8.6 **ADAPTATION OF THE QUIC-PLUME MODEL FOR HEAVY GAS DISPERSION AROUND BUILDINGS**

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1. Introduction

There is a growing concern about the threat of a malicious release of harmful substances to the air in order to cause harm to the population. In order to help decision-makers assess the consequences of such an attack, accurate predictions of the transport and dispersion of airborne contaminants in cities are needed. The complex flows produced by buildings pose difficult challenges to dispersion modelers. Among features of concern are channeling of plumes down street channels, circular transport within street canyon vortices, upwind transport, intermittent transport from street level to roof level within spiral vortices that develop on the downwind side of tall buildings, and the retention of toxic materials trapped between buildings.

A number of groups have developed computational fluid dynamics models that have been applied to neighborhood-scale problems and have explicitly resolved hundreds of buildings in their simulations. However, CFD models are computationally intensive and for some applications turn-around time is of the essence. For example, planning and assessment studies in which hundreds of cases must be analyzed or emergency response scenarios in which plume transport must be computed quickly. For many applications, where quick turn-around is needed (e.g., emergency response) or where many simulations must be run (e.g., vulnerability assessments), a fast response modeling system is required. Fast running models are not only needed for emergency response and post-event applications, but for scenarios in which many cases must be run or immediate feedback is needed.

We have developed the QUIC (Quick Urban & Industrial Complex) dispersion modeling system to fill that need. It can relatively quickly compute the dispersion of airborne contaminants released near buildings. It is comprised of QUIC-URB, a model that computes a 3D mass consistent wind field for flows around buildings (Pardyjak and Brown, 2001), QUIC-PLUME, a model that describes dispersion near buildings (Williams et al., 2003), and a graphical user interface QUIC-GUI (Boswell et al., 2004). The QUIC dispersion code is currently being used for building-scale to neighborhood-scale transport and diffusion

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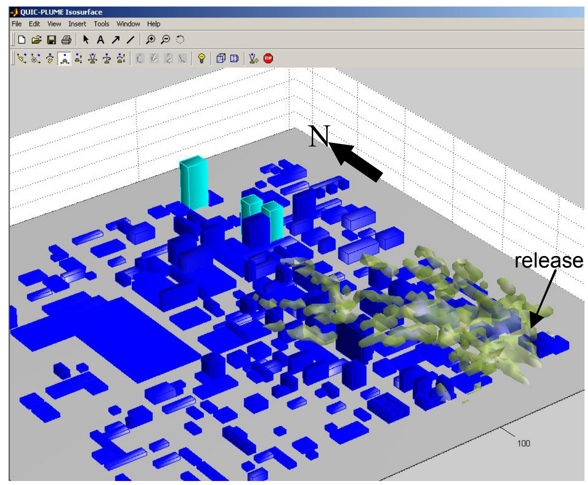


Figure 1. A QUIC simulation of plume dispersal in Salt Lake City under the influence of southeast winds. Shown are the estimated contaminant isopleths for a release near street level.

problems with domains on the order of several kilometers. Figure 1 illustrates the modeled dispersion for a release in downtown Salt Lake City.

The QUIC-PLUME dispersion model uses an enhanced random-walk methodology that is designed to describe transport in a complex environment with buildings. It also includes a non-local mixing formulation that better describes the turbulent mixing that occurs in building wakes or cavities.

We have tested the model against wind-tunnel measurements of a release near the back wall of a high-rise building. The measurements show that the material drifts towards the back wall before it spreads in the down axis direction. Despite the severe nature of this test the model performed well with the vast bulk of the simulations lying within a factor of two of the measurements along the back wall and in a plane extending along the axis of the building in the downwind direction. We have described the model and its performance (Williams et al, 2004) elsewhere. However, the model in its earlier formulation was not designed to treat the dispersion of dense gases.

This paper describes the modifications of QUIC-PLUME random-walk dispersion model formulation for treatment of heavy gas dispersion and shows comparisons of model-computed concentrations with measurements from a continuous release and an instantaneous release in open terrain. It also shows comparisons between measurements and simulations for a dense gas in a wind tunnel experiment in which there were obstacles in the flow.

