velocity u_{ri}

$$u_i'=u_i+u_{ri} \tag{8}$$

to describe the motion relative to the flow field resulting from turbulent diffusion. A prescription for the probability distribution of u_{ri} is required. By calculating the history for a large number of particles, the ensemble solution is approached. This method appears less sensitive to spatial resolution than Eulerian models or Sklarew's method. The influence of the grid size is due to the required interpolation of the flow properties at the grid nodes in order to determine the local properties at the particle positions. Provided an adequate interpolation scheme can be found, the stochastic approach may alleviate the numerical diffusion errors caused by a coarse grid. The remaining problems are the specification of the equations for particle motion and the number of particles required for a simulation.

Extension of particle transport to nonhomogeneous conditions

In the model recommended by Hotchkiss and Hirt [21], the turbulent diffusion is accounted for by assigning to each particle at each time step a random displacement of Gaussian probability with standard deviation

$$\sigma_i = \sqrt{2\,\eta_{M,i}\,dt} \tag{9}$$

The method was originally restricted to applications where the eddy diffusivity was constant [21]. It can be shown that this description (eqn. 9) is consistent with macroscopic gas cloud dispersion in the limiting case of a uniform spatial field and constant eddy diffusivity. In the application of interest here, the eddy diffusivities vary strongly in time and space due to the presence of the ground, obstacles and the (transient) heavy gas effect [1]. In earlier work [24,25], successful application of the method was reported for pollutant sources above ground level. When near-ground sources were tested or whenever the range of application was extended to the near-ground region, the results were not satisfactory [24,25]. This can be attributed to particle drift towards areas of lower diffusivity when eqn. (9) is applied. In the atmospheric surface layer, this leads to unrealistic concentration build-up at ground level. Several authors [26–28] have attempted to overcome this deficiency by adding an asymmetry term (skewness term) to the displacement scheme for nonhomogeneous conditions. From the theory of continuous stochastic processes, Durbin [29] presents the following particle displacement equation for application under nonhomogeneous conditions:

$$dz = \frac{\partial \eta_M(z)}{\partial z}\,dt + \sqrt{2\,\eta_M(z)\,dw_t} \tag{10}$$

where the increment dw_t has a Gaussian distribution:

$$P(\mathrm{d}w)_t = \frac{e^{-(\mathrm{d}w_t)^2/2\ \mathrm{d}t}}{\sqrt{2\,\pi\ \mathrm{d}t}}$$

with standard deviation $\sqrt{\mathrm{d}t}$. Equation (10) is identical to eqn. (9) in homogeneous conditions where the bias term $(\partial \eta_M(z)/\partial z)\ \mathrm{d}t$ vanishes. Under non-homogeneous conditions, eqn. (10) indicates that particles will be subject to a Lagrangian mean vertical velocity:

$$\frac{\mathrm{d}\bar{z}}{\mathrm{d}t} = \frac{\partial \eta_{\mathrm{M}}\ (z)}{\partial z} \tag{11}$$

This result can also be deduced analytically from the turbulent diffusion equation in the limiting case of an instantaneous plane source of passive material released at ground level in the neutral surface layer. When the Monin–Obukhov relationship for the vertical eddy diffusivity is adopted (i.e. $\eta_{\mathrm{M}}(z) = ku_* z$), the following analytic solution is obtained in this hypothetical case [11]

$$c(z,t) = \frac{Q}{k\,u_*\,t} \exp\left(\frac{z}{k\,u_*\,t}\right) \tag{12}$$

If mean cloud height is defined as

$$\bar{z} = \frac{\int_0^\infty z\,c\,\mathrm{d}z}{\int_0^\infty c\,\mathrm{d}z} \tag{13}$$

substitution of eqn. (12) into eqn. (13) yields:

$$\frac{\mathrm{d}\bar{z}}{\mathrm{d}t} = k\,u_* = \frac{\mathrm{d}\,\eta_{\mathrm{M}}}{\mathrm{d}z} \tag{14}$$

which is consistent with eqn. (11) and eqn. (10). Equation (11) means that the Lagrangian mean velocity of a cloud of particles is non-zero under non-homogeneous conditions, even though the Eulerian mean vertical velocity may be zero. For a cloud of particles released at the surface ($z = 0$), some will eventually rise above the surface, so that the mean height of all particles is increasing.

