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ANALYSIS AND SIMULATION OF THORNEY ISLAND TRIAL 34

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Summary

Results of Thorney Island Trial 34, which approximated an instantaneous release of heavy gas in zero wind conditions, are summarized. The gravity spreading and cloud dilution are predicted by laboratory scale instantaneous releases in calm air. The laboratory scale model experiment and Trial 34 are simulated with the MARIAH-II mathematical model which has been modified to incorporate a simplified second-order turbulence closure.

Introduction

The Gas Research Institute (U.S.A.)* sponsored a research program at the University of Arkansas to evaluate four 3-D mathematical models for atmospheric dispersion of LNG vapor clouds [1]. The four models were SIGMET-N [2], ZEPHYR [3], MARIAH-II [4] and FEM3 [5]. Determination of the models' applicability to the desription of gravity-driven flow and the associated air entrainment which initially dilutes rapidly formed heavy gas clouds was a principal task of the evaluation project. Havens and Spicer [6] reported laboratory experimental measurements of gravity spreading and dilution of right cylindrical volumes (35–500 l) of Freon-air instantaneously released in calm air. The Thorney Island Phase I trials provided field data on gravity spreading and dilution of instantaneously released right cylindrical volumes (nominally 2000 m^3) of Freon-nitrogen. The Phase I trials were conducted in a range of meteorological conditions. However, the initial gravity flow-dominated phase

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of the trials, during which the cloud was diluted to concentrations between 1 and 10%, was not strongly affected by the meteorological conditions [6], and this early phase of the experiments is predicted well by Froude number scaling of Havens and Spicer's laboratory experiments. An attempt was made to conduct a Thorney Island trial under as calm wind condition as possible to provide additional verification of the laboratory experiment scaling and to provide data from a field experiment which could be simulated with a two-dimensional (cylindrical coordinate) version of the complex mathematical models. The MARIAH-II model was used for the simulations reported here because it has been selected as the vehicle for evaluating a proposed turbulence closure, and because it is the only model (of the four) for which a 2-D cylindrical coordinate version has been developed. This paper compares the results of GRI-sponsored Trial 34 with a MARIAH-II simulation of the trial. Data from a laboratory scale (55 l) Freon release in calm air are also compared with the trial results and with the results of a MARIAH-II simulation.

Description of the experiments

Laboratory experiments

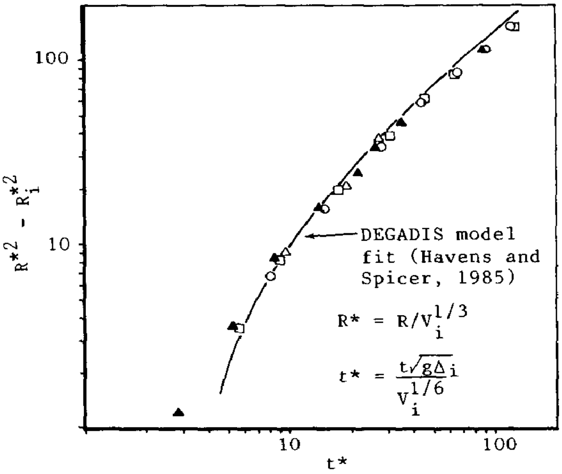
Havens and Spicer [6] reported laboratory, instantaneous releases of isothermal heavy gas volumes (35–500 l) with initial densities from 2.65 kg/m^3 to 5.0 kg/m^3. The data describe the gravity spread and air entrainment which occurs following such gravity-dominated-flow releases. Figures 1 and 2 indicate the position of the cloud spreading front (as determined from onset of measured gas concentration) and the peak-measured concentration as functions of time (or cloud front position) for the laboratory scale releases.

Thorney Island Trial 34

Trial 34 has been described by McQuaid [7]. Table 1 summarizes the important conditions.

Description of the MARIAH-II model

The MARIAH-II model is described in the final report to GRI [1]. The model incorporates simplified forms of the Navier–Stokes and energy balance equations with initial and boundary conditions describing a specified ambient flow (which can be zero) and the placement of contaminant gas into that flow. The Boussinesq approximation is invoked in the momentum balance equation, neglecting variations in density except in the buoyancy force terms. The equations are approximated with finite differences. The advection terms are calculated using the second-order Crowley method [8,9] with the FRAM (Filtering Remedy and Method) technique [10] to damp local oscillations.