2. Background

Several fast-response dispersion models of varying levels of fidelity have been developed to explicitly account for the effects of buildings. Several are intended for use around a single building so are not directly applicable to neighborhood-scale dispersion problems. Recently, several codes have been developed to treat these scales. The Urban Dispersion Model is a Gaussian puff model that utilizes simple algorithms for puff-building interaction (Hall et al., 2000). Although the model does not produce wind fields around buildings, it accounts for mixing in the lee of the building and some channeling effects. Comparisons to concentration measurements from the URBAN 2000 tracer experiment performed in Salt Lake City showed reasonable agreement for many cases if local winds near the source are appropriately accounted for. A potential flow model called MIDAS-AT has been advertised for dispersion applications in urban areas (http://www.plg-ec.com/), however, we have not been able to obtain reports or open-literature publications. In principle, a potential flow model can produce velocity fields around groups of buildings, but with the restriction that the flow must be irrotational. It appears that the dispersion model is of a random-walk type.

Röckle (1990) developed a diagnostic mass consistent wind model for computing the 3D flow field around isolated buildings and groups of buildings. The model utilizes empirical algorithms for determining initial wind fields in the cavity, wake, and upstream recirculation zones for single buildings, but it also includes algorithms for velocity fields in between buildings. A mass consistent wind field is then produced similar to the approach used in traditional diagnostic wind modeling, except that special treatment of boundary conditions is needed at building walls. The computed wind field is not restricted to being irrotational as in potential flow models. Several different approaches have been used to compute the dispersion of airborne contaminants, including Eulerian finite difference methods and random-walk models (Kaplan and Dinar, 1996). Whatever solution method is used for obtaining the concentration fields, the approach for obtaining turbulence variables is of special importance given that the diagnostic wind model approach only provides mean wind fields.

The Röckle-style model has been evaluated for a handful of cases. For a street intersection defined by four adjacent courtyards, Röckle et al. (1998) showed reasonable agreement between model-computed wind fields and wind-tunnel measurements for various inflow wind angles. Kaplan and Dinar (1996) qualitatively compared the model solutions to CFD model results for flow around two and three buildings and to wind-tunnel measurements of concentration on street canyon walls. Using a wind-tunnel study of an industrial complex, Röckle (1990) found that the model-computed wind directions and wind speed agreed fairly well at several points within the complex for various inflow wind directions.

Surprisingly, the urban diagnostic wind model approach has not been extensively tested for the single building case. We have found one example, in which Gross et al. (1994) compared turbulent intensity predictions with a few measurements made downwind of a cube. To help resolve this deficiency, Pardyjak and Brown (2002) compared model-computed wind fields to centerline velocities measured in the USEPA meteorological wind tunnel (Snyder and Lawson, 1994) for rectilinear buildings of varying width, height, and downwind length with a prevailing wind normal to the building face. Bagal et al. (2003) evaluated the upstream rotor for a single building for several different aspect ratios. In this paper, we will evaluate the concentration fields produced by the QUIC model for a point-source release in uniform and shear flow, and for the case of a release in the lee of tall building.

Several models have been designed to deal with the complexities of dense gas dispersion (Hanna,?). Dense gas dispersion poses a challenge because the transport is determined by a combination of ambient winds and self-induced winds. A heavy gas release under light wind conditions will produce a radial outflow as density gradients accelerate the material away from the center of the release. In addition, the density gradients produce sharply reduced turbulence within the transported material because the pronounced density gradients suppress vertical transport. Consequently, the flow is determined by a balance between the ambient conditions and the self-induced behavior.

There are other complexities associated with dense gas flows associated with the nature of the sources and, frequently, the phase changes that occur in the flow. At present the model is being adapted to treat the dispersion and transport of dense gases for which there are no phase changes or temperature changes.

Dense gas dispersion poses a particularly difficult problem for a random-particle transport code. Specifically, random-particle transport is normally treated with the assumption that the transport of one pollutant parcel is unaffected by the transport of any other pollutant parcel. However, for dense gas transport, the presence of other parcels produces the self-generated flows that influence the behavior of parcels in the vicinity.There are basically two approaches to deal with this problem: (1) the density driven flows can be estimated by some kind of bulk-flow model and those motions can be added the ambient motions for the transport, or (2) the local densities can be estimated based on the particle densities and local accelerations associated with density differences can be added to the particle transport. The latter approach has the advantage that it can treat the more complex situations that arise when buildings alter the flow. However, the local density approach has had little testing.

