

CFD SIMULATION OF LNG SPILLAGE

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Abstract. LNG (Liquid Natural Gas) accidental cryogenic spillage is one of the major safety concerns of Floating LNG facilities-FLNG. Superstructures such as topsides, deck and hull shall be properly protected against these risks. Modelling approach may be an efficient way for a better knowledge of the overall problem. The objective of the project is then to develop a 3D CFD model able to simulate all the physics of the spillage process. For this purpose, the CFD software EOLE of Principia is considered. Academic validations have been performed and are presented in the paper.

1 INTRODUCTION

Stakes of Quantitative Risk Assessment and safety studies performed in FLNG detailed engineering require our knowledge and modelling capabilities to be improved. The following complex physical phenomena which occur during cryogenic LNG releases from topsides leak point down to the sea water contact, need especially to be investigate in order to better quantify the extent of these phenomena and evaluate protection requirements (figure 1):

- 1) LNG jet fragmentation (liquid jet breakup), vaporization, rainout.
- 2) LNG pool formation, spreading and coalescence, heat transfer to the LNG pool and vaporization on solid structures leading to LNG vapour dispersion.
- 3) FLNG deck overtopping, drip and fall along hull vertical structures.
- 4) LNG pool formation on seawater and spreading.
- 5) LNG pool vaporization and dispersion from sea level.

A 3D CFD software has been developed to sequentially simulate all the physics. It is based on a URANS model using coupled VOF and mixture models to simulate all dynamic/thermodynamic processes of LNG multi-phases flows, more specifically:

- LNG/water, LNG/air and water/air interfaces mechanisms (VOF model including surface tension).
- Two-phase dispersed LNG droplets in continuous air phase (mixture model).
- LNG vaporization (vaporization/condensation source term in VOF and mixture models).

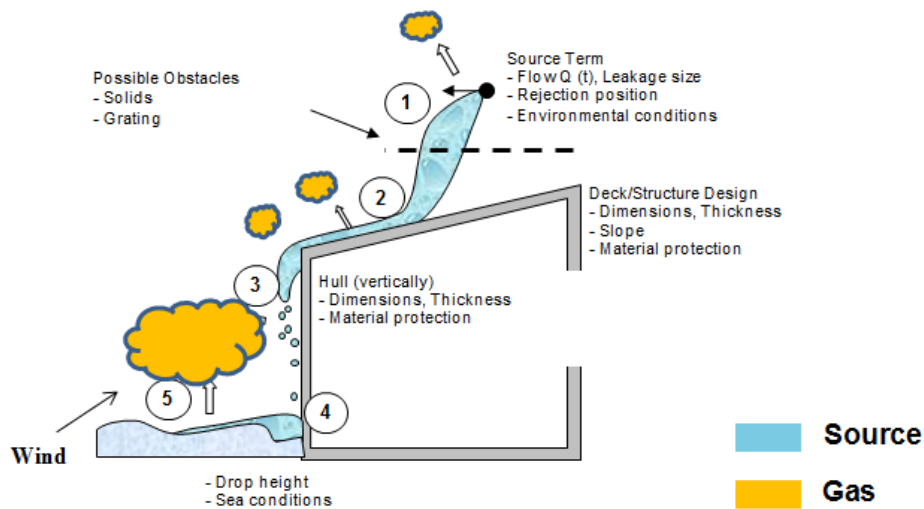


Figure 1: Sketch of the different mechanisms from the leak in FLNG topsides (1) down to the pool spreading/vaporization on sea water (4) and vapour dispersion (5)

Academic validations have been performed following a step-by-step approach allowing to investigate the different mechanisms separately:

- Jet mechanisms (mechanical fragmentation – thermodynamic flashing – rainout).
- LNG pool spreading and vaporization on solid substrate.
- LNG pool spreading and vaporization on water.

The paper presents the theoretical description of the numerical model and some examples of academic validation results.

2 NUMERICAL MODELLING

2.1 General description

For liquid jet and pool modelling, the main characteristics of a CFD model required to simulate all the physics of the problem are the following:

- Navier-Stokes equations in each fluid to account for dynamical interactions between the fluids.
- Stable and fragmented liquid jet: fluids interface model allowing to capture complex processes like fragmentation, coalescence, impact on structure (choice of the VOF model particularly well adapted to represent all these physics). For a fragmented jet, interface instabilities developing on the liquid jet interface (due to the shear stress with the air flow) and the induced fragmentation process needs to be computed by the model. From this primary break-up of the jet, the issued bigger ligaments (and

droplets) are directly computed in the mesh by the VOF model. In addition, the surface tension force has also to be included because it may be not negligible with respect to inertia especially for the smaller ligaments.

