CFD Simulation of Vapor Dispersion from LNG Jetting and Flashing Releases

Filippo Gavelli [a,1], Scott Davis [a], Olav Roald Hansen [a], Mathieu Ichard [b]

[a] *GexCon US,* [b] *GexCon AS*

Abstract

Accidental releases of liquefied natural gas (LNG) from high-pressure piping have recently become a matter of growing interest. In the context of U.S. onshore LNG facility sitin, for example, LNG terminal developers have been required to demonstrate that the flammable vapor cloud (to the ½ LFL concentration) due to "jetting" and "flashing" from pressurized LNG releases will not extend beyond the property boundaries.

The physical phenomena that occur as pressurized LNG flows from a breach are rather complex; as the release typically begins as a flashing jet that forms a gas-aerosol mixture as it expands to atmospheric pressure, which is followed by the rain-out or evaporation of the liquid droplets. The resulting vapor cloud, therefore, is likely to have very different characteristics from the "traditional" vapor cloud from a spill into an impoundment.

Integral models are available that can calculate the formation and dispersion of the vapor cloud from a high-pressure release in the absence of obstacles or significant terrain features. In many practical cases, however, obstacles are likely to be present along the path of the two-phase jet (e.g., flange guards, nearby equipment, pipe racks, etc.) or along the path of the vapor cloud (e.g., buildings, vapor barriers, etc.). In order to properly account for the effect of these obstacles, a more sophisticated modeling approach is necessary.

This paper discusses the simulation of high-pressure LNG releases using the computational fluid dynamics (CFD) model FLACS. FLACS can overcome the limitations of simpler models by: 1) accounting for the effects of obstacles and complex geometry on the flow of air and vapors; 2) simulating the behavior of the two-phase jet release from the source location. Case studies are presented to demonstrate the application of FLACS to different high-pressure LNG release scenarios.

Background

The analysis of LNG vapor dispersion hazards, particularly in the context of onshore facility siting, is typically focused on the consequences of atmospheric pressure releases, such as would result from a guillotine break to a storage tank withdrawal line. However, other types of leaks are possible in an LNG facility and their consequences need to be evaluated to ensure they do not affect the plant siting requirements. A scenario that has recently been brought up within the permitting process for several U.S. facilities is that of a high-pressure LNG release, for example,

---

[1] Corresponding author: fgavelli@gexcon.com

from the sendout line to the LNG vaporizers. In those instances, LNG terminal developers have been required to demonstrate that the flammable vapor cloud (to the ½ LFL concentration) due to "jetting" and "flashing" from pressurized LNG releases will not extend beyond the property boundaries.

The physical phenomena that occur as pressurized LNG flows from a breach are rather complex and include:

- Flashing (if the pressurized liquid is at temperatures above the atmospheric boiling point);
- Atomization of the liquid stream as it expands to atmospheric pressure;
- Entrainment of air by the liquid particle jet;
- Droplet evaporation; and
- Rainout (i.e., deposition of liquid droplets that reach the ground or hit objects before evaporating).

Semi-empirical correlations have been developed from experiments involving high-pressure releases [1, 2], so that quantities such as the flashing rate, air entrainment rate, vaporization and rainout can be predicted. These quantities can be used to calculate the source term for vapor dispersion in models, such as SLAB [3] or PHAST [4]. This type of approach is generally adequate provided that:

- The leak forms a unidirectional jet;
- The high-pressure jet can expand and fully evaporate without encountering any obstacles;
- The resulting vapor cloud can disperse downwind without encountering any obstacles.

In many practical cases, however, obstacles are likely to be present along the path of the two-phase jet (e.g., flange guards, nearby equipment, pipe racks, etc.) or along the path of the vapor cloud (e.g., buildings, vapor barriers, etc.). In order to properly account for the effect of these obstacles, a more sophisticated modeling approach is necessary.