In one approach (Gaffen et al, 1987) had excellent success in simulating dense gas dispersion with a random-particle transport model. However, they simulated the elevated release of a dense gas in a wind tunnel. They were able to achieve good results by adding a vertical acceleration associated with a buoyancy force and using modified eddy-viscosities. They did not address the flows associated with horizontal density gradients that play an important role for surface releases of dense gases.

3. Model Description

We will only briefly describe the QUIC-URB wind model in this paper. The underlying code is based on the work of Röckle (1990). It uses empirical algorithms and mass conservation to quickly compute the mean 3D flow field around building complexes. The size, shape, and velocity field for the upstream rotor, cavity, wake, and street canyon vortex are specified, and then a mass consistent wind field is produced similar to the approach used in traditional diagnostic wind modeling (e.g., Sherman, 1978), except that special treatment of boundary conditions is needed at building walls. Improvements to the original Röckle model are described in Bagal et al. (2003), Gowardhan (2003) and Pardyjak et al. (2003). Further details can be found in Pardyjak et al. (2004)

QUIC-PLUME uses a stochastic Lagrangian random-walk approach to estimate concentrations in a 3D gridded domain. The model is designed to use mean wind fields produced by the QUIC-URB model. Parcels, representing aerosols or gases, are transported with a vector sum of mean winds from QUIC-URB plus turbulent fluctuating winds computed using the random-walk equations. Turbulence parameters needed in the random-walk equations are estimated from vertical and horizontal gradients in the mean wind. A detailed description of the theory is described in a companion document (Williams and Brown, 2004).

3.1 Random-walk equations.

Lagrangian random-walk models describe dispersion by simulating the releases of air parcels and moving them with an instantaneous wind composed of a mean wind plus a turbulent wind. The equations that describe the parcel positions are:

$$x(t+\Delta t) = x(t) + \overline{U}\Delta t + \frac{u'(t+\Delta t) + u'(t)}{2}\Delta t \ , \qquad (1)$$

$$y(t+\Delta t) = y(t) + \overline{V}\Delta t + \frac{v'(t+\Delta t) + v'(t)}{2}\Delta t \ , \qquad (2)$$

and

$$z(t+\Delta t) = z(t) + \overline{W}\Delta t + \frac{w'(t+\Delta t) + w'(t)}{2}\Delta t \ , \qquad (3)$$

where *x, y,* and *z* are the longitudinal, lateral, and vertical position coordinates of the particle, $\overline{U}$, $\overline{V}$, and $\overline{W}$ are the x, y, and z components of the mean wind, u' , v' , and w' are the turbulent components of the instantaneous wind, and Δt is the time step.

The temporal evolution of the fluctuating components of the wind are calculated from:

$$u'(t+\Delta t) = u'(t) + du \ , \qquad (4)$$

$$v'(t+\Delta t) = v'(t) + dv \ , \qquad (5)$$

and,

$$w'(t+\Delta t) = w'(t) + dw \ . \qquad (6)$$

Traditionally, a three term random-walk equation for the vertical velocity has been used in the air quality community for describing vertical dispersion (e.g., references):

$$dw = -\frac{C_o\varepsilon}{2}\lambda_{33}w'dt + \frac{1}{2}\left(1+\lambda_{33}w'^2\right)\frac{\partial\tau_{33}}{\partial z}dt + \left(C_o\varepsilon dt\right)^{1/2} dW_3(t), \qquad (7)$$

where the constant C_o is the universal constant for the Lagrangian structure function, ε is the mean rate of turbulence kinetic energy dissipation, and $dW_3(t)$ is a random number generator with uncorrelated, normally distributed variables with mean of zero and standard deviation of one. The first term on the right is called the memory term, the second term is the drift term and the third term is the random acceleration term. Comparisons to plume dispersion experiments over flat surfaces have shown reasonable agreement. As we will show later, we have found poor agreement with the traditional random-walk equation for a release near the backside of a tall building. This is in part due to the assumptions that go into the derivation of equation (7) which do not hold for flows around buildings, namely the mean lateral and vertical winds $\overline{V}$ and $\overline{W}$ are zero and the mean horizontal winds are uniform (i.e., contain no gradients).