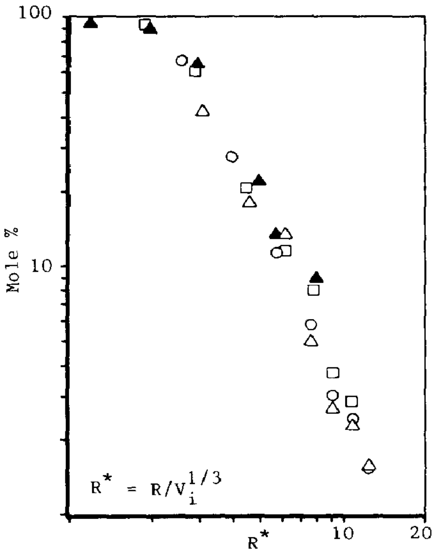


Fig. 1. Cloud front position versus time, Freon-12, $(H/D)_i = 1.0$, instantaneous release. Gas volume released: △ 0.035 m^3, ○ 0.054 m^3, □ 0.135 m^3, and ▲ 0.530 m^3.

Fig. 2. Maximum ground-level concentration versus distance from center, Freon-12, $(H/D)_i = 1.0$, instantaneous release. Gas volume released: △ 0.035 m^3, ○ 0.054 m^3, □ 0.135 m^3, and ▲ 0.530 m^3.

The diffusion terms are calculated implicitly, with the resulting linear equation system solved using the incomplete Cholesky conjugate gradient method [11].

The turbulence submodel originally used in MARIAH-II has been replaced with a local turbulence model derived from a second-order formulation incorporating the following simplifying approximations [12]:

- The theory is local, implying that all turbulent quantities are point functions depending on the state of the mean field; time- and space-derivatives of turbulence variables are neglected.

TABLE 1

Thorney Island Trial 34 conditions

Volume released	2110 m^3
Height-to-diameter ratio (initial)	~1.0
Relative (gas/air) density (initial)	1.83
Mean wind speed at 10 m	1.1 m/s
Mean wind heading (angle from centerline)	−20 degrees
Ambient air temperature at 9 m	9.1°C
Atmospheric stability	F

- The mean velocity field employed in the turbulence terms is simplified to retain dominant terms describing a stratified boundary layer; turbulent kinetic energy is strongly dependent on the magnitude of the shear of the flow field $S = [(\partial u/\partial y)^2 + (\partial v/\partial y)^2]^{1/2}$ and the gradient Richardson number $Ri = -[g(\partial \rho/\partial y)/\rho S^2]$.
- A length scale measured from the boundary is invoked. (In the simulations reported here, the length scale is the distance from the nearest solid boundary).

The formulation incorporating the above simplifications retains enough generality to describe a tensor diffusivity and to provide estimates of the variance of concentration. It is a generalization of methods developed [13] to describe the diffusivity of a trace constituent in a stratified boundary layer and to model the mixed layer dynamics of a water body [14]. The model can be evaluated numerically in closed form through solution of a quadratic equation for a scaled turbulence kinetic energy. Consequently, it is relatively inexpensive to evaluate and does not require additional storage for time-dependent quantities. When the distribution of concentrations is multidimensional, it is desirable to account for diffusion in the horizontal as well as the vertical direction. Under these conditions the local turbulence model results in a Fickian diffusion approximation. The diffusivities depend in a simple way on the components of the vertical derivative of horizontal wind as required by tensor covariance. In addition, they depend on the turbulence kinetic energy, the magnitude of the vertical shear of the wind, and the gradient Richardson number. A critical value of the Richardson number exists above which the diffusivity vanishes. The constituent added to the atmosphere is not restricted to be passive. Coefficients of turbulent viscosity and Prandtl and Schmidt numbers thus derived constitute a zero-equation formulation having a rather general dependence on local values of the mean flow solution.

Two-dimensional (Cartesian or cylindrical coordinate) versions of MARIAH-II have been developed. The 2-D cylindrical coordinate version was used for the calculations reported here.