This paper discusses the simulation of high-pressure LNG releases using the computational fluid dynamics (CFD) model FLACS. FLACS provides the following advantages when applied to the simulation of vapor dispersion from high-pressure LNG releases:

1. It is a CFD model capable of simulating the effects of obstacles and complex geometry on the flow of air and vapors;
2. It has been validated for LNG vapor dispersion; and
3. It includes a two-phase module capable of simulating the high-pressure jetting and flashing release from the source.

The paper will discuss the validation of the two-phase jet module for FLACS and will include examples to demonstrate the applicability of FLACS to "jetting and flashing" scenarios.

FLACS

The FLACS CFD model was developed in the early 1980s to simulate gas explosions in offshore platforms. The conservation equations are solved on a Cartesian grid using a finite volume method. The k-ε turbulence model is used to close the equations for fluid motion, with some modifications made for atmospheric boundary layer turbulence and dispersion applications [5-7]. A distributed porosity concept is implemented in FLACS to handle complex geometries, and turbulence production terms are parameterized for sub-grid objects[8]. At the upwind boundary of the domain, vertical profiles of wind speed and direction, temperature, turbulent kinetic energy and eddy dissipation rate are imposed according to the atmospheric stability class or to the Monin-Obukhov and surface roughness lengths. The vapor dispersion capabilities of FLACS have been validated against several field experiments involving both dense gas and passive gas releases, including CO_2 releases in an array of flat ‘‘billboard’’-shaped obstructions (the Kit Fox experiments) and tracer gas releases in an array of rectangular storage containers in the Mock Urban Setting Test (MUST) experiments [5]. More recently, FLACS was also validated against the 33 experimental tests included in the Model Validation Database for LNG vapor dispersion models [9].

Two alternative models can be used with FLACS to simulate the vapor cloud dispersion from a pressurized flashing jet release. The simpler method consists of a “flash” utility, which allows the user to define a pseudo-release location, where the release can be assumed to start as a single-phase jet (after flashing), for which the effects of droplet rain-out and evaporation, and air entrainment have been included [10]. At the single-phase pseudo-source location, the jet is a mixture of gas and air at a temperature below that of the source liquid, due to the droplets' evaporative cooling effect. The jet mass flow rate is larger than the leak flow rate, due to air entrainment, and the area of the pseudo-source is also increased. The “flash” utility, however, assumes that there is no impingement on objects during the jet evaporation and expansion process (which can take place over distances on the order of 10-20 m). When obstacles are closer than the “flash” utility allows, a different approach may be followed. The alternative approach consists of a “two-phase module”, which allows the aerosol phase of the high-pressure release to be tracked within the three-dimensional computational domain, as the aerosol spreads and vaporizes. The depressurization and flashing of the high-pressure release are first calculated, and a pseudo-source for the two-phase (gas and aerosol) atmospheric-pressure jet is defined. The two-phase pseudo-source is located very close to the actual leak, effectively eliminating the restriction on object impingement that applies to the “flash” utility. The two-phase, atmospheric pressure jet is then used as the source for the CFD simulations. An accurate representation of the jet dispersion requires the behavior of the evaporating droplets to be modeled. In FLACS, the droplet evaporation and jet cooling effects that characterize this phase are implemented through the homogeneous equilibrium model [11]. This includes accounting for rain-out, liquid pool spreading and evaporation.

The two-phase flashing jet dispersion model was validated against experimental data from the INERIS experiments [12] as well as from the Desert Tortoise test series [13]. In the Desert Tortoise simulations, for example, rain-out predictions by the model were found to be within 30% of the observations in three of the four tests. Statistical Performance Measures to assess the performance of the model reported an over-prediction of 25% in the maximum gas concentration at different sensor locations, with 94% of all predictions falling within a factor of two of the experimental data.

Case Studies

Two high-pressure LNG release scenarios are examined in this paper. The first scenario consists of a guillotine break to a small-diameter horizontal high-pressure pipe connection, for the purpose of demonstrating the effect of obstructions on the dispersion of the flammable vapor cloud from a jetting and flashing release. The second scenario consists of a circumferential flange leak in a horizontal high-pressure pipe, for the purpose of demonstrating the application of FLACS' two-phase module to a multidirectional pressurized LNG release.