- Co-existence of different kinds of interface (LNG/air, LNG/water, air/water) so need to duplicate a VOF methodology for each kind of interface [1].
- Two-phase jet: when the jet is fully fragmented the flow appears as a dispersed droplets phase evolving in a continuous air phase. For the smaller droplets which have size “under cell size discretization”, the VOF model is no longer able to represent them in the mesh, so a coupling with an eulerian “mixture” model for these smaller structures is required. In this model the phases are treated as interpenetrating continua, meaning without interfaces between phases. A volume fraction function for the small droplets is introduced allowing to characterize the mixing of the secondary phase (droplets) into the continuous phase (air, gas...). Then the droplets are represented in the mesh by this function as for the VOF but on the contrary of the VOF method which is based on a specific transport equation for sharp discontinuities (the interfaces), the eulerian “mixture” model is a classical transport equation (including an added term to account for drag and buoyancy of the droplets, when there is a relative velocity between phases).
- Local representation of the fluid characteristics (density, viscosity, thermal transfer) in each cell of the mesh. For a cell containing several fluids, the mean characteristics of the mixture are deduced from the volume fraction of the different fluids.
- Vaporization: the energy equation $mC_p \frac{dT}{dt} = Q - L\dot{q}$ is locally solved (with Q the heat flux, L the latent heat of vaporization and \dot{q} the vaporization rate). This equation allows more particularly translating the fall of temperature due to the latent heat absorbed in transforming the liquid into gas, during vaporization process. The vaporization term \dot{q} is also integrated as a source term in the VOF (and mixture) equation representing LNG (see §2.2). Note that a similar VOF modified model for cavitation problem has already been developed in the software [2].
- LNG vapour dispersion in air computed from a convection-diffusion scalar equation. The vaporization term \dot{q} is integrated as a source term in this equation.
- Buoyancy effects (natural convection) computed from density gradients in the fluids: LNG in water (about half density of water), LNG vapour in air.
- Equation of state for each fluid, especially for LNG which depends on pressure and temperature.
- Turbulence mixing especially for a LNG jet penetrating in water (development of vortices). The turbulence greatly increases the vaporization rate.
- Thermal interaction between fluids (LNG/water, LNG/air, water/air). The heat transfer between fluids is computed from the direct resolution of the energy equation considering the local properties of the different fluids and their volume fraction in each cell of the mesh. In this model there is no need to introduce empirical heat transfer coefficient.
- Thermal interaction between fluids and solid which can be simulated from a simple thermal boundary condition or, in a more accurate, way from a direct calculation of

the thermal fluid/solid coupling. In this case, the solid is discretized (meshing) as for the fluid, and the solid characteristics have to be included in the model.

- Influence of the substrate (especially roughness for solid substrates) on the dynamic boundary layer (shear stress) and the velocity of the liquid, and the thermal boundary layers which lead the thermal transfer between solid and fluid (or between two fluids). Increase of the surface exchange with roughness for solid substrate.
- Dynamic (pressure) impact of the liquid on structures.
- Thermal load on structures in contact with LNG.
- Changing of the composition of LNG during vaporization (variation of the saturation temperature, T_{sat}). But to simplify matters, it could be acceptable to model LNG as pure methane.
- Environmental conditions: influence of wind, waves and currents.

2.2 System of equations

The model includes classical Navier-Stokes system plus specific models:

- Mass conservation
- Momentum
- Energy
- k- ϵ turbulence model
- Equation of state for the fluid
- Multi-interfaces model: a VOF equation for LNG/water (or air) interface and for water/air interface
- Transport concentration of vaporized gas
- Mixture model: concentration of dispersed phase (for the smaller droplets)

The following paragraphs present these specific models.

Multi-interfaces model

It is used to simulate LNG/air, LNG/water and water/air interfaces.

The VOF method introduces a discrete function F (value included between 0 and 1) in each cell which represents the fraction of the cell occupied by the liquid. The fraction $1-F$ of the cell volume is occupied by the gas.

The transport of the fraction F , so the motion of the interface in the fixed mesh, can be ensured by a classical eulerian method.

