COMPUTATIONAL FLUID DYNAMICS METHODS OF CALCULATING GAS DISPERSION IN A BUILDING OR OUTSIDE AS A RESULT OF GAS LEAKS

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ABSTRACT

The NIST Fire Dynamics Simulator (FDS) computer program has been used to predict the dispersion of gases inside buildings and outdoors for a variety of scenarios. The authors present examples of applications of FDS for dispersion of gases. The examples include dispersion of vapor from a gasoline spill in a room, a natural gas leak in a pizza restaurant, gas plumes from underground leakage, comparison of a natural gas leak to a propane tank rupture in a shipping/receiving area, and a simple assessment of odorant transport in natural gas dispersion.

INTRODUCTION

The Fire Dynamics Simulator (FDS) computer model has been developed by the National Institute of Standards and Technology (NIST). Although FDS was developed primarily for simulation of fire phenomena (1), (2), (3), (4), and (5), it is a more general computational fluid dynamics computer code suitable for application in a much wider range of fluid dynamics problems. The FDS model is unique in that it is free to the public, and it enjoys continual funding support and technical evolution through the efforts of NIST and other researchers. In recent years the FDS model has increased our understanding of complex fire phenomena and has even been used to model the early fire development in the 911 incident (6).

Although FDS was developed for predicting fire dynamics, it has wider applicability. Of specific importance with respect to this paper, FDS has been used to model dispersion of gases inside and outside of buildings. Mniszewski and Pape (7) have used FDS for pure dispersion analyses without combustion and compared predicted results to experiments and analytical predictions. FDS has also been used for indoor air quality calculations by Musser, et al. (8) In the area of Computational Wind Engineering, Rehm, McGrattan, and Baum, have tested FDS (9) (10).

The authors use the FDS model extensively for applications such as these. The FDS model has been tested against experimental data for a variety of situations, however the preponderance of such validation tests have been concerned with the prediction of fire effects. This paper is concerned with prediction of gas dispersion using FDS. Several examples of dispersion modeling using FDS are presented. With proper validation, this modeling technique should be of value in many gas industry applications, particularly those involving public safety studies.

As FDS is free to the public, continually being improved and updated and user-friendly, this sophisticated and powerful computational fluid dynamics modeling tool is available for anyone who takes the time to learn it, in contrast to other CFD models which may be more costly to learn and use.

DESCRIPTION OF THE FDS MODEL

FDS is a computational fluid dynamics (CFD) model developed at the National Institute of Standards and Technology (NIST). Computational fluid dynamics is the mathematical solution of the equations that describe fluid motion. FDS stands for Fire Dynamics Simulator. Although the FDS code has been developed for prediction of fire behavior, it is applicable for general fluid dynamics computations, such as wind flow around obstacles. The FDS code is a Navier-Stokes equation solver for low Mach numbers. The FDS equations describe the motion of a fluid, such as air, and include conservation of mass, momentum, and energy relations. Analyses presented in this paper were accomplished using Versions 1.0 through 4.0 of the code.

The FDS computer code is described in detail in a number of references (1), (2), (3), (4) and (5). As described in these documents, FDS solves the fluid dynamics equations for low Mach number flows. The governing equations are the equations for conservation of mass, momentum, and energy, where energy conservation is included in the equation for flow divergence. The simplified equations that are solved numerically are given below:

Mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \tag{1}$$

Momentum:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla \tilde{p} - (\rho - \rho_\infty)\mathbf{g} = \mathbf{f} + \nabla \cdot \tau \tag{2}$$

Divergence Constraint:

$$\nabla \cdot \mathbf{u} = \frac{1}{\rho c_p T}\left(\nabla \cdot k\nabla T + \nabla \cdot \sum_l \int c_{p,l} dT \rho D_l \nabla Y_l - \nabla \cdot q_r + \dot{q}''' \right) + \left(\frac{1}{\rho c_p T} - \frac{1}{p_0} \right) \frac{dp_0}{dt} \tag{3}$$

where ρ is mass density, ρ_∞ is the ambient density, t is time, **u** is velocity (bold indicates vector quantities), $\tilde{p}$ is the perturbation pressure, p_0 is the background pressure, c_p is specific heat, T is temperature, k is thermal conductivity, D_l is diffusivity for specie l, Y_l is the mass fraction for specie l, **g** is gravitational acceleration, **f** is the body force (excluding gravity), and τ is the shear stress. For the low Mach Number form, pressure is written as the average background pressure added to the hydrodynamic pressure and a flow-induced perturbation pressure, $\tilde{p}$. The equation of state in the model is the ideal gas law.