Scenario 1: Guillotine break

The leak scenario consists of a guillotine break to a 5 cm diameter horizontal connection to a 30 cm diameter pipe carrying LNG. The pipe runs horizontally at 10 m elevation; the pipe pressure is 10 barg and the LNG is at -150°C. The leak is assumed to continue at the nominal flow rate (i.e., with no drop in pressure inside the pipe) for 180 s and the simulation is continued until 200 s. Ambient conditions are assumed to be as follows: 20°C temperature, 2.0 m/s wind speed at 10 m elevation, and stable atmosphere (Pasquill-Gifford class "F"); the effects of humidity are neglected.

The two-phase flashing jet emerging from the breach is allowed to expand, entrain air and evaporate without encountering any obstructions. The scenario is solved by first calculating the characteristics of the two-phase jet, as well as those of a pseudo-source at the location where the liquid droplets have completely evaporated (i.e., where the two-phase jet has become single-phase). The flashing jet entrainment and evaporation calculations are performed using the "flash" utility included in FLACS, whose output is summarized in Table 1. The single-phase jet pseudo-source provides the inlet boundary condition for the three-dimensional vapor cloud dispersion simulation.

Table 1. Flashing jet and vaporized jet characteristics

	Flashing jet	Vaporized jet
Distance from breach	0 m	6.76 m
Flow area	19.6 cm^2	4116 cm^2
Mass flow rate	37.84 kg/s	135.51 kg/s
Temperature	-150°C	-171.1°C
Mass fraction of flashed vapor	6.87%	-
Gas-air equivalence ratio	∞	6.68

Two different cases are considered for the dispersion of the vapor cloud from the single-phase jet source:

1. No obstacles;
2. A vapor barrier (4 m tall and 200 m wide) is placed perpendicular to the wind direction, approximately 150 m downwind of the high-pressure release.

Figures 1 through 3 compare the size of the vapor cloud (to the 50% of LFL concentration) for the unobstructed dispersion (top) and obstructed dispersion (bottom) at different times. Figure 1 shows that, early in the simulation, the presence of the vapor barrier has no noticeable influence on the growth of the vapor cloud. As the cloud approaches the barrier, the momentum of the vapor cloud causes it to impinge against the barrier with limited lateral spread (Figure 2), unlike the typical behavior of low-momentum vapor clouds from atmospheric pressure releases. However, even though portion of the vapor cloud flows over the barrier, the presence of the vapor barrier reduces the maximum downwind distance reached by the ½-LFL cloud from approximately 310 m (unobstructed case) to approximately 165 m (obstructed case).

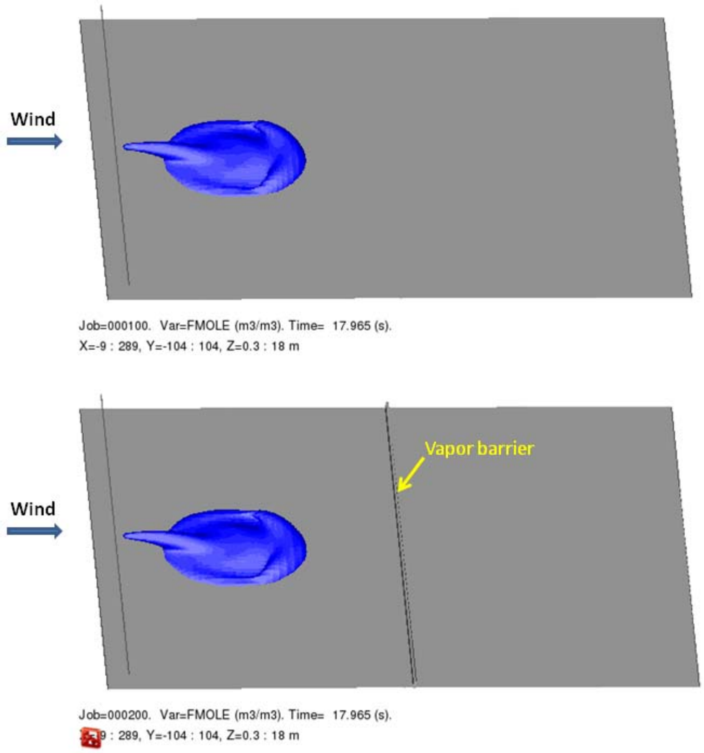

Figure 1. ½-LFL vapor cloud dispersion from high-pressure release, after approximately 18 s: unobstructed case (top) vs. obstructed case (bottom).

