

NUMERICAL SIMULATION OF THE MITIGATION  
OF HF CLOUD CONCENTRATIONS BY MEANS OF  
VAPOR BARRIERS AND WATER SPRAY CURTAINS

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**ABSTRACT** Laboratory and field data on barrier influence on dense gas dispersion were used to develop entrainment models to incorporate into integral numerical models. Barrier performance was predicted for a typical Hydrogen Fluoride spill for a wide range of vapor barrier heights, spill sizes, meteorological conditions and release configurations.

## 1. Introduction

Recent disastrous accidents (e.g., Bhopal [1984], Chernobyl [1986], Kerr-McGee [1986]) have focused attention on the potential risks of large and small scale releases of flammable or toxic gases. This paper examines numerically the effectiveness of vapor barriers in diluting and delaying heavier-than-air vapor clouds. Puttock, Blackmore and Colenbrander [1] identified over 22 field experiment programs on dense gas emissions. Subsequently, further field measurements have been performed on the release of Freon-air mixtures at Thorney Island, the release of hydrocarbon fuels at Maplin Sands, and the release of hydrocarbon fuels, ammonia, rocket fuels, and even HF at the DOE Liquefied Gaseous Fuels Test Facility at Frenchman's Flats, Nevada. A number of these experiments have also been simulated in fluid modeling facilities (Meroney [2]). Meroney et al. [3] recently examined eleven data sets from field and laboratory experiments dealing with the influence of vapor barrier fences and water spray curtains on the dispersion of dense gas clouds. Tests were paired into sets of data which reflected the dilution of the cloud with and without the barriers present. Peak concentration ratios, cloud arrival time ratios, peak arrival time ratios, and departure time ratios were calculated for each test pair.

## 2. Prediction of Dense Gas Dilution

When the flow situation is steady and diffusion in one direction is weak with respect to advection, it is possible to integrate over a plume cross-section and calculate plume width, average height, and cross-section averaged velocities, concentrations, temperatures, and humidity. Such a "box" type model is numerically very fast since the conservation equations reduce to a set of coupled ordinary differential equations. Alternatively when vapor generation is transient, and there are opportunities for upwind flow, a set of coupled partial differential equations of only two dimensions and time can be created by integrating the conservation equations over just the depth. Such a "shallow layer" or "slab" type model provides information about time- and space-dependent cloud widths, heights, and depth-averaged velocities, concentrations, temperatures, and humidities.

A box model (DENS62: Meroney and Lohmeyer, [4]; Meroney, [5]; and Andriev et al.[6]) and a slab model (SPRAY23: Meroney and Lohmeyer [7], and Meroney, [8]) have been adapted to consider HF dilution by water sprays (DENS65, SPRAY65) and vapor barrier fences (FENCE65, FENCE23).

### 2.1 Entrainment Models for Vapor Barriers and Water Spray Curtains

Both numerical models normally use the concept of an entrainment velocity,  $w_e$ , across the upper cloud surface to mix the cloud with ambient air. The entrainment velocity is a semi-empirical function of boundary-layer and cloud variables such that,

$$w_e = f(U_g, u_*, w_*, Ri_*), \quad (1)$$

where  $U_g$  = plume frontal velocity,  $u_*$  = friction velocity,  $w_*$  = convective velocity,  $Ri_*$  = local Richardson number.

Reductions in cloud concentrations can occur through chemical reaction between the cloud and water spray. For example, HF reacts with the liquid water and leaves the cloud as the water deposits on the ground. Laboratory and field tests described by Blewitt et al. [9] measured HF removal ranging from 9 to 80%. The entrainment models used to account for water-spray curtain dilution were described earlier by Meroney and Neff [10].

The following simple model is proposed to described the increased entrainment resulting from a vapor barrier fence:

$$(w_e)_{\text{fence}} = C_D U(H)(1 - P)(1 - (x - x_f)/(30H)), \quad (2)$$

where  $x$  is distance downwind of the source,  $x_f$  is fence location, and the relation is not used downwind of  $x_f$ . This model was used in the numerical models to compare with selected field and model data.

