CFD-Modeling of LNG Dispersion Experiments

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Introduction

The CFD-tool FLACS was developed from 1980 to model hydrocarbon gas explosions in process facilities. In order to also predict the gas build-up, very, the functionality very soon was extended to include dispersion. During three decades extensive validation against experiments has been given high priority in the FLACS development. FLACS is now considered to be a leading CFD-tool for gas explosion modeling, the modeling of hydrogen dispersion and explosion, dust explosion modeling and for dispersion modeling in offshore and onshore congested process areas.

With support from Norsk Hydro, Total, Statoil and Petroleum Safety Authority Norway (PSA), and in cooperation with DNV, a LNG-development and validation project for FLACS has been carried out recently. The first phase of the project was a validation activity in which 8 tests from Burro and 3 tests from Coyote experiments performed at China Lake (USA), and 4 tests from Maplin Sands (UK) have been simulated. Predicted downwind maximum gas concentrations at various distances have been compared to experiments showing good correlation. This validation activity will be presented in the current paper. Models have been further developed to extend the pool simulation capabilities to allow the formation and spread of a pool with local evaporation rates based on heat from ground, wind speed, local vapor pressure. These models will be described, and simulation examples will be shown. The combination of a good description of physical models and the ability to take into account buildings, terrain or process plants is essential for a proper consequence modeling of LNG-releases.

LNG-Vapor Dispersion Validation Study

The first part of this paper describes a validation study of FLACS simulating the dispersion downwind of LNG-releases. During previous FLACS development projects there has been a massive validation against explosion experiments, but also ventilation and dispersion studies both with natural gas (Phase 3B [1]), releases of buoyant or dense gas [2], and tracer gases [3]. In the study described here, releases of up to 100 kg/s or more LNG was released into a pond in Burro/Coyote tests [4] or river Maplin Sands [5]. In the modeling a simplified approach for the LNG pool has been assumed, in which natural gas is released with low momentum above ground at boiling point temperature. The ground is modeled flat, for Burro & Coyote the pool location is slightly lower than the terrain, in addition to this two buildings used for instrumentation and gas storage were also modeled. Burro & Coyote geometry model can be seen in Figure 1.

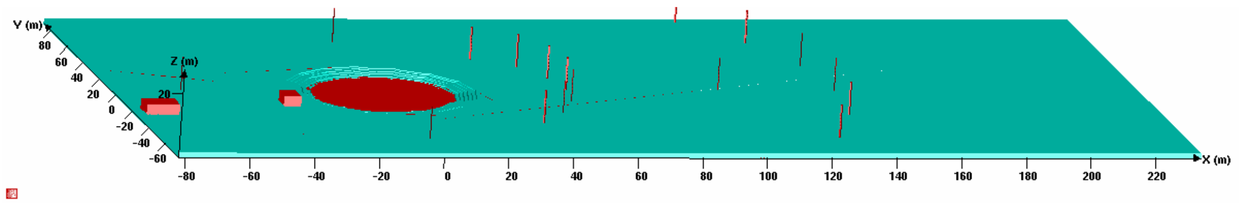


Figure 1 Burro & Coyote geometry model in FLACS [4]

In the simulations the proper wind direction was simulated, with assumption of some meandering of wind. In Figure 2 simulated gas plume (> 1%) is compared with observations in Burro test 7. In Figure 3 the observed temperature reduction due to the LNG release at 57m monitor point is compared to simulation.

