CFD modeling of dense gas cloud dispersion over irregular terrain

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1 INTRODUCTION

Computational techniques for dense gas cloud dispersion generally fall into four categories depending on the simplicity of the models—box models (volume integrated), slab models (cross-section integrated) shallow layer (depth integrated), and full 3-d field models (K or advanced turbulence models) (Duijm et al., 1997).

Box and slab models require the stipulation of boundary entrainment rates which are normally prescribed in terms of local relative cloud velocities (U and Re) frontal velocities (u_g), boundary friction (u_*) stratification (Ri_*, Gr) and for cold gases the temperature potential (T^*) or convective velocity (w_*) such that the entrainment velocity, $w_e = f(u_g, u_*, w_*, Ri_*, Re$. (Meroney, 1983, 1984a, 1984b, 1985) Empirical coefficients in these solution procedures are assigned based on comparison with field or model experiments; hence, the results are often dependent on the data set used to calibrate the calculation scheme.

Volume integration of the equations of motion, energy and mass species result in sets of ordinary differential equations in time which may be solved by standard Runga-Kutta solution procedures; hence, they are extremely fast (Meroney, 1983, 1984c (Dens4)). Box models have been modified to include the effect of simple up- or downwind terrain slope (Deaves and Hall, 1990; Kukkonen, and Nikmo, 1992). Unfortunately, these box model relationships can not deal with the effects of irregular terrain, nonhomogeneous surface heating, obstacles, or water spray mitigation.

Cross-section integrated models permit more accurate calculation of lateral, downwind and upstream motion of dense gas clouds. Integration of the equations of motion, energy and mass species in the vertical and lateral directions result in equations for the layer-averaged lateral and longitudinal momentum, mass continuity, concentration and enthalpy equations for longitudinally varying depth and width and cross-section-averaged densities, temperatures, velocities, and concentrations (Havens and Spicer, 1985; Meroney, 1984a, 1984b (Dens20)). The resulting partial differential equations have dependent variables in longitudinal direction and time. Assuming winds aligned with local slopes, fence like obstacles or water spray curtains aligned perpendicular to the wind, and slopes and surface conditions which do not vary laterally, it is possible to calculate up- and downwind cloud variations due to slope effects.

True depth-integrated or shallow-layers models integrate the equations only in the vertical direction assuming similarity in the variation of important flow properties. Depth averaged values of these quantities must therefore be defined in terms of their vertical distributions and a characteristic parameter (depth, average velocity, average temperature, etc.) The resulting 2-dimensional partial differential equations may vary in longitudinal and lateral directions and time. Thus, nonhomogeneous surface elevations, roughness, temperature, etc. are permitted, and a wide variety of obstacles, water spray arrangements, and fence configurations may be considered (Hankin and Britter, 1999; Hankin, 2004; Lee and Meroney, 1988 (DENST); Venetsanaos, et. al., 2003). Nonsymmetrical clouds are generated with winds directed obliquely to terrain slopes, channeling can be produced along gulley shapes and canyons, and gravity fronts are demonstrated although wave breaking and vertical overtopping over buildings and fences are unlikely to be faithfully reproduced.

Finally, solution of the full 3-dimensional equations of motion, energy, and species concentration are possible using a CFD code which solves the full set of partial differential equations in space and time (Eg., FLUENT, CFX, FLOW-3D, STARCD, etc.). One no longer presumes similarity in vertical profiles in plume properties (velocity, concentration, species concentration, etc.), entrainment velocities and dilution are not specified but calculated as a result of the joint effects of advection and turbulence. Specification of appropriate inflow conditions, surface boundary conditions, material properties and an appropriate turbulence model become crucial. The turbulence models should include components which adjust for the damping effects of thermal or density stratification on turbulent generation and dissipation. Perturbations produced by complex terrain, tunnels, 3-dimensional objects, water sprays, heat sources, water surfaces, etc. may hypothetically be incorporated only limited by domain resolution, computer capacity, and computational time. Several modelers have calculated dense plume dispersion using CFD techniques, but little is published that includes complex terrain effects:

- Scariali et al. (2005) used CFX-4.4 to calculate mesoscale size transport of chlorine plumes for a hypothetical industrial accident in eastern Sicily. They assumed initial plume collapse configuration was not important over the long distance and time scales examined.
- Meroney (2010) used Fluent to calculate dense gas dispersion in mock urban environments including single and multiple building obstructions.

The goal of this paper will be to compare modeling results for instantaneous dense gas clouds dispersing over several simple terrain configurations: a flat homogeneous terrain, a sloped terrain, and a simple wedge-shaped gulley in a flat terrain. Earlier results for box, cross-section averaged, and depth-averaged models will be compared to a full CFD simulation using FLUENT 12.

2 NUMERICAL PREDICTION OF DENSE CLOUD BEHAVIOR

All calculations were performed with the commercial code FLUENT 12© in a rectangular domain H x L x W m in which an initial volume of dense gas was placed on the surface at a release point. Inlet velocity and turbulence fields were set to produce a stationary homogeneous flow in the absence of the dense cloud or gorge configurations (Blocken et al., 2007) by calculating a preliminary clean domain boundary layer flow. Side domain walls were set to a symmetric condition, the top surface velocity was specified to fit the inlet velocity profile, and a standard outflow condition was used. Both realizable kappa-epsilon and Discrete Eddy Simulation (DES) turbulence models were tested using standard wall functions.

