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ADVANCES IN DENSE GAS DISPERSION MODELING OF ACCIDENTAL RELEASES OVER ROUGH SURFACES DURING STABLE CONDITIONS

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INTRODUCTION

A major, cooperative research project will be completed in 1997 from which an improved understanding will be gained about the dispersion of accidental, dense gas releases at industrial sites (i.e., high surface roughness) during low-wind stable meteorological conditions. The plans for this project were presented by Hanna and Steinberg (1995). Most previous research was limited to releases over smooth surfaces in nearly-neutral conditions (Hanna et al., 1993).

More specifically, the goals of this research program include the following:

- Determine the effects of a wide range of surface roughness on dense gas dispersion (DGD),
- Explore the effects of a wide range of atmospheric conditions of most concern to DGD modeling, from near neutral stability with wind speed (at a height of 1 m) of about 5 m/s, to quite stable with wind speed of about 1.5 m/s (corresponding to Pasquill "F" conditions),
- Determine the effects of wind shear and along-wind dispersion on concentration magnitude and duration downwind of short-duration releases,
- Measure the effect of plume Richardson number, Ri^* = 0 (passive plume) to about 20,

- Determine whether there are significant atmospheric stability effects on vertical DGD by repeating some of the above in a stably stratified wind tunnel flow,
- Determine more precisely the Reynolds number and Peclet number limits of good simulations of full-scale scenarios in wind tunnels.

The major elements of this research program include the following:

- Studies in several wind tunnels of vertical entrainment into dense gas clouds flowing over surfaces with roughness elements ranging in size from smaller to taller than the cloud height,
- Exploration of methods to simulate dense gas releases under a stable atmospheric boundary layer in an environmental wind tunnel by achieving appropriate parameter ranges for a flow with a Monin-Obukhov length sufficiently small and a roughness length sufficiently large,
- Development of a demonstration data-set from a series of field experiments including both short duration and continuous dense gas release during neutral to very stable atmospheric conditions for surface conditions ranging from (1) smooth, (2) uniform roughness, to (3) a combination of uniform roughness and localized very large roughness.
- Modification of scientific algorithms (e.g., vertical entrainment parameterizations) used in dense gas dispersion models and evaluations of the revised models.

An integrated philosophy was used to coordinate the field and wind tunnel elements of this project in order to enhance the usefulness of the overall data sets. As the wind tunnel experiments are now largely complete, an overview of these experiments is given. Also, some preliminary results from the completed neutral wind tunnel tests are provided, such as entrainment rate as a function of the plume Richardson number. The main field experiment known as "Kit Fox" was completed during the summer of 1995. A description of these experiments as well as a summary of the data collected are presented.

INTEGRATED EXPERIMENTAL DESIGN

We believe that the scientific conclusions of dense gas diffusion (DGD) studies would be greatly strengthened if both field and wind tunnel experiments were carried out in an integrated fashion. Wind tunnel studies are cheaper, faster, and more controllable, but for DGD the low tunnel speeds required for Richardson number (Ri) similarity impose simulation limits that are not well defined. This is especially so for DGD in stable conditions, but we saw possibilities of using advanced facilities for this purpose for the first time. Flow visualizations and plume measurements over a range of Reynolds numbers, comparisons with similar field runs, and comparison of measured dimensionless plume entrainment rates with field-validated values could both increase confidence in wind tunnel DGD studies and better define the limits of this tool.

The first step was to use neutral wind tunnels, at speeds ensuring full turbulence, to design two standard roughness arrays for use in both types of experiments. A "uniform roughness array" (URA) was developed in the wind tunnel at the U.S. Environmental Protection Agency (EPA) Fluid Modeling Facility (FMF) by measuring wind and turbulence profiles over candidate arrays (Snyder, 1995). The object was to maximize z_0/H_r, the ratio of roughness length to element height, while maintaining low element density, since we needed to cover 37,000 m^2 of field with the design. The URA is intended to represent the general effects of non-smooth land surfaces on DGD. An "equivalent roughness pattern" (ERP) was developed in the Cermak-Petersen-Peterka (CPP) wind tunnel to represent the downwind effects of a concentrated area of very large roughness, e.g. an industrial complex (Petersen and Cochran, 1995a and b). Scale models of refinery complexes were used to establish target values of downwind turbulence and passive diffusion. For maximum roughness efficiency, flat baffles facing the wind were chosen for both arrays. In both the wind tunnel and the field experiments, a line of tall spires was set up perpendicular to the wind in the approach flow in order to generate additional turbulence (the spires were 5 m tall in the field).