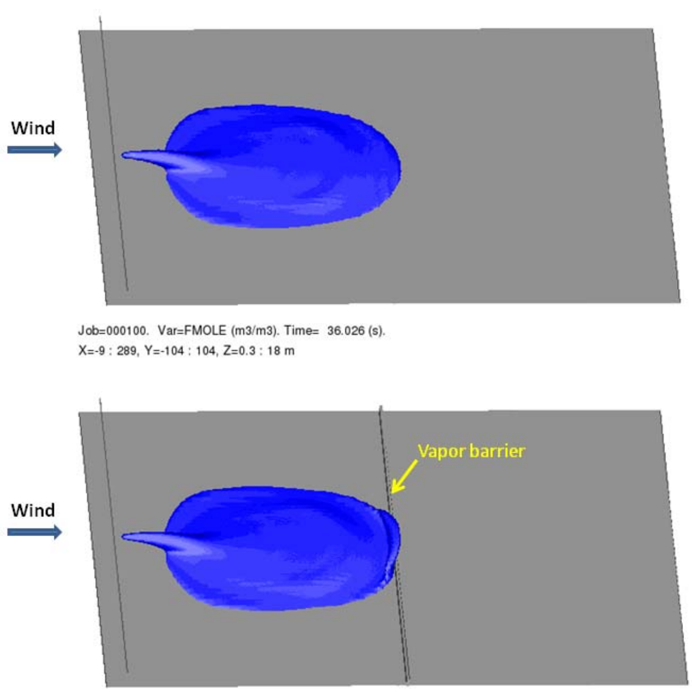

Figure 2. ½-LFL vapor cloud dispersion from high-pressure release, after approximately 36 s: unobstructed case (top) vs. obstructed case (bottom).

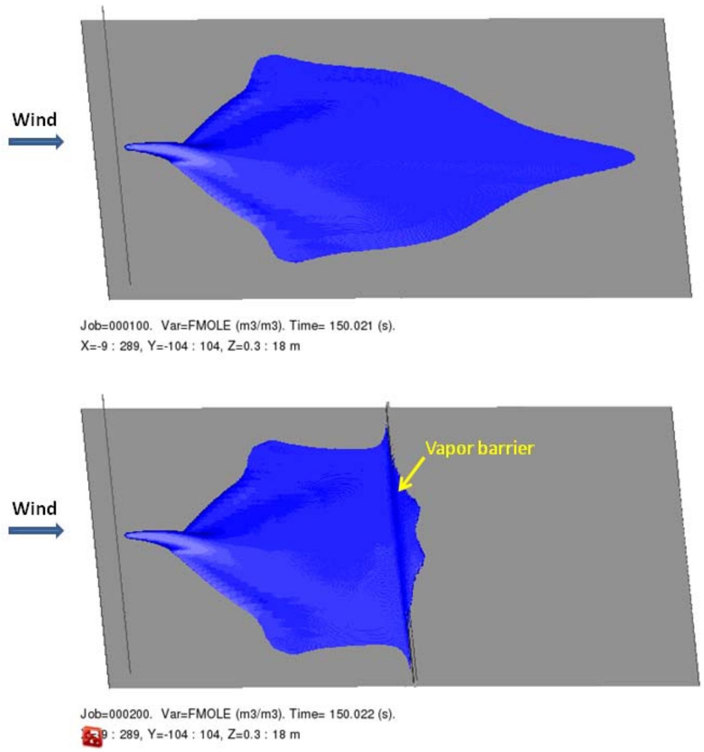

Figure 3. ½-LFL vapor cloud dispersion from high-pressure release, after approximately 150 s: unobstructed case (top) vs. obstructed case (bottom).

