UCRL--90150

DE84 005210

UCRL- 90150
PREPRINT

CONF-830802--1-Summ.

SIMULATIONS AND PARAMETER VARIATION STUDIES OF HEAVY GAS DISPERSION USING THE SLAB MODEL - CONDENSED

David L. Morgan, Jr.
Edward J. Kansa
Louise K. Morris

NOTICE
PORTIONS OF THIS REPORT ARE ILLEGIBLE.
It has been reproduced from the best available copy to permit the broadest possible availability.

This paper was prepared for submittal to the IUTAM Symposium, organized by the Delft University of Technology, "Atmospheric Dispersion of Heavy Gases and Small Particles", The Hague, The Netherlands, August 29 - September 2, 1983.

December 1983

Lawrence Livermore National Laboratory

This is a preprint of a paper intended for publication in a journal or proceedings. Since changes may be made before publication, this preprint is made available with the understanding that it will not be cited or reproduced without the permission of the author.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

SIMULATIONS AND PARAMETER VARIATION STUDIES OF HEAVY GAS DISPERSION USING THE SLAB MODEL - CONDENSED*

D.L. MORGAN, JR.; E.J. KANSA; L.K. MORRIS
Liquefied Gaseous Fuels Program
Lawrence Livermore National Laboratory
Livermore, California

Summary

We are employing the SLAB model in ongoing studies of the atmospheric dispersion of heavy gases. SLAB computer simulations of four of the Burro series large-scale 40-m^3 liquefied natural gas (LNG) spill experiments at China Lake, California [1] have been successful in predicting distances to the lower flammability limit (LFL) [2]. We have used this model in simulations of three of the Coyote series of experiments [3] as well as in parameter variation and sensitivity studies [4] and improved simulations of some of the Burro tests. The parameters studied include source rate, wind speed, atmospheric stability, type of source gas, and source duration, as well as the parameters important to certain physics submodels.

The SLAB Model

The SLAB model is a one-dimensional model describing diffusion and gravity flow of a heavy gas released into the atmosphere [2, 4-6]. The properties of the air-gas cloud are treated explicitly in their dependence on downwind distance (x) and time. The properties are slab-averaged in the horizontal (y) and vertical (z) crosswind directions.

Five coupled, partial differential equations (PDEs) of the model express the conservation of air and gas masses, downwind and horizontal momenta, and thermal energy. They are derived by averaging the Navier-Stokes conservation equations over y and z within the limits of the cloud. With the use of the hydrostatic approximation for pressure, these equations relate cloud motion, density, and temperature to the forces that affect them: gravity, the mixing in of air, heat flow from the ground, ground friction, air resistance, and the source gas. Another PDE defines the cloud

---

*Work performed under the auspices of the USDOE by LLNL under contract number W-7405-ENG-48 and the Gas Research Institute.

width by stating that the downwind-Lagrangian speed of the cloud edge in the y-direction is the material speed (v_g) plus the horizontal air-entrainment speed (v_e). Together with the ideal gas law this equation provides the additional information necessary for defining the size and shape of the cloud. Thus, the SLAB model is quasi-three-dimensional. Algebraic submodels are employed to calculate turbulent diffusion (using entrainment), heat flow, friction, height-dependent wind speed, and crosswind gas concentration. In the averaging, it is assumed that concentration and temperature are independent of y and z, while the downwind cloud speed is independent of y and has a prescribed power law dependence on z. The speed in the y-direction is assumed to be proportional to $|y|$. Since the model cloud is symmetric about $y = 0$, it is only necessary to consider one half of the cloud. This is done in defining the dependent variables of the SLAB equations which are (per unit downwind distance for all but B):

m = total mass of air and heavy gas,
m_1 = mass of heavy gas,
ε = thermal energy,
P_x = downwind component of momentum,
P_y = mean horizontal crosswind component of momentum, and
B = width of the half-cloud.

The variables, height (h), density (ρ), temperature (T), cloud speed (u), and volume concentration (C_o), as well as v_g can be related to the above variables, e.g.,

$$C_o = \frac{m_1}{m_1 + (m - m_1)M_s/M_a} \quad , \quad u = P_x/m, \quad v_g = 2\ P_y/m,$$

where M_s and M_a are the molecular weights of the source gas and air. A formula based on experimental and theoretical information is employed to obtain the concentration distribution in a crosswind plane:

$$C = C_o\ e^{-z/h\ -\ \pi y^2/4B^2} \quad ,$$

where it is assumed that the maximum concentration in the crosswind plane is equal to C_o.