An earlier 1993 smooth-surface field experiment at DOE's Spills Test Facility provided experience with a dense array of collocated CO_2 (real-time) sensors and bag samplers for CO_2 and SF_6(Egami et al., 1995). The CO_2 sensors were available with spans of 0.2 to 10% CO_2, allowing practical arc distances of about 25 to 225 m for the planned release rates. The real-time sensors allowed us to make multiple releases during favorable conditions, to measure concentration fluctuations, and to detect the passage time and peak concentrations at each arc for short duration releases (20 s). The most relevant 1995 Kit Fox field experiments had three primary goals. The first goal was to study the effect of roughness on DGD using three different surface conditions: the baseline smooth desert, the URA alone, and the URA+ERP arrays together to simulate effects of an industrial release. The second goal was to study DGD during much lower wind speeds and more stable conditions than attempted previously. The third goal was to study the effects of wind shear and along-wind dispersion on short-duration releases. The 1993 tests and continuous meteorological monitoring established that the best time to capture neutral to very stable conditions, with diminishing winds predominantly from a narrow sector, was one hour prior to and following sunset. The 1995 Kit Fox series included releases with winds at a height of 1 m of 5 m/s down to 1 m/s and stabilities from Pasquill D to F and beyond, meeting or exceeding our expectations.

Wind tunnels were used for simulations of full-scale, point source releases and for idealized DGD studies. The CPP planning studies mentioned above can be compared with actual field tests, for both continuous and 10-s releases, made with u (1m) near 5 and 2.5 m/s. However, because of the scale-down of tunnel speed required for Ri similarity, lower speed simulations were not possible because laminarization and flow instabilities would occur; this is a serious limitation in all DGD wind tunnel studies. Measurements of continuous point source DGD were also made at four wind speeds in the EPA FMF tunnel over a roughness array identical to the URA. Three series of idealized studies in three different tunnels complete our wind tunnel program. These focus on vertical entrainment because that is the most weakly supported element of present DGD modeling, especially with no previous studies over rough surfaces. To reduce the need for three dimensional measurements, which are very time consuming, and to maintain near constant plume Ri, a line source spanning the tunnel was used. The EPA FMF wind tunnel studies focused on the URA array (Snyder, 1996). Two scales were used, with elements 5 cm high and 5/6 cm high, to study entrainment for plumes both shallow and deep compared to the roughness and to better establish the minimum Reynolds number required for full-turbulence simulation. A purposely similar program for the 5 cm elements was carried out in the wind tunnel at the University of Arkansas Chemical Hazards Research Center (CHRC)(Havens et al., 1996); it used an identical physical setup but different instrumentation to check on the replicability of results. In addition, a series using roughness of a very different geometry was carried out to test the generalizability of entrainment parameterizations, e.g., ones in terms of friction velocity. Finally, a similar series of measurements over a URA type array, 2 cm high, is now in progress at EnFlo (University of Surrey) to study the effect of strong ambient stability on DGD. This is the first such attempt, and has required development of new instrumentation to measure surface heat flux.

FIELD EXPERIMENTS

The primary objective of the field experiments was to capture a matrix of finite and continuous duration releases under neutral to stable meteorological conditions over three different surface roughness configurations. To meet the objectives of the project, the field tests were designed to incorporate the results of the exploratory wind tunnel studies mentioned above, the 1993 CO_2 dispersion experiments (Egami et al., 1995), and the predictions of expected plume concentrations and geometry by dense gas models. It was necessary to measure gas concentrations, meteorological data, and source data at one second intervals prior to, during, and after release of the surrogate dense gas for three types of surface roughness: 1) the flat unobstructed desert surface, 2) the URA, and 3) the URA+ERP. When the URA and ERP roughness elements were in place, a line of spires was placed 89 m upwind of the source, in order to enhance the development of turbulence in the boundary layer over the roughness elements. These so-called Irwin spires were also used in the wind tunnel experiments. Details concerning the locations and sizes of the spires and the ERP and URA elements are given in Table 1. Because the time window available for the experiments was limited, the sequence of the surface roughness configurations used for the experiments was ordered from high (URA+ERP) to low (smooth desert). As the roughness configurations were changed, the array of meteorological towers was kept fixed, but the 95 CO_2 sensors had to be positioned lower and partially respanned for higher concentrations for anticipated changes in DGD during the smooth desert tests.