Numerical procedures for particle models

In order to advect and diffuse the pseudo-particles, the local mean and turbulent flow properties have to be known at the particle positions. This requires interpolation using values at surrounding grid nodes. Two basic procedures have been commonly applied: bivariate linear interpolation [4,30] and second-order interpolation [31]. The latter has been shown to result in increased accuracy near extrema and in perturbed flow fields. However, Chan's formula [31] cannot be applied close to solid boundaries, e.g. whenever a particle is at a height below half the vertical step size. In this case ($z_{\mathrm{p}} < 0.5\ \Delta z$), the particle

motion is handled by profile functions which in this case are consistent with known similarity close to the ground and match the flow properties at the first vertical node point. If the particle rises above 0.5 Δz during subsequent cycles, it is handed over again to the interpolation scheme.

Additional limitations must be observed in defining the time step for the particle transport scheme. We have imposed the requirement that material must not be permitted to advect and diffuse across more than one computational cell in a single time step. Such constraints are equivalent to the stability requirements for the explicit Eulerian flow field model.

In order to simulate the turbulent diffusion properly, it is essential that the random number generating technique is adequate. Uniform random numbers are commonly generated by a multiplicative congruential generator [32]. To generate random numbers of a particular non-uniform distribution, the hit-or-miss method can be applied [33]. For the specific case of a Gaussian distribution, the following standard transformation method allows derivation of normally distributed numbers R_G from uniform random numbers R_U $(0<R_U<1)$.

$$R_{G,1}=\sqrt{-2\ln R_{U,1}}\cos(2\pi R_{U,2})$$

$$R_{G,2}=\sqrt{-2\ln R_{U,1}}\sin(2\pi R_{U,2})$$

We have checked the above procedures by generating sequences of random numbers and comparing the result against the expected distribution by means of a χ^2-statistical test.

Numerical filtering can be applied to reduce the "graininess" of the predicted concentration distribution which results from the use of a discrete number of particles. A transition of a particle from one Eulerian cell to another leads to a jump change in concentration, causing statistical fluctuations in the concentration prediction. Numerical filtering is applied to smooth these fluctuations. The length and time scales imposed by the flow field discretization constitute a lower limit of (implicit) numerical filtering. The upper limit on filter size depends on the desired relevant scale range of the specific problem. The several filtering procedures that can be applied have been summarized by McRae et al. [15]. We have used a first-order Kalman time filter:

$$k\frac{dc_F}{dt}+c_F=c_o$$

where c_o represents the unfiltered concentration and c_F the filtered value. The filter size is characterized by k, which is the reciprocal of a time constant τ. The default size of the filter k_D is taken as twice the node spacing:

