LNG Safety Research: FEM3A Model Development

Quarterly Report
10-01-04 – 12-31-04

For:
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Contract: DE-FG26-04NT42030

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February 21, 2005

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1. ABSTRACT

This quarterly report for DE-FG26-04NT42030 covers a period from October 1, 2004 to December 31, 2004. On December 9, 2004 a meeting was held in Morgantown to re-scope the LNG safety modeling project such that the work would complement the DOE's efforts relative to the development of the intended LNG-Fluent model.

It was noted and discussed at the December 9th meeting that the fundamental research being performed on surface to cloud heat transfer and low wind speed issues will be relevant to the development of the DOE LNG/Fluent Model. In general, it was decided that all research to be performed from December 9th through the remainder of the contract is to be focused on the development of the DOE LNG/Fluent model. In addition, all GTI activities for dissemination and transfer of FEM3A will cease and dissemination activities will focus on the new DOE LNG/Fluent model. The proposed new scope of work is presented in section 4 of this report.

The work reported in the present document relates to the original scope of work which was in effect during the reporting period. The future work will be re-scoped to meet the requirements of the new scope of work.

During the report period work was underway to address numerical problems present during simulation of low-wind-speed, stable, atmospheric conditions with FEM3A. Steps 1 and 2 in the plan outlined in the first Quarterly report are complete and steps 3 and 4 are in progress. During this quarter, the University of Arkansas has been investigating the effect upon numerical stability of the heat transfer model used to predict the surface-to-cloud heat transfer, which can be important for LNG vapor dispersion. Previously, no consideration has been given to ground cooling as a result of heat transfer to the colder gas cloud in FEM3A. Details of work performed are given in section 3.

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2. EXECUTIVE SUMMARY

During the report period work was underway to address numerical problems present during simulation of low-wind-speed, stable, atmospheric conditions with FEM3A. Steps 1 and 2 in the plan outlined in the first Quarterly report are complete and steps 3 and 4 are in progress. During this quarter, the University of Arkansas has been investigating the effect upon numerical stability of the heat transfer model used to predict the surface-to-cloud heat transfer, which can be important for LNG vapor dispersion. Previously, no consideration has been given to ground cooling as a result of heat transfer to the colder gas cloud in FEM3A. Details of work performed are given in section 3.

3. EXPERIMENTAL

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 show 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).

<u>Task C – Adapting the FEM3A Model for More General Application</u>
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.

1.0 PROGRAM TIME SCHEDULE

Tasks A and B will be pursued concurrently because they are coupled. However preparations for Task A, which are computational in nature, will be 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.

	Q1	Q2	**Q3**	Q4	Q5	Q6	Q7	Q8
<u>Task A</u>								

Numerical Stability	X	X	**X**					
Task B								
Model Verification		X	**X**	X	X	X	X	X
Task C								
General Application							X	X

2.0 WORK PERFORMED DURING OCTOBER-DECEMBER (QUARTER 3)

Primary effort has continued on Task A. Equipment repair and replacement tasks necessary to begin experiments under Task B are complete.
Efforts continue 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 - no problems anticipated)
2. Same as (1) with LNG release (this will introduce the additional complication of dense gas insertion into the boundary layer – no problems anticipated)
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

Steps 1 and 2 are complete and steps 3 and 4 are in progress. 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 has been given to ground cooling as a result of heat transfer to the colder gas cloud. The present effort is directed to describing the ground surface temperature decrease as a function of time. Kunsch and Fannelop (1995) considered how to model the decreasing surface temperature using an analytical approximation for the temperature distribution in a semi-infinite solid. A similar approach was also reported by Eckert and Drake (1972). Eckert and Drake show that the analytical approach is valid for a step change in cloud temperature. The numerically integrated form of the equations suggested by Kunsch and Fannelop agree with the analytical solution of Eckert and Drake. Luikov (1968) provides the analytical solution for the ground-to-cloud heat transfer to a passing cloud of constant temperature (as observed in the Desert Tortoise test described below). We are focusing on two issues:

- FEM3A has treated the ground surface temperature as constant. Nielsen and Ott (1999) analyzed the temperature, concentration, and heat transfer measurements for one particular ammonia release in the Desert Tortoise test series. In the test they analyzed, the ammonia cloud was present over the sensors located 100 m downwind of the source for approximately 180 s. While the cloud was present, the temperature and concentration at 1 m elevation were essentially constant. However, the inferred surface heat flux was not constant while the cloud was present as would be predicted by the surface heat transfer model used currently in FEM3A. Even though the cloud was present for only 180 s, the surface heat flux after 180 s was approximately 60% of the original value - due to cooling of the ground surface. Since the temperature of an LNG cloud would be much lower than that considered by Nielsen and Ott, the decrease in heat transfer due to ground cooling would be expected to be more significant for an LNG vapor cloud.

- FEM3A assumes a heat transfer model that is based on a forced convection model. Under low wind speed regulatory conditions, ground-to-cloud heat transfer for an LNG cloud may be more appropriately described with a natural convection model.