The FDS model has two solution options for capturing turbulence. These are direct numerical simulation (DNS) and large eddy simulation (LES). All simulations presented in this report used the LES approach. Large eddy simulation allows direct numerical solution of the larger scale fluid motion (including large turbulent eddies) but greatly reduces the required computational time by calculating the sub-grid scale viscosity using an eddy viscosity based (in FDS) on the Smagorinsky viscosity model. (11) (12) The ability to use larger grid elements and account for the sub-grid mixing using the Smagorinsky viscosity allows solution of complex three-dimensional problems in practical computational times and memory requirements. Large eddy simulation is now an option in many CFD codes, as well as FDS.

Diffusion is treated similarly for all gas species in the model, where diffusion coefficients are the same. This tends to put into question the usefulness of the model in quiescent applications. However, it is reassuring that in most fuel-gas leakage scenarios, the mass transfer of the subject gas tends to be dominated by the bulk movement from the gas release, turbulent mixing and buoyancy effects, not diffusion. Thus, it is expected that in most cases, the physics of the model will approximate the real world reasonably well.

The primary limitation of the code is its validity for low Mach numbers. This requires that the maximum flow velocities be well below the speed of sound in the medium being analyzed. When considering the fact that the speed of sound in air at ambient conditions is about 340 m/s (1100 ft/s), this is not really a practical restriction for a wide variety of problems, particularly involving fire development, dispersion of gases and wind flow around structures. For dispersion analyses, the low Mach number restriction may be significant if it is necessary to model the details of a high velocity gas jet very near a leak, but generally the detailed leak flow right at the source is not important as long as the overall leak flow rate is accounted for.

The geometries of structures in FDS simulations must be represented as composites made of rectangular solid blocks. This is sometimes listed as a limitation of the FDS code because curved surfaces are approximated by a stair-step arrangement. However, when this restriction is balanced against the simplifications and consequent efficiency that results, the block structure is well worth it.

Figures 1 and 2 are examples of results from FDS analyses of fire (what FDS was original designed for). Figure 1 is the simple burning of an item under a hood, showing the flow of hot gases using tracer particles and heating of a nearby surface. Figure 2 shows a kitchen range fire in a townhouse. Flame plumes are shown spreading through the rooms. Many options are available to allow for displaying quite a number of parameters, including temperature, smoke density, heat release, gas concentrations, etc.

FDS VALIDATION

A great deal of effort has been expended by NIST in the last several years in the validation of the FDS model involving fire phenomena. The current edition of the FDS Technical Reference Guide (4) provides a long list references from many sources citing validation cases and application techniques. Much of the validation work has been concerned with fire phenomena. Mniszewski and Pape (7) have tested FDS for pure dispersion analyses without combustion and compared predicted results to experiments and analytical predictions. Musser, et al. (8) have used FDS for indoor air quality calculations. Rehm, McGrattan, and Baum, have tested FDS (9) (10) for prediction of wind flow around buildings.

The FDS version 4 User's Guide (13) states that "Although FDS was designed specifically for fire simulations, it can be used for other fluid flow simulations that do not include fire or heat addition of any kind". This guide also presents an example of a release of helium into a compartment filled with air. Dr. McGratten of NIST is the main architect of the FDS software. He has encouraged the authors in the use of the model for dispersion applications, and has provided useful guidance on how to implement it properly.

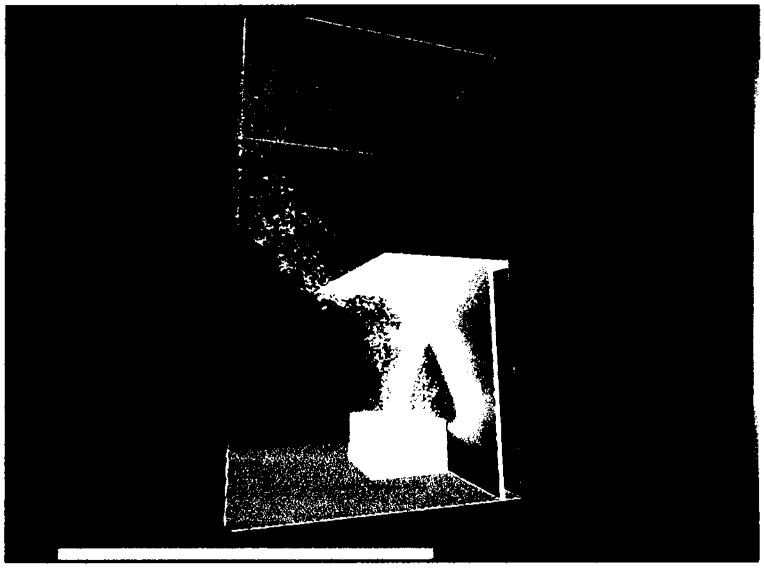

Figure 1. Idealized Fire Experiment Simulation.