$$k_D=\frac{2\,\Delta x}{u}$$

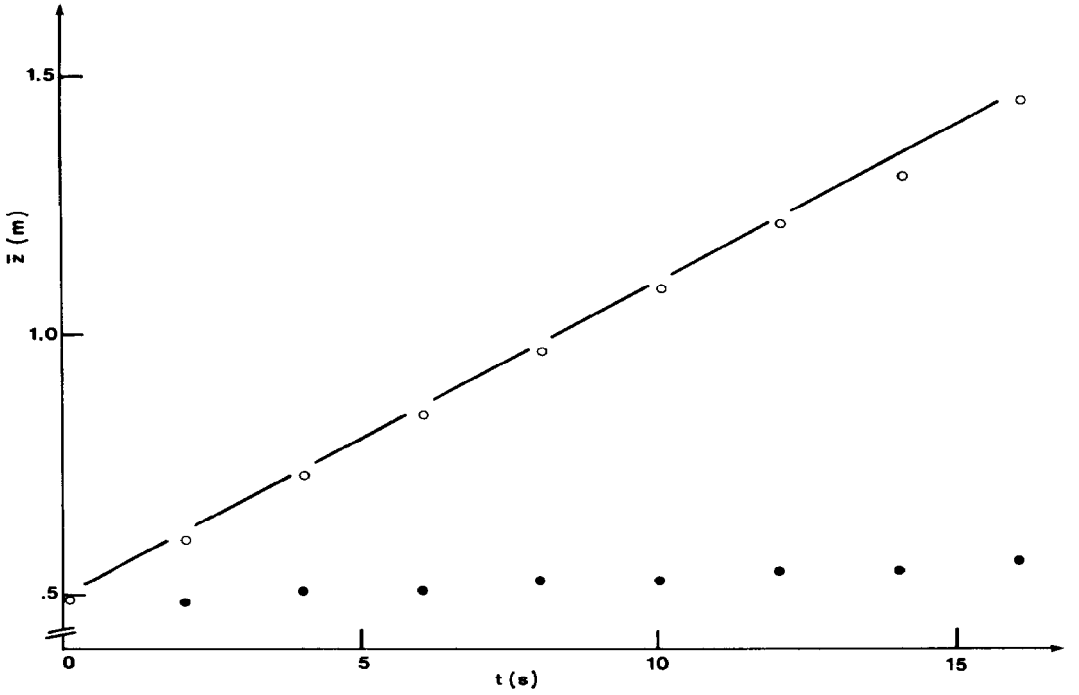

Fig. 2. Effect of skewness term on mean particle height: • - eqn. (9); o - eqn. (10); -- - similarity prediction.

In simulations of accidental releases, this corresponds to a time scale of the order of seconds.

Computational evaluation

Several numerical experiments have been conducted to evaluate the particle diffusion model. In the first test, an instantaneous, passive source in a neutral surface layer ($u_* = 0.15$ m/s) is simulated for comparison with the known analytic solution [11]. Figure 2 shows the computed evolution of the average particle height. The result based on similarity theory [11] is reproduced correctly. The figure also shows the importance of the skewness term for this simulation.

In the second test, a passive instantaneous source in a uniform flow is modeled. The initial concentration distribution is uniform with height. In a correct dispersion model, the homogeneous concentration distribution should be preserved. In this case, one hundred particles were introduced in each of thirty vertical cells. The vertical ambient diffusivity profile is chosen to represent an unstable surface layer (characteristics $u_* = 0.277$ m/s, $L = -50$ m, $z_0 = 0.02$ m). Using eqn. (9), i.e. ignoring the bias term, results in rapid accumulation of