Turbulent mass diffusion is modeled by entrainment of air into the cloud surface. The entrainment rate depends on the air-cloud density and velocity differences and on the friction and convection velocities of the cloud. As the cloud becomes dilute the entrainment rate approaches ambient. Our formulae for the vertical and horizontal entrainment speeds, w_e and v_e, are fitted to experimental data and were derived by Morgan, Ermak, and Zeman [4-6]. The submodel formulae for w_e and v_e are:

$$w_e = \frac{0.4\ w}{D}, \qquad v_e = (1.8)^2\ \frac{h}{B}\ w_e\ ,$$

where

$$w = (u_*^2 + 0.02\ (\delta u)^2 + 0.27\ w_*^2)^{1/2},$$

$$D = \begin{cases} 1 + 0.28\ \mathrm{Ri} & \text{for Ri} \geq 0\ , \\ (1 - 0.90\ \mathrm{Ri})^{-1/4} & \text{for Ri} < 0\ , \end{cases}$$

where u_* is the cloud friction velocity, δu is a density-adjusted cloud-air velocity difference, and w_* is the convection scale velocity. Ri is the Richardson number for the cloud, $g(1-\rho_a/\rho)\ h/w^2$, where ρ_a is the air density, but its value is adjusted to approach the ambient value as the cloud becomes dilute.

We use an empirical formula for heat flux from the ground, based on measurements made during the Burro series [1]:

$$j \simeq 0.0125\ C_p\ \rho(T_a - T),$$

where C_p is the specific heat of the cloud and T_a the air temperature. The formulae for the fluxes of horizontal momentum from the cloud into the ground (the effect of the ground friction) follow from atmospheric surface boundary layer theory [5]:

$$\tau_x = \rho u_*{}^2 u/(u^2 + v^2)^{1/2}, \quad \tau_y = \rho u_*{}^2\ v/(u^2 + v^2)^{1/2},$$

where $v = P_y/m$ is the mean horizontal crosswind cloud speed.

The SLAB code employs a height-dependent wind speed u_a. The speed of the air entrained into the cloud is assumed to be equal to the ambient wind speed at $z = h$:

$$u_a = u_{a2}(h/h_2)^n,$$

where u_{a2} is the measured average wind speed at $h_2 = 2$ m. The exponent is chosen to match the variation of wind speed with z for the conditions of interest.

The theory of the SLAB model was initially developed by Zeman [5]. The current theoretical form was derived by Ermak and Morgan [2,6]. The SLAB computer model was developed by Morgan and Morris [6] and is described in detail in [4] and [6].

Simulations

We have conducted simulations of seven of the Burro and Coyote tests. The principal spill and meteorological parameters describing these experiments are given in the following table.

LNG Spill Tests

	B3	B7	B8	B9	C3	C5	C6
LNG Volume (m^3)	34.0	39.4	28.4	24.2	14.6	28.0	22.8
Spill Rate (m^3/min)	12.2	13.6	16.0	18.4	13.5	17.1	16.6
Wind Speed (m/s)	5.4	8.4	1.8	5.7	6.0	9.7	4.6
Ambient Richardson No. at 2m	-0.22	-0.02	+0.12	-0.01	-0.32	-0.08	+0.03

Figure 1 shows the maximum observed values of 10-s averaged LNG vapor concentration (by volume) observed at various downwind distances from the source for six of the seven tests. From such information the maximum distances to the LFL (C = 5%) can be determined (least squares linear fit on a log-log plot, emphasizing points near the LFL). These distances are shown in Fig. 2, where they are compared to SLAB predictions. The comparisons show good agreement, with Burro 8 being the weakest which we believe is due to the relatively high ambient stability, low wind speed, and high spill rate resulting in terrain-influenced gravity flow and cloud bifurcation[7]. The SLAB model cannot predict such effects. It is also possible that the entrainment and heat flow submodels may not be sufficiently accurate for Burro 8.

