LNG Safety Research: FEM3A Model Development

Quarterly Report
04-01-05 to 06-30-05

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ABSTRACT

This quarterly report for DE-FG26-04NT42030 covers a period from April 1, 2005 to June 31, 2005. GTI's activities during the report quarter were limited to administrative work. The work at the University of Arkansas continued in line with the initial scope of work and identified the questions regarding surface to cloud heat transfer as being largely responsible for the instability problems previously encountered. Drs. Havens and Spicer have successfully completed simulations at the required low wind speed of 2 m/s at 10 m elevation, with both D stability and F stability conditions, with the presence of LNG vapor release, but without the presence of dike/tank obstacle features. Complete report from University of Arkansas is included as Appendix A.

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EXECUTIVE SUMMARY

During this quarter, University of Arkansas completed their investigation of the effect upon numerical stability of the heat transfer model used to predict the surface-to-cloud heat transfer, that effort being directed to describing the ground surface temperature decrease as a function of time. They identified the questions regarding surface to cloud heat transfer as being largely responsible for the instability problems previously encountered, and have successfully completed simulations at the required low wind speed of 2 m/s at 10 m elevation, with both D stability and F stability conditions, with the presence of LNG vapor release, but without the presence of dike/tank obstacle features. University of Arkansas researchers now move to inclusion of the effects, under low wind speed and stable conditions, of the presence of dike and tank obstacles to the flow. Consequently, substantial progress toward the resolution of the instability problems has been made, and the project is on schedule to complete this important task.

EXPERIMENTAL

Primary effort has continued and substantial progress has been made. Equipment has been readied for measurement of wind tunnel turbulence spectra requested by NETL, as well as initiation of near-field measurements of gas concentration (within the dike/tank assembly), as agreed upon at a recent meeting at the University of Arkansas with NETL representatives.

RESULTS AND DISCUSSION

Development and utilization of new modeling methods for surface to cloud heat transfer appear to have been the key to overcoming the instability problems previously experienced in simulations of LNG vapor releases under the regulatory conditions required; 2 m/s wind speed at 10 m elevation, with F stability. Work during the quarter demonstrated successful completion of the simulation of the test case LNG vapor releases with 2 m/s wind speed at 10 m elevation, with both D and F atmospheric stability, respectively, without the presence of dike/tank assemblies.

CONCLUSION

The surface to cloud heat transfer was identified as being largely responsible for the instability problems previously encountered, and simulations at the required low wind speed of 2 m/s at 10 m elevation, with both D stability and F stability conditions, with the presence of LNG vapor release, but without the presence of dike/tank obstacle features were successfully completed.

APPENDIX A

Report by Dr. Jerry Havens and Dr. Tom Spicer
University of Arkansas

July, 2005

Vapor Dispersion and Thermal Hazard Modeling

Fifth Quarterly Report
(April - June, 2005)

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For
GAS TECHNOLOGY INSTITUTE
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K100029184 (Subcontract)

GTI Project Manager
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1.0 RESEARCH SUMMARY

Title	Vapor Dispersion and Thermal Hazard Modeling
Contractor	University of Arkansas GTI Contract Number: K100029184
Principal Investigators	Jerry Havens Tom Spicer
Contract Period	April 2004 – March 2006
Objective	To develop the FEM3A model for application to general scenarios involving dispersion problems with obstacles and terrain features of realistic complexity, and for very low wind speed, stable weather conditions as required for LNG vapor dispersion application specified in 49 CFR 193.
Technical Perspective	The dispersion model DEGADIS specified in 49 CFR 193 is limited to application for dispersion over smooth, level terrain free of obstacles (such as buildings, tanks, or dikes). There is a need for a dispersion model that allows consideration of the effects of terrain features and obstacles on the dispersion of LNG vapor clouds.
Project Milestones	<ul style="list-style-type: none"> A. Simulation of Low-Wind-Speed Stable Atmospheric Conditions. A. Verification for Dispersion over Rough Surfaces, With And Without Obstacles. B. Adapting the FEM3A Model for General Application
Results In Quarter 4	Work has continued to address numerical problems experienced with simulation of low-wind-speed, stable, atmospheric conditions with FEM3A. Steps 1 through 5 in the plan outlined in the first Quarterly report were completed and steps 6-8 are in progress. During this quarter, we completed our investigation of the effect upon numerical stability of the heat transfer model used to predict the surface-to-cloud heat transfer, that effort being directed to describing the ground surface temperature decrease as a function of time. We have identified these questions regarding surface to cloud heat transfer as being largely responsible for the instability problems previously encountered, and we have successfully completed simulations at the required low wind speed of 2 m/s at 10 m elevation, with both D stability and F stability conditions,

