CFD Modelling of Vertical LNG Tanks Adopted in Heavy Trucks Refuelling Stations

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In the present study, a Computational Fluid Dynamics (CFD) model was set up to analyse the dynamic behaviour of LNG (Liquefied Natural Gas) tanks adopted in heavy trucks refuelling stations in normal operating conditions or during process upsets. The CFD model was based on the Volume-Of-Fluid (VOF) method to simulate the transient behaviour of a multi-phase flow in a 100 m\textsuperscript{3} vertical cylindrical tank. The model first considered a fully insulated vessel, and subsequently it was modified to take into account possible damages of the insulation layer, this being a critical upset scenario. The CFD model allowed predicting the dynamic pressure build up in the damaged tank, thus obtaining key indications for the evaluation of the vessel mechanical resistance and set up of safety measures. The model also provided the prediction of vapor temperature with respect to time and external heat source, that is a key issue to assess the effectiveness of the thermal insulation.

1. Introduction

The use of liquefied Natural Gas (LNG) as heavy truck fuel is expanding due to its multiple benefits; indeed LNG is nowadays considered as the best mass market alternative to diesel for long-distance transport (BMVI, 2017). In Italy, the demand for final user utilization of this fuel was about 16,400 t (36,500 m\textsuperscript{3}) in 2015, 12 % of which was provided to refuelling stations supplying LNG to heavy road vehicles. Those numbers show a doubled demand of LNG compared to the 2014 request (REF-E, 2016). The growing market of the LNG-fuelled trucks is also supported by a large number of companies, which are ordering fleets of heavy trucks fed with LNG (LNG World News, 2018). Nevertheless, due to its flammable properties, severe fires and explosions may be generated after the release of LNG, thus introducing relevant safety issues and the operability of the LNG storage vessels (Zhang, 2014). LNG is stored in extreme temperature conditions, typical operating conditions provides for storage pressure between 1 and 9.3 bar and saturation conditions. This implies a storage temperature from -162 to -125 °C (Sharafian et al., 2016). A critical phenomenon affecting LNG, and, more in general, cryogenic fluids in storage equipment, is the thermal stratification of the liquid phase, which leads to a self-induced pressurization phenomenon (Gursu et al., 1993). Such stratification is due to a buoyancy driven flow, caused by the more rapid temperature increase of the liquid in contact with the vessel walls heated by external environment with respect to the bulk fluid. Natural convective heat transfer with the surrounding air and solar radiation are the main contribution to the temperature increment and boil-off gas generation, that is the vapor that is formed due to natural evaporation in the tanks driving the pressurization rate. Several studies were devoted to the analysis of natural convective flow and thermal stratification in cryogenic tanks during self-pressurization. Barsi and Kassemi (2008) investigated a liquid hydrogen (LH\textsubscript{2}) tank coupling a CFD model with a lumped model. Fu et al. (2014) also analysed a LH\textsubscript{2} tank through a CFD model focusing on the effects of different rib design solutions. Kassim and Kartuzova (2016) analysed the influence of the accommodation coefficient in a tank filled with liquid nitrogen (LN\textsubscript{2}) with different CFD model configurations and different geometries. Choi et al. (2017) developed a multiphase CFD model and shaped a small-scale vertical tanks performing simulations on both LNG and LN\textsubscript{2}, with different heat...
fluxes and different filling levels. Khelifi-Touhami et al. (2010) and Rho et al. (2013) both studied small-scale vertical tank filled with LNG in atmospheric and pressurized conditions, respectively. However, the latter works focussed only on the liquid domain. Moreover, scale effect associated with real scale geometries inducing complex convective flows possibly leading to preferential patterns in the liquid stratification were not systematically evaluated.

In the present work, a CFD model is developed to predict the thermal stratification and the dynamic pressure build up in a 100 m$^3$ tank storing LNG. The CFD model is based on the Volume-Of-Fluid (VOF) method. The study aims at providing reference data for a real scale storage tank, in both fully insulated and damaged insulation cases, in order to support the safe operation of LNG storage tanks.

The paper is structured as follows: Section 2 gives an overview of relevant safety issues affecting LNG storage tanks; Section 3 reports details on the CFD model; in Section 4 the case-studies are defined; results of the numerical implementation are given in Section 5, together with the discussion about the outcomes and potential developments of the present work; finally, conclusions are given in Section 6.