Simulations with the MARIAH-II model

Laboratory experiments

Figure 3 shows a MARIAH-II prediction of the development of a 55 l Freon-12 release with an initial height-to-diameter ratio of 1.0. The cloud profile (half of the radially symmetric section), defined by the 1% volume fraction, is shown at zero time and 0.5, 1, 2, 3, 4, 5, and 6 s after release. The simulation was made with 1 cm square (two-dimensional) grid spacing. The initial grid size was 75 cells vertically and 200 cells radially. The grid size was changed at simulation time 2 s to 40 cells vertically and 500 cells radially. The simulation of 6 s real time required approximately 60 h computing time on a Digital Equip-

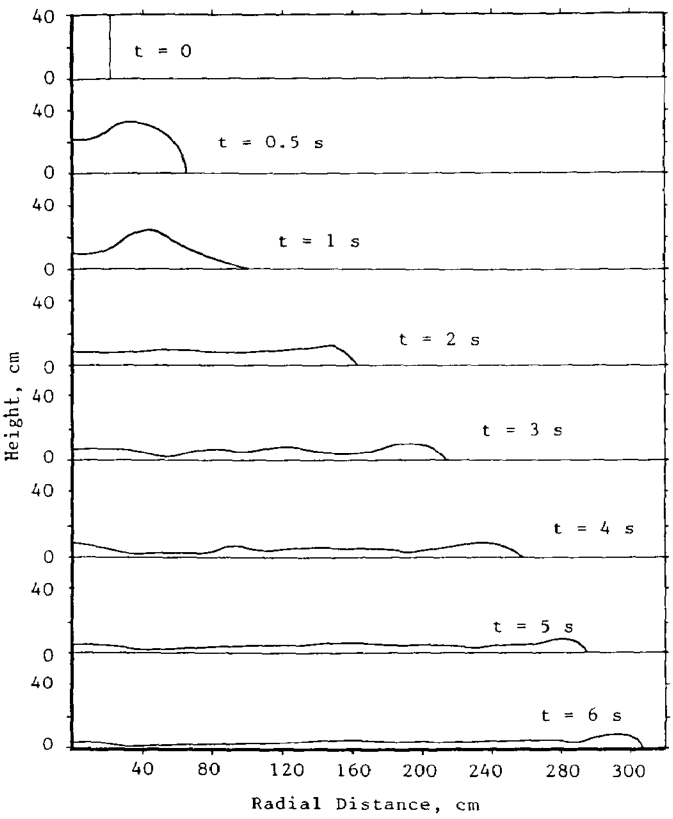


Fig. 3. Laboratory, calm-air, 55-l Freon-12 release, $(H/D)_i = 1.0$ – MARIAH-II prediction of cloud boundary (defined by 1% volume fraction) vs. time.

ment Company VAX 11-730 machine. Figure 4 shows the predicted vs. measured radial cloud extent for the same release.

Figure 5 shows MARIAH-II-predicted and measured maximum values of the gas cloud concentration and the cloud spatial average gas concentration as a function of time for the 55-l Freon-12 release. The predicted cloud average gas concentrations were obtained by spatial averaging the MARIAH-II prediction using cloud boundary concentration limits of 1% and 2.5%. The DEGADIS model cloud average concentration prediction [6] is shown for comparison.

Thorney Island Trial No. 34

Figure 6 shows a MARIAH-II simulation of a 2110 m^3 Freon-nitrogen (relative density = 1.83) release, with an initial height-to-diameter ratio of 1.0.

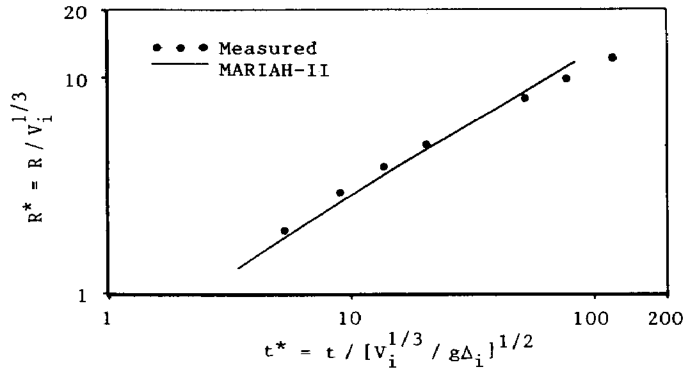


Fig. 4. Laboratory, calm-air, 55-l Freon-12 release, $(H/D)_i = 1.0$ - MARIAH-II prediction of cloud radial extent.