This example demonstrated how coupling the one-dimensional flashing jet calculations with a three-dimensional CFD model allows one to account for and benefit from the effect of obstacles (including passive mitigation features) on vapor cloud dispersion.

Scenario 2: Flange leak

The leak scenario assumes a complete gasket loss in a flange for a 30 cm diameter pipe carrying LNG. The pipe runs horizontally at 10 m elevation; the pipe pressure is 10 barg and the LNG is at -150°C. The leak is assumed to continue at the nominal flow rate (i.e., with no drop in pressure inside the pipe) for 180 s and the simulation is continued until 200 s. Ambient conditions are assumed to be as follows: 20°C temperature, 2.0 m/s wind speed at 10 m elevation, and stable atmosphere (Pasquill-Gifford class “F”); the effects of humidity are neglected.

The complete loss of a gasket results in a radial leak around the circumference of the flange, with a total flow area of approximately 29.9 cm^2. The resulting flow rate is approximately 92 kg/s, with a liquid volume fraction of approximately 4.5%, and is assumed to remain constant for 180 s. This case has been simulated with the FLACS’s two-phase module and Figures 4 and 5 show the volume fraction isocontours for the liquid (top) and the vapor (bottom), respectively, 1 s and 30 s after the beginning of the leak.

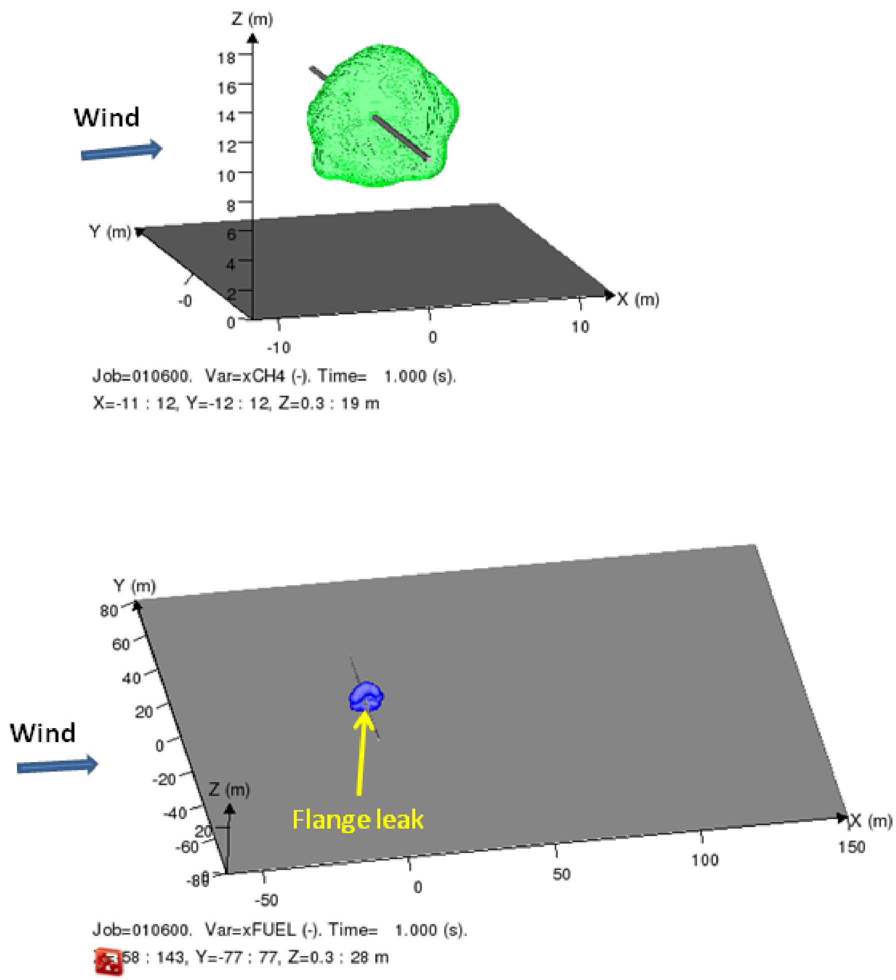

Figure 4. Liquid (top; 0.01% volume fraction, which after evaporation would correspond to an equivalent vapor cloud at approximately LFL) and vapor (bottom; 2.5% volume fraction) volume fraction from high-pressure flange leak, after approximately 1 s. Note that the top image is zoomed to the leak location to show the liquid volume fraction distribution more clearly.