## 2.2 Calibration of the Vapor Barrier Fence Entrainment Model

Data from the pre-Falcon model tests performed by Neff and Meroney [11] were used to calibrate the vapor barrier fence entrainment model. Run No. 2 (9.4 m fence, no vortex generator, enclosure alone) was selected to compare with Run No. 10 (no enclosure). Figure 1 compares the results of calculations by FENC62 when the coefficient  $CD = 0.1$ . Variations in virtual distance between 60 and 44 m, and variations in the entrainment coefficient over a two-fold range did not significantly improve agreement. Best agreement occurred for Trial No. 10 data when the initial source width without a fence was set to 44 meters. A small dike existed about the model water spray pond, which may have inhibited lateral spread at the source.

## 2.3 Calibration of the Vapor Removal Model

Deposition measurements suggested that the water sprays removed 10-25%, 44%, and 47% of the Hydrogen Fluoride during Goldfish Trials 4, 5, and 6, respectively. The water spray systems were

designed to produce small droplets to enhance chemical reactions, rather than strong dilution. DENS65 was used to predict cloud concentrations with the reduction mode on but water spray entrainment set to zero. Figures 2 compares program predictions of cloud concentrations against measured values for Goldfish Trial No. 6.

### 3. Sensitivity Study

The effects of fence location were determined to be similar to that of water spray curtain location. Fences are more effective in terms of initial dilution, when they are placed nearer the source. Fence dilution effects did not persist beyond 1000 m, when the fence was placed less than 400 m downwind of the source.

#### 3.1 Fence Barriers

The fence entrainment model permits the entrainment velocity to increase with fence height velocity. Since wind profiles increase with height, then the dilution rate should increase with fence height. The FENC62 model assumes that a logarithmic velocity profile exists, such that wind speed is determined by surface roughness and friction velocity. Figure 3 displays a set of concentration curves for fence heights ranging from 3 to 12 meters. The entrainment velocity does not turn off abruptly like the water spray model, but decreases linearly out to a distance of 30 fence heights. The resulting displacement of the concentration profile is cusp shaped rather than triangular, and the dilution effect is small after about 200 fence heights. The effect of fence height on cloud height is displayed in Figure 4. The cloud height approaches the cloud height in the absence of a barrier after 1000 meters or about 200 fence heights.

Increased wind speeds result in larger entrainment rates, but this is compensated by the tendency for the plume to pass through the fence wake more quickly. Given a constant fence height of 3 meters located 100 meters downwind of the source for a range of wind speeds varying from 1 to 8 m/sec, the increased entrainment and

shortened time in the wake balance out to produce no net change in dilution rate. Plume height also remains constant. These calculations agree with other experiences in building aerodynamics, where it is found that perturbation of gas plumes by obstacles seems to be velocity independent. Concentrations decay at higher wind speeds inversely with the speed, but this is an independent effect of source dilution by the ambient wind, not an effect of a fence.

Cloud height downwind of an obstacle is expected to be independent of wind speed, since a sharp edged geometry will produce similar streamline patterns over a range of velocities. Model results suggest that the perturbation produced by a fence is constant, but the model fails to allow for a constant height wake region.

### 3.2 Water Spray Curtain Barriers

Water spray curtain tests were performed during the Goldfish Trials No. 4, 5, and 6. These tests included chemical reactions between the HF and the water spray and subsequent deposition of the HF on the ground. Goldfish Trial No. 1 conditions are used below to examine the effect of various spray placement and water spray reduction and entrainment rate alternatives.

SPRAY65 was used to predict the joint effects of water spray dilution and deposition on an HF cloud. Figure 5 displays the effect of placing a single spray which produces 80% deposition at 100m followed by a second spray of similar strength at 300 m. Notice that spray deposition produces a parallel shift of the concentration decay curve. A second spray produces a second shift of equivalent width. The decrease in concentration persists at all subsequent downstream distances.