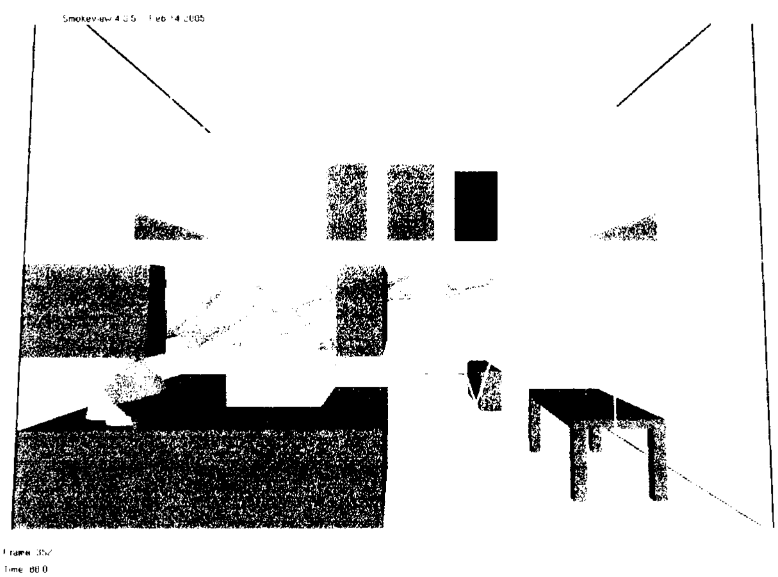

Figure 2. Example of FDS for Fire Development Analysis.

Suggested Additional Experimental Validations. Although there has been some testing of the FDS computer code for dispersion analysis, for gas industry applications it would be desirable to conduct a number of highly instrumented experimental validations involving some typical natural gas leak scenarios. One suggested approach might include:

1. Indoor/ typical residential single-family home/ 2 story with basement – leak scenario involving a failed flexible connector at the kitchen range

2. Indoor commercial facility – leak scenario involving a ruptured 1 ½" gas pipe
3. Outdoor Scenario - leak scenarios involving underground pipe rupture at various flow rates

While there are safety concerns in using undiluted natural gas for such testing, the use of diluted gas testing or use of an appropriate simulant gas may help qualm public concern and allow testing in real buildings. With natural gas source concentrations kept below the LEL at perhaps 50% LEL for safety, the mass transfer phenomena should be reasonably similar to sources at undiluted concentrations. If a simulant gas were used, molecular weight and diffusion characteristics would have to be considered and proper scaling of results evaluated. A reasonable array of gas sensors would be necessary throughout each testing volume. Infiltration would need to be considered in indoor testing to some degree. Such additional testing, with corresponding validation analyses using FDS, would increase confidence in the predictions of FDS for such cases.

Propane leak scenarios can be considered similarly.

EXAMPLES OF DISPERSION ANALYSES USING FDS

Several examples of gas dispersion simulations were discussed previously by Mniszewski and Pape in (7). The cases discussed at that time (not repeated here) include the following:

- Comparison with One Room Model Perfect Mixing Theory

Perfect mixing theory predictions were compared to FDS simulation results for dispersion of gas inside a single room. Calculations were completed for dispersion within the room with and without room forced ventilation. Whereas perfect mixing theory is based on formation of two distinct layers, FDS predicts a more gradual transition from the concentrations within the upper spaces of the room and the lower spaces.

- Comparison with Theory for Vapor Dispersion in a Wind

Predictions of dispersion in an imposed wind of vapors leaking from a component in a chemical process plant (e.g. a valve or pump) were compared to concentration profiles produced from an idealized point source of vapors, for which there was an analytic solution. Except near to the source, where geometry effect are significant, the FDS results compared quite good to the ideal point source solution.