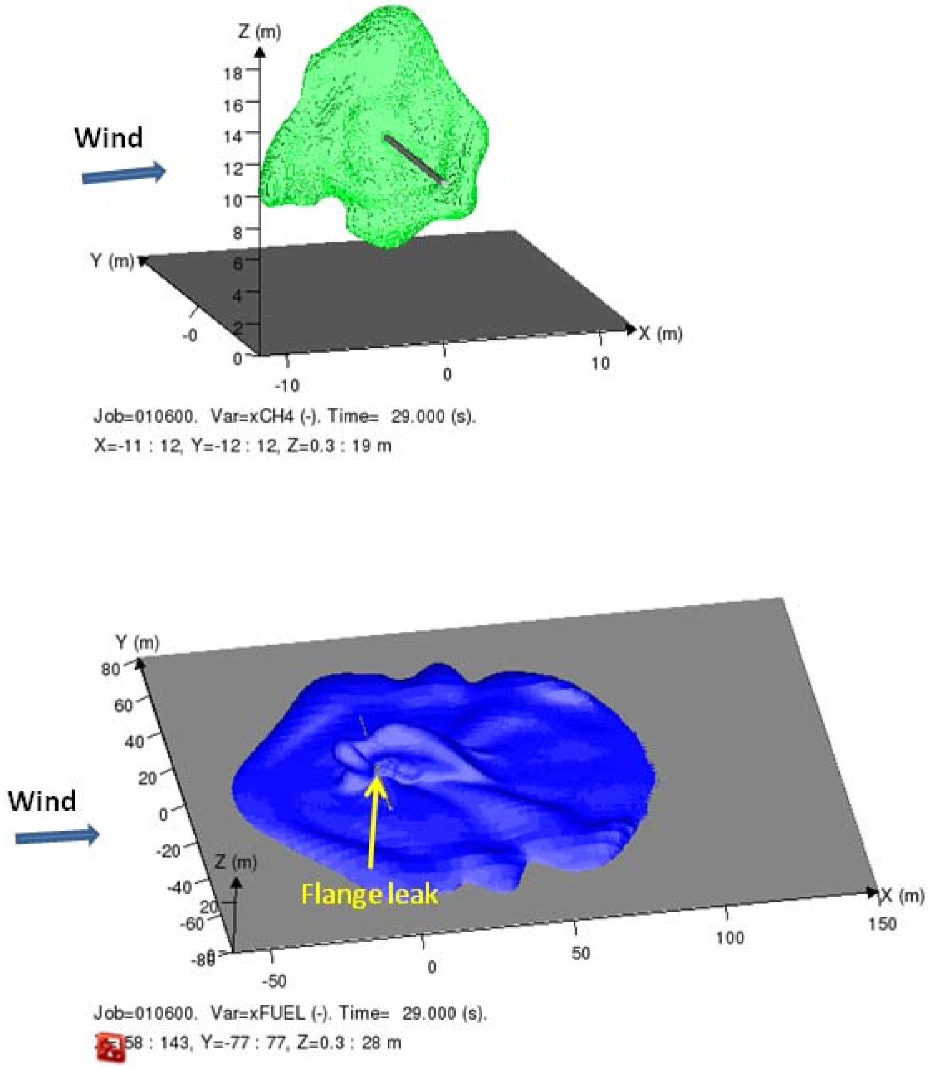

Figure 5. Liquid (top; 0.01% volume fraction, which after evaporation would correspond to an equivalent vapor cloud at approximately LFL) and vapor (bottom; 2.5% volume fraction) volume fraction from high-pressure flange leak, after approximately 30 s. Note that the top image is zoomed to the leak location to show the liquid volume fraction distribution more clearly.