2. Safety issues in LNG storage operations

The most critical unit in LNG refuelling station is the main LNG tank, due to the high inventory, up to 43 t of flammable substance. Due to the extremely low temperature conditions (e.g., -160 °C temperature) operational problems are mostly related to the boil-off gas (BOG) generation, that is the vapour that is formed due to evaporation in the tanks driving the pressurization rate. In normal operating conditions, the tank undergoes to a self-pressurization phenomenon due to natural convective heat transfer with the surrounding air and solar radiation. The latter are the main contribution to the temperature increment and BOG generation. Thus, the performance of the insulation system plays a central role in the minimization of the BOG generation. The more efficient is the coating system, the less BOG production is achieved in the storage tank (Hofmann, 2006). External heat sources such as external fire induce a more severe heat-up of the tank (Landucci et al., 2013), but this event is out of the scope of the present study. In particular, only the self-pressurization due to process upsets and failure is analysed in the present work, being a key issue in the design of refuelling stations. A review published by Sharafian et al. (2017) pointed out that the 44 % of the total LNG heavy-duty trucks refuelling stations have no BOG management, worldwide. This means that, to fit pressure requirements upon delivery, the BOG must be lowered or be released to the atmosphere. In this framework, the aim of the present study is the investigation of the influence of a thermal insulation layer under vacuum on the self-pressurization in LNG tanks typically adopted in heavy-trucks refuelling stations, comparing the tank performance in presence of effective or damaged insulation.

3. Model

3.1 Reference geometry

The industrial case-study implemented in the present work considers a 100 m$^3$ cryogenic LNG tank adopted in the typical configurations of heavy trucks refuelling stations. The tank consists of:

- an inner tank, in direct contact with the cryogenic lading,
- an insulation layer under vacuum,
- an outer vessel, in contact with the external environment.

The reference geometry considers the standard features of the existing stations. For both the inner and the outer tank, stainless steel type 304 was considered as construction material (Marquardt et al., 2002); and expanded perlite under vacuum (pressure < 0.1 Pa) was assumed to fill the space between the two vessels (Sholtens et al., 2008). Details of the geometry are summarized in Table 1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>SI Units</th>
<th>Inner Tank</th>
<th>Outer Tank</th>
<th>Insulation Layer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>m$^3$</td>
<td>99.6</td>
<td>39.4</td>
<td>-</td>
</tr>
<tr>
<td>Height</td>
<td>mm</td>
<td>16,770</td>
<td>18,300</td>
<td>-</td>
</tr>
<tr>
<td>Diameter</td>
<td>mm</td>
<td>2,750</td>
<td>3,000</td>
<td>-</td>
</tr>
<tr>
<td>Thickness</td>
<td>mm</td>
<td>12.65</td>
<td>2.54</td>
<td>247</td>
</tr>
</tbody>
</table>

3.2 CFD model set-up

A multiphase CFD model was developed on ANSYS Fluent 16 to analyse the behaviour of the LNG tank described in Section 3.1 exposed to external heat source (i.e., heat flux from the external environment).
The CFD model aimed at solving the governing equations of continuity, momentum, energy and turbulence with respect, among other boundary conditions, to the heat flux entering the stored fluid. The latter incoming thermal power is due to conductive heat transfer from the environment through the tank layers (i.e., outer tank shell, insulation layer, and inner tank shell) and it was applied as thermal boundary condition in the model. A 2-dimensional domain was considered due to the symmetry associated with the vertical cylindrical tank configuration. Then, a fully block-structured grid was generated with ANSYS ICEM; the grid was refined in correspondence of the regions with high gradients, i.e. near the walls and the liquid-vapour interface. Hence, despite the 2-dimensional domain, a large number of cells, i.e. 440,000, was used. The computational domain and grid are shown in Figure 1. The LNG was represented as pure methane: the vapour properties were computed as functions of the temperature; whereas, the liquid properties were assumed as constants. The initial flow conditions consisted of a steady liquid up to a prescribed initial liquid filling level and a steady vapour in the remainder of the vessel.

The transient biphasic fluid dynamic problem was solved through the Volume-Of-Fluid method. The model is suitable for immiscible fluids as it well represents the shape and the evolution of the surface of interface between the phases. The model assumes that each cell may contain just one phase or the interface. This is determined by the volume fraction $\alpha$ of, say, the liquid phase, identifying three cases: 1) for $\alpha_L = 0$ the cell is full of vapor; 2) for $\alpha_L = 1$ the cell is full of liquid; 3) for $0 < \alpha_L < 1$ the cell contains the vapor-liquid interface. Hence, in each cell the conservative equations (continuity, momentum, energy and turbulence) are solved using the properties (density, specific heat and thermal conductivity) of the phase present, i.e. computation of density is shown in Eq(1).

\[
\rho = \alpha_L \cdot \rho_L + (1 - \alpha_L) \cdot \rho_V
\]  
\[
\frac{\partial (\alpha_L \rho_L)}{\partial t} + \nabla (\alpha_L \rho_L v) = m_{LV} - m_{VL}
\]  

Where: the subscripts L and V indicate that the variable is referred to the liquid or vapor phase, respectively; $t$ is the time; $\rho$ is the density; $v$ is the velocity, and $m_{LV}$ and $m_{VL}$ are the mass fluxes at the liquid-vapor interface in case of evaporation and condensation, respectively. Here, the mass and heat transfers at the liquid-vapor interface due to evaporation-condensation were taken into account through the model of Lee (1979). The Shear-Stress Transport (SST) $k-\omega$ model was implemented to account for the turbulence.

