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# A Concept for Treating Dense-Gas Dispersion Under Realistic Conditions of Terrain and Variable Winds

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## ABSTRACT

A method is presented for including dense-gas effects in an existing advection-diffusion (particle-in-cell) type model capable of dispersion simulations over terrain and with time-varying synoptic winds. The physical processes associated with dense-gas dispersion affect both the windfield and the turbulent diffusivity. We propose to include these effects by perturbing the ambient windfield and diffusivity within the local region of the dense-gas cloud. The perturbed local windfield will be calculated by using a vertical or layer averaging approach and will be nested between the windfield and dispersion calculations. The ambient diffusivity will be replaced by an adapted form of a dense-gas, $K$-theory diffusivity that has the property that it approaches the ambient diffusivity level as the cloud density approaches the ambient value.

For numerical models, the low-lying nature of dense-gas clouds often presents a problem with resolution in the vertical direction. This is largely overcome in the proposed approach by: 1) the use of vertical averaging and assumed vertical cloud profiles to calculate the dense-gas perturbations on the flow field and diffusivity, and 2) the use of the particle-in-cell technique with a Monte Carlo (stochostic) displacement equation that does not rely on the concentration gradient to calculate the trajectories of the concentration marker particles.

These dense-gas dispersion modifications attempt to preserve the main features of the advection-diffusion, particle-in-cell model and, thereby, minimize the impact on the existing code. All of the changes can be implemented by either modifying an existing subroutine or adding a new one.

## INTRODUCTION

The manufacture, transportation, and use of hazardous chemicals is increasing world-wide, and with this increase also come an increase in the frequency of serious chemical accidents. In the industrialized countries, over 200 chemical accidents, causing significant damage to human health, environment, or property, occur each year. In the U.S. alone, the Environmental Protection Agency (EPA) has recorded at least 6928 accidents with acutely toxic chemicals in the past five years. These accidents killed 135 and injured nearly 1500 people. In addition, increasing population and, particularly, population expansion around existing chemical facilities, raises the potential for a severe accident. These conditions emphasize the need for realistic simulations of toxic and dense-gas releases for both emergency response and planning purposes.

A popular approach to simulating the atmospheric dispersion of a trace release under realistic conditions of terrain and variable winds is to use an advection-diffusion type model. For example, the LLNL Atmospheric Release Advisory Capability (ARAC)[1,2] emergency response system uses a two-model system called MATHEW-ADPIC[3,4] that is based on the advection-diffusion approach. MATHEW generates three-dimensional, mass-consistent windfields over terrain using a limited number of wind observations. These windfields are input to ADPIC, a particle-in-cell advection-diffusion model, which simulates the dispersion of a trace release by calculating the trajectories of "marker particles." While this system of models has been validated against numerous field tests of trace gas releases, it, and all other advection-diffusion type models, does not include the necessary physics for the simulation of the atmospheric dispersion of denser-than-air releases.

Over the past decade, there has been extensive study of the atmospheric dispersion of dense-gas releases including both field-scale dispersion experiments and the development of computational models. However, none of the models appear to be directly applicable to an operational emergency response situation requiring dispersion simulations over terrain and with variable winds. Most of the models (SLAB, HEGADAS, DEGADIS, etc.)[5-7] are intended to be used to simulate dense-gas dispersion over flat terrain with constant winds. Several three-dimensional (FEM3, MARIAH, HEAVYGAS)[5-7] and two-dimensional (Lee and Meroney[8]) conservation equation models have been developed that treat variable terrain, but assume a constant synoptic wind speed and direction. Furthermore, and perhaps more importantly for operational uses, these codes require a knowledgeable user, large amounts of computer time, and often large computers. Thus, the need exists to incorporate the phenomena of dense-gas dispersion into models capable of dispersion simulations under realistic conditions.

In this paper, we describe a method for including dense-gas effects in the MATHEW-ADPIC model. This model is typical of advection- diffusion type models that are capable of simulations over terrain and with time-varying synoptic winds. The physical processes associated with dense-gas dispersion affect both the windfield and the turbulent diffusivity. We propose to include these effects by perturbing the ambient windfield and diffusivity within the local region of the dense-gas cloud. The perturbed local windfield will be calculated by using a vertical or layer averaging approach and will be nested between the windfield (MATHEW) and dispersion (ADPIC) calculations. In addition, the ambient diffusivity will be replaced by an adapted form of a dense-gas, $K$-theory diffusivity which has the property that it approaches the ambient diffusivity level as the cloud density approaches the ambient value.