Thus a transport equation is solved for the VOF function giving the kinematic motion of the liquid/gas interface in the eulerian mesh, induced by the fluid velocity \vec{V} :

$$\frac{\partial F}{\partial t} + \vec{V} \cdot \text{div}(F) = 0 \quad (1)$$

The interface location is first determined by calculating the normal vector \mathbf{n} of the interface, related to the gradient of volume fraction F by $\vec{n} = \frac{\nabla F}{\|\nabla F\|}$. With the knowledge of the interface orientation and the local fluid velocity, the volume of fluid transferring into the neighbouring cells is evaluated and the volume fraction F updated.

In the case of a LNG pool spreading on a liquid substrate (water), two liquid phases of high density (LNG and water) are in presence of lower density phase (air). Two VOF equations introducing two discrete functions F_1 and F_2 are required to track the kinematic motion of the two liquid interfaces:

- LNG interface motion is calculated using $\frac{\partial F_1}{\partial t} + \vec{V} \cdot \text{div}(F_1) = 0$. The discrete function F_1 (value between 0 and 1) is the fraction of the cell occupied by the LNG. The fraction $1-F_1$ of the cell volume is occupied either by the air and/or the water.
- Water interface motion is calculated using $\frac{\partial F_2}{\partial t} + \vec{V} \cdot \text{div}(F_2) = 0$. The discrete function F_2 (value between 0 and 1) is the fraction of the cell occupied by water. The fraction $1-F_2$ of the cell volume is occupied either by the air and/or the LNG.

To prevent the two liquid phases LNG and water from penetrating into each other (non miscible fluids of different density), LNG and water interface motions are constrained such as $F_1 + F_2 = 1$.

Density (ρ), viscosity (μ), thermal conductivity (K) and specific heat (C_v) are calculated using the volume fractions F_1 and F_2 (with subscript l and v corresponding to liquid and vapour).

$$\begin{aligned}
 \rho &= F_1 \rho_{l \text{ LNG}} + F_2 \rho_{l \text{ water}} + (1 - (F_1 + F_2)) \rho_{v \text{ air}} \\
 \mu &= F_1 \mu_{l \text{ LNG}} + F_2 \mu_{l \text{ water}} + (1 - (F_1 + F_2)) \mu_{v \text{ air}} \\
 K &= F_1 K_{l \text{ LNG}} + F_2 K_{l \text{ water}} + (1 - (F_1 + F_2)) K_{v \text{ air}} \\
 C_v &= F_1 C_{v \text{ LNG}} + F_2 C_{v \text{ water}} + (1 - (F_1 + F_2)) C_{v \text{ air}}
 \end{aligned} \tag{2}$$

Mass transfer

When thermodynamic process occurs, a source term has to be considered to account for the mass transfer \dot{q} between phases: respectively vaporization of liquid and condensation of gas, depending of the temperature of the fluid with respect to the saturation temperature T_{sat} .

By assuming that phase change occurs at a quasi-thermo-equilibrium state and at a constant pressure, and that the transfer rate \dot{q} is mainly led by the local temperature T_c (temperature in a given cell of the mesh), the saturation temperature T_{sat} and the volumetric fraction of liquid (phase F) and gas (phase $1-F$), the mass transfer term is written:

- Vaporization of liquid: $T_c \geq T_{sat}$

$$\dot{q} = r_l F \rho_l \left(\frac{T_c - T_{sat}}{T_{sat}} \right) \quad (3)$$

- Condensation of gas: $T_c < T_{sat}$

$$\dot{q} = r_v (1 - F) \rho_v \left(\frac{T_c - T_{sat}}{T_{sat}} \right) \quad (4)$$

Hence the VOF equation including the mass transfer process is written:

$$\frac{\partial F}{\partial t} + \vec{V} \cdot \text{div}(F) = \frac{\dot{q}}{\rho} \quad (5)$$

In this equation, depending on its sign, \dot{q} is the production rate of vapour LNG or of liquid LNG.

In the mass transfer term, r_l and r_v are empirical coefficients which may be tuned.

The mass transfer source term is also included in the energy equation to account for the amount of heat released when liquid evaporates:

$$\frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\vec{V}(\rho E + p)) = \nabla[(K + K_t)\nabla T] + L \times \dot{q} \quad (6)$$

with K_t the turbulent thermal conductivity and L the latent heat.