As reviewed by Rodean (1996), the general set of equations for du, dv, and dw can be derived from the Folker-Planck equations and the well-mixed condition and result in equations with a large number of terms. For the QUIC-PLUME model, we have taken a simplified form of the full set of equations and applied a local coordinate rotation in order to remove some of the approximations inherent in equation (7).

$$du = \left\{ \frac{-C_o \varepsilon}{2} \left[\lambda_{11} u' + \lambda_{13} w' \right] + \frac{\partial \overline{U}}{\partial z} w' + \frac{1}{2} \frac{\partial \tau_{13}}{\partial z} \right\} dt + \left\{ \frac{\partial \tau_{11}}{\partial z} \left[\lambda_{11} u' + \lambda_{13} w' \right] + \frac{\partial \tau_{13}}{\partial z} \left[\lambda_{13} u' + \lambda_{33} w' \right] \right\} \frac{w'}{2} dt + \left(C_o \varepsilon dt \right)^{1/2} dW_1(t), \quad (8)$$

$$dv = \left[-\frac{C_o \varepsilon}{2} \left(\lambda_{22} v' \right) + \frac{\partial \tau_{22}}{\partial z} \left(\lambda_{22} v' \right) \frac{w'}{2} \right] dt + \left(C_o \varepsilon dt \right)^{1/2} dW_2(t), \quad (9)$$

and

$$dw = \left\{ -\frac{C_o \varepsilon}{2} \left[\lambda_{13} u' + \lambda_{33} w' \right] + \frac{1}{2} \frac{\partial \tau_{33}}{\partial z} \right\} dt + \left\{ \frac{\partial \tau_{13}}{\partial z} \left[\lambda_{11} u' + \lambda_{13} w' \right] + \frac{\partial \tau_{33}}{\partial z} \left[\lambda_{13} u' + \lambda_{33} w' \right] \right\} \frac{w'}{2} dt + \left(C_o \varepsilon dt \right)^{1/2} dW_3(t), \quad (10)$$

where

$$\lambda_{11} = \left(\tau_{11} - \tau_{13}^2 / \tau_{33} \right)^{-1}, \quad \lambda_{22} = \tau_{22}^{-1},$$

$$\lambda_{13} = \left(\tau_{13} - \tau_{11} \tau_{33} / \tau_{13} \right)^{-1}, \quad \lambda_{33} = \left(\tau_{33} - \tau_{13}^2 / \tau_{11} \right)^{-1},$$

$$\tau_{11} = \sigma_u^2, \quad \tau_{22} = \sigma_v^2, \quad \text{and} \quad \tau_{33} = \sigma_w^2.$$

Note that the τ's refer to kinematic stresses, i.e., shear or normal stress divided by density.

The details of the local coordinate system, the treatment of non-local mixing, and reflection are described elsewhere (Williams and Brown, 2004).

3.6 Adaptation for dense-gas dispersion

Average concentrations, normalized to unit release, are estimated by summing over all particles that are found within the sampling box *i,j,k* during the concentration averaging time t_{ave}:

$$\chi_{i,j,k} = \sum \frac{Q \Delta t_c}{n_{tot} dx_b dy_b dz_b t_{ave}},$$

where n_{tot} is the total number of particles released during the computations, dx_b, dy_b, and dz_b are the x, y, and z dimensions of the sampling box, respectively, and Δt_c is the particle time step. For dense gas dispersion we use a similar expression to calculate the gas density at each time step:

$$\rho = \rho_{dg} \frac{d}{d_{\max}} + \rho_{air} \left(1 - \frac{d}{d_{\max}} \right),$$

Where d is the local particle density:

$$d = \frac{n}{dx * dy * dz_{rho}}.$$

We use the horizontal resolution of the QUIC-URB model in the definition of the particle density, but we use a finer resolution in the vertical characterized by dz_{rho} in the vertical to better resolve density differences that are important in the self-induced flows. The initial particle density in the source region is $d_{\max}$ while the initial mass density of the heavy gas is ρ_{dg}. We calculate the cell specific densities in the domain where $z < z_\rho$, for heights above z_ρ we calculate the minimum density associated with a single particle in a QUIC-URB unit volume as:

$$\rho_{\min} = \rho_{dg} \frac{1}{d_{\max}} + \rho_{air} \left(1 - \frac{1}{d_{\max}} \right).$$