## ADVECTION - DIFFUSION MODEL

The two-model system MATHEW-ADPIC consists of the MATHEW[3] model, which generates three-dimensional, mass-consistent windfields over terrain surfaces by interpolation of wind observations, and the ADPIC[4] particle-in-cell, advection and diffusion model that calculates the time-dependent spatial evolution of the emission over the domain of interest. The particle-in-cell numerical integration technique represents the emission concentration by Lagrangian-marker particles inside a fixed Eulerian grid[9-11]. The marker particle trajectories are calculated from a displacement equation derived from the advection-diffusion equation. Consequently, the distribution of marker particles in time and space represents, in a statistical sense, the concentration distribution of the released emission.

ADPIC solves the advection-diffusion equation in the flux conservative form (pseudo-velocity technique) for a given nondivergent advection field. The pseudo velocity method is obtained from a transformation of the advection-diffusion equation

$$\frac{\partial \chi}{\partial t} + \bar{U}_a \cdot \nabla \chi = \nabla \cdot (K \nabla \chi) , \tag{1}$$

where $\chi$ is concentration, $\bar{U}_a$ is the nondivergent ($\nabla \cdot \bar{U}_a = 0$) advection velocity field, and $K$ is the diffusion coefficient. By making the assumption of incompressibility ($\nabla \cdot \bar{U}_a = 0$), the $\bar{U}_a \cdot \nabla \chi$ term can be replaced by $\nabla \cdot (\chi \bar{U}_a)$ and Equation (1) can be rewritten in the flux conservative (pseudo-velocity) form

$$\frac{\partial \chi}{\partial t} + \nabla \cdot \left[ \chi \left( \bar{U}_a - \frac{K}{\chi} \nabla \chi \right) \right] = \frac{\partial \chi}{\partial t} + \nabla \cdot (\chi \bar{U}_p) = 0 , \tag{2}$$

where $\bar{U}_p = \bar{U}_a + \bar{U}_d$ is the pseudo-transport velocity and $\bar{U}_d = -(K/\chi)\nabla \chi$ is the diffusivity velocity.

The advection field $\bar{U}_a$ is supplied by the MATHEW code. MATHEW produces a three-dimensional, mass-consistent windfield from a spatially sparse windfield data set that has been interpolated and extrapolated onto an Eulerian grid. The interpolated-extrapolated windfield is then adjusted in a weighted least-squares sense [12-14] to satisfy the continuity equation ($\nabla \cdot \bar{U}_a = 0$) within the specified volume.

The grid mesh used by the model is an Eulerian grid consisting of three-dimensional rectangular cells. The concentration is defined at the cell centers and the velocities are defined at the cell corners. The locations of the marker particles, which represent the dispersing cloud, are defined by their individual coordinates within the fixed grid.

Solution of the advection-diffusion equation to obtain the evaluation of the dispersing cloud concentration is performed by a numerical integration in time involving three steps. First, the concentration $\chi(t)$ at the cell centers is used to calculate the diffusivity velocities $\bar{U}_d$, which are then added to the advection velocity $\bar{U}_a$ to yield the pseudo-velocity $\bar{U}_p$ at each cell corner. Second, each marker particle is transported for one time step $\Delta t$ with a velocity $\bar{U}_p$, which is calculated from the pseudo-velocities $\bar{U}_p$ at the cell corners by a linear interpolation. The new particle coordinate $\bar{R}(t + \Delta t)$ is obtained from the displacement equation

$$\bar{R}(t + \Delta t) = \bar{R}(t) + \bar{U}_p \cdot \Delta t . \tag{3}$$

In the third step, the new concentration distribution $\chi(t + \Delta t)$ is calculated from the new particle positions. This three-step procedure is continually repeated throughout the simulation.