An additional convection-diffusion equation is introduced for the transport concentration of vaporized LNG (methane) in air:

$$\frac{\partial(\rho C)}{\partial t} + \nabla(\rho \vec{V} C) = \nabla[\rho(D_c + D_t)\nabla C] + \dot{q} \quad (7)$$

with C the concentration of LNG vapour phase in the air phase, D_c mass molecular diffusivity (methane in air) and D_t turbulent massic diffusivity.

As in the VOF equation \dot{q} deals with the production/condensation rate of vapour LNG.

Mixture model for the smaller droplets

The simulation of very small droplets with the interface VOF method may be possible using very refined grids but the problem is the issued very large CPU time consuming of such simulation. In the aim to remain on coarse grids and so to limit CPU time, an eulerian mixture model is activated for the simulation of smaller droplets, issued from the fragmentation of the jet, which are “under cell size discretization”.

The mixture model accounts for a dispersed (secondary) phase, the smaller droplets, moving in a continuous phase (air for instance). Like the VOF model the volume fractions of each phase for a control volume can be equal to any value between 0 and 1, depending on the space occupied by one phase with respect to the other. But the main difference with the VOF method is that the model allows the phases to be interpenetrating, so without interface between phases.

The model assumes local equilibrium but can take into account different velocities of the phases (concept of slip velocity).

It solves the Navier-Stokes equations for the mixture, for which the local properties of the fluid (density, viscosity,...) are deduced, as for VOF, from the local volume fraction of each phase. But an additional volume fraction equation of the secondary phase (droplets) is introduced, possibly including algebraic expressions of source terms to account for relative velocity between phases if the phases move at different velocities, and for vaporization.

Several formulations exist to represent slip velocity between phases, which include drag and buoyancy effects.

This volume fraction equation for the secondary phase is written:

$$\frac{\partial(\rho S)}{\partial t} + \nabla(\rho \vec{V} S) = T + \dot{q} \quad (8)$$

Where:

- S is the concentration of the liquid (droplets) in a cell
- T is a source term accounting for possible slip velocity between phases (including drag and buoyancy effect)
- \dot{q} is the vaporization rate of droplets given by same kind of formulation as in the VOF equation

Coupling VOF/mixture model

The mixture model is activated when the smallest structures issued from the atomisation of large liquid ligaments (computed with the VOF methodology) become under size cell. For this, it is necessary to introduce a criterion based on the VOF value in each cell, able to find the smaller structures in the mesh, so the isolated liquid cells (droplets) having gaseous neighbouring cells. These cells must be simulated with the mixture model and not with the VOF model.

All the equations are solved simultaneously but the mixture model will propagate the small droplets only from the cells where the criterion is verified, so cells for which the concentration S of the droplets will be initialized with the VOF value of the corresponding cell.

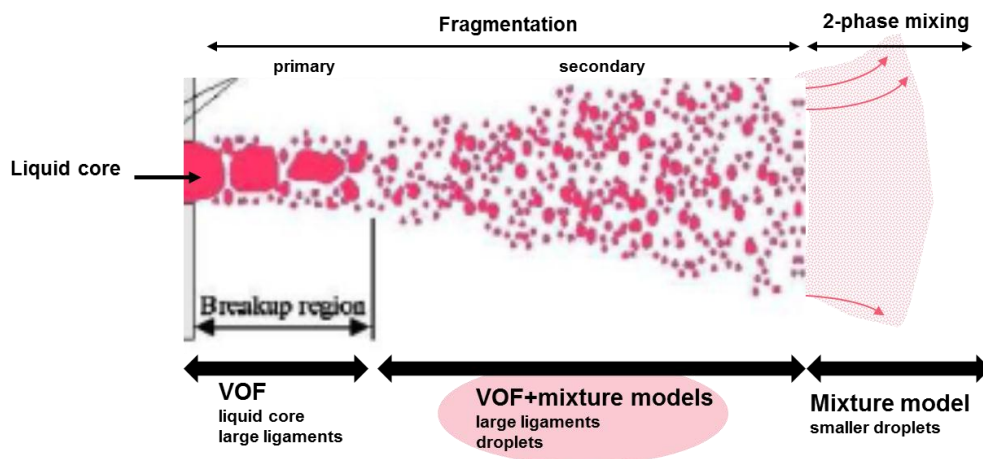


Figure 2: Sketch showing the coupling between the different models

3 ACADEMIC VALIDATIONS

Depending on availability of open publications on experimental tests results, both qualitative and quantitative academic validations are performed.