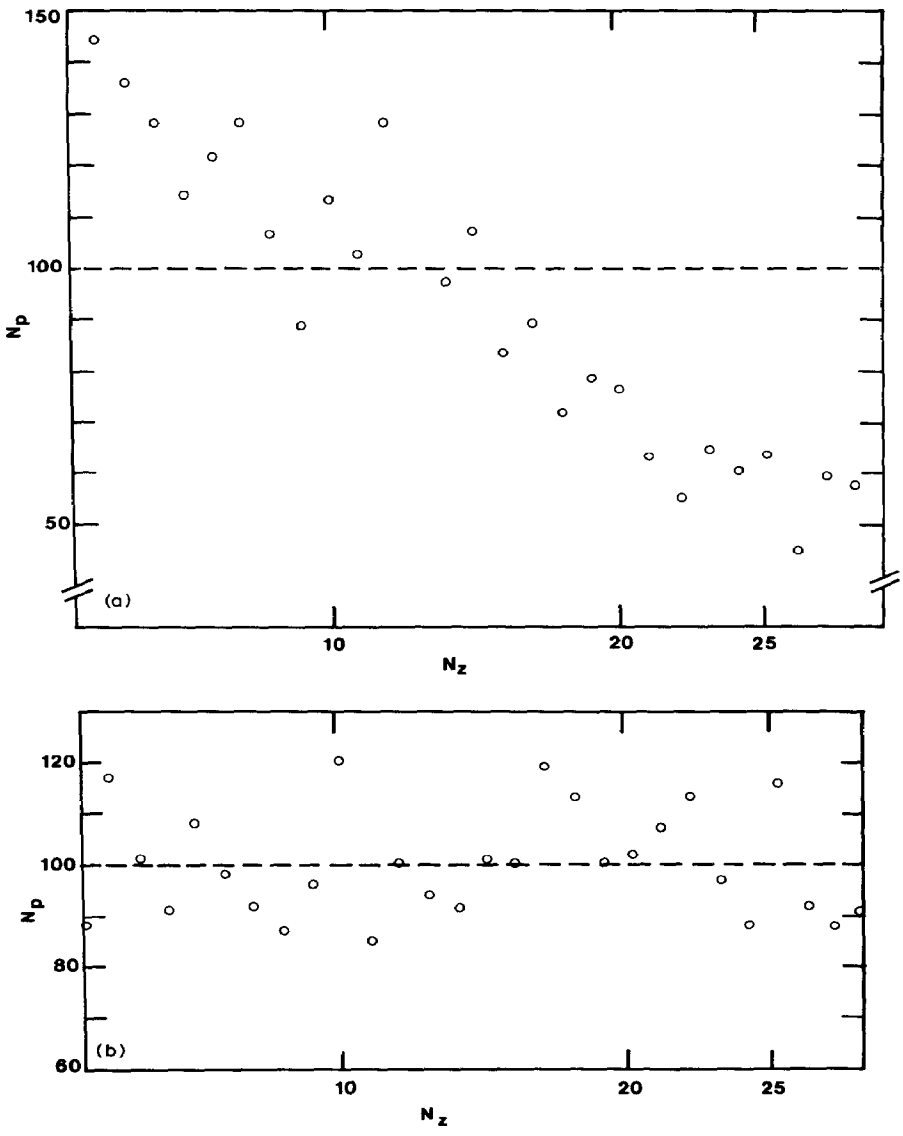

Fig. 3. Calculation of vertical particle distribution after 20 s for a height-independent source: a – without skewness term; b – with skewness term.

particles near the ground. Figure 3a shows the corresponding profile after 20 s. The assumption of a uniform homogeneous turbulence field is obviously unsuitable for accidental releases with stratification effect and the presence of the ground. On the other hand, the result of eqn. (10) does not exhibit such

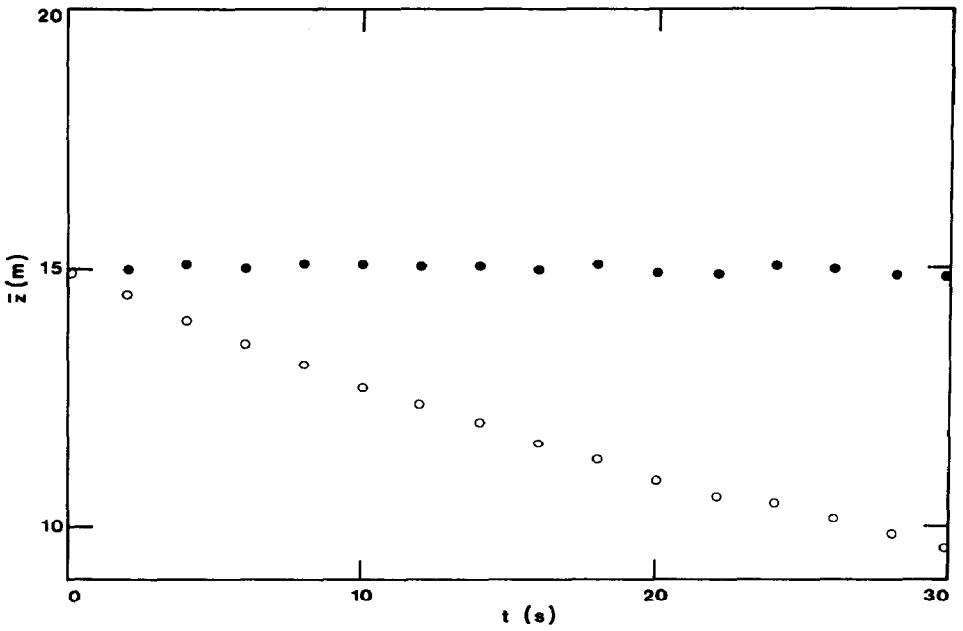

Fig. 4. Evolution of mean particle height for a height-independent source: o – without skewness term; • – with skewness term.

erroneous behavior. The vertical particle distribution remains uniform as expected (Fig. 3b). The observed scatter is due to the finite number of particles. For the same conditions, the evolution of the mean particle height can also be computed (Fig. 4). We again observe that the result obtained without the skewness term is not acceptable.