## DENSE-GAS DISPERSION EFFECTS

The dispersion of a dense-gas in the atmosphere involves physical processes not encountered in trace gas dispersion. In a trace gas release, the quantity of material released to the atmosphere is too small to have any significant effect upon the atmospheric flow into which it is mixing. Consequently, trace gas dispersion is controlled solely by the advective and diffusive properties of the ambient atmosphere. On the other hand, a dense-gas release behaves more like an independent, continuous cloud whose physical properties (density, temperature, turbulence level) are significantly different than those of the ambient atmosphere. More importantly, the dispersion of a dense-gas cloud is controlled by these in-cloud conditions rather than the ambient conditions.

Four major effects are observed in the dispersion of dense-gas clouds released at ground level that are not observed in dispersion of trace emissions. The first is a reduction of turbulent mixing of the vapor cloud with the ambient atmosphere due to stable stratification of the dense layer. The second is the generation of gravity-spreading and self-induced vortices due to density gradients in the horizontal direction. These two effects (reduced cloud-air mixing and gravity-spreading) result in a lower and significantly wider cloud than is observed when a trace or neutral density gas is released. The third, like the second, is also a gravity flow effect that occurs in sloped terrain. Dense-gas clouds tend to follow the downhill slope independent of the wind direction and can become "trapped" in valleys or low spots. In addition to these effects, dense-gas clouds initially travel downwind at a slower rate than the ambient wind speed due to the lack of mixing between the dense-gas cloud and the ambient atmosphere.

All of these effects are most pronounced when the ambient wind speed is low and the atmospheric stability conditions are stable. As the cloud mixes with the surrounding ambient atmosphere, the cloud becomes more dilute, the in-cloud properties approach ambient levels, and the above mentioned effects begin to play a less significant role. Eventually, after a considerable amount of dilution, the orginally dense-gas cloud begins to disperse like a trace gas cloud where dispersion is primarily controlled by the ambient wind speed and atmospheric stability.

## DENSE-GAS MODIFICATIONS

Our main interest in modifying the MATHEW-ADPIC model is to be able to calulate the dispersion of a denser-than-air release over ranges in time and space where the effects of terrain and changes in the ambient windfield are important. (When our concern is limited to the source region where variations in terrain and the windfield can usually be neglected, it will be more expedient to use codes that neglect these effects.) From a practical point-of-view, we would like to preserve the main features of the MATHEW-ADPIC models as much as possible while including the major physical processes associated with dense-gas behavior. These processes are (1) gravity flows that cause slumping and horizontal spreading of the dense-gas cloud as well as flows that tend to follow the downward slope of terrain, (2) flow field modification that allows the ambient air to flow over or around the dense-gas cloud in the initial stages before the cloud mixes with the surrounding air, and (3) suppression of turbulence and mixing of the cloud with the surrounding air due to the stable density stratification of the denser-than-air cloud.

With these goals in mind, we have employed several assumptions that have guided our approach to incorporating dense-gas dispersion effects into the MATHEW-ADPIC advection-diffusion model. They are:

1. The dense-gas effect upon the flow field can be treated as a perturbation of the ambient windfield where the flow field within the dense-gas cloud is modified due to gravity flow and the flow field outside the cloud remains essentially unchanged from the ambient.
2. The gravity flow field within the cloud is in a quasi-steady state so that the gravity flow velocity can be obtained from a balance between the gravitation force terms and the dissapative terms due to air entrainment into the cloud and ground friction. Similarly, the turbulent diffusivity can be expressed in terms of the local equilibrium properties (such as density, friction velocity, cloud height, etc.).
3. The dense-gas cloud can be treated as a relatively thin layer whose behavior can be described in terms of its layer- (vertically-) averaged properties and the thickness (cloud height) of the layer.
4. Mixing of the cloud with the surrounding air is an adiabatic process so that the cloud density and temperature can be expressed in terms of the cloud concentration. (In the future, we plan to allow for non-adiabatic processes such as ground heating.)