The field tests were conducted at the U.S. Department of Energy (DOE) Spill Test Facility in Nevada. Storage tanks were filled with CO_2 vaporized from a portable liquid tank to a maximum pressure of 8.85 atmospheres. A 329 m release line extended from the tank farm to a sub-surface box which had a quick-acting (<1 sec) sliding door that exposed a 1.5 m x 1.5 m opening at ground level; this provided a low-momentum source. Since concentrations are inversely related to surface roughness, flow rates were adjusted to 4 kg/s for the URA+ERP surface, 1.5 kg/s for the URA surface, and 1.0 kg/s for the smooth surface, to keep arc concentrations within the optimum ranges of the sensors.

Table 1. Description of Locations and Sizes of Roughness Elements Used in Field Experiments.

Field Roughness Element	Farthest Upwind Location with Respect to the Source	Spatial Coverage	Number of Elements	Element Width	Element Height	Element Lateral Spacing	Element Downwind Spacing
Spires	89m	upwind edge of URA	36	0.458m bottom 0.12m top	4.87m	3.25m	not applicable
ERP	50m	39m x 85m	75	2.4m	2.4m	6.1m	8.5m
URA	89m	120m x 314m	6,600	0.8m	0.2m	2.4m	2.4m

Solid state infrared CO_2 chemical sensors were deployed at four different downwind arrays (25, 50, 100, and 225 m from the source). The first three arrays each had three towers with vertical arrays of five sensors plus additional ground level sensors, while the 225 m array consisted of only ground level sensors. Meteorological instruments, consisting of propeller/vane anemometers and temperature probes, were located on three towers, one 20 m in front of the spires, one 6 m in front of the ERP, and one 50 m downwind of the source. Towers with sonic anemometers were located 20 m upwind of the spires, 6 m upwind of the ERP, 7.5 m upwind of the source, and 50 m downwind of the source. An eight level 24 m tower with propeller/vane anemometers and temperature sensors was located approximately 100 m upwind of the source and 180 m off the centerline of the test grid.

Releases were made during 13 evenings from August 22 to September 15. At least partially successful data capture was obtained for 14 URA+ERP releases, predominately during "D" and "E" Pasquill stabilities, as determined from atmospheric Richardson numbers. For the URA surface, we count about 33 successful data captures, including about 6 each in the "E" and "F" stabilities. For the smooth surface, we count about 23 successful data captures; 7 of these were "F" stability and 3 can possibly be considered "G" stabilities. For each surface condition, about 1/3 of the releases were continuous (2 to 6 minutes) and 2/3 were short-duration (20 seconds).

The analysis of the Kit Fox field experiments is only in a preliminary stage, since the data are still being calibrated and subjected to QA/QC procedures. However, one or two runs from each stability class, roughness class, and source duration class have been analyzed and compared with the predictions of an updated version of the HEGADAS model. The results of the analyses demonstrate that 1) vertical entrainment (and hence ground-level concentrations) are strongly affected by changes in the underlying roughness, 2) ambient wind speed has the largest effect on dense gas dispersion and subsequent distribution of concentrations, 3) theoretical scaling relations developed in the wind tunnels and used in models such as HEGADAS are verified by the field observations, and 4) along-wind dispersion (for the finite duration releases) is enhanced by wind shear near the ground. The comparisons of limited observations with model predictions suggest that the updated algorithms in HEGADAS properly account for these effects.