3.1 Sub-cooled liquid jet

A free jet simulation impacting a free surface is concerned (see figure 3). We are interested in the ability of the model to capture physics such as jet spreading, jet impact and buoyancy. In this test case two different liquids and different kinds of interface are considered:

- Liquid in tank = liquid 1 (below the free surface in grey) with density ρ_1
- Liquid jet = liquid 2 (in black) with density $\rho_2 < \rho_1$
- Interface:
 - liquid 1 / liquid 2
 - liquid 1 / air
 - liquid 2 / air

The velocity of the jet at the inlet is imposed at 2m/s, up to $t=3s$.

Due to dynamic effects the jet firstly penetrates in liquid 2 (figure 3). Then because of its lighter density the pool remains in the surface layer.

It is concluded qualitatively that the buoyancy effects between 2 different immiscible liquids are correctly reproduced by the model.

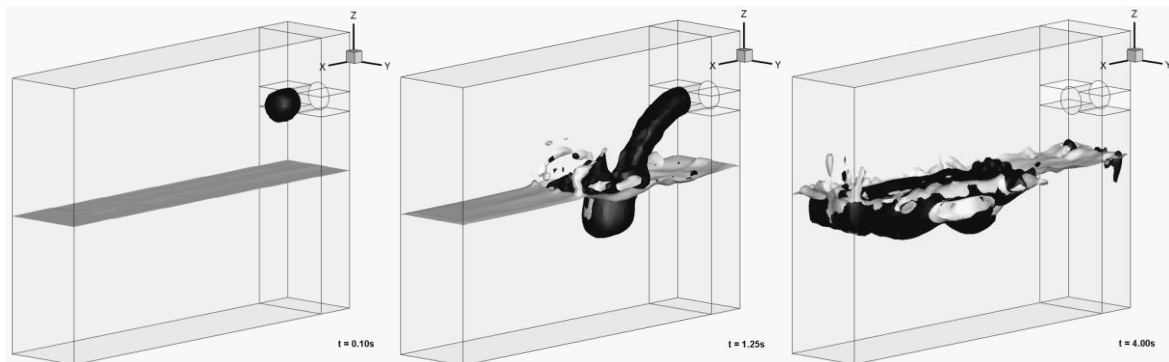


Figure 3: Interaction jet/free surface

The same test case is now considered but with a difference related on the accounting of vaporization effect of the liquid 2 (LNG here) in contact with the warmer liquid 1 (water here at 20°C). The comparison of results issued without and with vaporization shows that thermodynamic effects logically reduce the dynamic of the jet when penetrating into the water, because light vapour progressively replaces heavy LNG and disperses into the air volume (figure 4, right column). The phenomenon is still visible even later (figure 5), with an intensification of the cloud dispersion (figure 5).