The flashing jet correlations typically used for high-pressure releases (as in Example 1 above) cannot be applied to the radial leak pattern in this scenario without drastic and potentially very conservative assumptions. For example, if the vapor cloud dispersion is calculated using an integral model, only a single, unidirectional jet can be simulated: an intuitive, but not necessarily conservative approach would be to split the radial flow into two horizontal components – upwind and downwind – and to calculate the vapor cloud dispersion only for the downwind component.

In Figure 6, the vapor cloud dispersion from a single, horizontal flashing jet at half the leak flow rate (calculated as in example 1) is compared with the more realistic radial leak pattern simulated using FLACS' two-phase module. In the radial leak simulation, the two-phase jet emerges with zero net momentum in the downwind direction, which results in a wider and slower moving vapor cloud that dissipates below ½-LFL within a shorter distance than in the horizontal jet simulation.

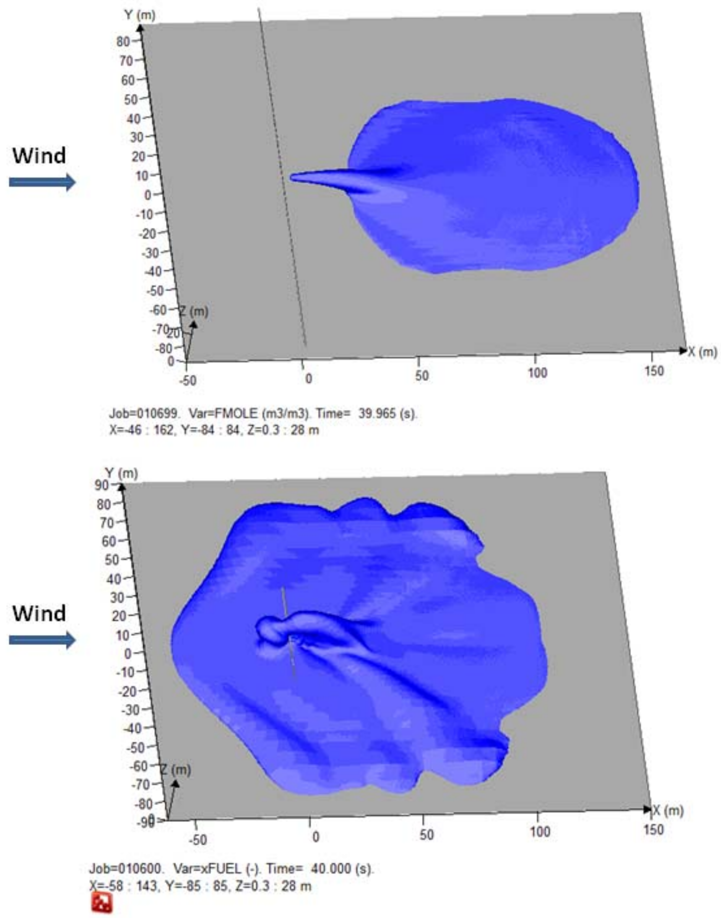

Figure 6. ½-LFL vapor cloud dispersion from high-pressure flange leak, after approximately 40 s: horizontal flashing jet (top) vs. two-phase radial leak (bottom). Note that the horizontal flashing jet (top image) represents only half of the total LNG spill flow rate.

Conclusions

This paper demonstrates the application of the CFD model FLACS to high-pressure releases of LNG, for the purpose of determining the vapor dispersion hazard distances for facility siting. FLACS provides the following advantages when applied to the simulation of vapor dispersion from high-pressure LNG releases:

1. It is a CFD model capable of simulating the effects of obstacles and complex geometry on the flow of air and vapors;
2. It has been validated for LNG vapor dispersion; and

3. It includes a two-phase module capable of simulating the high-pressure jetting and flashing release from the source.

The examples provided in this paper show the potentially significant benefits of performing vapor dispersion calculations from high-pressure releases using a CFD tool like FLACS, in terms of reducing the size of exclusion zones by performing more realistic simulations or by taking proper credit for passive mitigation features (e.g., vapor barriers).