VERTICAL ENTRAINMENT STUDIES IN NEUTRAL WIND TUNNELS

At the time of writing, the two programs of vertical diffusion measurements in neutral wind tunnels are complete, data reports are available (Havens et al., 1996: Snyder, 1996), and data analyses are in progress. The stable boundary layer program at the University of Surrey is scheduled for completion by late spring of 1997. As described in the "Design" section, the wind tunnel at the EPA FMF was used to investigate DGD over the "URA" array at two contrasting scales with element heights $H_r = 5/6$ and 5 cm. The small and large versions are designated "WH4-12S" and "WH4-12L" (see Fig. 1), with "4" referring to the ratio of roughness element width to H_r and "12" referring to the ratio of element spacing to H_r. Closely coordinated experiments were run in the CHRC wind tunnel, which was especially designed for dense gas studies. At CHRC, two significantly different roughness geometries were run, one identical to the WH4-12L array above and one designated as the "WH1-8" array with $H_r = 3.8$ cm. On the basis of earlier wind tunnel studies, the ratio z_0/H_r for the 4-12 array is about three times that of the 1-8 array; thus, the 4-12 array is far more efficient for generating increased turbulence intensity.

It is expected that when the plume depth, h, is large compared with H_r, the roughness effects may be parameterized through a single variable, z_o. However, when the elements are the same height or larger than the plume depth, entrainment will be affected by the shapes, sizes and spacings of the individual elements. Hence, the dual-scale experiments in the EPA FMF wind tunnel were designed to study plume growth both when $h >> H_r$ and when $h < H_r$ or $h \sim H_r$. The contrasting geometry studies in the CHRC wind tunnel focused on how the geometry of the elements affect entrainment rates in the latter situation. The WH4-12L array was run at both laboratories with ostensibly identical flow rates and free flow speeds. The EPA study included additional measurements to elucidate Reynolds number effects.

In both facilities, a "line" source supplied a metered rate of carbon dioxide at negligible vertical velocity through a bed of fine gravel contained within a rectangular box. This box stretched the entire width of the EPA tunnel. Because the CHRC tunnel was much wider than the EPA tunnel, interior sidewalls were used to obtain the same effective width, and the line source was identical. Its width (streamwise direction) was 10 cm. The flow structure was measured with hot-wire anemometry (EPA) and laser-doppler anemometry (CHRC). A small fraction of ethane (C_2H_6) was mixed with the carbon dioxide (CO_2) so that the downwind concentration fields could be measured with flame ionization detectors.

Prior to analyses of these wind tunnel and field data, an international group of scientific advisors agreed on certain definitions and conventions. For example, in analyzing boundary-layer profiles, we agreed to assume that the von Kármán constant $k = 0.4$. We define effective mean plume speed, $\bar{u}$, from the vertical profile of wind speed, $u(z)$, weighted by the concentration profile: $\bar{u} = \int uCdz \div \int Cdz$; when available, crosswind integrated or summed C is used. As a practical matter, $u(z)$ is measured outside the plume. A characteristic plume depth is defined by $h = \int Cdz \div C_s$, where C_s is the surface concentration. Vertical entrainment velocity is defined simply as $w_e = d(\bar{u}h)/dx$. Thus, when the mass flux of plume gas or tracer is conserved ($\int uCdz = Q$), then $w_e = QdC_s^{-1}/dx$, a relatively simple determination. All velocities are scaled by the friction velocity, u_*, which is measured outside the plume. The basic Richardson number definition is $Ri^* = g'h/u^{*2}$, where g' is reduced gravity ($g\Delta\rho/\rho_a$). For the two-dimensional, line source plumes used above we can derive $Ri^* = B_o/(\bar{u}\, u^{*2})$, where $B_o = g_o'Q_o/C_o$ is the line-source buoyancy flux.,

Some preliminary results, from just the EPA FMF wind tunnel, are shown in Fig. 1; we have plotted w_e/u^* versus Ri^*. One encouraging result is that, at the passive limit ($Ri^* = 0$, plotted at 0.1 in Fig. 1), our data agree well with the best available field data, Project Prairie Grass, when these data are analyzed exactly the same way: $w_e/u^* \approx 0.65$. Previously published values for this limit range from 0.4 to 1.0. Another encouraging result is the reasonably good agreement between the small and large array, provided that the tunnel speed for the small array was not dropped below 1 m/s. When it was dropped further, concentration measurements became erratic and the plume appeared to laminarize. Therefore, to maintain full-scale similarity, it appears that the minimum roughness Reynolds number for laboratory studies over sharp-edged roughness is $Re^* = u^*z_o/\nu = 1.5$. Compared to common DGD models, e.g., DEGADIS, these w_e/u^* are about 30% larger at small Ri^*. However, in a range where the models are more frequently used, $Ri^* = 0.3$ to 3, the agreement is reasonably good.