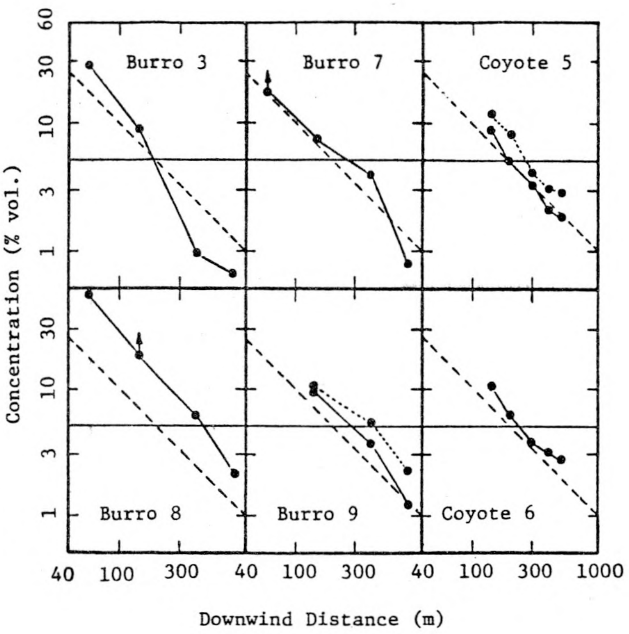

Fig. 1. Maximum values of 10-s averaged data. Dotted lines indicate data in which RPT effects have not been removed. The solid horizontal line is the 5% LFL. The dashed line is for visual reference (C[%] = 1000/x[m]). Arrows indicate instrument saturation. The results for Coyote 3 are simular to those for Burro 3.

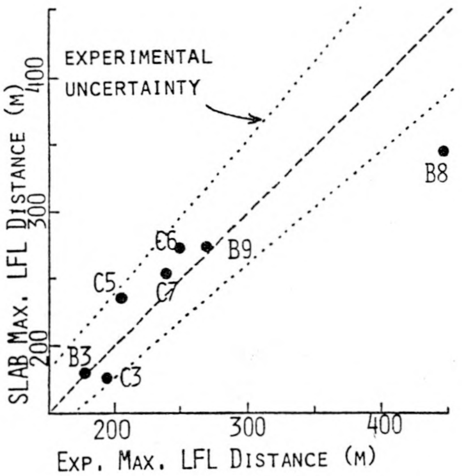

Fig. 2. SLAB vs experiment LFL distance comparison.

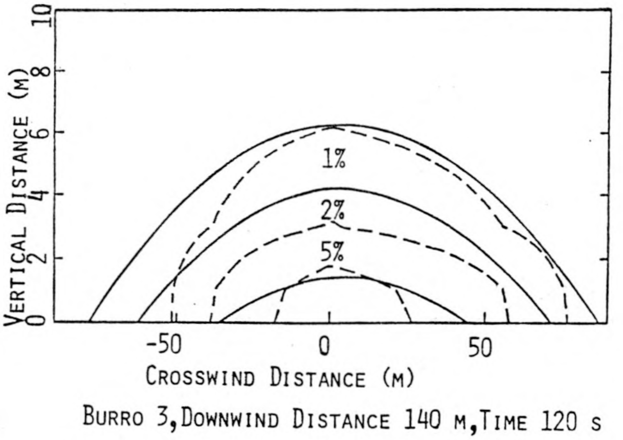

Fig. 3. SLAB (solid) vs experiment (dashed) ccrosswind concentration comparison.

Figure 3 is an example of a comparison between crosswind concentration contours calculated by SLAB and from experimental data. The good agreement is typical of most comparisons excluding the bifurcated cloud of Burro 8.

Figure 4 shows typical examples of SLAB vs experiment, time-history comparisons for 1 m above the surface. Two comparisons at 3 m (Coyote 5) are included. In each case, the SLAB centerline (y = 0) concentration for the indicated height above ground and downwind distance is compared to experimentally determined concentrations for all sensors in a horizontal crosswind row at the same height and distance. Such a comparison is made due to