- Comparison with Experiment for Propane Migration in a Room

FDS was used to simulate an experiment for which there appeared to be a good description of the setup and results in a paper in the literature. The experiment involved dispersion of a 50:50 mixture of propane and carbon dioxide in a room with air infiltration. FDS over-predicted the experimental gas concentrations, which may have resulted from an oversimplification of the distribution of air infiltration.

Dispersion of Vapors from a Gasoline Spill in a Room

Several experiments were performed inside an enclosure simulating a closed garage with a water heater in a corner. In the center of the floor, there was a gasoline spill or a release of a simulant (carbon dioxide). Initially, the enclosure was kept closed, either with or without room forced ventilation. At six minutes into the experiment, forced ventilation was introduced through a slot at floor level at the opposite end of the enclosure, simulating cracking open a garage door with outside wind. Figure 3 shows the concentrations of gasoline vapors before and after the outside wind was introduced through the slot. The FDS predictions of time for flammable concentrations to reach the water heater combustion chamber matched the time to explosion in the gasoline tests reasonably well.

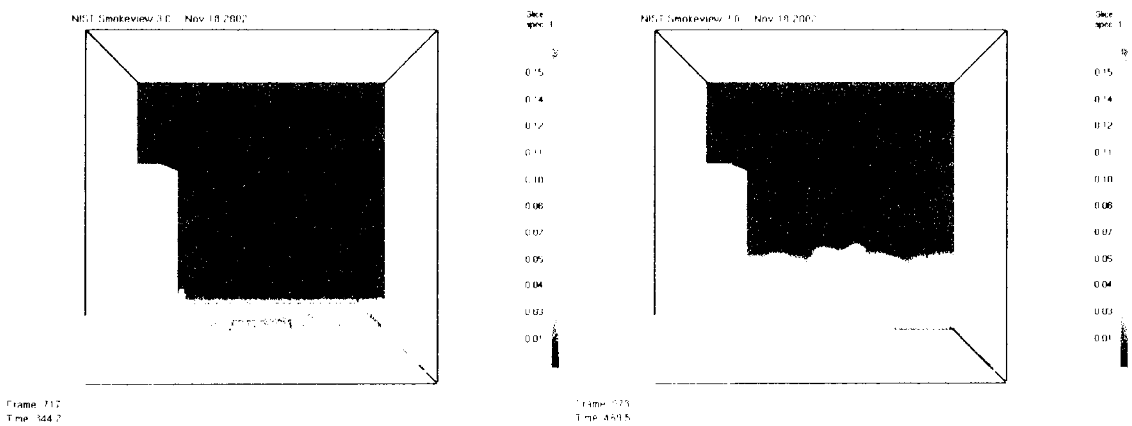

Figure 3. Gasoline Spill in Room With Water Heater.

Natural Gas Dispersion in a Pizza Restaurant

This example involves an underground natural gas leak caused by external forces, adjacent to an old commercial building with a granite block foundation. Iterative modeling was utilized to establish the rate of leakage into the basement, using the known timing between leak initiation and the explosion, and the probable ignition source (furnace pilot) location as constraints. Figure 4 is a vertical slice of gas concentrations for one leak rate scenario showing concentration distribution of natural gas throughout the building. The gas concentration is shown to be highest near the source of the outside leak in the basement, while open stairway doors allow gas to rise and fill grade level areas.