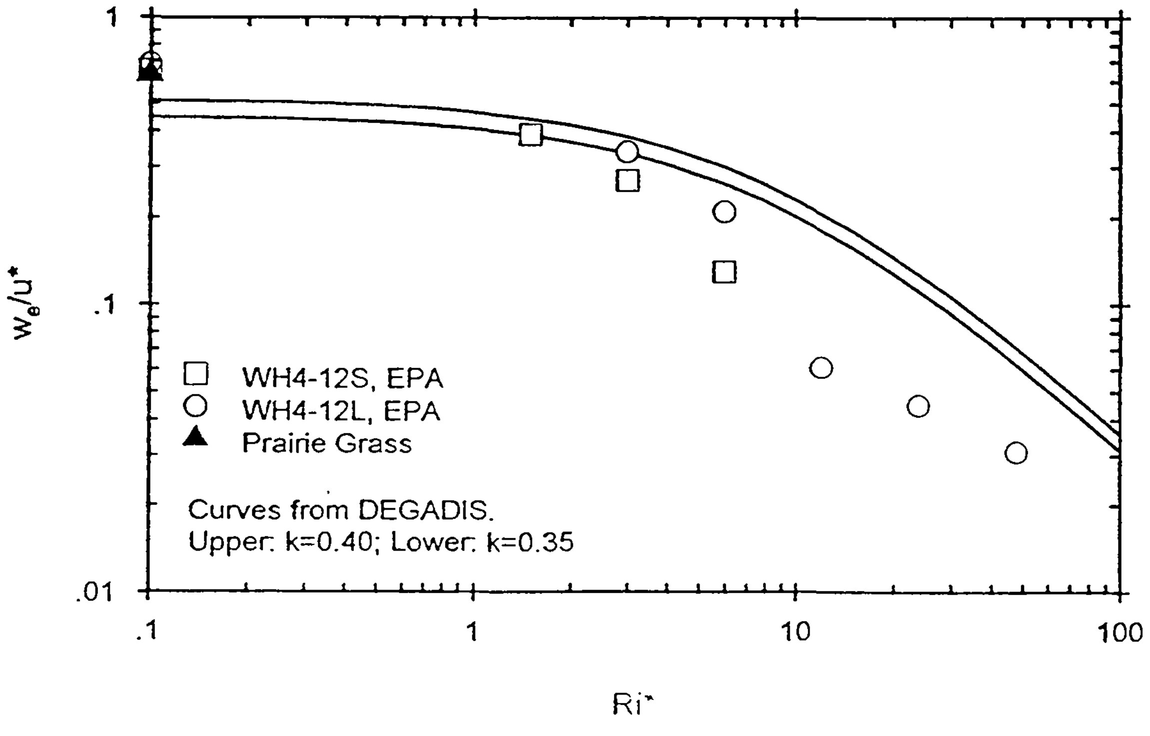

Figure 1. Entrainment velocities deduced from EPA FMF neutral wind-tunnel measurements.

PLUME STUDIES IN STABLE BOUNDARY LAYERS

Entrainment studies with dense gas plumes in stable ambient conditions are being investigated in the University of Surrey's EnFlo stratified flow wind tunnel. The objective is the same as for the neutral experiments, except that the entrainment experiments are conducted in moderately stable conditions.

Initial work concentrated on demonstrating that suitable, moderately stable boundary layers could be established, as determined by comparison of profiles of mean velocity and temperature, turbulence intensities, heat fluxes and temperature fluctuations with relationships based on measurements in the atmospheric boundary layer.