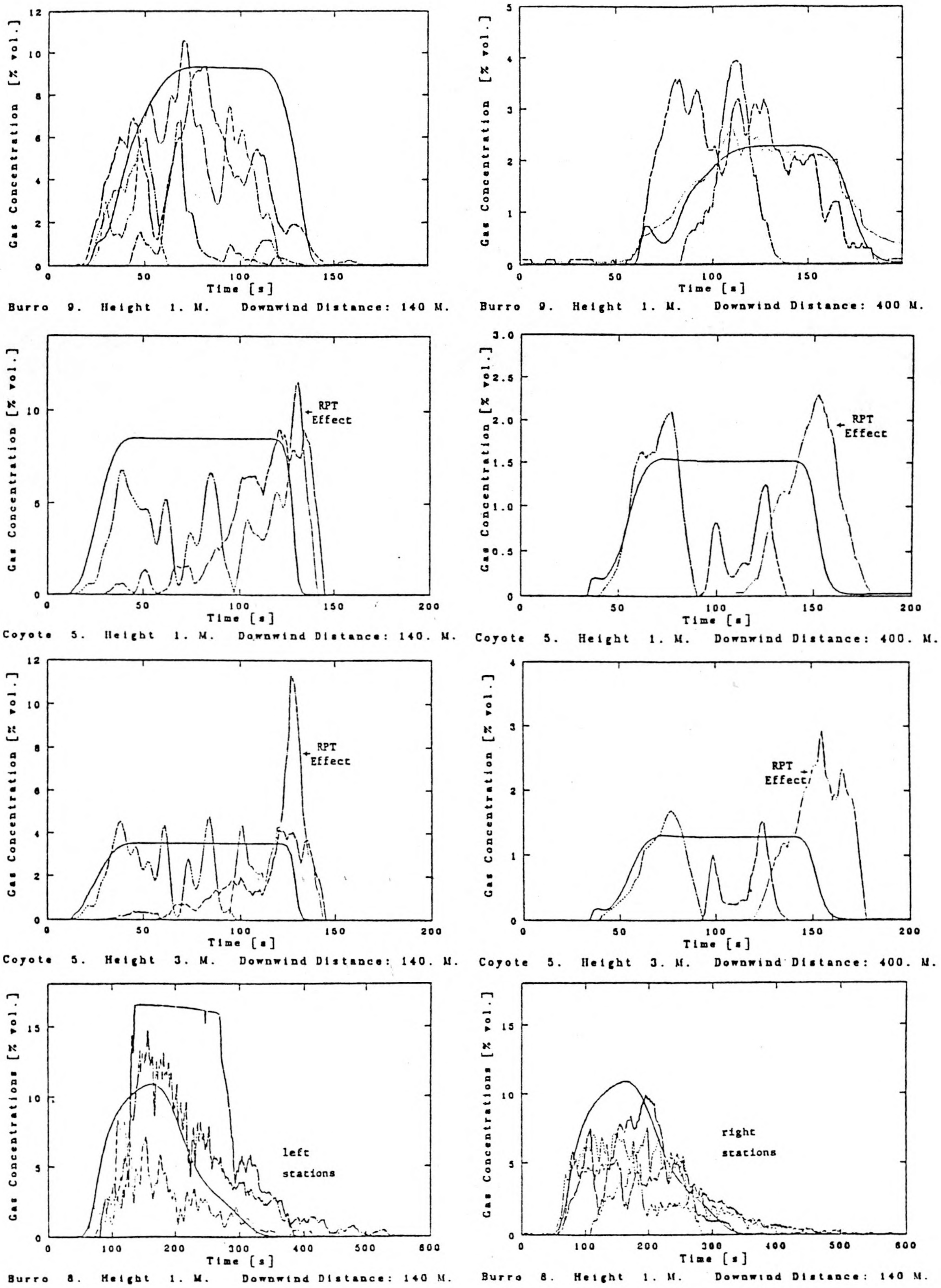

Fig. 4. Examples of SLAB (solid curve) vs experiment concentration time history comparisons.

meander of the cloud centerline. When the centerline passes over a sensor, the resulting concentration peak is the mean centerline concentration except for the presence of relatively smaller turbulent variations in the 10-s averaged data. Thus a correct model result would probably fall slightly below the highest concentration peaks.

In Burro 9 and Coyote 5, RPT explosions [8] released puffs of LNG vapor that momentarily increased concentrations downwind. Such phenomena were not modeled by SLAB. Their presence is noted in the Coyote 5 comparisons where the effect was substantial.

