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Application of dispersion models to flammable cloud analyses

Thomas O. Spicer *, Jerry Havens

Chemical Hazards Research Center, University of Arkansas, 700 West 20th Street, Fayetteville, AR 72701, USA

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Abstract

The accidental release of flammable gases may result in a gas cloud which presents a hazard due to heat exposure (from burning), mechanical damage due to generated overpressures (from explosion), or both. The damage potential in such incidents depends not only on the material released but also on the spatial gas distribution as a function of time and the degree of confinement.

Estimates of the temporal and spatial distribution of gas clouds formed from accidental releases can be made using physical (wind or water tunnel) models or mathematical models. This article discusses the application of mathematical dispersion models to the prediction of the spatial and temporal distribution of gas in the vicinity of an accidental release. A primary objective of such analyses is to estimate the amount of gas which exists at concentrations above the lower flammability limit and the amount of gas which exists at concentrations between the upper and lower flammability limits.

Based on experiments performed by Shell Research Limited on the ignition of denser-than-air flammable clouds, examples of the application of the DEGADIS and FEM3A models are described, and the sensitivity of DEGADIS model predictions to gas release rate and windspeed is examined.

Keywords: Dense gas dispersion; Flammability; Vapor cloud fire; Vapor cloud explosion

1. Introduction

Many flammable gases form denser-than-air gas clouds when accidentally released to the atmosphere. The behavior of denser-than-air gas clouds differs significantly from the

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* Corresponding author. Tel: (501) 575-2055; Fax: (501) 575-8718; E-mail: tos@engr.uark.edu

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behavior of passive clouds in two important aspects: denser-than-air clouds can displace the atmospheric flow field and can exhibit significant upwind and lateral spread; and dilution of the denser-than-air gas cloud with air by atmospheric turbulence is reduced because of the stable density stratification present. For low momentum releases of flammable gas (such as from boiling liquefied natural gas or propane), which forms a boiling liquid pool, the intensity of these denser-than-air effects can be quantified with a Release Richardson number:

$$Ri_c = \frac{g}{u_*^2}\left(\frac{\rho_i - \rho_a}{\rho_a}\right)\frac{E}{\rho_i u D}$$

where E is the release rate (kg s^{-1}), ρ_i is the initial density of the flammable gas (kg m^{-3}) released to the atmosphere, D is the diameter of the area source (m), u is the ambient windspeed typically at 10 m elevation (m s^{-1}), u_* is the friction velocity (m s^{-1}), ρ_a is the ambient air density (kg m^{-3}), and g is the acceleration due to gravity. When spill conditions are such that $Ri_c > 1$, denser-than-air effects are important, and a passive dispersion model should not be used to predict the cloud properties. This article uses two available models which take these effects into account: DEGADIS and FEM3A.

Developed through research sponsored by the U.S. Coast Guard, Gas Research Institute, and the U.S. Environmental Protection Agency, DEGADIS models denser-than-air effects for low-momentum, ground-level releases and for vertical jet releases by making suitable assumptions so that the governing system of partial differential equations is simplified to a system of ordinary differential equations [1,2]. DEGADIS is consistent with (established) passive dispersion principles as the cloud density approaches ambient density.

Developed by Lawrence Livermore National Laboratory [3,4], FEM3A solves the governing partial differential equations using a (weak) Galerkin finite element solution technique in space and a finite difference solution technique in time. FEM3A allows for terrain and obstacle effects to be modeled. The present version of FEM3A has two turbulence closure submodels: a planetary boundary layer model similar to the model used in DEGADIS (and consistent with passive dispersion principles), and an isotropic k-ϵ turbulence closure model.

There are several methods which have been proposed to quantify the potential for damage associated with the accidental release of a flammable gas. All of these techniques, from the most simple [5,6] through the more complicated (such as the multi-energy method) [7] to the very complex [8] require some estimate of the flammable gas distribution when it encounters an ignition source. DEGADIS and FEM3A can be used to estimate the spatial distribution of a flammable gas cloud as a function of time. By integration of the assumed concentration profiles, DEGADIS provides estimates of the mass of flammable gas above the lower limit of concern (LLC – typically taken to be the lower flammable limit LFL) and the mass of flammable gas between the upper limit of concern (ULC – typically taken to be the upper flammable limit UFL) and the LLC. By integration of the calculated concentration distribution, FEM3A can provide estimates of the same parameters.