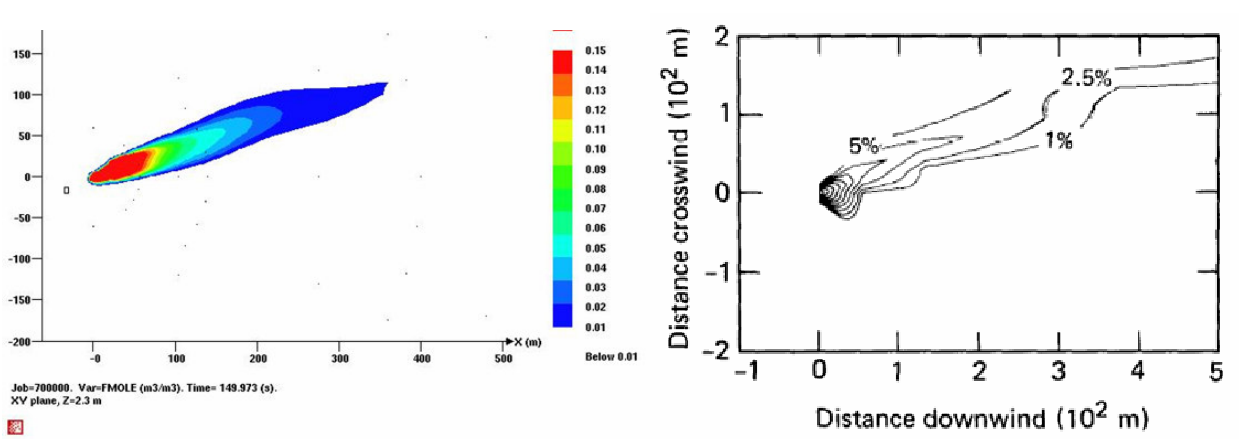


Figure 2 Example of plume comparison Burro 7 simulation (left) versus contour plots based on experimental recordings [4]

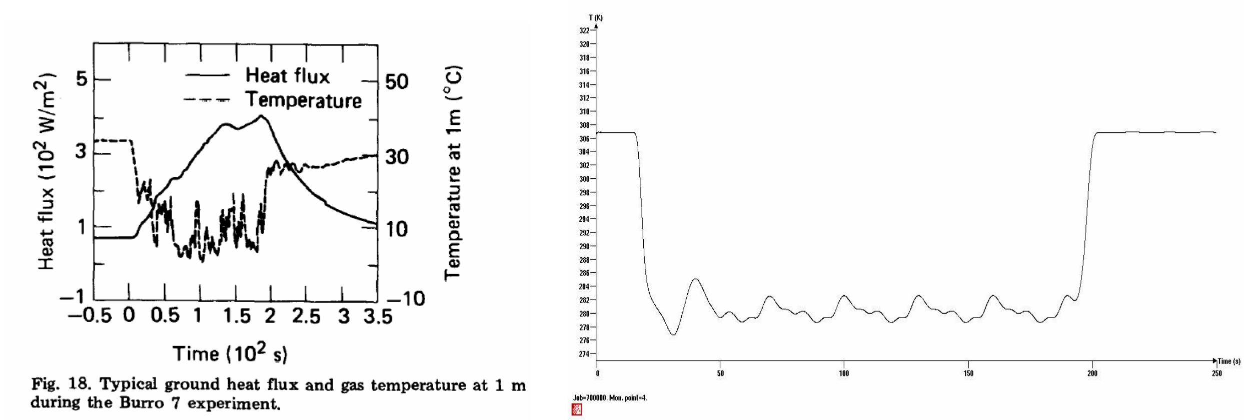


Figure 3 Example of observed temperature reduction at 57m sensor in Burro 7 experiment (left) versus simulation (right) [4]

In the Burro & Coyote validation study a very detailed curve-by-curve comparison for sensors at each monitor arch and elevation (1m, 3m and 8m) was carried out. One example of such comparison plots are shown in Figure 4, where curve comparisons for Coyote 6 experiment and simulation are compared a 1m elevation 140m, 200m and 400m from the release. Similar plots are produced for all 11 Burro and Coyote tests for all monitor point elevations. A numerical comparison of maximum reported concentrations at each sensor and arc was also carried out, with different averaging times 0s, 10s, 30s and 60s. The parabola plots in Figure 5 are using this information with 10s averaging for Burro & Coyote, each point in the plot is a geometric variance versus geometric mean observation taking into account maximum averaged observation at each of 2-3 downwind arcs (each with measurements at 5-7 different positions and 2-3 elevations). In Figure 6 a similar parabola plot is shown for simulation of Maplin Sands experiments, here each point in the parabola is the result of 2-7 downwind observations. For MS 29 observations at 7 different distances were available, and these are compared with FLACS simulations on a coarse grid (4m x 4m x 0.5m) and fine grid (2m x 2m x 0.25m) resolution.