The SLAB time-history curves compare well with experimental data for Coyote 5 and Burro 9. The same is true for Burro 8 except for the very high concentration measured by the G11 sensor at 1 m (the nearly flat top of this curve is due to instrument saturation) and the fact that the cloud tended to arrive and depart somewhat later than predicted by SLAB. Both of these differences are probably due to terrain-influenced gravity flow. The G11 station was 4m lower than the average elevation of the 140 m row.

Parameter Study

Results of the parameter study using SLAB show the effects of individual variations of five parameters about values that define an LNG base case: rate 135 kg/sec; wind speed 5.7 m/s; neutral atmospheric stability. The base case is similar to Burro 9 except a value of 0.05 is used for the friction coefficient c_f, instead of 0.08 as subsequently recommended by Zeman [private communication] and the source remains on until steady state is reached (c_f affects the entrainment rate since u_* is taken to be proportional to it).

Results for variations in wind speed, stability, and in source rate, type, and duration are in Ref. [4]. Except for possibly wind speed, they agree with physical expectation. The effects on concentration, height, and width of the cloud, due to resulting variations in gravity flow, turbulent mixing, and cloud heating, are seen.

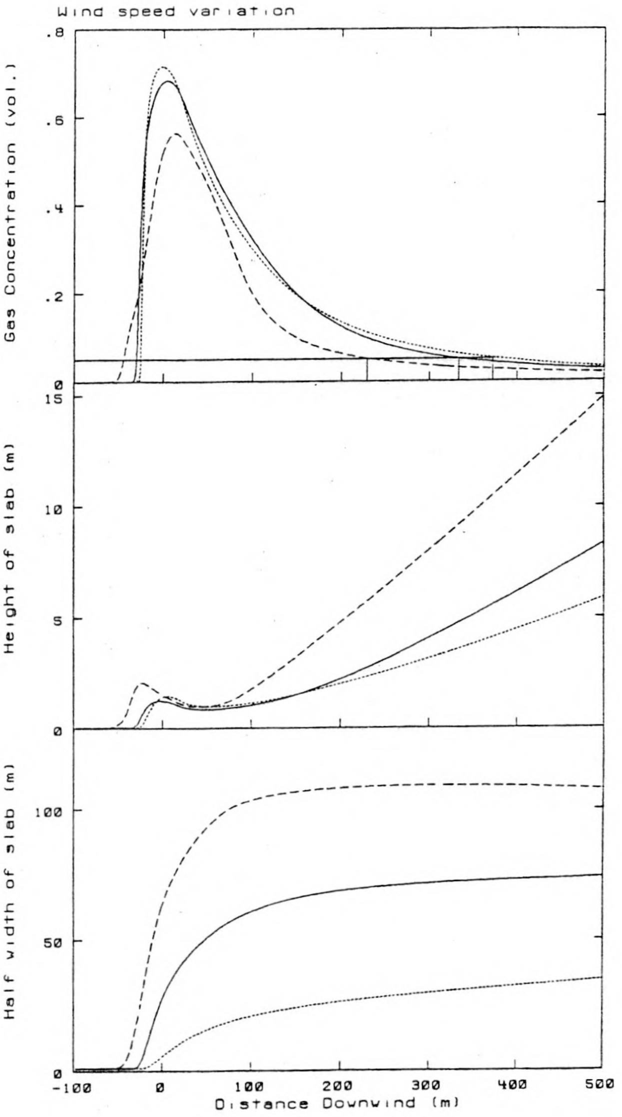

Fig. 5. SLAB predicted effects of wind speed variation on LNG vapor dispersion (3m/s dashed; 5.7 m/s solid; 15 m/s dotted). Ambient stability, source rate, and other parameters are held constant. The horizontal line in the concentration plot is the 5% LFL. The effects of wind speed variation are markedly different from the wind speed effects on the dispersion of trace pollutants, where cloud height and width are independent of wind speed and concentration is inversely proportional to wind speed.

The results for wind speed variation (stability is held constant) are shown in Fig. 5. Increasing u_{a2} reduces the height and width of the cloud (they are constant for trace pollutants), since the air-cloud density difference leads to entrainment speeds that are much less than proportional to u_{a2}. This decreased dependence of entrainment on wind speed is sufficient, in the SLAB model, to lead to the higher values of downwind concentration for higher wind speed shown in the figure. This result is in contrast to trace pollutant dispersion where concentration is inversely proportional to wind speed. In light of the approximate nature of SLAB's entrainment formulation, the exact magnitude of this difference in wind speed dependence is uncertain, but it is clear that such a difference exists. Our experimental data may indicate a slight inverse dependence of concentration on wind speed for constant source rate and ambient stability, but they are definately inconsistent with the inverse proportionality for trace pollutants.