with the presence of LNG vapor release, but without the presence of dike/tank obstacle features. We now move to inclusion of the effects, under low wind speed and stable conditions, of the presence of dike and tank obstacles to the flow. Consequently, substantial progress toward the resolution of the instability problems has been made, and we believe we are on schedule to complete this important task.

We also met this quarter with representatives from DOE-NETL, to discuss plans for experimental work during the next quarter; specifically to obtain spectral data on wind tunnel turbulence applicable to the data sets being investigated by NETL and to initiate planning for detailed near-field measurements of gas concentration which will be useful for further CFD model validation efforts.

2.0 PROGRAM OBJECTIVE

The primary objective of this research is to develop the FEM3A dispersion model for application to general scenarios involving dispersion problems with obstacle and terrain features of realistic complexity, and for very low wind speed, stable weather conditions as required for LNG vapor dispersion application specified in 49 CFR 193. The program involves three principal tasks:

Task A – Simulation of Low-Wind-Speed Stable Atmospheric Conditions

It has been necessary to validate the FEM3A model with data from neutral (stability) wind tunnel boundary layer experiments, since suitable experimental facilities for simulating a stable boundary layer (at the required scale) in a wind tunnel do not exist. However, the regulatory code (49 CFR 193) requires the model prediction to be made for very low wind speed, stable weather conditions. The FEM3A code has not been applied previously for such conditions, and calculations at the University of Arkansas had shown that FEM3A simulations of stably stratified conditions are subject to numerical stability problems. We are confident that such problems can be eliminated, and research is underway to modify the turbulence closure model and to verify the model changes by conducting experiments in the University of Arkansas Ultra Low Speed wind tunnel. This is a high priority requirement since the normal application of the code for compliance with the regulation, as well as for application to counter-terrorism issues, requires the simulation to be made for such conditions, which most often are worst-case.

Task B – Verification for Dispersion over Rough Surfaces, With and Without Obstacles

Previous experiments in the CHRC wind tunnel to validate the FEM3A model for prediction of the effect of the presence of tank and dike structures utilized a smooth wind tunnel floor. Recent research work in the CHRC wind tunnel indicates that the presence of the smooth floor combined with the low wind speeds required to simulate the dense gas effects involved in LNG vapor dispersion can result in the tendency for the boundary layer near the floor to laminarize. Under such conditions the wind tunnel flow is not similar to the atmospheric wind flow because field conditions are normally fully turbulent (laminarization does not normally occur at field scale). There are strong indications that the experimental data from the wind tunnel would be more applicable to field conditions, and therefore more useful for model validation, when the floor is artificially roughened.

The primary purpose of this task will be to repeat and extend former experiments using uniform roughness elements covering the wind tunnel floor to create turbulence properties similar to field scale wind conditions. The roughness that will be used has already been characterized in a related research program; consequently, only the gas concentration measurements will have to be repeated. The resulting data set(s) will be a valuable addition to the data archives demonstrating the FEM3A model for application to LNG vapor dispersion prediction.

Data from this Task will be used to verify the FEM3A model for applications involving dispersion over rough surfaces (for example, suburban housing) with and without the presence of obstacles such as tank and/or dike structures and industrial buildings. The product of this task

will be an advanced turbulence closure model (for describing the turbulent mixing involved in the dispersion process) that will allow for more realistic description of dispersion problems with obstacle and terrain features of greater complexity (the real world).