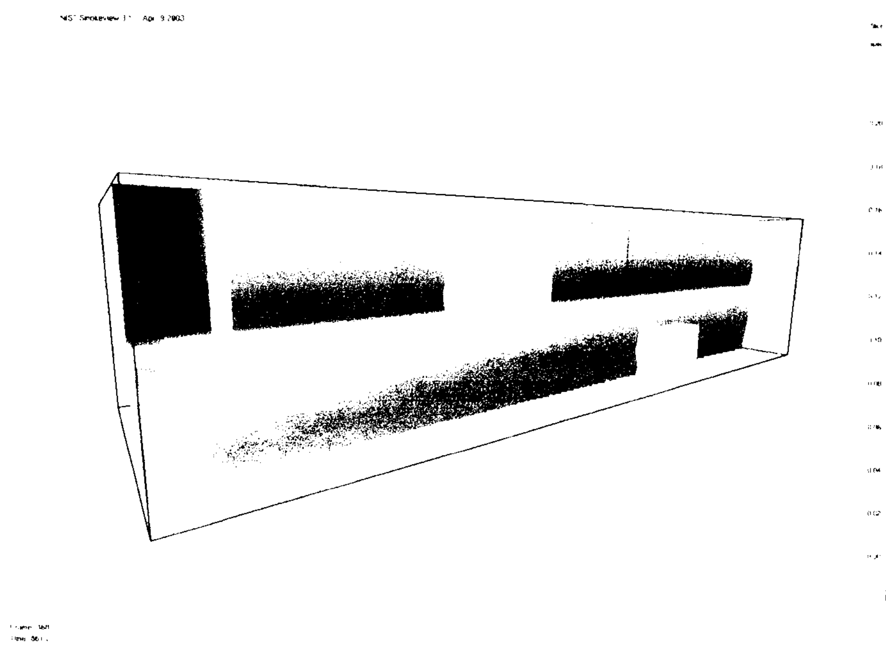

Figure 4. Gas Dispersion in a Pizza Restaurant.

<u>Gas Plumes from Underground Leakage</u>

This example involves the possible use of modeling to estimate the above ground gas plume available from a variety of underground leak sizes and wind conditions. Figure 5 shows an example of results from a 1270 CFH natural gas leak distributed over a square meter, with a wind speed of 2.24 mph (0.1 m/s). Such results may allow a field engineer to estimate leakage rate below by simply measuring some points within the gas plume and wind conditions.

<u>Natural Gas Versus Propane Dispersion in a Shipping/Receiving Area</u>

An explosion occurred inside the shipping/receiving area of a food processing facility. The shipping/receiving area was covered by a peaked roof, but it was otherwise open to the outdoors and wind penetration. Figure 6 shows the facility with the white roofed at the middle covering the shipping/receiving area. Figure 7 shows the layout of the facility with the roof removed. The shipping/receiving area had two forklift trucks in the rear left corner and the propane tank on one was being changed. One possible cause scenario involved an overfilled propane tank rupturing. A second cause scenario that was evaluated involved a natural gas leak emanating from a floor crack at the right-hand side of the shipping/receiving area, behind a plywood partition. Figure 8 shows the results for the natural gas case, and Figure 9 shows the results for the propane tank rupture. Clearly, the propane tank rupture was capable of producing a large flammable cloud whereas the natural gas leak produced concentrations in the space well below the lower explosion limit.