2. Shell Research Ltd. experiments at Spadeadam

Evans and Puttock [9] reported a series of experiments aimed at determining the time-averaged concentration (as a fraction of the LFL) where a gas cloud would become flammable. In a series of eight experiments conducted at Spadeadam (UK), propane was released at a constant rate into a water-filled bund in the corner of a level concrete pad 100 m on edge. A movable trolley carried five sets of igniters and gas concentration sensors all at 0.5 m elevation; an infrared camera was used to detect ignition of dispersing propane. In the experiments, the trolley was moved toward the propane source starting sufficiently far downwind to not ignite the cloud. Ignitions were classified as "small flames" (4 to 16 m diameter zone of hot gases), "large flames" (greater than 16 m diameter zone of hot gases), and "sustained flames" (flame which travelled back to the source).

In three of the tests, the wind direction changed so that the propane plume meandered away from the movable trolley. In the remaining tests, the windspeed ranged from 2 to 7 m s^{-1}; the spill rate was reported to be 4.9 kg s^{-1} to 5.85 kg s^{-1}. "Sustained flames" were reported for downwind distances from 55 m to 79 m. Using assumed ambient conditions (15°C, 1 atm, 75% humidity, *D* stability), a typical surface roughness of 2 cm, and a propane boil-off rate of 0.12 kg $m^2 s^{-1}$, the Release Richardson number ranged between 3 and 110 indicating denser-than-air effects were important.

Evans and Puttock pointed out that peak concentrations observed immediately before "sustained flames" should be adjusted to take into account the fact that the (time-averaged) mean concentration at that same location would be lower. As the mean concentration should be used for comparison with mathematical model predictions, Evans and Puttock argued that the mean concentration limit below which "small flames" are not predicted (mathematically) is 0.6 LFL and the mean concentration limit below which "sustained flames" are not predicted (mathematically) is 0.9 LFL (based on previous work with the same gas sensor at Maplin Sands [10]). (For propane, LFL is 2.1%, and UFL is 9.5%.)

3. DEGADIS simulations of Shell experiments

DEGADIS simulations were made using an average release rate (5.4 kg s^{-1}) and the windspeed extremes of 2 m s^{-1} and 7 m s^{-1}. As shown in Table 1, the (steady-state) DEGADIS-predicted distance to 0.9 LFL at 0.5 m elevation was 80 m for 2 m s^{-1} windspeed and 47 m for 7 m s^{-1} windspeed which is in agreement with the reported range of "sustained flames" (55 m to 79 m corresponding to 0.9 LFL at 0.5 m elevation). Although the windspeed changed by a factor of 3.5, the predicted distance to 0.9 LFL changed by only a factor of 1.7. Fig. 1 shows the DEGADIS-predicted development of the 0.9 LFL contour (at 0.5 m elevation) as a function of time for both cases. The low windspeed (high Richardson number) case clearly shows the upwind and lateral spreading characteristic of a denser-than-air gas cloud. Because of slower advection speeds, the low windspeed case also takes longer to reach its steady-state extent (120 s vs. 30 s for the 7 m s^{-1} case).

Table 1
DEGADIS simulation of propane releases at Spadeadam

Windspeed at 10 m ($\mathrm{m\ s^{-1}}$)	Extent of 0.9 LFL at 0.5 m (m)	Maximum mass of propane above 0.9 LFL (kg)	Maximum mass of propane between UFL and 0.9 LFL (kg)
2	80	390	220
7	47	47	35

The estimated mass of propane above 0.9 LFL and the estimated mass of propane between UFL and 0.9 LFL for the steady-state plumes are also shown in Table 1. As might be anticipated from the area coverage for the two cases shown in Fig. 1, the estimated mass of propane above 0.9 LFL for the low windspeed case is nearly an order of magnitude larger than the same estimate for the high windspeed case.