For particles above z_ρ, we treat them as isolated and undergoing a downward acceleration of:

$$g \left(\frac{\rho_{\min} - \rho_{air}}{\rho_{\min}} \right),$$

So that the particle is displaced by the amount:

$$-g \left(\frac{\rho_{\min} - \rho_{air}}{\rho_{\min}} \right) \frac{\Delta t^2}{2}.$$

This follows the approach of Gaffen (Gaffen et al,1987).

Within the density-resolved region $z > z_{rho}$, we first calculate the column-integrated densities as:

$$d_{col} = \sum_{z_k}^{z_{rho}} \rho_k \Delta z_{z_{rho}},$$

The pressure gradient is calculated from the column-integrated densities as:

$$\frac{\partial P}{\partial y} = -g \frac{d_{coli,j+1} - d_{coli,j-1}}{2dy}.$$

We assume that local bulk velocities will be aligned with the local pressure gradient. We calculate a conversion factor between the local pressure gradient and the local bulk velocities, based on relationships that describe the out flowing winds from instantaneous releases:

$$\frac{dR}{dt} = \left[g \frac{\rho_{dg} - \rho_a}{\rho_a} V^{1/3} \right]^{1/2},$$

and the corresponding relationship for continuous releases of:

$$u_e \frac{dR}{dx} = \left[g \left(\frac{\rho_{dg} - \rho_a}{\rho_a} \right) h \right]^{1/2},$$

as described by Hanna and Drivas (Hanna and Drivas, 1987). These two relationships are essentially the same when we note that $V^{1/3}$ is h and,

$$u_e \frac{dR}{dX} = \frac{dR}{dt}.$$

We assume that the outflow velocity on the perimeter of the dense gas is in the direction of $-\nabla P$ on the perimeter. We then form two sums, One describes the outflow direction weighted perimeter length as:

$$L_{per} = \sum_i - \vec{f}_i \bullet \frac{\nabla P_i}{|\nabla P_i|},$$

where $\vec{f}_i$ represents the face of a boundary cell with a magnitude of the cell length and a direction normal to the cell boundary so that the right-hand boundary of a cell would have magnitude dy and direction in the plus x direction while the top boundary would have length dx and direction in the plus y direction. Points in walls or facing outward toward walls are excluded from the sum. The second sum describes the pressure gradient weighted by the perimeter cell lengths as:

$$DP_{per} = \sum_i - \vec{f}_i \bullet \nabla P_i.$$

The constant used to convert the local pressure gradient into the local wind is then:

$$P_{const,k} = \frac{dR}{dt} \bullet \frac{L_{per}}{DP_{per}},$$

The subscript k is used to indicate that this procedure is used for each height level in the density-resolved layer. In the calculation of the average outflow velocity only the heights in or above the k level are used. The bulk cell winds are then:

$$u_{bulk} = -P_{const,k} \bullet \frac{\partial P}{\partial x},$$

and,

$$v_{bulk} = -P_{const,k} \bullet \frac{\partial P}{\partial y}.$$

While for the vertical downward acceleration we use:

$$w_{acc} = g \left(\frac{\rho_k - \rho_{k-1}}{\rho_k} \right),$$

If the upper cell density ρ_k, is greater than the lower cell density ρ_{k-1}.

The resulting position changes are:

$$\Delta z = \Delta z - w_{acc} \frac{\Delta t^2}{2},$$

$$\Delta y = \Delta y + v_{bulk} \Delta t,$$

and

$$\Delta x = \Delta x + u_{biulk} \Delta t.$$

We also adjust the turbulence using an approach suggested by Gaffen et al (Gaffen, et al,1987). In their approach they modified the eddy viscosity, while we make a similar modification to the local friction velocity. First, we estimate u_{*p} in regions of dense gas as:

$$u_{*p} = 1.26 u_*^3 / \left(g \left(1 - \frac{\rho_{air}}{\rho_{dg}} \right) \right),$$

and then the new local

$$u_{*l} = C u_{*p} + (1 - C) u_*,$$

where C is fractional concentration of the heavy gas.