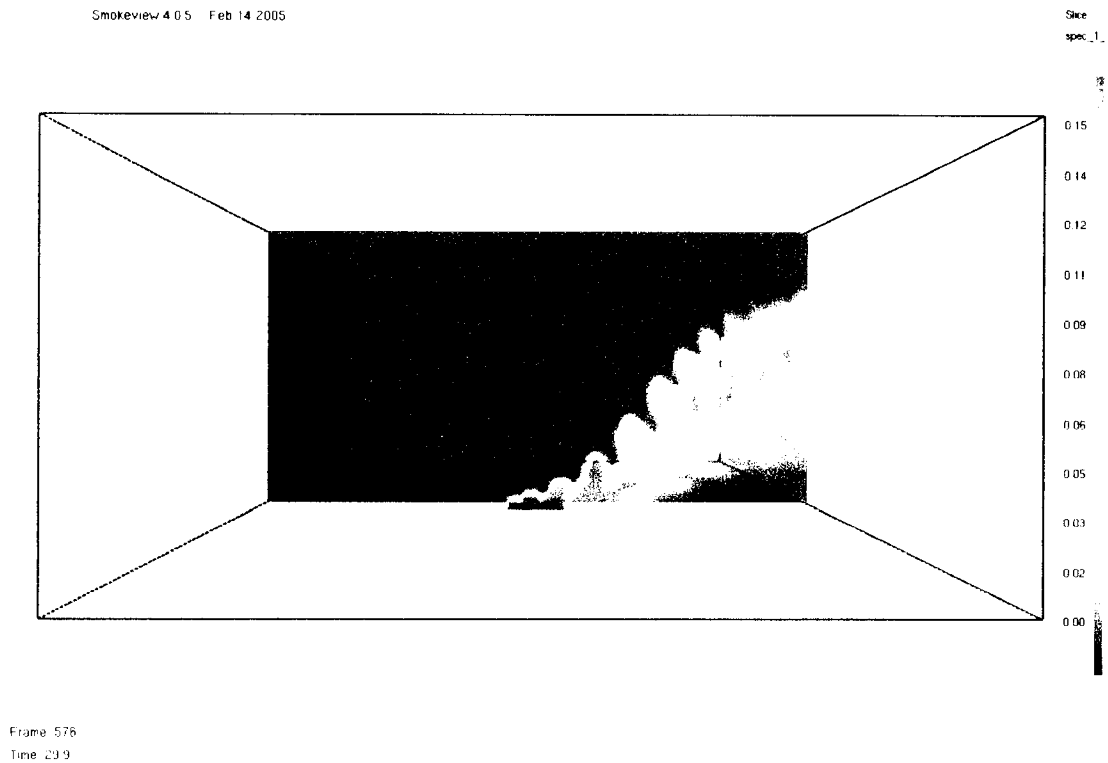

Figure 5. Dispersion of Gas From An Underground Leak.

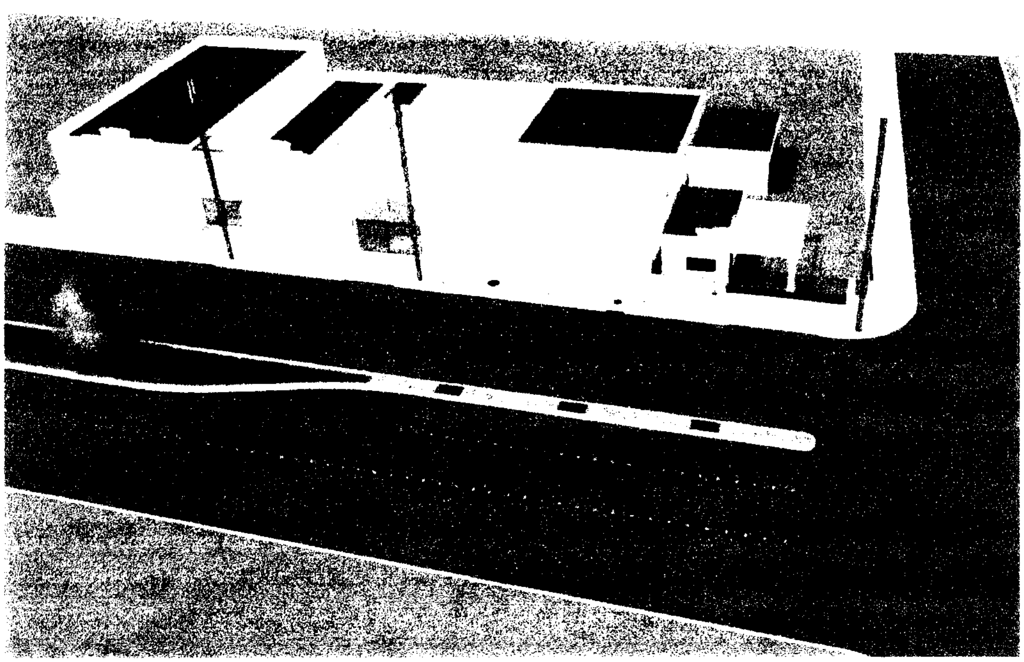

Figure 6. Food Processing Facility.