In terms of the MATHEW-ADPIC advection-diffusion model, inclusion of dense-gas dispersion effects requires modification of the ambient windfield $\bar{U}_a$ and the ambient vertical diffusivity $K_z$. The dense-gas perturbation of the local windfield is to be calculated using a two-dimensional extension of the one-dimensional SLAB[15] model approach. The SLAB concept is based on the assumption that the dense-gas cloud is relatively thin in comparison to its horizontal dimensions. Consequently, cloud behavior is assumed to be described by the layer- (height-) averaged cloud properties and the thickness (cloud height) of the layer. Thus, all of the cloud properties (concentration, density, velocity, etc.) are expressed as vertically averaged quantities such as

$$\rho(x,y) = \frac{1}{h} \cdot \int_o^h dz \cdot \rho(x,y,z) \ , \tag{4a}$$

where $\rho$ is density and $h = h(x,y)$ is the cloud height. (In a particle-in-cell code, cloud height is defined in terms of an average of the individual marker particle heights in each grid cell.) To achieve a three-dimensional description of the dense-gas cloud, vertical profiles are assumed for the cloud properties. Using the above example,

$$\rho(x,y,z) = \rho(x,y) \cdot f(z) \ , \tag{4b}$$

where $f(z)$ is a convenient function of height such as a Gaussian or exponential function. In the full SLAB model, the complete set of conservation equations are solved in this vertically averaged form; here, we will be concerned with only the three components of the flow field (velocity).

Treating gravity flow as a perturbation to the ambient windfield and recognizing that the initial cloud velocity is either zero (evaporating pool or instantaneous release) or some non-zero value $\bar{U}_s$ (horizontal jet release) that is generally different than the ambient value, the horizontal components of the local windfield $\bar{U}$ within the cloud can be expressed as

$$\bar{U} = \bar{U}_a + \bar{U}_d + \bar{U}_g \tag{5}$$

where $\bar{U}_a$ = ambient windfield (MATHEW)
$\bar{U}_d = m \cdot (\bar{U}_s - \bar{U}_a)$ = displacement flow field
$\bar{U}_g$ = gravity flow field
$m$ = mass fraction

The horizontal velocities $\bar{U}$, $\bar{U}_a$, $\bar{U}_d$, $\bar{U}_g$ and the mass fraction $m$ are all vertically averaged quantities [see Eq. (4a)]. The perturbations to the ambient flow $\bar{U}_d$ and $\bar{U}_g$ are assumed to have a vertical dependence $g(z)$ [see Eq. (4b)] where $g(z)$ is selected to qualitatively represent the actual vertical profile. The displacement flow field tends to force the ambient streamlines over the dense-gas cloud during the initial dispersion period when $m \approx 1$ and becomes neglibible as air is entrained into the cloud and the mass concentration approaches zero.

The horizontal components of the gravity flow field are obtained by equating the gravitational force terms (using the hydrostatic approximation) to the dissipative terms due to air entrainment and ground friction, yielding

$$\begin{aligned} \rho\omega_e U_g &= -\frac{d}{dx}\left[0.5g(\rho-\rho_a)h^2\right] - g(\rho-\rho_a)h\frac{dH}{dx} - \rho u_f U_g \\ \rho\omega_e V_g &= -\frac{d}{dy}\left[0.5g(\rho-\rho_a)h^2\right] - g(\rho-\rho_a)h\frac{dH}{dy} - \rho u_f V_g \end{aligned} \tag{6}$$

where $\omega_e$ = entrainment rate
$g$ = acceleration of gravity
$h$ = cloud height above terrain
$H$ = terrain height
$u_f$ = friction velocity coefficient

Again, $U_g$, $V_g$, and $\rho$ are vertically-averaged. The entrainment rate $\omega_e$ is the rate at which air mixes into the dense-gas cloud from above and is taken to be proportional to the vertical diffusivity $K_z(h)$ divided by the cloud height $h$.

The vertical components of the displacement and gravity flow field are obtained from the non-divergence condition for the flow field ($\nabla \cdot \bar{U} = 0$) applied in MATHEW. Thus,

$$\omega_i = -\left(\frac{\partial U_i}{\partial x} + \frac{\partial V_i}{\partial y}\right) \cdot \int_o^z dz\ g(z) \tag{7}$$

where sub "$i$" corresponds to either the displacement field or the gravity flow field, and $U_i$, $V_i$ are the horizontal components of these two flow fields, respectively. By choosing $g(z)$ judiciously, both $g(z)$ and the integral of $g(z)$ can be analytical functions.