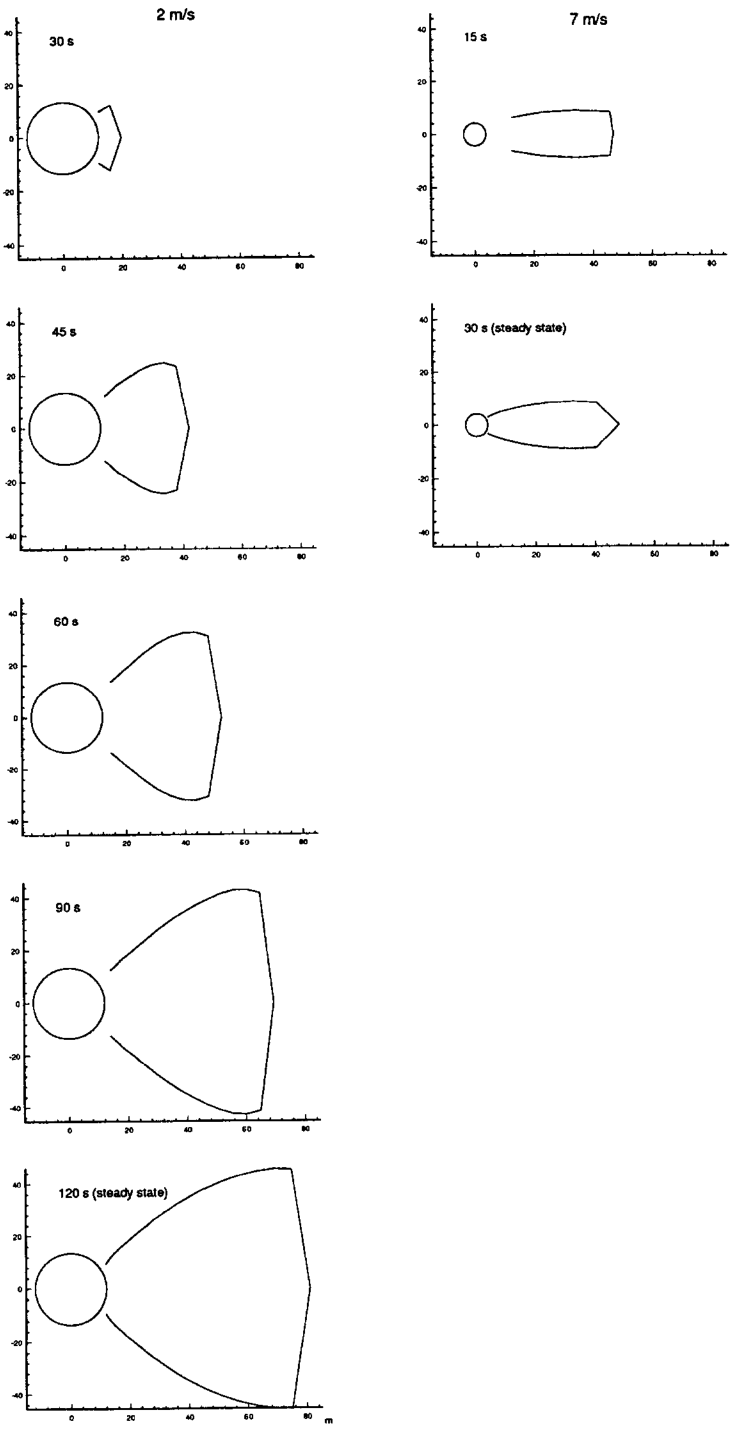
Fig. 2 shows the development of the estimated cloud mass and extent as a function of time for the low windspeed case. The steady-state DEGADIS simulation was used to determine steady-state conditions. The cloud development in time is simulated with DEGADIS using a series of pseudo steady-state observers which travel with the mean cloud advection speed; the transient cloud development was calculated until the steady-state conditions were met (120 s). Fig. 2 also shows a reference line with slope equal to the release rate (5.4 kg $\mathrm{s^{-1}}$). After the initial development of the cloud, the rate of growth of the mass above 0.9 LFL should be expected to approach that of the release rate for early times and to decrease as the plume approaches steady state which is shown in Fig. 2. Fig. 2 also shows that the mass between UFL and 0.9 LFL starts near zero after the initial development of the cloud and has a characteristic sigmoidal shape approaching steady state faster than the mass above LLC.