Discretization requirements

A method is needed for estimating the required number of particles for a simulation. Therefore calculations were performed with varying particle numbers for a given scenario. An example of such an analysis is shown in Fig. 5, representing predictions with increasing number of particles. The latter are based on a passive release of 153.2 kg/s during 2 s in a neutral surface layer ($u_* = 0.42$ m/s, $z_0 = 0.02$ m). The results show agreement at higher concentration levels with substantial scatter at lower concentrations. Given the operational characteristics of our specific particle model, our sensitivity study indicates the lowest concentration level that can be represented with a given number of particles (N_p) and a given spatial discretization of the Eulerian

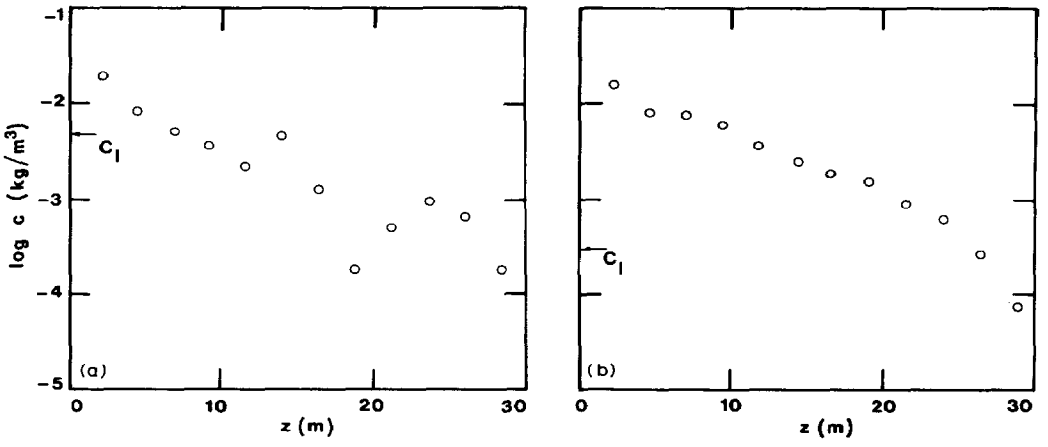

Fig. 5. Sensitivity test for particle number: a - $N_p = 500$; b - $N_p = 8000$.

flow field ($\Delta x, \Delta y, \Delta z$):

$$c_l = \frac{Q_T}{N_p \, \Delta_x \, \Delta_y \, \Delta_z} \tag{15}$$

where Q_T represents the integrated amount of mass. The limiting concentration c_l is also shown in Figs. 5a-b for the range of particle numbers investigated. Equation (15) can be used to provide an estimate of the minimum required number of particles for a given spill scenario, spatial discretization, and lower concentration level of interest to the user.

Finally, we consider the spatial resolution needed. Figures 6 and 7, respectively, show a calculation for dispersion around a 2-D obstacle and for a heavy gas release. The surface layer conditions are identical in both cases ($u_* = 0.257$ m/s, $z_0 = 0.02$ m, $L = \infty$). Figure 6 represents the concentration profile for a 2-D wall with a height of 10 m on a distance of 30 m from a ground level passive source ($Q = 300$ kg/s, $t = 10$ s). Figure 7 shows the results for an instantaneous release of a heavy gas ($\rho_g = 3$ kg/m^3, $Q = 3000$ kg) at ground level. We observe that grid-independent solutions can be obtained with affordable mesh sizes in both cases. The major advantage of the particle scheme therefore is the absence of numerical diffusion errors for an affordable spatial discretization. These less severe spatial resolution requirements (relative to conventional finite difference schemes, see Fig. 1) also compensate for the additional computational cost incurred with the particle treatment.