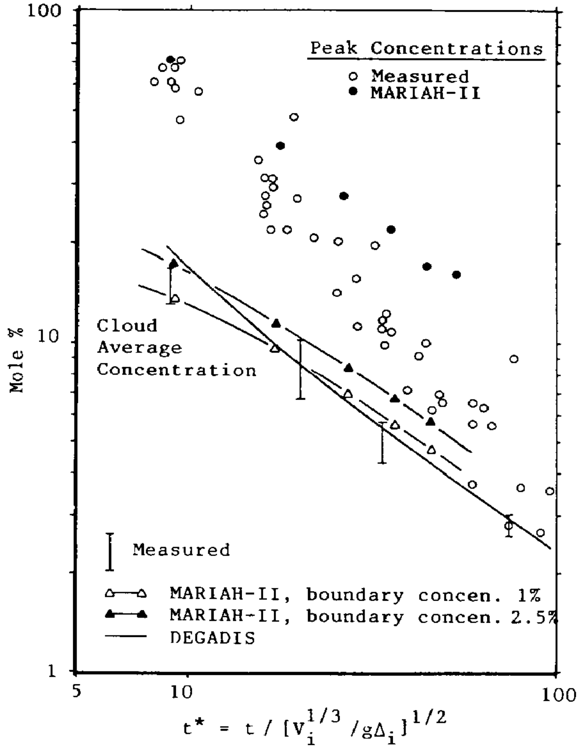


Fig. 5. Laboratory, calm-air, 55-l Freon-12 release, $(H/D)_i = 1.0$ – Measured and predicted cloud maximum and volume-averaged gas concentrations.

The simulation was made with 1/3 m square (two-dimensional) grid spacing. The initial grid size was 75 cells vertically and 200 cells radially. The grid size was changed at simulation time 24 seconds to 40 cells vertically and 500 cells

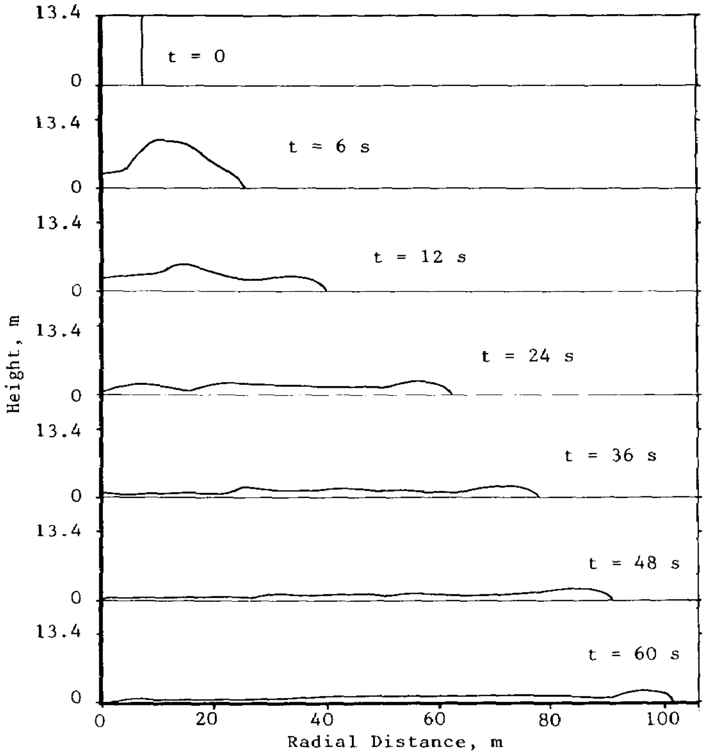


Fig. 6. Thorney Island Trial 34 – MARIAH-II prediction of cloud boundary (defined by 1% volume fraction) vs. time.

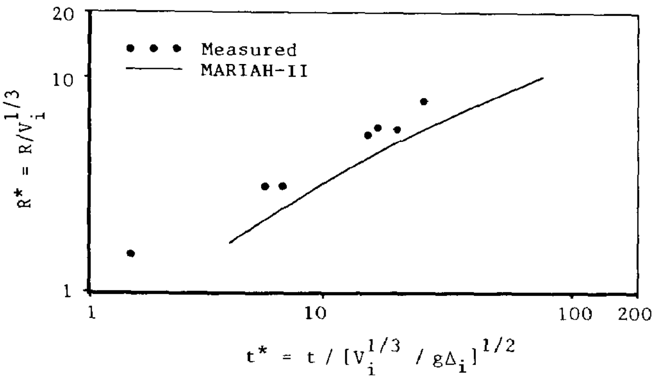


Fig. 7. Thorney Island Trial 34 – MARIAH-II prediction of cloud radial extent.

radially. The simulation of 72 seconds real time required approximately 100 h computing time on a Digital Equipment Company VAX 11-730 machine. The cloud profile (half of the radially symmetric section), defined by the 1% vol-