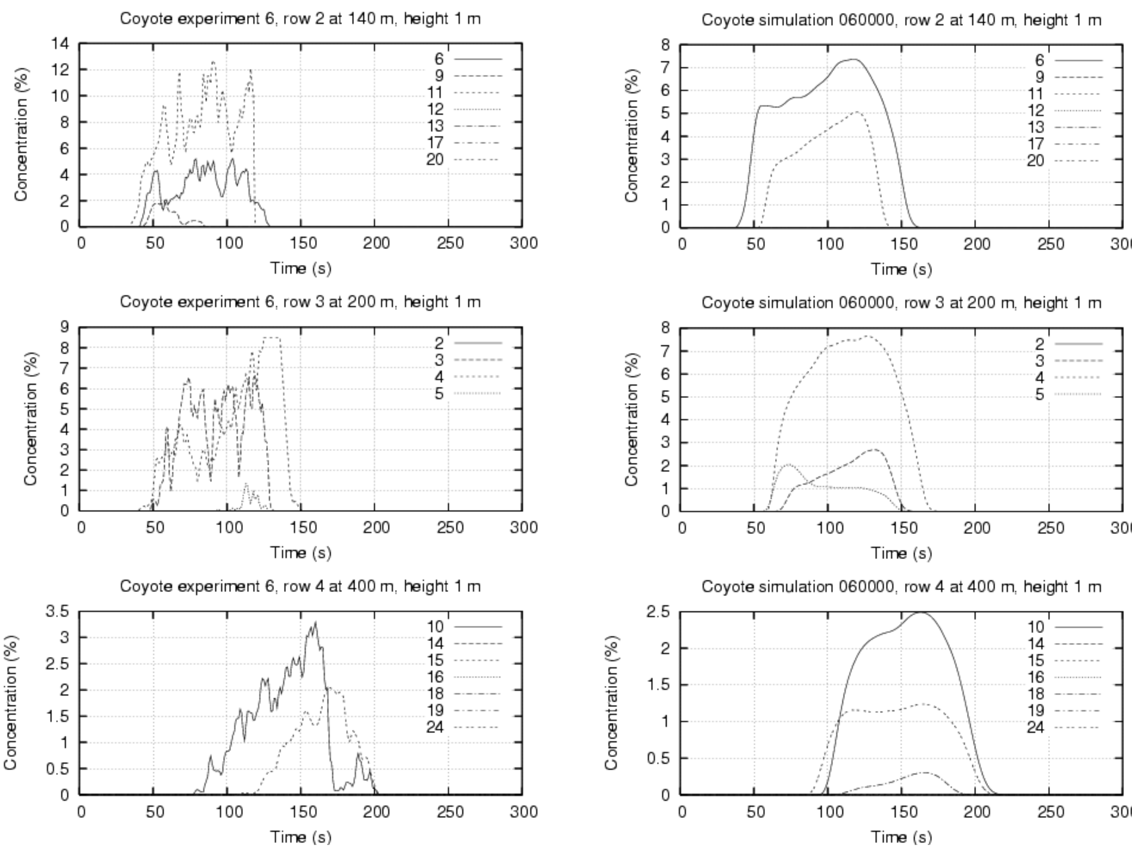
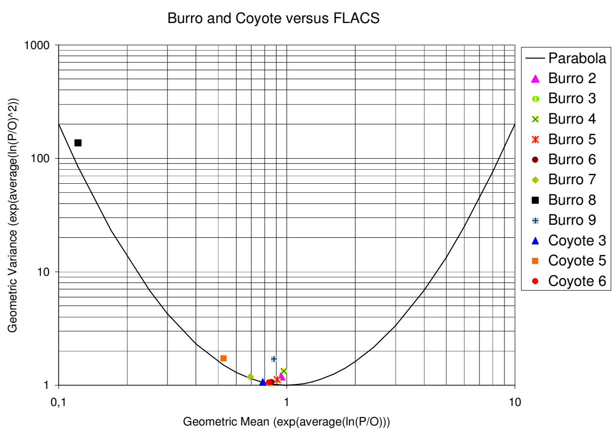


Figure 4 Example of monitor arc comparisons, observed concentrations for Coyote test 6 measurement arcs at 140m, 200m and 400m compared to simulated concentrations.