We have also tested the sensitivity of our results to the friction coefficient value c_f, the choice made for the heat flow submodel, and to inclusion of the retarding force of surface friction on motion of the cloud. Details of these tests are given in Ref. [4]. A base case similar to the above was employed. We find that the recommended value of $C_f = 0.08$ gives good agreement with experiment but values of 0.04 and 0.12 give poor agreement. Employing a theoretical ground heat flow model in place of our empirical model also significantly reduces agreement [4]. In contrast, taking the surface friction to be zero has no signifcant effect on our results. Thus, at least for the conditions of the base case, accurate submodels for entrainment and heat flow are important for accurate modeling of LNG vapor dispersion, but the retarding force of surface friction is not.

Conclusions

The SLAB model has achieved good agreement with experimental data in predicting gas concentration levels measured in the seven Burro and Coyote vapor dispersion experiments it simulated. In the most difficult case (Burro 8), SLAB did reasonably well in predicting those features for which it was designed.

The dependence of SLAB model results on source rate, atmospheric stability, source type, and source duration is physically reasonable. The dependence of downwind concentration on wind speed indicates less of a dependence in heavy gas dispersion than the inverse proportionality in trace pollutant dispersion. This alteration is significant and worthy of further investigation.

The choice of model for heat flow from the ground into the cloud is found to be quite significant to the dispersion of the cold

LNG vapor. The level of air entrainment, which is somewhat uncertain, is also quite significant, and it is therefore important to formulate accurate entrainment/turbulence models for heavy gas dispersion. For the cases studied, the retarding effects of ground friction on the cloud appear to be of much less significance.

References

1. Koopman, R.P.; Cederwall, R.T.; Ermak, D.L.; Goldwire, H.C. Jr.; Hogan, W.J.; McClure, J.W.; McRae, T.G.; Morgan, D.L.; Rodean, H.C.; Shinn, J.H.: Analysis of Burro series 40-m^3 LNG spill experiments. J. Haz. Mat. 6 (1982) 43-83.

2. Ermak, D.L.; Chan, S.T.; Morgan, D.L.; Morris, L.K.: A comparison of dense gas dispersion simulations with the Burro series LNG spill test results. J. Haz. Mat. 6 (1982) 129-160.

3. Goldwire, H.C., Jr.; Rodean, H.C.; Cederwall, R.T.; Kansa, E.J.; Koopman, R.P.; McClure, J.W.; McRae, T.G.; Morris, L.K.; Kamppinen, L.M.; Kiefer, R.D.; Urtiew, P.A.; Lind, C.D.: Coyote series data report, LLNL/NWC 1981 LNG spill tests, dispersion, vapor burn, and rapid phase transition. UCID-19953, LLNL, Livermore, Calif. (1983).

4. Morgan, D.L., Jr; Kansa, E.J.; Morris, L.K.: Simulations and parameter variation studies of heavy gas dispersion using the SLAB model. UCRL-88516, LLNL, Livermore, Calif. (expanded version of this report).

5. Zeman, O.: The dynamics and modeling of heavier-than-air cold gas releases. Atmos. Environ. 16 (1982) 741-751.

6. Morgan, D.L. Jr.; Morris, L.K.; Ermak, D.L.: SLAB: a time-dependent computer model for the dispersion of heavy gases released in the atmosphere. UCRL-53383, LLNL, Livermore, Calif. (1983).

7. Chan, S.T.; Rodean, H.C; Ermak, D.L.: Numerical Simulations of Atmospheric Releases of Heavy Gases Over Variable Terrain. UCRL-87256, LLNL, Livermore, Calif, (1982)

8. McRae, T.G.: Preliminary analysis of RPT explosions observed in the LLNL/NWC LNG spill tests. UCRL-87564, LLNL, Livermore, Calif. (1982).

DISCLAIMER

Technical Information Department · Lawrence Livermore Laboratory
University of California · Livermore, California 94550