We have also modified the code to accept a new geometry for the source. There are two variations: (1) for a continuous release it is a cone with a volume equivalent to cylinder with a volume equal to a time steps flow of the material and with a specified radius, and (2) for an instantaneous release it is a cone with a volume equivalent to that of a cylinder of specified height and volume equal to the release. In the case of the instantaneous source the volume is approximately by a collection of uniform density cells. If there are buildings within the release area, cells will be chosen as close to the release point as possible without having to pass through a wall. For the continuous source there is no provision to wrap around buildings, but there is an additional imposed velocity normal to the cone surface of a magnitude such that one time steps flow will pass through it at each time step. The cones have the same height as the original cylinder, but the radius is expanded to achieve the same volume as the cylinder.

The height of the cone for a continuous release is equal to the velocity of the release multiplied by the time step. The imposed outflow velocity is maintained for the transit time of the wind at the first grid cell from across the specified radius. The imposed outflow is an attempt to maintain approximate continuity. The choice of a cone instead a cylinder is made to make flow better behaved during the early evolution of the self-induced flow.

4. Model Evaluation

Three separate experiments were used to test the model. The first two were open air releases in flat terrain, while the third was a wind tunnel experiment that included the effect of obstacles on the flow. Both of the open air experiments were part of the Heavy Gas Dispersion Trials project carried out by the British Health and Safety Executive. We selected two of the trials for simulation: the continuous release trial #45 and the instantaneous release trial 8. In both cases 2000 cubic meters of a mixture of Freon and nitrogen was released. In the case trial 45 the release was continuous with a release rate of 5 cubic meters per second.

Trial #	Date	Wind speed	Stability class	Volume released	Initial Relative Density
8	9/9/82	2.4	D	2000	1.63
45	6/9/84	2.1	E/F	2000	2.0

The wind speeds were based on measurements at a 10 meter height. Figure 1 reports the comparison between measured and modeled concentrations highest concentrations. The simulated concentrations are within a factor of two of the measured maximum

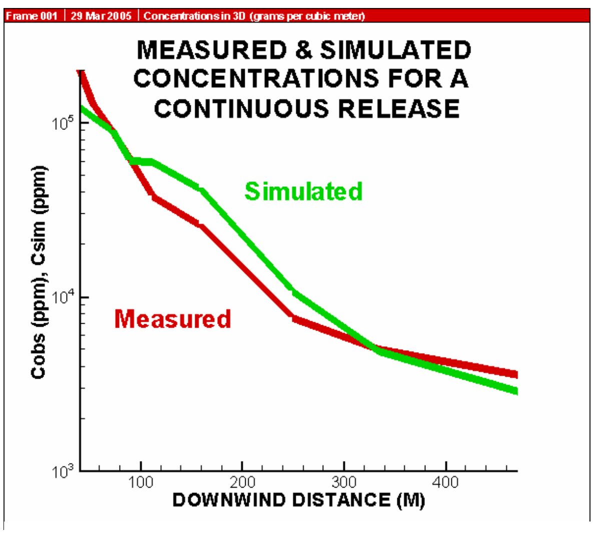


Figure 2. Comparison between maximum measured and simulated concentrations.

concentrations. While this is a generally accepted measure of good performance, it is not definitive in this circumstance. Hanna and others (Hanna, et al, 1991) report similar performance for a Gaussian-plume model that does not treat dense-gas phenomena at all. Consequently it is possible to achieve good behavior by this measure even though the actual dispersion has an entirely different character than that depicted by the model itself.