In general good simulation results are seen. Wind conditions in experiment are not controlled, and tend always to be more chaotic than assumed in simulation model. One consequence of this is that it is difficult to compare average concentrations at downwind arcs since significant wind fluctuations are seen. When using short averaging times, and considering maximum reported concentration at each downwind arc, for two reasons some underprediction in simulations should be expected. The first reason is that the higher variability of the wind in the experiment will also make the reported concentrations oscillate more than in simulations, and with short averaging time this gives a somewhat high concentration reported from experiment. Second, with the lower wind fluctuations assumed in the simulations, we will to a greater extent fail to hit measurement points with the highest concentrations (plume falls between sensors). For these reasons, the weak underprediction of concentration level shown in Figure 5 is considered fully acceptable. For the one scenario with low wind (Burro 8, 1.8m/s) a factor of 10 underprediction of concentration are seen at measurement points. However, when comparing downwind extent of flammable gas concentration, very good results are seen. The explanation to this deviation is simply that in simulations the dense gas cloud was mainly below the 1m sensors, whereas in the experiment sporadically higher concentrations reached the sensors likely due to much more local variability in the wind.



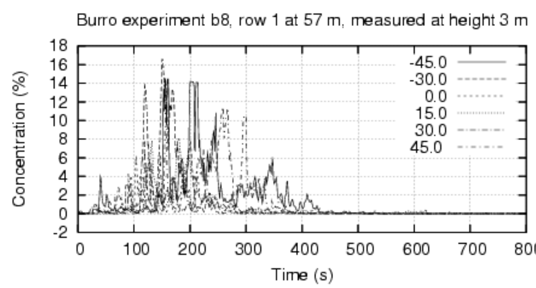
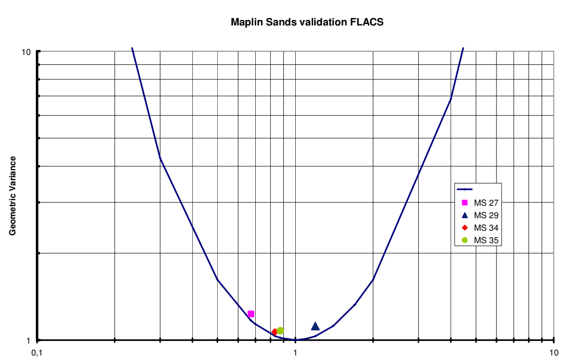


Figure 5 Geometric variance versus geometric mean for all 8 Burro and 3 Coyote experiments, each point is based on maximum observations at 6 different arc distances/elevations. In the right picture an example of sensor observation from Burro 8, with high concentrations only seen sporadically.



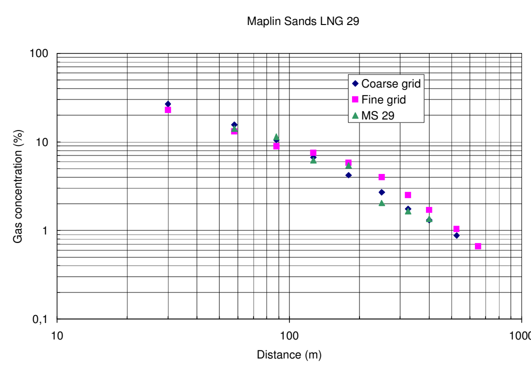


Figure 6 Geometric variance versus geometric mean for all 4 Maplin Sands experiments simulated (left plot), observations [from Hanna] at 2-7 different downwind distances are compared. For Maplin Sands test 29 (29 kg/s LNG with 7.4 m/s wind) 7 observations with increasing distance were available and compared to simulation results (right plot) with fine grid and coarse grid.

Development of LNG pool models and humidity effects

In 2002 an LNG pool evaporation model was developed for FLACS [6]. The model took into account several parameters like heat flux from ground, solar influx, wind parameters and more. Limitations of the model were that the pool had a fixed size and shape (circular or ring), and would not include LNG added to the pool during the simulation. In the current work a further development of these models are performed.