Task C – Adapting the FEM3A Model for More General Application

As more complex applications of the FEM3A model are proposed, it is anticipated that there will be additional questions that can best be addressed by experimentation in the CHRC wind tunnel. The major advantage of this approach is that the specific questions regarding the application of the model to different scenarios can be addressed experimentally without having to recreate all of the experimental conditions in the real scenario, and without the high cost and insufficient controllability that is inherent in larger scale field tests. FEM3A simulations of more complex scenarios will inevitably require experimental verification efforts, and the continued availability of the CHRC wind tunnel for such verification is a necessary adjunct for the successful standardization of the FEM3A model for general application. Examples of complex scenarios that will be considered are evaluation of vapor fences for containment of flammable gases and aerosols, scenarios containing multiple obstacles, and major terrain features.

3.0 PROGRAM TIME SCHEDULE

Tasks A and B were pursued concurrently because they are coupled. However preparations for Task A, which are computational in nature, were initiated first, with concurrent experimental validation efforts immediately following. Tasks A and B are expected to require six quarters for completion. Task C will be the primary effort during the last two Quarters, but it will require continuing experimental verification work.

	<u>Q1</u>	<u>Q2</u>	<u>Q3</u>	<u>Q4</u>	<u>Q5</u>	<u>Q6</u>	<u>Q7</u>	<u>Q8</u>
<u>Task A</u>								
Numerical Stability	X	X	X	X	X			
<u>Task B</u>								
Model Verification		X	X	X	X	X	X	X
<u>Task C</u>								
General Application							X	X

4.0 WORK PERFORMED DURING APRIL - JUNE (QUARTER 5)

Primary effort has continued, and substantial progress has been made on Task A. Equipment has been readied for measurement of wind tunnel turbulence spectra requested by NETL, as well as initiation of near-field measurements of gas concentration (within the dike/tank assembly), as agreed upon at a recent meeting at the University of Arkansas with NETL representatives.

CHRC efforts continued to fix the numerical stability problem for application of FEM3A to low wind speed, stable atmospheric conditions. Our approach uses as a base case the field scale release conditions for which we have carried out the experimental verification of FEM3A thus far. The base-case is the tank and high-dike configuration described in previous reports with a continuous, steady, release of 0.6 cubic meters LNG per second into the annular space around the tank. Simulation of worst case regulatory conditions is the requirement: 2 m/s wind (at 10 meters elevation), stable atmosphere (Pasquill-Gifford Stability Class F), relative humidity 50%, and 3 cm surface roughness. A methodical approach is underway, with introduction of potential problem areas one at a time:

1. Simulation of a base case, with no gas release and with no obstacles, and regulatory conditions - except for D stability (this is a base case to ensure the code's handling of the simulation of the wind field)
2. Same as (1) with LNG release (this will introduce the additional complication of dense gas insertion into the boundary layer)
3. Same as (1) with F stability (this will introduce the additional complication of the F stability condition, but without the complications of alteration of the flow by obstacles)
4. Same as (3) but with LNG release (adding the complication of the insertion of the LNG into the boundary layer)
5. Same as (1) with Dike and Tank (testing the code for handling the simulation of the wind field around obstacles – no problems anticipated)
6. Same as (5) with LNG release
7. Same as (5) but with F stability (testing the code for handling the simulation of the wind field around obstacles, with stable atmospheric conditions)
8. Same as (7) with LNG release

We have made very substantial progress, having completed during this quarter the program described above through step 5. The simulations in steps 1 and 2 were field scale, obstacle-free simulations made with 2 m/s wind (at 10 m elevation), 3 cm surface roughness, D stability, for a 10 minute release of 272 kg/s LNG (0.6 m³/s LNG). As described in Quarterly Report No. 2, these simulations initially indicated a numerical instability that began at the inflow boundary and propagated down the domain. This instability problem was overcome by limiting the upwind (x-direction) aspect ratio to 25; the upwind aspect ratio is the ratio of the maximum alongwind (x-direction) grid spacing to the minimum vertical grid spacing. Guidance in Volume 5 suggested that the maximum aspect ratio should not exceed 50. Simulations showed that the aspect ratio limit of 50 was adequate downwind of the source and in the lateral direction, so the changes (aspect ratio) appear to result from the requirement for simulation at the lower (regulatory worst-case) wind speed. The initially specified grid also showed discontinuities in the concentration profile when a gas release was simulated; this problem was overcome by reducing the minimum vertical grid spacing to 0.3 m. This experience indicates that the minimum vertical grid spacing may need to be further decreased when the F stability simulations are considered.