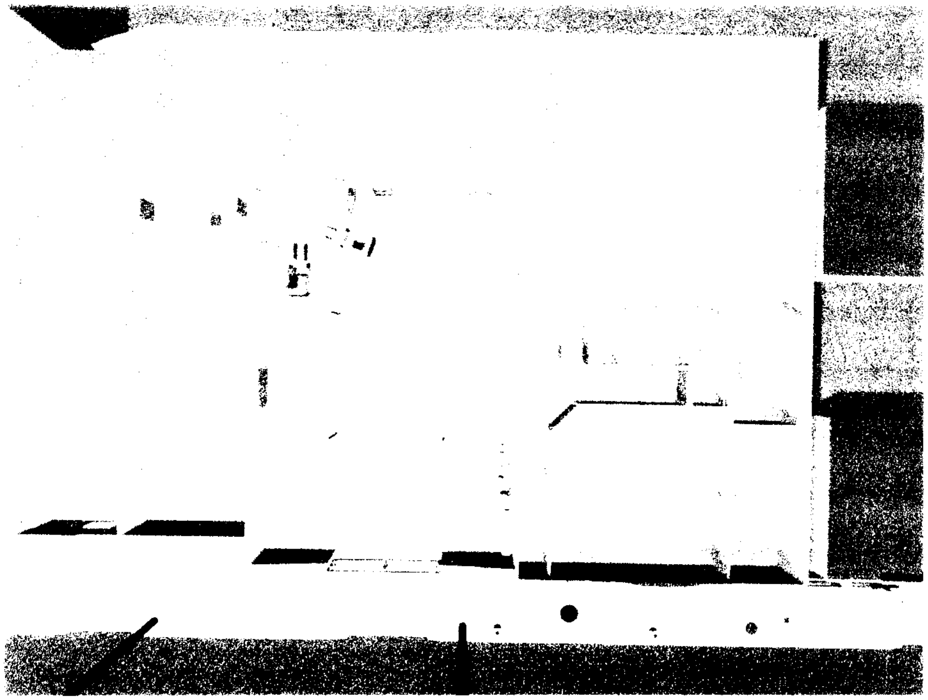

Figure 7. Facility Layout.

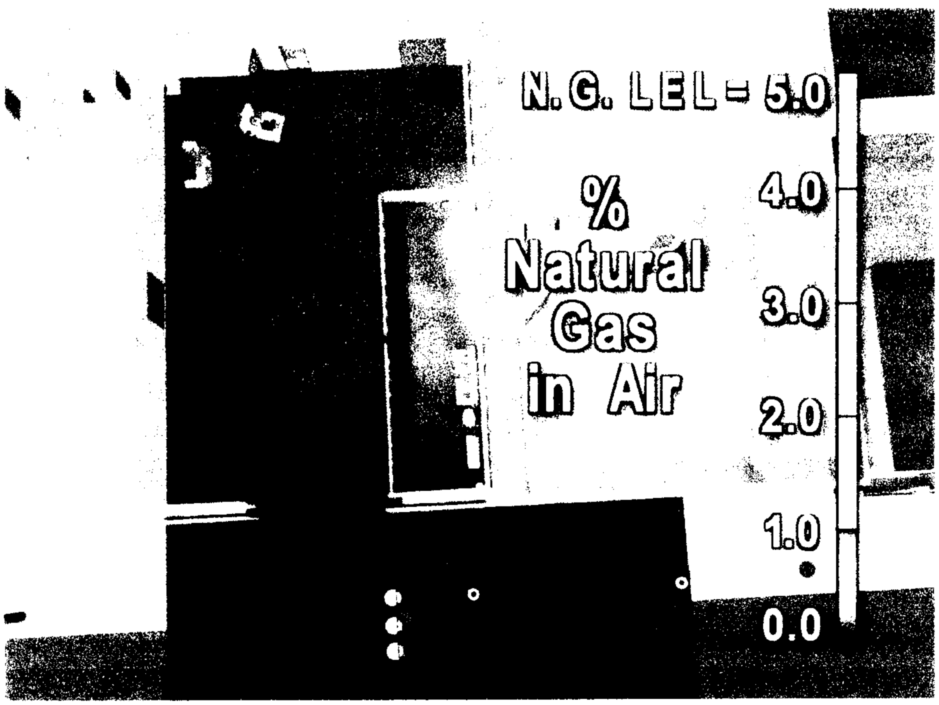

Figure 8. Natural Gas Leak Scenario.

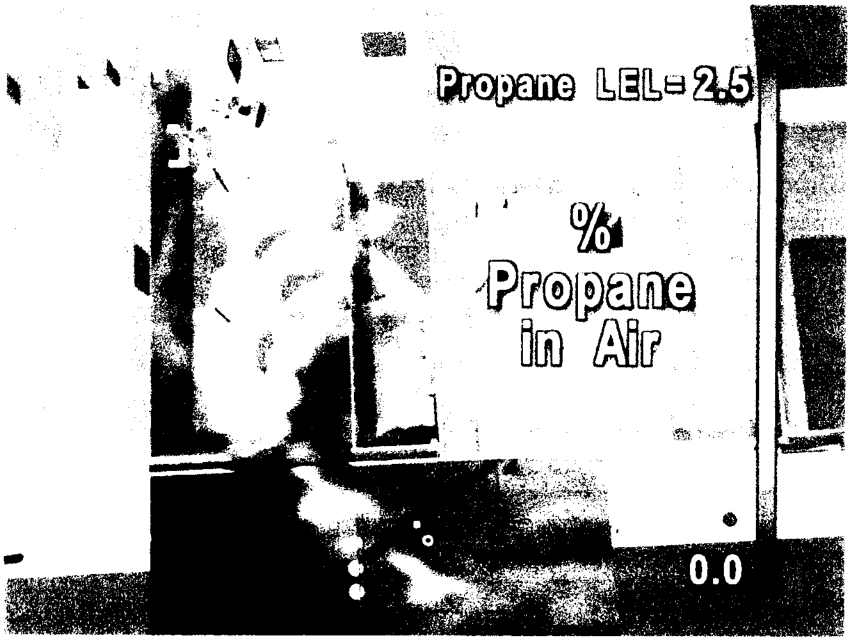

Figure 9. Propane Tank Rupture Scenario.