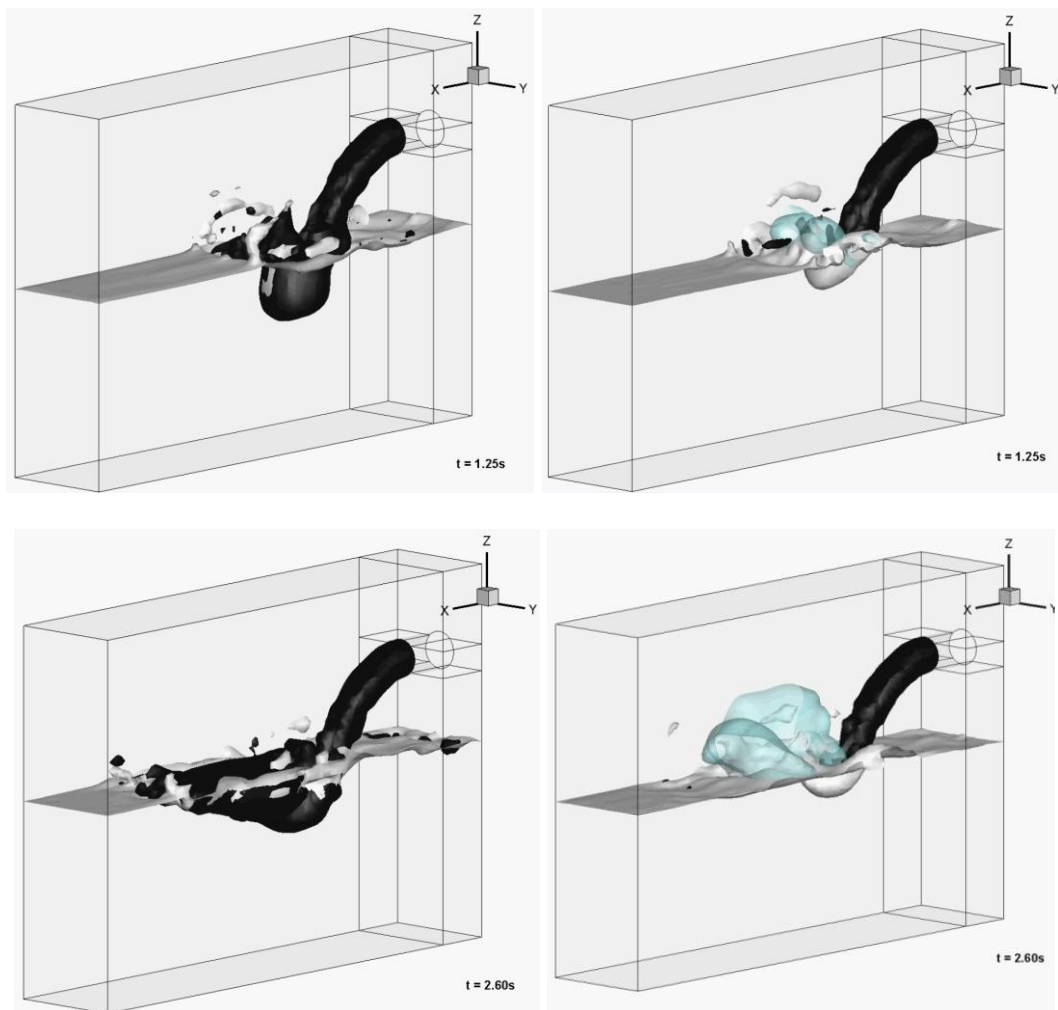


Figure 4: Interaction jet/free surface without vaporization (left) and with vaporization where vapour appears in light blue (right)

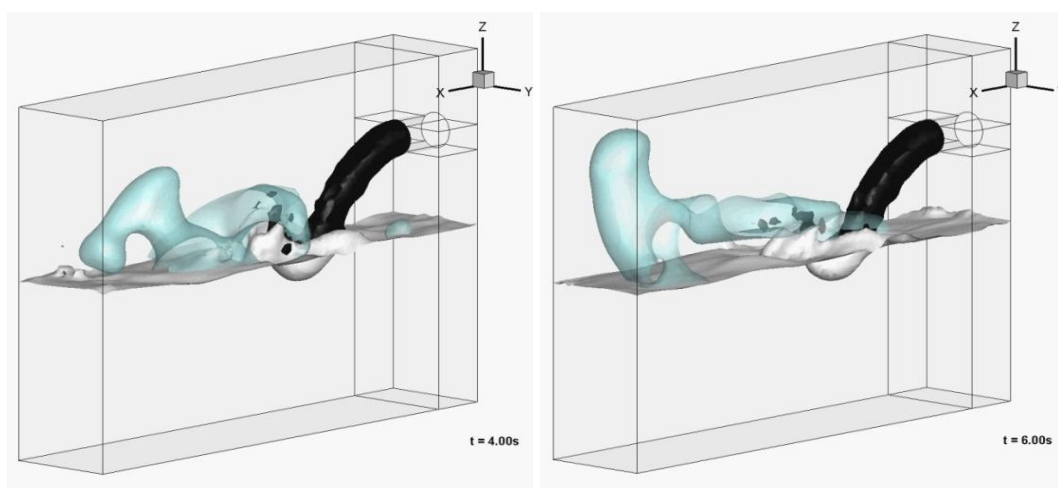


Figure 5: Vapour dispersion

3.2 Jet fragmentation (with VOF model)

The following example concerns the study of the mechanical fragmentation of a liquid jet spreading from a nozzle (diameter=2mm, length=1mm) at a velocity of 34 m/s. The flow is isothermal.

Kelvin-Helmholtz instabilities develop along the interface and initiate the fragmentation [4]. Local high velocities occur near the free surface due to strong interactions (development of vortices) between liquid and aerodynamic flows.