A pool will spread until it reaches a steady state where the evaporation balances the leak or obstacles hinder the pool spread. A LNG pool is driven by gravitational forces in form of differences in the pool height and the shape of the ground and friction resist the spread. For LNG, it is assumed that the surface tension can be neglected. In several pool-spread models, a circular or semi-circular pool is considered [7]. It is, however, easy to imagine scenarios where a more general description of the pool spread will be more realistic. Woodward [8] described the pool spread by transport equations for the pool height, radial velocity and temperature on an annular grid, and it is straightforward to write the governing equations in [8] for any grid.

In real life, the source of the leak, for instance a storage tank or a LNG tanker, will setup a non-uniform flow field above the pool. Expressions based on boundary layer theory are therefore used to calculate the convective heat and mass transfer in grid cell separately. The equation solved for the pool height is given by:

$$\frac{\partial h}{\partial t} + \frac{\partial h u_i}{\partial x_i} = \frac{\dot{m}_L - \dot{m}_V}{\rho_l} \qquad (1)$$

and the momentum equation is written as:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = F_{g,i} + F_{\tau,i} \qquad (2)$$

The gravity term is written as:

$$F_{g,i} = g\Delta \frac{\partial (h+z)}{\partial x_i} \Bigg/ \sqrt{\left(\frac{\partial (h+z)}{\partial x_i}\right)^2 + 1} \qquad (3)$$

where also the height of the ground above a reference level *z* has been included. Δ equals 1 for solid grounds and $\Delta = (1 - \rho_l / \rho_w)$ for spill on water. The shear stress can be given by the general formula:

$$F_{\tau,i} = \frac{1}{2} f_f u_i |\vec{u}| \qquad (4)$$

where the friction factor is follows the expression for flows on fully rough surfaces.

The equation for the specific enthalpy is given by:

$$\frac{\partial \theta}{\partial t} + u_i \frac{\partial \theta}{\partial x_i} = \frac{\dot{m}_L}{h}\left(\theta_L - \theta\right) + \dot{q}_c + \dot{q}_{rad} + \dot{q}_{ground} + \dot{q}_{evap} + \dot{q}_{boil} \quad (5)$$

The first term on the right hand side is due to the leak. The model for the convective heat and mass transfer is based on boundary layer theory, dividing the boundary layer into a viscous region and a log-region. The convective heat transfer is given by [9]:

$$\dot{q}_c = \frac{\rho_g C_\mu^{1/4} k^{1/2} c_{p,g} T_g \ln \frac{T_l}{T_g}}{T^+} \quad (6)$$

where $T^+ = \Pr y^+$ in the viscous region and $T^+ = E^+ \Pr + \Pr_t / \kappa \ln\left(y^+ / E^+\right)$ else.

Analogue to the heat transfer, the expression for the mass transfer is written as [10]:

$$\dot{m}_c = \frac{\rho_g C_\mu^{1/4} k^{1/2} \frac{P_0}{RT_l} \min\left\{-\ln\left(\frac{1 - x_{sat}}{1 - x}\right),\ 3.1534\right\}}{x^+}$$

where the *Stefan flow* has been taken into account. Stefan flow might be important for large mass fluxes [11]. $x^+ = \mathrm{Sc}\, y^+$ in the viscous region and $x^+ = E^+ \mathrm{Sc} + \mathrm{Sc}_t / \kappa \ln\left(y^+ / E^+\right)$ outside. The modeling of the radiative heat transfer, heat from ground and heat loss due to evaporation and boiling is described in [6]. The governing equations for the pool are discretized on a non-uniform Cartesian staggered grid in two dimensions with a finite volume method. An upstream scheme is employed for the convective terms in the momentum equation, while a central difference scheme is used for the enthalpy equation. The equations are solved explicitly in time.

In Figure 7 results from a simulation using the improved pool models are shown. A 1000 kg/s LNG release from a cylindrical tank onto the ground is modeled, and the LNG-pool spreads on the ground falls into the sea. The development of methane vapor cloud volume above stoichiometry is also shown.