4. FEM3A simulations of Shell experiments

Using the guidelines in Spicer [11], FEM3A simulations were also made as described in Table 2 using the average release rate (5.4 kg $\mathrm{s^{-1}}$) and the windspeed extremes of 2 m $\mathrm{s^{-1}}$ and 7 m $\mathrm{s^{-1}}$. As shown in Table 3, the (steady-state) FEM3A-predicted distance to 0.9 LFL at 0.5 m elevation was 180 m for 2 m $\mathrm{s^{-1}}$ windspeed and 65 m for 7 m $\mathrm{s^{-1}}$ windspeed. In FEM3A, the predicted distance to 0.9 LFL changed by a factor of 2.8 when the windspeed changed by a factor of 3.5.

The estimated mass of propane above 0.9 LFL and the estimated mass of propane between UFL and 0.9 LFL for the steady-state plumes are also shown in Table 3. Similarly to the DEGADIS predictions, the estimated mass of propane above 0.9 LFL

Fig. 1. Development of the 0.9 LFL concentration contour (at 0.5 m elevation) as a function of time for windspeeds of 2 m $\mathrm{s^{-1}}$ and 7 m $\mathrm{s^{-1}}$.


2 m/s
7 m/s
30 s
15 s
45 s
30 s (steady state)
60 s
90 s
120 s (steady state)
40
20
0
-20
-40
0
20
40
60
80
m

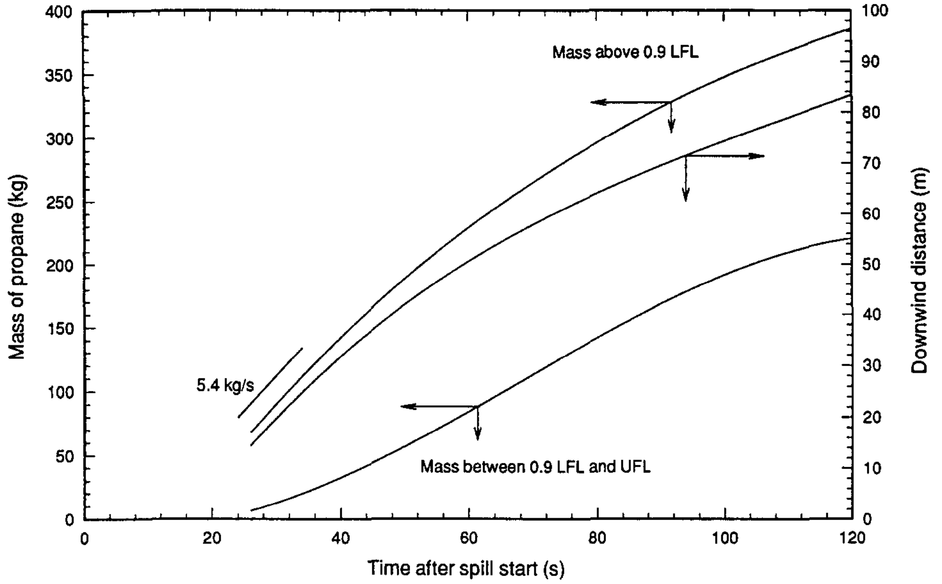


Fig. 2. DEGADIS-estimated cloud mass and extent as a function of time for the low windspeed (2m s^{-1}) case.

for the low windspeed case is over an order of magnitude larger than the same estimate for the high windspeed case.

Fig. 3 shows the development of the estimated cloud mass as a function of time for

Table 2
FEM3A parameters for Spadeadam simulations

	2m s^{-1} case	7m s^{-1} case
Alongwind nodes	56	46
extent (m)	−35 to 170	−35 to 120
minimum element size (m)	1.1	1.1
maximum element size (m)	5.0	5.0
Vertical nodes	20	20
extent (m)	0 to 30	0 to 30
minimum element size (m)	0.25	0.25
maximum element size (m)	2.0	2.0
Lateral nodes	18	18
extent (m)	−50 to 0	−50 to 0
minimum element size (m)	1.1	1.1
maximum element size (m)	5.0	5.0
Minimum vertical diffusivity (m^2 s^{-1})	0.0026	0.009
Minimum horizontal diffusivity (m^2 s^{-1})	0.042	0.146
Computation time step (s)	0.010	0.0025
Simulation time for steady state (s)	600	60
Execution time (CPU hs^{-1}) [a]	0.11	0.33

[a] Calculations were performed on a Digital Equipment Corporation DEC 3000 Model 400 workstation (rated at 111 SPECfp92) with 96 megabytes RAM.