Figure 3 describes the particles distribution for a dense-gas release and it is clear that the behavior is much different than that shown in figure 4 for a neutrally-buoyant plume. Figure 5 displays the position of particles in the vertical plane, while Figure 6 reports

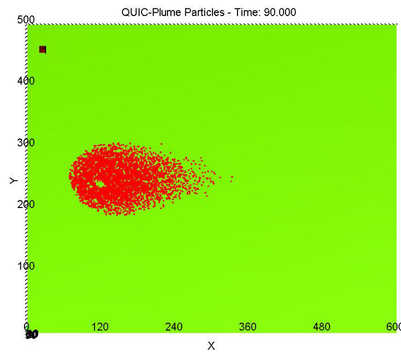


Figure 3. Random particle-positions 90 seconds after the start of a continuous release of a dense gas

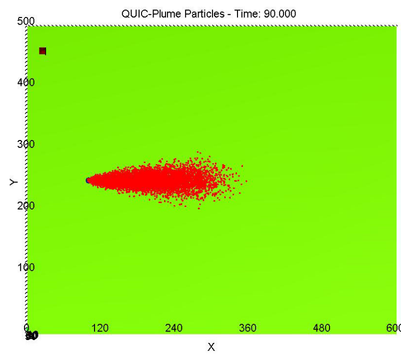


Figure 4. Random particle-positions 90 seconds after the start of a continuous release of a neutrally buoyant gas.

particle positions for a neutrally buoyant plume with the same release characteristics.

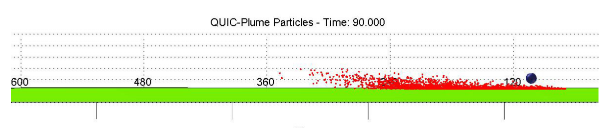


Figure 5. Vertical distribution of random particles from a dense gas release. The source position is on the right and the wind is from the left.

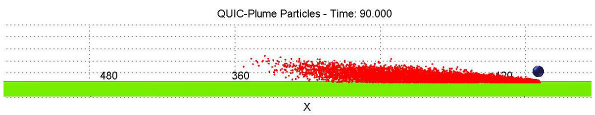


Figure 6. Vertical distribution of random particles from a neutrally-buoyant gas.

The instantaneous release, TI8, provided a different test of the model. The centerline values were not available but there was an approximate representation of the plume area available (Hanna and Drivas, 1987).

The definition of points within the plume area is unclear. In the case of the simulation, any concentrations above zero were counted as within the plume area; a definition that might overstate the area. On the other hand, when the plume becomes diluted there is a minimum concentration the can be represented as a non-zero value that corresponds to a single particle spending one time step in one receptor cell

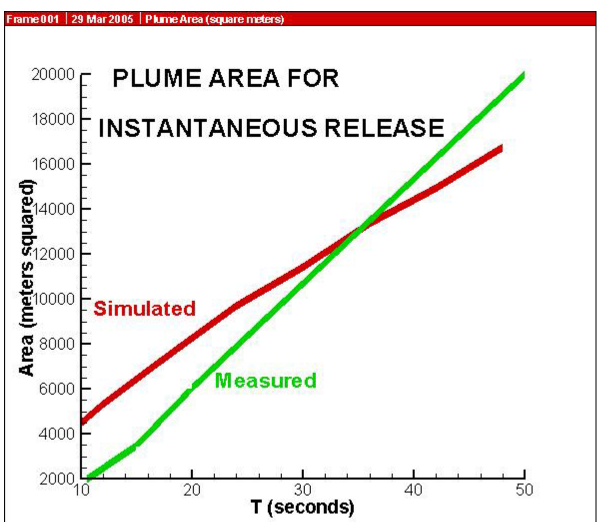
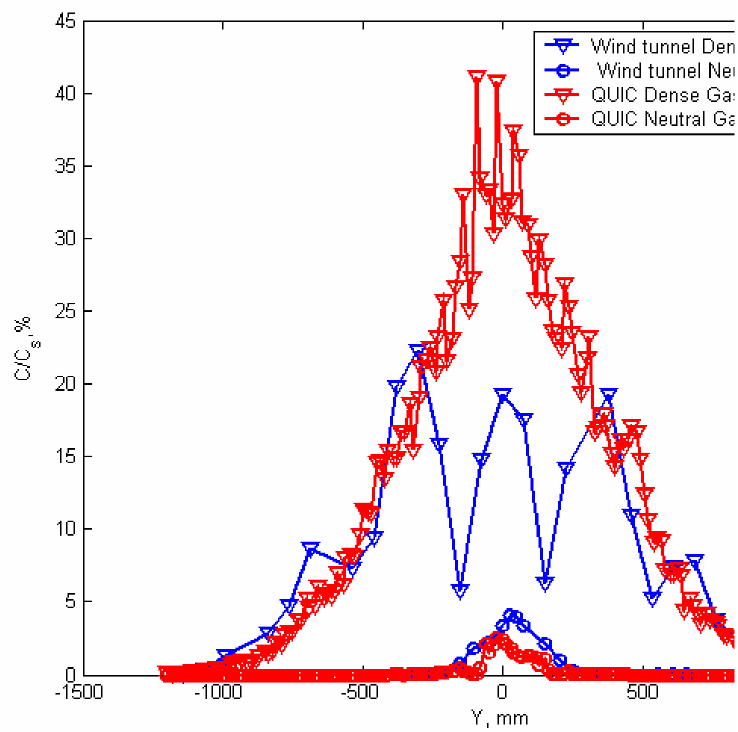