Alternatively consider the dilution effect of the water sprays. Figure 6 considers the effect of varying curtain location from 30 to 50 to 100 to 400 meters downwind of the spill center. A nominal spray entrainment rate of 6 m/sec was chosen for these calculations. The

concentrations are very similar with just slightly lower concentrations when the spray is further downwind. The magnitude of the reduction in concentrations when the barrier is farther from the source is not large, and any advantage in final concentrations would be outweighed by the greatly increased water consumption as the spray curtain width increases over the wider plume.

Figure 7 displays the effect of a water spray curtain on plume height when activated at various downwind distances. Near the source cloud height is increased 25-fold; whereas further downwind the same spray curtain only causes a 2.5-fold increase in height.

Calculations were performed for a ten-fold range of spray entrainment velocity. Given a constant spray location (100 m), wind speed (5.6 m/sec), and plume width, increased entrainment velocities result in proportional increases in dilution. As noted in Figure 8 a fairly substantial entrainment rate of 10 m/sec will result in about a ten-fold dilution for these conditions.

Increased wind speed advects the gas plume through the spray zone more quickly. Figures 9 exhibits the marked effects of wind speed on dilution effectiveness. Given a constant water spray entrainment rate of 6 m/sec, then a plume moving slowly through the spray curtain at 1 m/sec will receive about 12.5 times more dilution than a plume traveling at 10 m/sec. Cloud height increases by the same ratio.

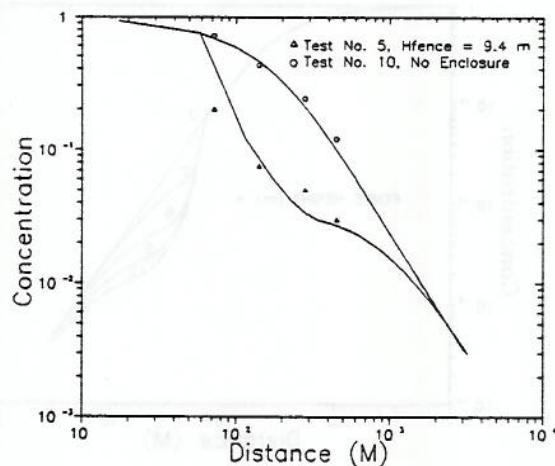
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**Figure 1** Predicted concentrations for Pre Falcon Tests No. 5 and 10.  $Q_L = 40 \text{ m}^3/\text{sec}$ ,  $U = 3.5 \text{ m/sec}$ ,  $T_s = 111 \text{ oK}$ ,  $T_{\text{amb}} = 300 \text{ oK}$ .

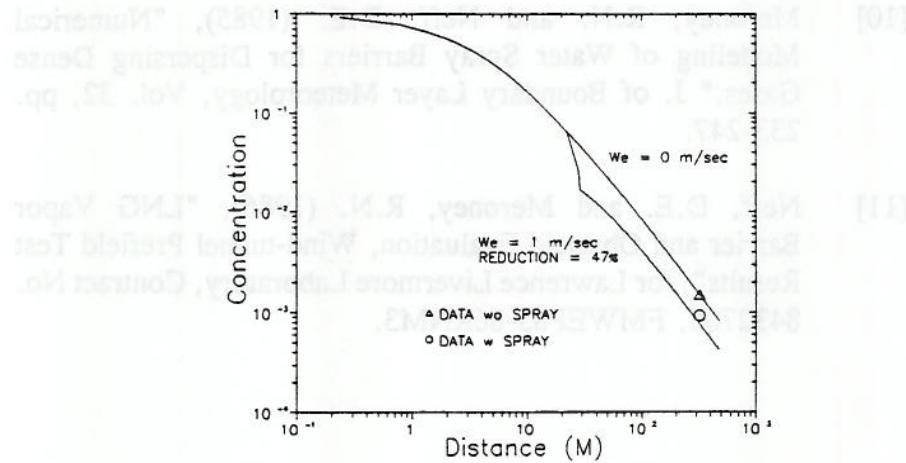


Figure 2 Comparison of observed and SPRAY 65 predicted plume centerline concentrations for Goldfish Test No. 6.  $Q_L = 33$  gallons/min,  $U = 5.4$  m/sec.