An additional advantage of the model accrues for application to the simulation of massive instantaneous heavy gas releases such as the Thorney Island Trials [10]. The calculation can be terminated when the average particle height becomes similar to the vertical step size, at which point there is inadequate

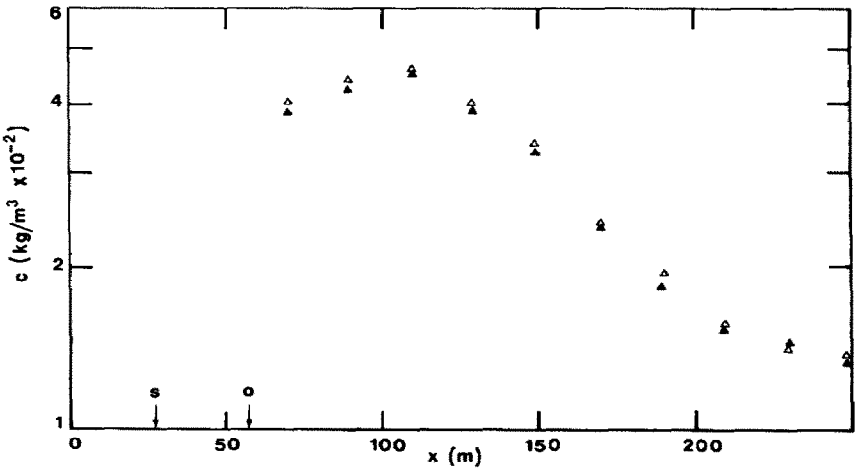

Fig. 6. Sensitivity of the dispersion calculation to spatial resolution, maximum centerline concentration at $z=3$ m after an obstacle: s - source; o - obstacle; △ - $\Delta z=2$m; ▲ - $\Delta z=1.25$ m.

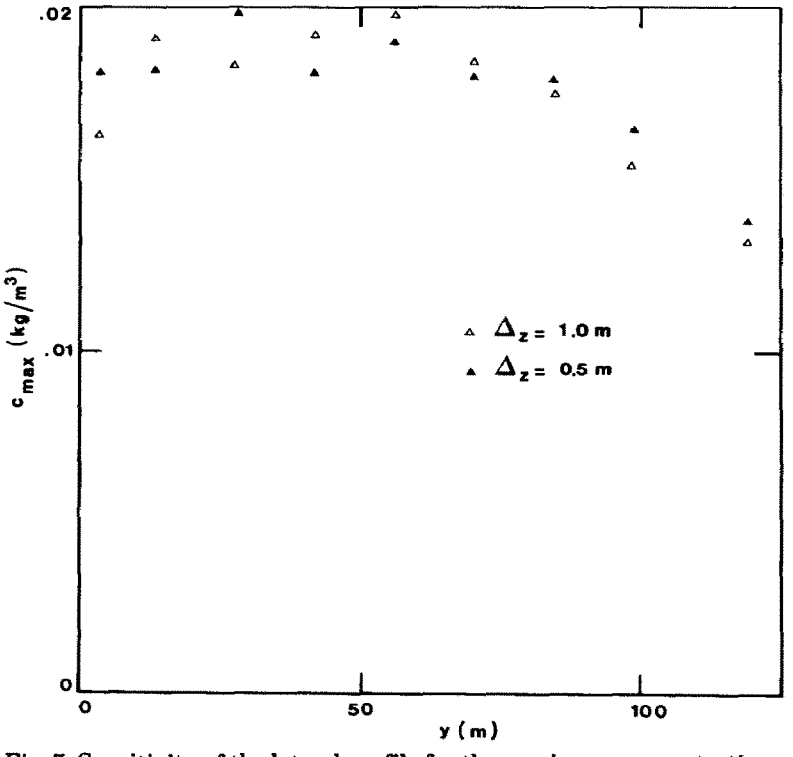

Fig. 7. Sensitivity of the lateral profile for the maximum concentration at ground level to vertical spatial resolution ($x=270$ m): △ - $\Delta z=1.0$ m; ▲ - $\Delta z=0.5$ m.