Table 3
FEM3A simulation of propane releases at Spadeadam

Windspeed at 10 m ($m\ s^{-1}$)	Extent of 0.9 LFL at 0.5 m (m)	Maximum mass of propane above 0.9 LFL (kg)	Maximum mass of propane between UFL and 0.9 LFL (kg)
2	180	1410	990
7	65	86	56

the low windspeed case. The FEM3A-predicted curves show the same characteristic behavior as the DEGADIS-predicted curves.

5. Sensitivity of DEGADIS predictions to release rate and windspeed

To investigate the sensitivity of model predictions to changes in release rate and windspeed, a series of DEGADIS simulations were made using the Spadeadam tests as a base case. Two additional release rates were chosen: (7/2)5.4 kg s^{-1} and 54 kg s^{-1}; the windspeed range was unchanged. Steady-state DEGADIS simulation results are shown in Table 4. (Note that the maximum extent of 0.9 LFL in Table 4 is different from that reported in Table 1 because the maximum extent is predicted at ground-level.)

Table 4 shows that the windspeed variation becomes more important as the release rate increases for all three quantities (maximum extent of 0.9 LFL and the plume mass above 0.9 LFL and between UFL and 0.9 LFL) for these simulations. Windspeed and

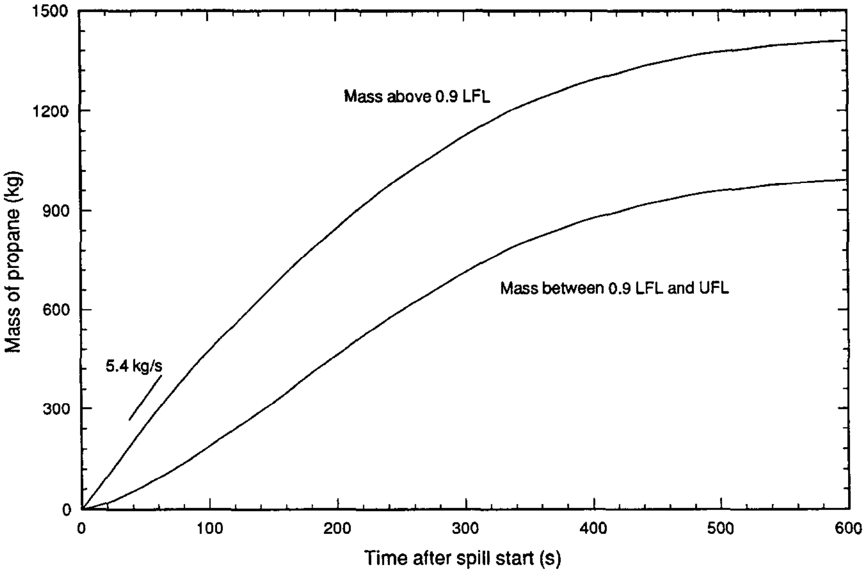


Fig. 3. FEM3A-estimated cloud mass as a function of time for the low windspeed (2 m s^{-1}) case.

Table 4
Sensitivity of DEGADIS simulations to changes in release rate and windspeed

Release rate (kg s^{-1})	Windspeed at 10 m (m s^{-1})	Maximum extent of 0.9 LFL (m)	Maximum mass of propane above 0.9 LFL (kg)	Maximum mass of propane between UFL and 0.9 LFL (kg)
5.4	2	100	390	220
	7	57	47	35
18.9	2	209	2590	1450
	7	105	296	210
54	2	388	12900	7110
	7	169	1390	940

release rate appear to be (approximately) equal in their relative importance for all three quantities. (The difference between a factor of 3.5 variation in windspeed and a factor of 3.5 variation in release rate is not very different, and the results for the 5.4 kg s^{-1}, 2 m s^{-1} case are not very different from the 18.9 kg s^{-1}, 7 m s^{-1} case for these three quantities (other simulation parameters were not compared).)