When modeling vapor cloud dispersion from releases of cryogenic liquids, the temperature effects when cooling the air must be taken into account. Air humidity may gradually condensate to mist when temperature is reduced, and thus influence the efficient heat capacity of the air. In Figure 8 an example is shown of the modeled heat capacity of air with humidity taking into account the condensation of water vapor. When implementing the models, we had access to a report from DNV describing how they used a similar approach when modeling with CFX [11].

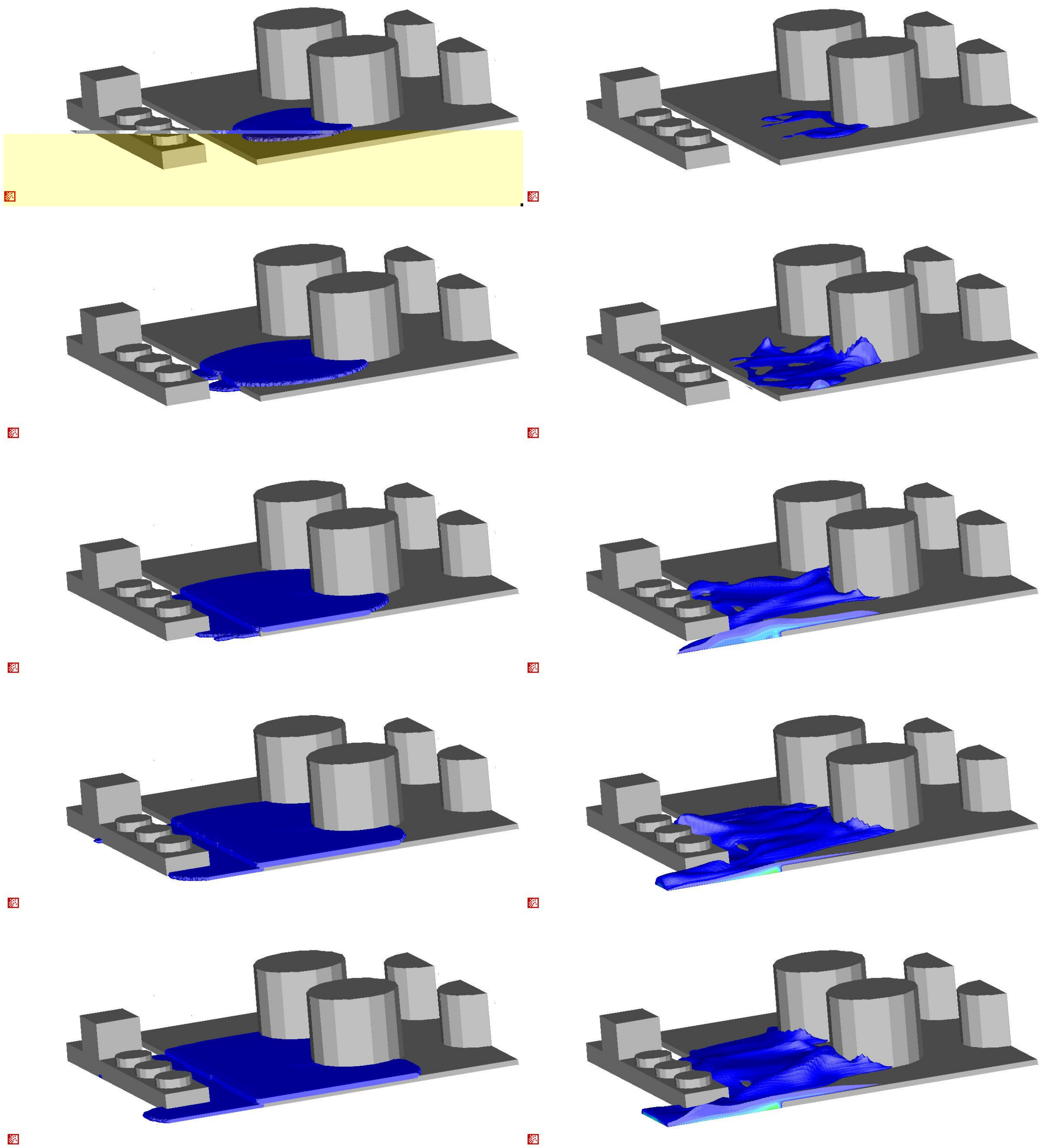


Figure 7 **Simulated 1000 kg/s LNG leak from tank with liquid pool development (left) and vapor cloud above stoichiometry (right), simulated wind speed is 5 m/s, pictures show 25s, 50s, 100s, 150s and 200s after start of release. A "simplified" LNG-carrier is included in the simulation.**