To complete the dense-gas modifications, the ambient vertical diffusivity is replaced with a dense-gas vertical diffusivity used in the FEM3[16] three-dimensional, conservation equation model for dense-gas dispersion. The new diffusivity within the surface layer is

$$K_z = \frac{k \cdot u_* \cdot z}{\Phi} \tag{8}$$

where $\Phi = 1 + 5 \cdot z/L$
$L^{-1} = L_a^{-1} + 2 \cdot g \cdot k^2 \cdot z \cdot (\rho - \rho_a)/(\rho \cdot h \cdot u_*^2)$
$k$ = Von Karman's constant
$u_*$ = friction velocity,

and is such that the diffusivity approaches the ambient value as the cloud density approaches the ambient level.

While the above equations completely describe the dense-gas modifications, a practical difficulty in implementing them still remains. The displacement equation, Equation (3), used in the particle-in-cell ADPIC code to track particle trajectories uses the diffusivity velocity $\bar{U}_d$ which requires the calculation of the concentration gradients [see Equation (2)]. This is a particular problem for simulating dense-gas dispersion since the low lying nature of dense-gas clouds will at times preclude (from a practical standpoint) the accurate determination of the vertical concentration gradient. To overcome this difficulty, we will use the following Monte Carlo (statistical) form of the displacement equation adapted from Boughton, et al.[17]

$$\begin{aligned} X(t+\Delta t) &= X(t) + U\cdot\Delta t + R_x(\Delta t) \\ Y(t+\Delta t) &= Y(t) + V\cdot\Delta t + R_y(\Delta t) \\ Z(t+\Delta t) &= Z(t) + W\cdot\Delta t + \nu_o\cdot\Delta t + R_z(\Delta t) \end{aligned} \tag{9a}$$

where $U, V,$ and $W$ are the three components of the local velocity and $R_x, R_y,$ and $R_z$ are three independent Gaussian random variables with the mean and mean square properties

$$\begin{aligned} < R_x >= 0, \quad < R_x^2 > &= 2\cdot K_x\cdot\Delta t \\ < R_y >= 0, \quad < R_y^2 > &= 2\cdot K_y\cdot\Delta t \\ < R_z >= 0, \quad < R_z^2 > &= 2\cdot K_o\cdot\Delta t + \nu_o^2\cdot\Delta t^2, \quad \text{where} \\ K_o &= K_z(Z_o),\ Z_o = Z(t), \\ \nu_o &= \frac{\partial K_z(Z_o)}{\partial Z}, \text{and} \\ < > &= \text{average value.} \end{aligned} \tag{9b}$$

In the new displacement equations, the diffusivity velocity term has been replaced with a Gaussian random term. Furthermore, in the vertical direction, the diffusivity has been assumed to depend on height and we have retained all terms up to the second order in the time step $\Delta t$. This Monte Carlo approach overcomes the cloud resolution difficulties since it does not require the concentration gradient to be determined. In addition, not calculating the concentration gradient also reduces the computing time for each cycle.

## CONCLUSION

Numerical integration of the dense-gas modified MATHEW-ADPIC advection-diffusion model follows essentially the same three-step process as before.

1. The first step begins with all the vertically-averaged cloud properties defined on a two-dimensional grid. These properties are then used to calculate the local perturbations to the ambient windfield $\bar{U}_a$, namely the displacement flow field $\bar{U}_d$ and the gravity flow field $\bar{U}_g$. As before, the concentration, density, temperature, etc., are defined at the cell centers and the velocities are defined at the cell corners.
2. In the second step, each marker particle is transported according to the Monte Carlo displacement equation, Equation (9).
3. And finally, the new vertically-averaged cloud properties (concentration, density, temperatue, etc.) are calculated from the new marker particle coordinates. In addition, the three-dimensional concentration distribution can also be calculated from the new particle coordinates. While this latter result is usually the result of main interest to the code user, it is not necessary for calculating the transport of the marker particles. Consequently, calculation of the three-dimensional concentration distribution does not have to be done during each time step and can be limited to those times when this result is requested.

The final step in implementing these dense-gas modifications to MATHEW-ADPIC is model evaluation. In addition to comparisons with experimental gravity flow dispersion experiments such as wind tunnel and field tests, it is essential to evaluate the numerical accuracy with which the code integrates the transport equations and, therefore, simulates the various models for the flow field and diffusivity. This will be done by simulating problems with a realistic height dependent windfield and diffusivity, and for which there is either a known analytic or numerical solution.

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