References

[1] Witlox, H.; Harper, M.; Bowen, P. & Cleary, V., "*Flashing Liquid Jets and Two-Phase Droplet Dispersion. I. Overview (Literature Survey, Experiments and Model Implementation / Validation)*", 8th Annual Symposium, Mary Kay O'Connor Process Safety Center, 2005

[2] Cleary, V.; Bowen, P. & Witlox, H., "*Flashing Liquid Jets and Two-Phase Droplet Dispersion. II. Experiments for derivation of droplet atomisation correlations*", 8th Annual Symposium, Mary Kay O'Connor Process Safety Center, 2005

[3] Ermak, D. L., "*User's Manual for SLAB: an Atmospheric Dispersion Model for Denser-than-Air Releases*", Lawrence Livermore National Laboratory, 1990, UCRL-MA-105607

[4] Witlox, H. M. & Holt, A., "*A unified model for jet, heavy and passive dispersion including droplet rainout and re-evaporation*", CCPS, 1999

[5] Hanna, S. R.; Hansen, O. R. & Dharmavaram, S., "*FLACS CFD air quality model performance evaluation with Kit Fox, MUST, Prairie Grass, and EMU observations*", Atmospheric Environment, 2004, 38, 4675-468

[6] Hanna, S. R.; Hansen, O. R.; Ichard, M. & Strimaitis, D., "*CFD model simulation of dispersion from chlorine railcar releases in industrial and urban areas*", Atmospheric Environment, 2009, 43, 262-270

[7] Dharmavaram, S., Hanna, S.R. & Hansen, O.R, "*Consequence analysis – using a CFD model for industrial sites*", Process Safety Progress, 2005, 24, 316–327.

[8] Arntzen, B.A., "*Modelling of turbulence and combustion for simulation of gas explosions in complex geometries*", PhD thesis, 1998, NTNU, Trondheim, Norway. ISBN 82-471-0358-3.

[9] Hansen, O.R., Ichard, M. & Davis, S.G., "*Validation of FLACS for Vapor Dispersion from LNG Spills: Model Evaluation Protocol*", Proc. 2009 Mary Kay O'Connor Process Safety Symposium

[10] Salvesen, H.C., "*Modeling Release of Liquefied Gas Under High Pressure*", CMR-95-F20062, Christian Michelsen Research, 1995, 33 pp.

[11] Kukkonen, J., Kulmala, M., Nikmo, J., Vesala, T., Webber, D.M. & Wren, T., "*The homogeneous equilibrium approximation in models of aerosol cloud dispersion*", Atmospheric Environment, 1994, Vol. 25, No. 17, pp. 2763-2776

[12] Ichard, M., Hansen, O. R. & Melheim, J. A., "*Modeling of flashing releases around buildings*", 90th AMS annual meeting, Phoenix, AZ, USA, 2009

[13] Ichard, M., Hansen, O. R. & Melheim, J. A., "*Releases of pressurized liquefied gases: Simulations of the Desert Tortoise test series with the CFD model FLACS*", 91st AMS annual meeting, Atlanta, GA, USA, 2010

Speaker's Bio

Dr. Filippo Gavelli is the Head of the Dispersion Consulting group at GexCon US, Inc. and specializes in the analysis of heat transfer and fluid flow phenomena, including multiphase flows and cryogenic fluids. He applies his engineering and CFD modeling expertise to the atmospheric dispersion of hazardous gaseous releases, and has extensive experience modeling Liquefied Natural Gas (LNG) vapor cloud dispersion. Dr. Gavelli is responsible for GexCon US' dispersion modeling activities, which include risk assessments and consequence modeling for chemical and petrochemical facilities, offshore installations, hazardous materials transportation and various other applications. He is the lead author of several LNG safety-related papers and has contributed to numerous LNG-related technical committees and expert panels.