In the wind tunnel, a standard 1 m high barrier wall and a vorticity generator system (spires) were mounted at the entrance to the working section. The inlet heaters were set to provide a uniform temperature profile at the start of the cooled floor section (i.e., at $x = 9$ m) with the temperature difference between the free flow above the boundary layer and the cooled floor panels being held constant. For most of the work the tunnel was run at a free stream speed, u_{ref}, of 1.35 m/s, with some additional runs at speeds of 1.2 and 1.5 m/s. The floor was covered with a "WH4-12" configuration of roughness elements of height $H_r = 20$ mm. This configuration is similar to the one used in the EPA and CHRC wind tunnels (see above), and used in the field as the URA roughness. A combination of LDA and cold-wire instrumentation was used to measure the full set of mean flow and turbulence profiles.

A well behaved, moderately stable boundary layer was simulated with u_{ref} set at 1.35 m/s, developing quite markedly to begin with, but slowly thereafter. Between $x = 16$ and 18 m, log-linear profiles were found to provide a very close fit to the mean velocity and temperature data up to a height of about $z = L$. The boundary layer depth, δ, was about 250 mm; this is shallow but sufficient for dense gas studies. The characteristic scaling ratios, δ/L, σ_u/u^*, σ_w/u^*, and σ_T/θ^* are listed in Table 2, where L is the Obukhov (stability) length, σ_u, σ_v, and σ_T are standard deviations of longitudinal and lateral turbulent velocities and temperature fluctuations, and θ_* is the turbulent temperature scale.

Table 2. Characteristic Properties of Stable Boundary Layer in EnFlo Wind Tunnel

x(m)	δ(mm)	δ/L	σ_u/u^*	σ_w/u^*	σ_T/θ^*
15	200	0.78	1.8 - 2.0	1.2 - 1.4	1.7 - 1.9
16	250	1.48	1.7 - 2.0	1.3 - 1.4	1.6 - 1.7
17	250	1.38	1.6 - 1.9	1.2 - 1.3	1.7 - 1.9
18	270	1.57	1.5 - 1.9	1.1 - 1.3	1.6 - 1.8

Since the scaling ratios in Table 2 satisfied the boundary layer criteria set forth by the project steering group, the stable boundary layer flow was judged suitable for the dense gas entrainment studies and the tunnel was then adapted for that phase of the work. This involved extending the fetch of cooled floor for sufficient plume development, and installing a supply system for a mixture of carbon dioxide and propane. A source arrangement identical to that used in the EPA and CHRC wind tunnels was also installed. The experimental program covers both two and three dimensional plume studies, with attention focussed mainly on the former. At conclusion, the entrainment velocity versus cloud Richardson number relationship will be evaluated as a function of ambient stability conditions.

SUMMARY

A multi-component cooperative research program consisting of both field and wind tunnel experiments was designed to answer basic questions concerning dense gas dispersion over a wide range of surface roughnesses and atmospheric stabilities. The field measurements are completed and the data should be cleared through the quality assurance process by late spring 1997. Two series of experiments on vertical DGD have been completed in two neutral wind tunnels and data reports are available; partial analyses concerning Richardson and Reynolds number effects were presented here, while more finalized analyses are near completion. A similar experiment in a stably stratified wind tunnel is near or at the end of the experimental phase, with a data report and data analyses due before the end of 1997. We believe that the totality of data collected under this program will be adequate to meet the goals stated at the outset of this paper.

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15. SUPPLEMENTARY NOTES

A major, cooperative research project should be completed in 1997 from which an improved understanding will be gained about the dispersion of accidental, dense gas releases at industrial sites (i.e., high surface roughness) during stable meteorological conditions. Most previous research focussed on releases over smooth surfaces in nearly neutral conditions. An integrated philosophy was used to design this project with will enhance the usefulness of the overall data. As the wind tunnel experiments are now largely complete, an overview of these experiments including techniques, scope, and data quality checks will be give. Also, some basic results from the completed neutral wind tunnel tests will be provided, such as entrainment rate as a function of the plume Richardson number. The main field experiment known as "Kit Fox" was completed during the summer of 1995. A description of these experiments as well as a summary of the data collected will be presented.

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