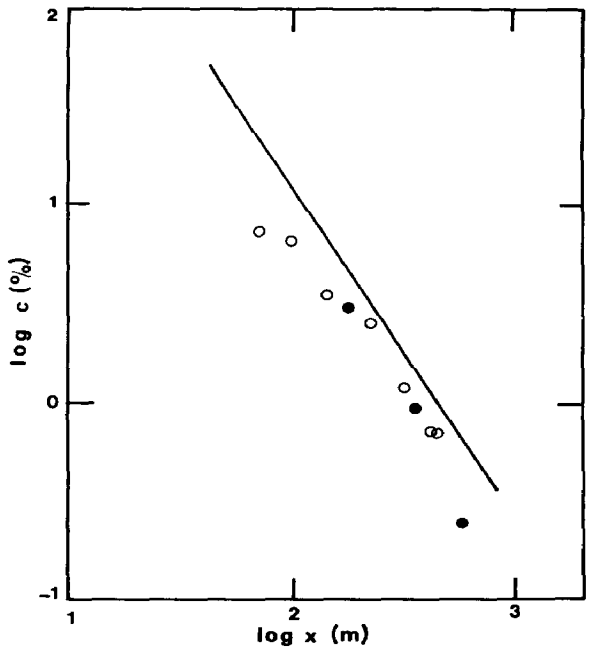

Fig. 8. Comparison of prediction against experimental data for heavy gas dispersion (Thorney Island exp. no. 13): • - center line data, o - near center line data, — - prediction; concentrations c in mol%.

spatial resolution. This condition can be detected more easily with a particle model because the particle distribution adds a level of detail at a smaller scale than the computational cell size. This is important in such simulations because the initial source size is not the smallest length scale of the problem for an instantaneous heavy gas release, in contrast to the typical evaporative releases where the resolution of the source area is most critical.

Up to now several aspects of the numerical procedure have been discussed separately without providing a global picture of its performance. It is impossible to separate completely the assessment of the numerical part from that of the physical model. A comparison between the simulation predictions and experimental evidence is discussed together with the physical model in [1]. The quality of the fit for a large scale test on heavy gas dispersion is illustrated in Fig. 8.

Conclusion

A Lagrangian particle technique for simulating the equations of atmospheric dispersion of heavy gases is described. It has been developed to alleviate numerical advection errors obtained with finite difference methods. Numerical

verification tests have been presented to check the consistency of the solution procedure and to provide examples of resolution requirements. The primary advantage of the procedure is the ability to control numerical diffusion errors adequately with affordable discretization. Comparison with a large scale experiment on heavy gas dispersion shows a good agreement.

Acknowledgements

Computer facilities have been provided by the von Karman Institute and the Solvay Central Research Center. The work was partially supported by the Bureau Technique International du Chlore. Stimulating discussions with Prof. M. Riethmuller (VKI) and Messrs. Van Diest and Vergison (Solvay) are gratefillu acknowledged. One of us (P.S.) acknowledge a fellowship from the Instituut tot Bevordering van Wetenschappelijk Onderzoek in Nijverheid en Landbouw (Belgium). Finally, we wish to thank V. Asfahl for the excellent manuscript preparation.

List of symbols

c	concentration (kg/m^3)
g	acceleration of gravity (m^2/s)
k	reciprocal of Kalman-filter time constant (s^{-1})
k_D	default value for k (s^{-1})
L	Monin–Obukhov length (m)
N_z	vertical computational cell number
N_F	total number of cells in computational domain
N_p	number of particles
P	pressure (N/m^2)
Pe	grid Peclet number
Q	source strength in eqn. 12 (kg/m^2)
Ri	gradient Richardson number
R_G	element of normally distributed random number sequence
R_U	element of uniformly distributed random number sequence
S_o	initial source size (m)
S	source term ($kg/m^3\,s$) in eqn. (6)
Sc_t	turbulent Schmidt number (–)
T	temperature (K)
t	time (s)
u,v,w	velocity components along coordinate direction (m/s)

u_*	friction velocity (m/s)
dw_t	increment defined by eqn. (10) ($s^{-1/2}$)
x,y,z	coordinates in mean wind, lateral, and vertical directions, respectively
$\bar{z}$	mean particle height (m)
z_0	roughness length (m)
ρ	density (kg/m^3)
$\bar{\eta}$	diffusivity (m^2/s)
σ	standard deviation of particle fluctuations (m)
τ	time constant (s)

Subscripts

a	"artificial" quantity as a consequence of the numerical scheme (in contrast to its physical counterpart)
F	filtered values
g	contaminant gas
l	lowest value
i or x,y,z	coordinate direction
max	maximum
m	coefficients of turbulent momentum transfer
M	values of turbulent mass transfer coefficients
o	unfiltered value
p	particle
r	randomized
s	source
T	thermal coefficients of turbulent transfer

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