Previously, no consideration had been given to ground cooling as a result of heat transfer to the colder gas cloud. Primary efforts during the fifth quarter have been directed to describing the ground surface temperature decrease as a function of time. A simplified model which can be

incorporated in FEM3A without substantial increase in computational resources has been developed and tested. The model under consideration describes the ground surface temperature and the thermal penetration depth as a function of time using an ordinary differential equation at each of the computational nodes on the ground surface. The ground-to-cloud heat flux added to an element on the bottom of the computational domain q (W/m^2) is modeled in FEM3A with a convective heat transfer coefficient h ($\text{W}/\text{m}^2\text{K}$) and a temperature driving force of $(T_g - T_1)$ where T_g is the ground surface temperature and T_1 is the lowest node in the computational domain (in the gas phase). In the original formulation of FEM3A, T_g was assumed to be constant, and based on observations discussed above, such an assumption would tend to overestimate the ground-to-cloud heat transfer.

The ground-to-cloud heat transfer must also account for heat transfer from the ground surface into the ground by conduction. Conduction through the ground surface is modeled with a thermal conductivity of the ground (or substrate) and the temperature gradient in the solid. The solution to such a problem has been extensively studied for boundary conditions such as a constant surface heat flux, a constant surface temperature, and a convective boundary condition assuming the fluid above the solid is at a constant temperature. None of these boundary conditions can model the situation under consideration since the fluid temperature above the solid (in this case the gas vapor/air mixture) is not constant. It has been demonstrated that the temperature profile in the solid can be approximated with

$$T_g - T_{go} = \frac{q\delta}{3k} \left(1 - \frac{x}{\delta} \right)^3 \quad (1)$$

where T_{go} is the initial ground temperature, k is the thermal conductivity of the ground, δ is the penetration depth of the temperature change, and x is the distance from the ground surface into the solid. Note that T_g , q , and δ are all time varying in Equation (1). Substituting this into the partial differential equation for conduction in the solid, the surface heat flux is described using

$$q = -k \frac{\partial}{\partial x}(T_g - T_{go}) \Big|_{x=0} = -\frac{3k}{\delta}(T_g - T_{go}) \quad (2)$$

Furthermore, substituting the temperature profile of Equation (1) in the integrated form of the heat conduction equation provides the way to describe T_g and δ

$$\frac{d}{dt}(\delta^2 q) = 12\alpha q \quad (3)$$

where α is the ground thermal diffusivity. Equation (3) can be integrated in time using the Euler scheme used in FEM3A for the quantity $(\delta^2 q)$. A second differential equation can be obtained by substituting Equation (2) into (3) as follows:

$$\frac{d}{dt}(\delta(T_g - T_{go})) = -\frac{4\alpha q}{k} \quad (4)$$

When integrating Equations (3) and (4), the surface heat flux q is modified to take into account radiative cooling present for simulating stable atmospheric conditions as follows:

$$q = h(T_g - T_1) + q_{rad} \quad (5)$$

where $q_{rad} > 0$ for stable conditions and is calculated based on atmospheric measurements.

Utilization of these methods for modeling surface to cloud heat transfer appear to have been the key to overcoming the instability problems previously experienced in simulations of LNG vapor releases under the regulatory conditions required; 2 m/s wind speed at 10 m elevation, with F stability.

The figures on the following page demonstrate successful completion of the simulation of the test case LNG vapor releases with 2 m/s wind speed at 10 m elevation, with both D and F atmospheric stability, respectively, without the presence of dike/tank assemblies.

0.6 cubic meters LNG per second for 10 minutes
2 m/s wind speed at 10 m elevation - D stability

0.6 cubic meters LNG per second for 10 minutes
2 m/s wind speed at 10 m elevation - F stability

5.0 PLANS FOR FUTURE WORK

Contract tasks are expected to be completed on schedule as shown in Section 3.0.