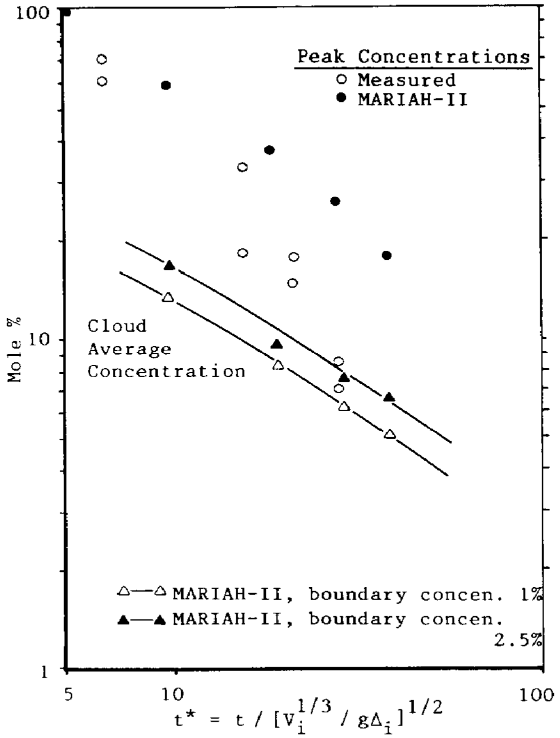


Fig. 8. Thorney Island Trial 34 - Measured and predicted cloud maximum and volume-averaged gas concentrations.

ume fraction, is shown at zero time and 6, 12, 24, 36, 48, and 60 s after release. Fig. 7 shows the predicted vs. measured radial cloud extent for the same release. The predicted radial extent of the cloud assumes no advection of the centroid, and allowance for advection of the cloud centroid by the ~ 1 m/s wind improves the agreement.

Figure 8 shows predicted and measured maximum values of the gas cloud concentration as a function of time for the 2110-m^3 release. The maximum (0.6 s average) concentrations were measured at 0.4 m height. The predicted cloud average gas concentrations, obtained by spatial averaging the MARIAH-II prediction using cloud boundary concentration limits of 1% and 2.5%, are also shown. The Trial 34 cloud spatial average concentration as a function of time has not been determined.

Conclusions

Cloud time-of-arrival and peak concentration vs. distance-from-release measurements from Thorney Island Trial 34 have been compared with similar measurements from laboratory-scale releases in calm air. The scaled field-observed times of arrival of the cloud are earlier than the laboratory measured times, but much of the difference may be attributable to the advection of the cloud by the slight wind present during the trial. The laboratory-scale peak concentration decay with distance is less than observed in Trial 34 and therefore provides a conservative estimate of the field test-observed distances to peak concentrations characteristic of hydrocarbon flammability limits.

MARIAH-II predictions of the gravity spreading and dilution of the laboratory-scale and Trial 34 experiments are in good agreement when scaled by the characteristic length and time $V_i^{1/3}$ and $V_i^{1/6}/(g\Delta_i)^{1/2}$, respectively. MARIAH-II predictions of the cloud volume-averaged concentration vs. time are in good agreement with the laboratory-scale observations; the cloud volume average concentration vs. time has not been determined for Trial 34. MARIAH-II predictions of the time of cloud arrival are in good agreement with the laboratory measurements. MARIAH-II predictions of the cloud time of arrival are later than were observed in the field trial, but are in reasonable agreement if allowance is made for cloud advection by the wind. MARIAH-II predictions of peak concentrations vs. time are higher than observed in both laboratory-scale and Trial 34 experiments.

Acknowledgements

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List of symbols

D	cloud diameter, m
g	gravitational acceleration, m/s^2
H	cloud height, m
R	cloud radius, m
R^*	dimensionless cloud radius, $R/V_i^{1/3}$
R_i^*	initial dimensionless cloud radius, $R_i/V_i^{1/3}$
t	time, s
t^*	dimensionless time, $t/[V_i^{1/3}/g\Delta_i]^{1/2}$
u	horizontal, along-wind velocity, m/s
v	horizontal, crosswind velocity, m/s
V	cloud volume, m^3
y	vertical coordinate, m

Greek symbols

ρ	cloud density, kg/m^3

ρ_a air density, kg/m^3
Δ reduced density, $(\rho-\rho_a)/\rho_a$

Subscripts
i initial

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