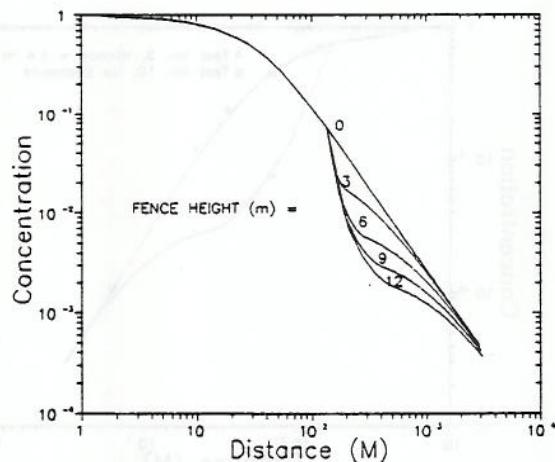


Figure 3 FENC62 predicted plume centerline concentrations for Goldfish Test No. 1, Fence heights = 0, 3, 6, 9, and 12 m/sec at  $X = 100$  m.

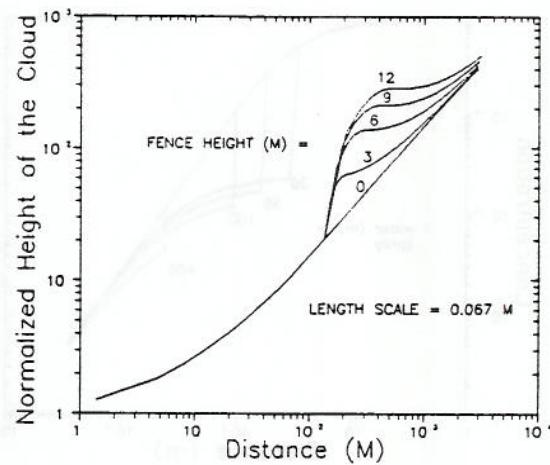


Figure 4 FENC62 predicted plume heights for Goldfish Test No. 1, Fence Heights = 0, 3, 6, 9, and 12 m at  $X = 100$  m.

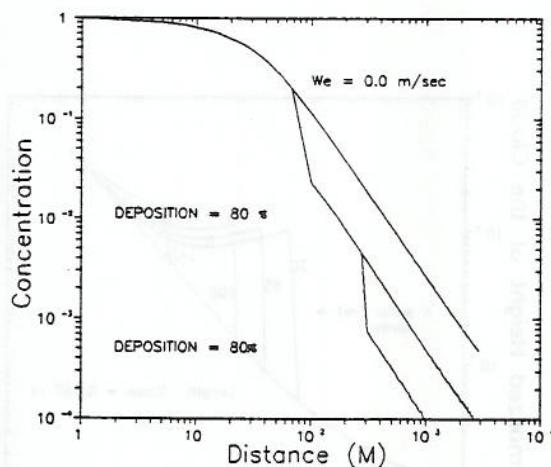


Figure 5 SPRAY65 predicted plume centerline concentrations for Goldfish Test No. 1, 80% HF removal by water spray at  $X = 100$  m and  $X = 300$  m.