6. Comparison of DEGADIS predictions with a passive gas dispersion model predictions

As indicated above, denser-than-air effects are important when $Ri_c > 1$, and Ri_c is a function of not only the density of the released material but also the windspeed and release rate. Accordingly, if the 7 m s^{-1} windspeed base case release rate (5.4 kg s^{-1}) is decreased to 0.8 kg s^{-1}, $Ri_c \simeq 1$, and a passive dispersion model should apply even though the released propane is denser than air. (DEGADIS or FEM3A can also be used in this case since both are designed to be consistent with established passive dispersion techniques.) Hesse [12] reported a method for estimating the mass of gas in a passive plume between specified concentration limits based on the Gaussian diffusion model with power law representations for dispersion coefficients. Hesse's method (including important author errata distributed at the meeting where the paper was presented) was

Table 5
Comparison of Hesse's method and DEGADIS for passive cases

	Release rate (kg s^{-1})	Maximum extent of 0.9 LFL (m)	Maximum mass of propane above 0.9 LFL (kg)	Maximum mass of propane between UFL and 0.9 LFL (kg)
Hesse	0.4	11	5.7	0.4
	0.8	17	17	1.2
DEGADIS	0.4	16	1.1	0.9
	0.8	21	3.0	2.4

applied to two low Richardson number cases (0.8 kg s^{-1} and 0.4 kg s^{-1}); Hesse's approach is compared with DEGADIS predictions in Table 5.

As indicated in Table 5, DEGADIS predictions are in reasonable agreement with passive model predictions when considering maximum downwind extent to 0.9 LFL. However, note that these distances are short (< 100 m) because of the small release rate (required for the release to be passive), and passive dispersion coefficients must be extrapolated for short distances. DEGADIS and passive model predictions differ by about a factor of two on the mass of propane between UFL and 0.9 LFL for these passive cases, but both models seem to have the same trend over this limited range. In Hesse's approach, the estimate of mass above 0.9 LFL must by necessity include integration of the concentration profile back to the release point where passive dispersion techniques are known to be incorrect; therefore, the estimate of mass above 0.9 LFL using Hesse's approach is likely to be less reasonable than the DEGADIS estimate. Because DEGADIS was designed to model near-source behavior, DEGADIS estimates of maximum extent and cloud mass are likely to be more reasonable for short downwind distances (< 100 m).

7. Conclusions

Whether considering the damage of an accidental release of a flammable gas because of fire or explosion, gas dispersion models can provide important information concerning the potential hazard.

Considering all uncertainties, DEGADIS and FEM3A predictions of flammable cloud extent are generally consistent with observations reported by Evans and Puttock for releases of propane at Spadeadam using the suggested criteria of 0.9 LFL for ''sustained flames.'' We note that it appears that DEGADIS predictions are closer to the observed range of ''sustained flames'' (based on Evans and Puttock's analysis) than FEM3A predictions in this very limited comparison; further study is warranted.

For DEGADIS and FEM3A, the predicted mass of gas above the lower limit of concern (0.9 LFL here) grows at a rate which initially is the same as the gas release rate and decreases as the plume approaches steady state. The cloud mass predicted by FEM3A was larger than the cloud mass predicted by DEGADIS (mainly due to the longer downwind extent predicted by FEM3A for the low windspeed case).

Based on DEGADIS simulations, windspeed and release rate are (roughly equivalent) important determinants of the mass of gas above the lower limit of concern (0.9 LFL) and between the upper and lower limits of concern (UFL and 0.9 LFL).

For sufficiently small releases where $Ri_c < 1$, passive dispersion techniques may be applicable for determining maximum downwind flammable extent and mass between upper and lower limits of concern (UFL and 0.9 LFL), but Hesse's approach (based on passive dispersion modelling) should not be used to estimate mass above a lower limit of concern (such as 0.9 LFL). Because DEGADIS was designed to model near-source behavior, DEGADIS estimates of maximum extent and cloud mass should be used for short downwind distances (< 100 m) and for estimates of mass above typical lower limits of concern for $Ri_c > 0$.

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