A qualitative comparison with experimental results confirms the instability development process leading to primary fragmentation (figure 6).

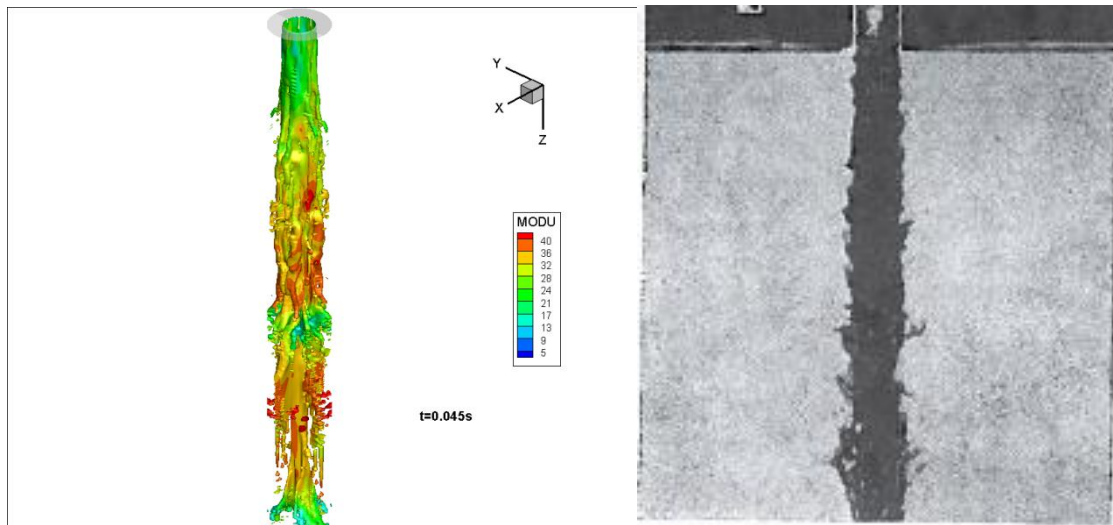


Figure 6: Qualitative comparison between CFD and experiments of jet atomization process

3.3 Two-phase jet (VOF and mixture models)

A qualitative test aims to ensure the numerical validation of the coupling between VOF and mixture models described above. A water jet spreads from a horizontal nozzle (diameter=2mm) involving droplet atomisation and two-phase droplet dispersion is concerned (figure 7).

Due to the high jet outlet velocity (34 m/s) and the water/air density difference, an important shear stress takes place at water/air interface. It follows a mechanical break-up appearing mainly at the tip jet extremities. Small droplets are formed and depending on the size criterion of the break-up ligaments are treated either by the VOF model or the mixture model.

The coupled VOF/mixture model needs now further quantitative validations.