Odorant Transport

The final case to be discussed was done to evaluate the propensity for odorant to separate from natural gas during dispersion in air. A simple cubical enclosure was considered. A small section of the floor was given a 100% concentration of methane, but no forced flow into the enclosure. Odorant was applied to the methane at concentrations up to 1% by volume. Figure 10 shows the result for this case, with the methane gas rising to the ceiling as a plume by natural convection due to its low density. When the methane source was at the ceiling it just collected beneath the ceiling. When the source was on the side wall, a wall plume rose to the ceiling. In all cases, odorant concentration was monitored. The odorant concentration remained identically at the fraction of the gas concentration at which it was injected, without deviation in any case. There was no separation of the odorant from the carrier gas.

CONCLUSIONS

Based on the variety of gas dispersion analyses that have been conducted, the following conclusions are reached:

- FDS is valid for conducting dispersion analyses
- Some of the validations of FDS for dispersion and examples of dispersion applications using FDS have been presented in this paper.
- More validation of FDS for dispersion problems is needed.
- Suggestions are provided for more detailed experimental validation.
- Benefits to the Gas Industry from these efforts will include better analysis tools for public safety studies.

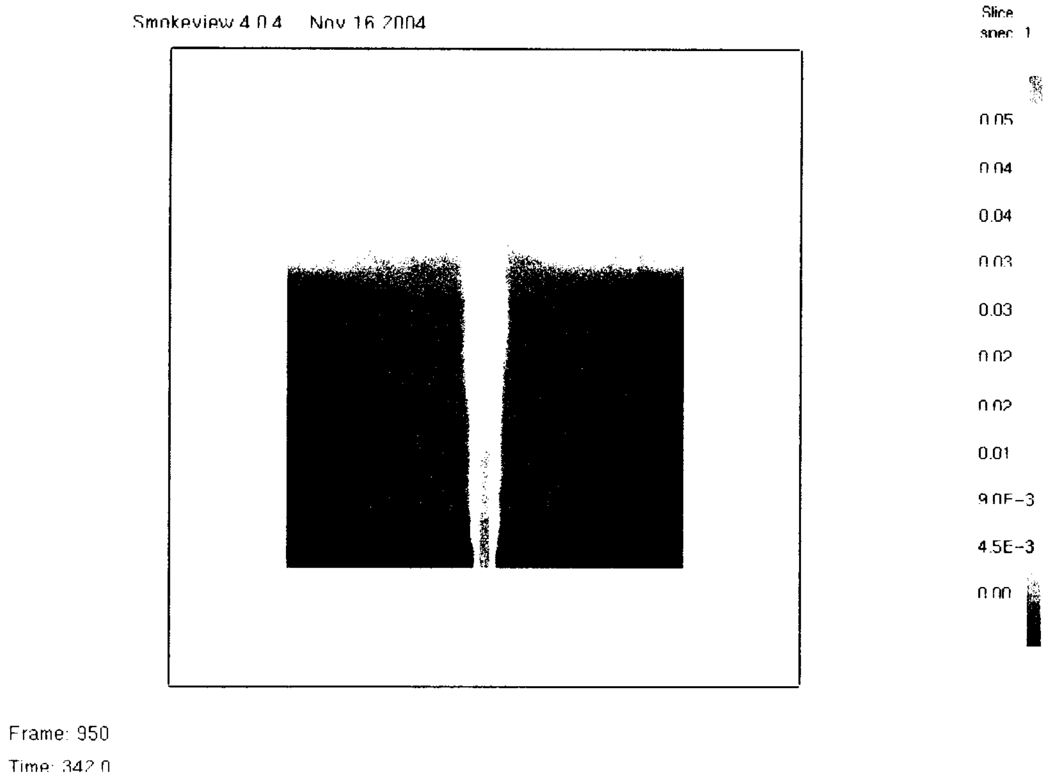

Figure 10. Methane Plume With Odorant Injected

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