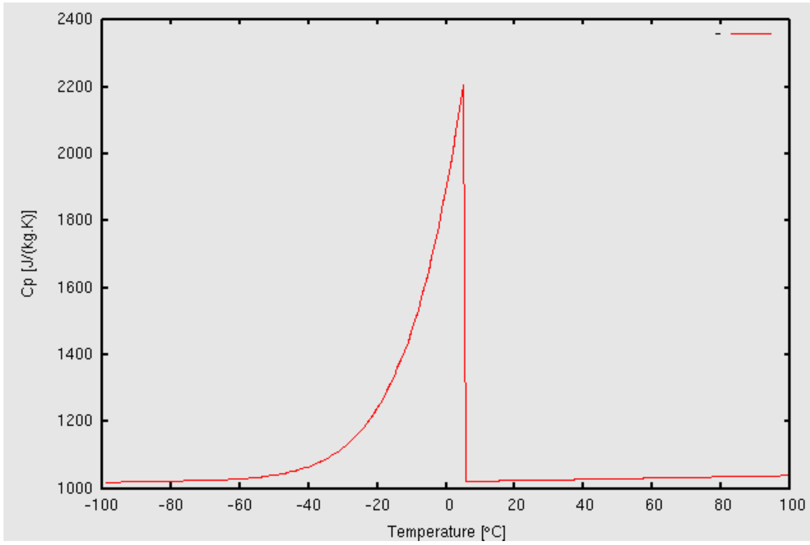


Figure 8 **Efficient heat capacity of air containing some water vapor, according to newly implemented models in FLACS. For certain release conditions, some additional humidity of air may make the evaporated cold natural gas buoyant.**

Further development tasks

Despite a newly developed pool model with potentially advanced possibilities, there will always be modeling aspects that can be improved. Through previous validation work it has been demonstrated that FLACS dispersion modeling is good once the LNG evaporates. Some elements that could be improved are the understanding of heat transfer phenomena, of the arbitrary atmosphere and stability classes (in particular Pasquill A, B and C), and more details on pool behavior e.g. when mitigation is applied. For most of these phenomena it is however difficult to describe reality very detailed.

When modeling with FLACS there are however limitations using Cartesian grids. Whereas process plants and buildings are generally well described using the distributed porosity concept of FLACS, dominating sloping elements like terrain will be less good modeled. In the presented validation study, most predictions were carried out with a flat terrain assumption. Still some calculations were performed with a realistic representation of the terrain. The sloping terrain will be represented as steps on a Cartesian grid giving a too high momentum loss. With large grid cell sizes in the vertical direction, this will influence the downwind predicted hazard distance. Future development work will aim at implementing numerical schemes that will minimize the momentum loss for sloping terrain. In the meantime a fine vertical grid resolution (much finer than height of gas cloud) will be recommended when modeling dense gas dispersion in a sloping terrain.

Since FLACS is primarily an explosion simulator, the explosion effects of the dispersed clouds from LNG-pools should be well taken care of. Another hazard in connection to LNG release scenarios will be fire. FLACS has in the past not been able to model fire scenarios (with precision). There is however an ongoing development which will improve the fire modeling capabilities of FLACS in future versions of the tool.

Acknowledgments

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Conclusion

FLACS is established as a very powerful CFD tool for gas dispersion, in particular for situations where detailed description of geometry details is of importance (process facilities, urban areas and more). Numerous validation activities have been carried out in the past, the current paper describes a validation activity simulating the dispersion from LNG-release experiments Burro, Coyote and Maplin Sands. Results are generally good, FLACS predicts downwind natural gas concentrations with reasonable precision assuming the released LNG quickly evaporates from a pool with boiling point temperature. A further improvement of pool models is described in the paper which hopefully will lead to a more realistic description of accident scenarios simulated in connection to risk assessments.

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