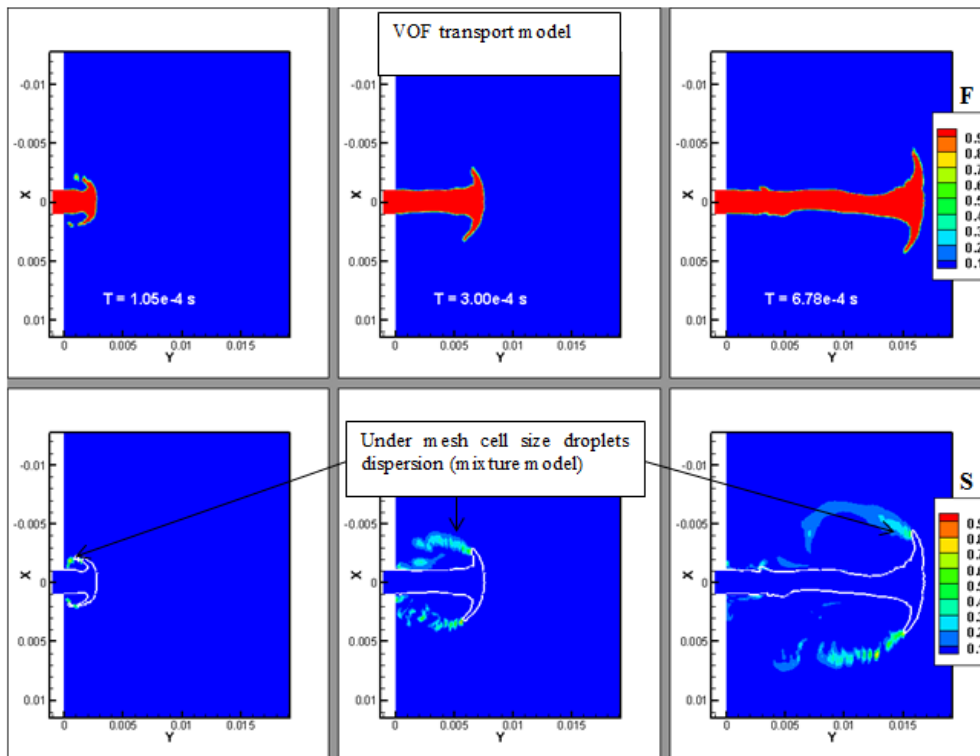


Figure 7: Example of VOF/mixture coupling - Mechanical break-up process of a high velocity jet into droplets

3.4 Validation of the vaporization model

Boiling occurs when LNG is spilled on a hot substrate (water, concrete) due to the high temperature difference of roughly 180 K. Mass transfer rate from the liquid phase to the vapour phase is a function of temperature difference as described in [3].

The “Bureau des Mines” experiments are used for validation of the numerical model [3]. Small scale experiments were conducted to calculate the vaporization rate of LNG on water: LNG is poured onto water in a 2×1×1 foot deep aquarium. The aquarium has a metal ramp just below the water surface which minimized the mixing of the cryogenic liquid with the water. The aquarium is positioned on a load cell and the weight as a function of time is recorded. The vaporized mass of LNG and the vaporization rate are deduced from these data. For comparison purpose, the same case is studied with the well-known PHAST hazard analysis software.

The time evolution of LNG volume (from which the LNG vaporized rate can be extracted) is shown on figure 8. It appears from these results that only CFD, which accounts for 3D effects (especially boiling effect at LNG/water interface and transport of temperature due to natural convection of the flow), gives very close results according to experiments and is able to reproduce a correct vaporization rate, whereas PHAST vaporization curve shows a too strong vaporization rate at the beginning and a vaporization delay after 10s.

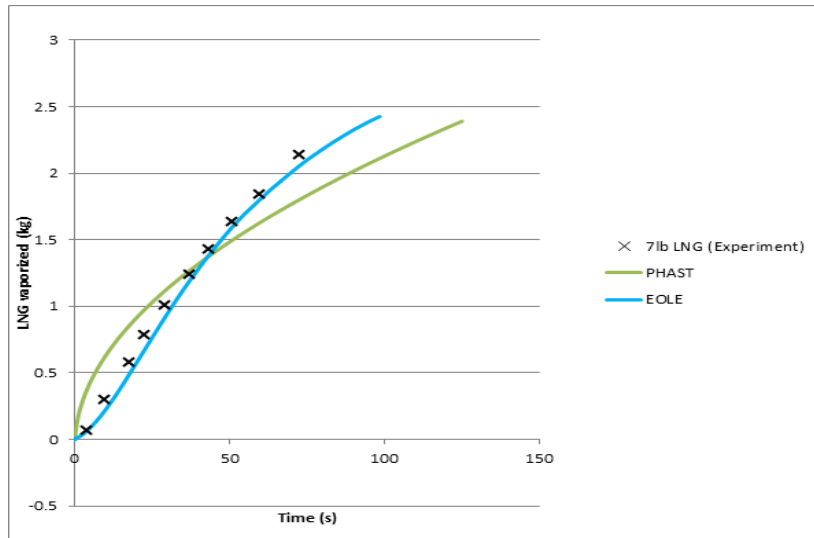


Figure 8: Time evolution of the LNG mass. Experiment vs. simulations (CFD and PHAST)

4 CONCLUSIONS

A CFD software, EOLE, has been developed to sequentially simulate all the physics of a potential leak of LNG from a FLNG facility. It is based on a URANS model using coupled VOF and mixture models to simulate all dynamic and thermal processes of LNG multi-phases flows. Academic validations have been performed following a step-by-step approach allowing to investigate the different mechanisms separately. This first validation work is promising but further validation, especially quantitative, are necessary. For this reason, a qualification program in association with several Oil and Gas operators was launched in late 2013. The purpose of this new program is to perform medium scale tests to quantitatively validate the physical models implemented into EOLE.

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