A simplified model is being considered which can be incorporated in FEM3A without substantial increase in computational resources. The present 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 present model is being compared with simplified problems which can be modeled analytically. When this comparison is complete, the model will be implemented in FEM3A for further evaluation. It is anticipated that the heat transfer effects now under consideration will become even more important as consideration is given to the potential for cloud liftoff, which can be a vapor-cloud-impact mitigation factor.

5.0 PLANS FOR FUTURE WORK

Plans for future work will be developed to meet the requirements of the revised scope of work.

6.0 LITERATURE CITED

Eckert, E.R.G., and R.M. Drake, Jr., "Analysis of Heat and Mass Transfer," McGraw-Hill, 1972.

Kunsch, J.P., and T.K. Fannelop, "Unsteady heat-transfer effects on the spreading and dilution of dense gas clouds," Journal of Hazardous Materials, 43, 169-193, 1995.

Luikov, A.V., "Analytical Heat Diffusion Theory," J.P. Hartnett, ed., Academic Press, 1968.

Nielsen, M., and S. Ott, "Heat transfer in large-scale heavy-gas dispersion,"

4. RESULTS AND DISCUSSIONS

On December 9th a meeting was held in Morgantown to rescope the LNG Safety modeling project. The project is to be re-scoped to focus efforts on research that would be useful to DOE in their development of an LNG modeling software using the Fluent model. It was therefore decided to redirect the FEM3A model to the LNG-Fluent model. Accordingly, a new scope of work was prepared and has been submitted. It is pending approval by DOE. The new scope of work is as follows:

4. PROPOSED REVISED SCOPE OF WORK (Version 12-20-04)
(LNG Safety Research: DOE LNG/Fluent Model Development)

A. OBJECTIVES

The objective of this research is to develop the DOE LNG/Fluent 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.

B. SCOPE OF WORK

This research will provide the DOE LNG/Fluent model with an advanced turbulence closure module for describing the turbulent mixing with air of denser-than-air gases or aerosols. This will allow for more realistic description of dispersion problems with obstacle and terrain features of real-world complexity. The resulting DOE LNG/Fluent model will be used for evaluating hazard consequence issues for LNG and other liquefied energy fuels.

Other improvements as identified by the research team and approved by DOE will also be incorporated into the DOE LNG/Fluent model.

C. TASKS TO BE PERFORMED

The following tasks will maintain and further develop the technical credibility of the DOE LNG/Fluent model and extend its use to more general hazard evaluation scenarios.

TASK 1.0 Technology Transfer

Task 1.0 Objective:
GTI will disseminate information about the DOE LNG/Fluent model to potential users through trade publications, workshops and GasTips (the DOE/GTI technology dissemination journal.) GTI will publish a report regarding the conclusions of the research program and the efficacy of the DOE LNG/Fluent model. Industry peer review of the model will be performed.

TASK 2.0 Coordination of Computer Modeling and Wind Tunnel Experiments

Task 2.0 Objective
GTI will coordinate model development activities with the University of Arkansas' Chemical Hazards Research Center (CHRC) and the NETL researchers. GTI will assess future model needs through interaction with the LNG industry and lead an effort to develop an effective more efficient model to operate.

Subtask 2.1 – Improve the DOE LNG/Fluent Advanced Turbulence Closure Module
CHRC will improve the DOE LNG/Fluent model by improving the advanced turbulence closure module it uses for describing the turbulent mixing with air of denser-than-air gases or aerosols. The improved turbulence closure module will enable more realistic description of LNG/nature gas dispersion with obstacle and terrain features of realistic complexity, and for very low wind speed and stable weather conditions.

Subtask 2.2 – Verification of Dispersion over Rough Surface, with and Without Obstacles Using the Improved Advanced Turbulence Closure Module
This subtask will repeat former experiments, conducted with a smooth floor, using uniform roughness elements covering the CHRC 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 in the tunnel; consequently only the gas concentration measurements will have to be repeated.

Data from this subtask will be used to verify the DOE LNG/Fluent improved turbulence closure module fog applications involving dispersion over rough surfaces (for example, suburban housing) with and without the existence of obstacles such as tanks and /or dike structures and industrial buildings.

Subtask 2.3 – Adapting the DOE LNG/Fluent Model for More General Applications
As more complex applications of the model arise, it is anticipated that there will be additional questions that can best be addressed by CHRC wind tunnel experimentation. 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 an insufficient controllability that is inherent in the larger scale field tests.

DOE LNG/Fluent simulations of more complex scenarios will 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 DOE LNG/Fluent model for general application. Complex scenarios that could be considered are evaluation of vapor fences for containment of flammable gases and aerosols, scenarios containing multiple obstacles, and important terrain features.

CHRC staff and NETL researcher will coordinate efforts as required upgrading the DOE LNG/Fluent model to a used and useful status. Efforts previously intended for upgrade of the FEM3A model will be redirected to the DOE LNG/Fluent model by this change of technical scope.