2.1 *Validation Experiments*

Porton Trial Test No 8 involved a release of 40 cubic meters of a Freon-air mixture (specific gravity = 2) instantaneously from a collapsing tent under calm conditions on a flat field (Picknett, 1981). Wind-tunnel experiments of Hall et al. (1982) and earlier predictions from box and cross-section averaged models (Meroney, 1984) are available. Figure 1 compares CFD predictions of ground concentration vs distance against full scale, wind tunnel, box models, section averaged and depth-averaged model results. Similarly Figure 2 compares cloud edge growth versus transport time.

Meroney and Lohmeyer (1983, 1984) Test No. 7 involved a release of 165 cubic centimeters of pure Freon (specific gravity = 4.17) from a suddenly rotated cylinder built into the floor of a small open-circuit wind tunnel. Wind speeds were 0.2 m/sec. Measurements were made of cloud arrival, cloud departure, and maximum concentration times. Box and DENST model predictions of the cloud behavior are also available (Meroney, 1983).

2.2 *Slope Experiments*

A hypothetical plume of the same characteristics as the Porton Trial Test No. 8 (no wind) was simulated as it disperses over a slope of 1:20. Lee and Meroney (1987) compared calculated behavior using box and depth-average models to the horizontal surface results. Figures 3 and 4 compare CFD predictions to maximum concentration versus distance and cloud transport up and down slope against time to depth-averaged model (DENST) results.

2.2 *V-Shaped Gorge*

Finally, a Porton Trial Test No. 8 cloud was released at the edge of a V-shaped gorge with side slopes of 1:4.14 and a down-slope gradient of 1:20. Again Lee and Meroney (1987) previously calculated this situation using their depth-averaged model (DENST). Figures 5 and 6 display ground-level concentrations as the cloud floods down the gorge producing a thumb that extends beyond the normal spread boundaries. Since heightened flow velocities increase dilution, the actual surface concentrations do not tend to exceed maximum levels seen without the gorge, but the values arrive earlier.

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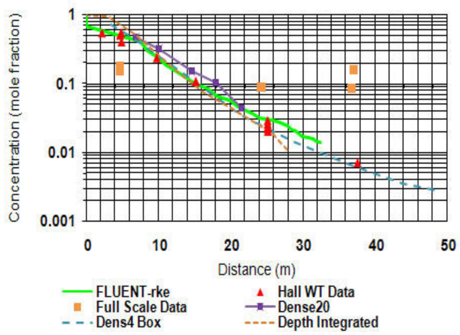

Figure 1: Porton Trial No. 8, gas cloud peak concentrations vs. distance.

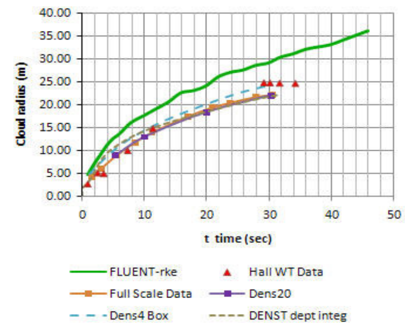

Figure 2: Porton Trial No. 8, gas cloud radius vs. time.

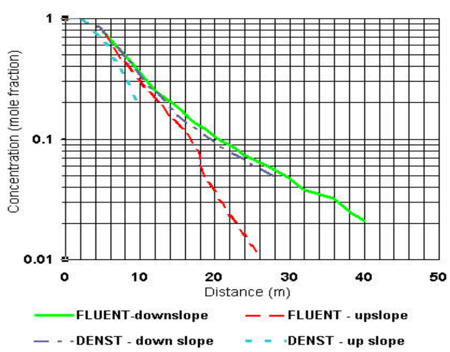

Figure 3: Hypothetical Porton Trial No. 8 spill on 1:20 slope, concentrations vs. distance.

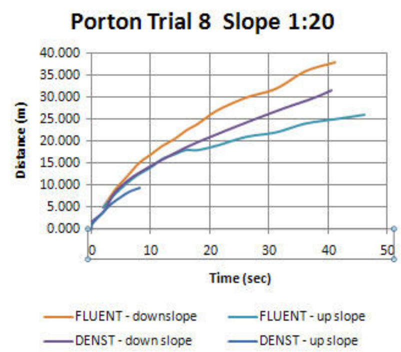

Figure 4: Hypothetical Porton Trial No. 8 spill on 1:20 slope, cloud radius vs time.

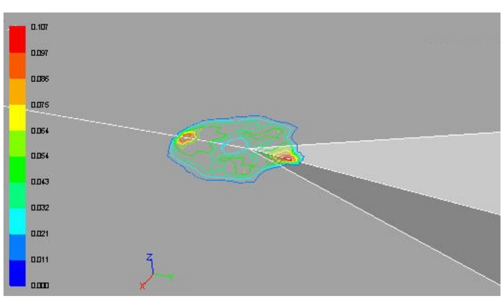

Figure 5: Hypothetical Porton Trial No. 8 spill surface concentrations with gorge slope 1:10, sidewall slope 1:4.14 at t = 40 sec.

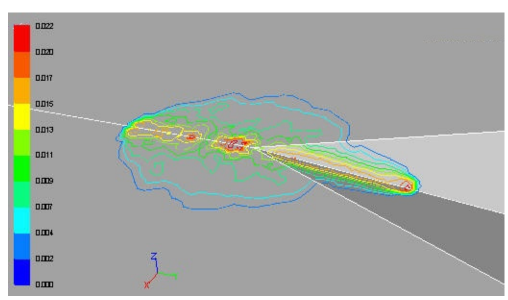

Figure 6: Same configuration at t = 10 sec.