Figure 7. Measured and simulated plume area for the Thorney Island trial #8.

The third experiment that was used to test the model involved a series of wind tunnel experiments in which a dense gas was released continuously into a section of a wind-tunnel that had grid of rectangular obstacles (Zhu, et al, 1995). Figure 8 describes the simulated concentrations and the geometry. In this instance the wind speed was 0.5 meters per second at a height of 0.5 meters. The release rate was 0.49 grams per second and the density of the material was 1.96 kg per cubic meter. Figure 9 reports the measured and simulated concentrations at a point 0.6 meters downwind of the release point. Figure 10 reports measured and simulated concentrations above a point along the plume center and 0.6 meters down axis from the source. In both cases the lowest wind speed, 0.5 m/s and the higher wind speed of 2. m/s are reported.



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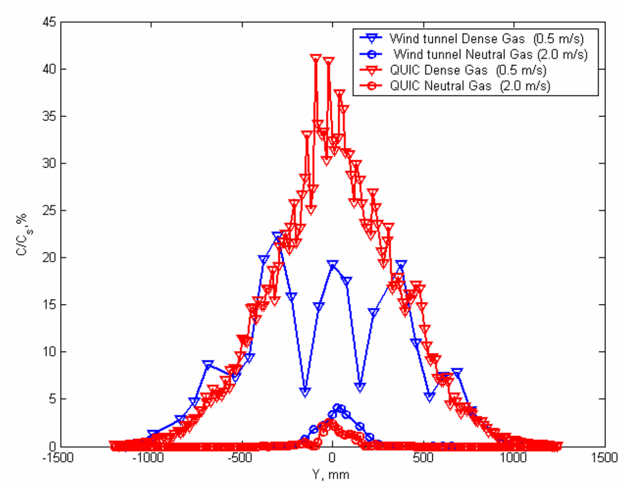

Figure 9. Comparison of measured (red) crosswind profiles with simulated (blue) ones for 0.5 m/s wind speed (top –inverted triangles) and 2.0 m/s wind speeds (bottom – circles) at 0.6 meters down wind.

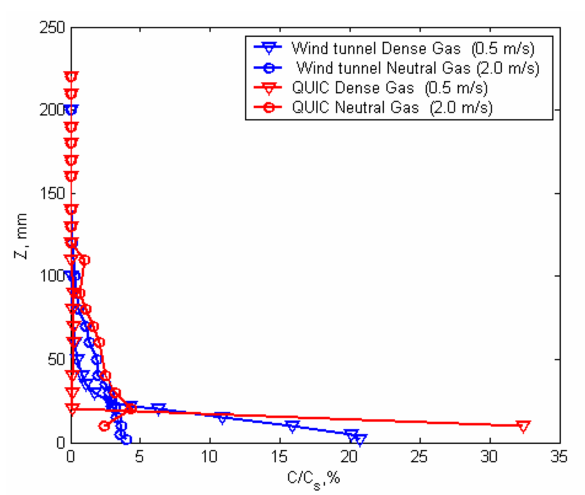

Figure 10. . Comparison of measured (red) vertical profiles with simulated (blue) ones for 0.5 m/s wind speed (top –inverted triangles) and 2.0 m/s wind speeds (bottom –circles) at 0.6 meters down wind and along plume center.

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