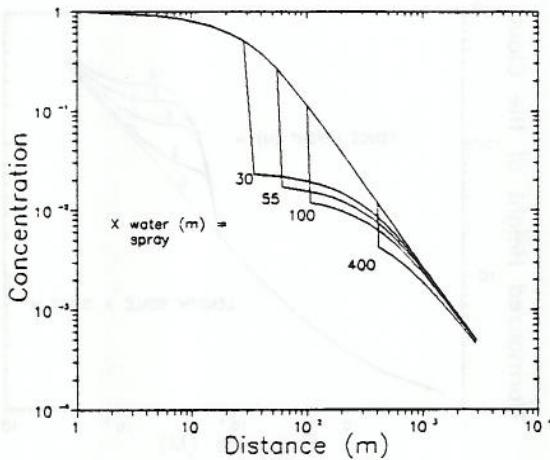


Figure 6 SPRAY62 Predicted plume centerline concentrations for Goldfish Test No. 1, Water Spray placed at  $X_{\text{spray}} = 30, 55, 100$  and 4, 6, 8 and 10 m/sec

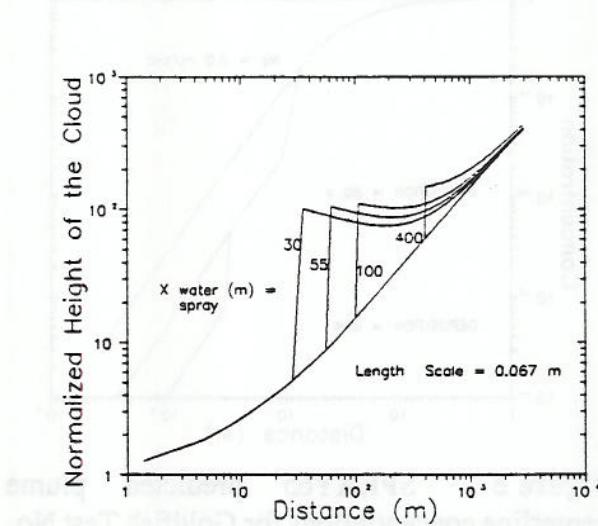


Figure 7 SPRAY62 predicted plume heights for Goldfish Test No. 1, Water spray placed at  $X_{\text{spray}} = 30, 55, 100$  and 400 m

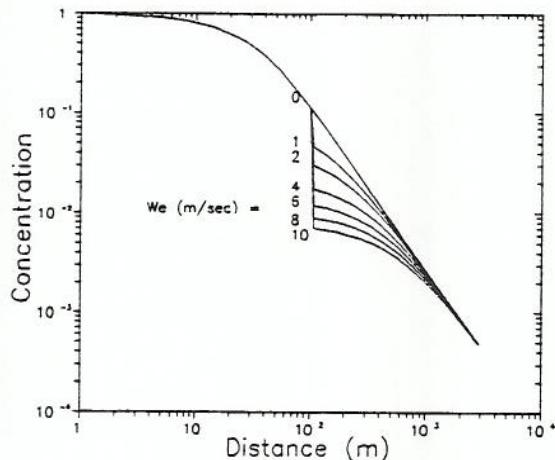


Figure 8 SPRAY62 predicted plume centerline concentrations for Goldfish Test No. 1,  $X_{\text{spray}} = 100$  m,  $W_e = 1, 2, 4, 6, 8$  and  $10$  m/sec

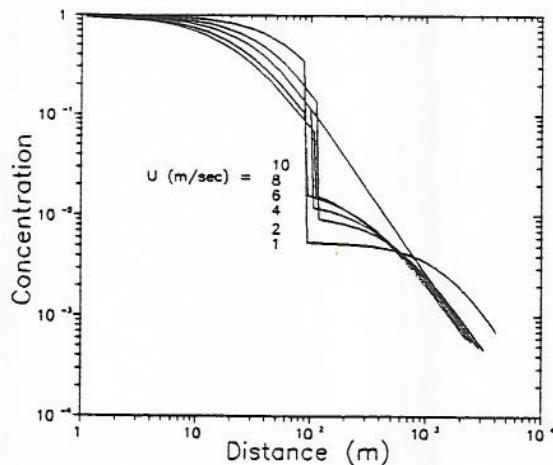


Figure 9 SPRAY62 predicted plume centerline concentrations for Goldfish Test No. 1,  $X_{\text{spray}} = 100$  m,  $W_e = 6$  m/sec,  $U = 1, 2, 4, 5, 6, 8$  and  $10$  m/sec