The pressure-based solver with an implicit time advancement was employed. The Courant number was between 0.25 and 1. The SIMPLE algorithm scheme was applied for the pressure-velocity coupling. The spatial discretization was carried out selecting: Least Squares Cell-Based for the gradient, Body Force Weighted for the pressure, Geometric Reconstruction for the volume fraction, and the Second Order Upwind for all other variables discretization. Normalized residuals for all equations were typically well below $10^{-6}$. Table 2 summarizes the model settings.

One hour of CPU time was needed to cover 4 s of real time when run on 16 threads. Simulations are run for a real-time of 2 h.

Figure 1: Schematization of the full-scale tank implemented in the numerical solver: a) mesh overview; b) mesh details.
Table 2: Summary of relevant set-up items implemented in the CFD model.

<table>
<thead>
<tr>
<th>Item</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal boundary conditions</td>
<td>Constant heat flux</td>
</tr>
<tr>
<td>Momentum boundary conditions</td>
<td>Stationary Wall &amp; No Slip</td>
</tr>
<tr>
<td>Time stepping method</td>
<td>Variable, with Courant number from 0.25 to 1</td>
</tr>
<tr>
<td>Convergence criteria</td>
<td>$10^{-6}$ for all criteria</td>
</tr>
<tr>
<td>Mathematical model</td>
<td>Shear-Stress Transport (SST) $k$-$\omega$</td>
</tr>
</tbody>
</table>

4. Case-studies definition

The present work analyses the transient behaviour of a cryogenic vessel adopted in heavy-truck refuelling stations exposed to external environment. The influence of the thermal coating performance on the dynamic behaviour of the tank is analysed through the numerical model defined in Section 3.2.

Two case-studies are defined in the present study, namely:

- **“Fully-insulated”** - a normal operating state, in which the perlite is under vacuum (pressure < 0.1 Pa);
- **“Damaged-insulation”** - an accidental condition, in which the perlite has lost the vacuum and its internal pressure equals the ambient pressure.

The main difference between the case studies is the thermal flux entering the LNG inside the tank. In case the insulation layer is totally damaged, the mechanism of heat transfer will result in a heat flux five times higher than in the normal operating condition. Thus, the two case studies are implemented in the software with the same set-up, and only the thermal boundary condition is modified. A summary of the relevant boundary conditions and the initial data is reported in Table 3, for the normal and damaged insulation cases.

Table 3: Summary of the case-studies implemented in the present analysis.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Fully insulated</th>
<th>Damaged insulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substance</td>
<td></td>
<td>Pure Methane</td>
<td>Pure Methane</td>
</tr>
<tr>
<td>Pressure</td>
<td>Pa</td>
<td>690,000</td>
<td>690,000</td>
</tr>
<tr>
<td>Temperature</td>
<td>K</td>
<td>141.4</td>
<td>141.4</td>
</tr>
<tr>
<td>Liquid Filling Level</td>
<td>%</td>
<td>90</td>
<td>90</td>
</tr>
<tr>
<td>Thermal Boundary Condition- Heat Flux</td>
<td>W/m²</td>
<td>4.3</td>
<td>23</td>
</tr>
</tbody>
</table>

5. Results and discussion

The 100 m³ LNG storage tank was implemented in the software with respect to the approach and boundary conditions reported in Section 3 and Section 4.

The results of the “Fully Insulated” and the “Damaged insulation” case studies are shown in following three figures: Figure 3 and Figure 4 show the temperature contours of the vapor and liquid phase, respectively, at different times of simulation, and Figure 5 reports the pressure of the top of the tank and the temperature of the vapor ullage during the heat-up period. During the simulation, data shown in the latter figure were recorded in a point fixed at 770 mm from the ceiling of the tank, in the vapor ullage space.

![Figure 3: Vapour temperature contours at three different times. The white point indicates the recording point of data shown in Figure 5.](image-url)
Fluid temperature contours clearly show a net stratification phenomenon in both liquid and vapor phase. However, the liquid temperature increase after 2 h of simulation is limited in both case-studies, and its magnitude is on the order of 1 K. On the other hand, temperature in the vapor space appreciably increases and highlights the differences between the fully insulated and the damaged insulation case. At the end of simulation time (2 h) and at the recording point, vapor temperature increased by more than 2 K in normal operating conditions, and by about 14 K in the compromised insulation state. At the top ceiling of the tank, vapor temperature shows its maximum increase of about 28 and 130 K in the effective and damaged insulation case, respectively. In the same way, pressure behavior during the heat-up shows a faster build-up of roughly five times in the damaged insulation state compared to the fully insulated case.

The preliminary results obtained show an example of the potentialities of the present code. The model may be extended considering different types of geometry, environmental conditions and damage states for the insulating coating. In this way, scale effects on the pressure heat up of cryogenic tanks may be derived. Moreover, different substances normally stored in cryogenic conditions (e.g., ethylene, propylene, hydrogen, etc.) may be also implemented in the model to investigate the effect of substance on the BOG formation and consequent pressure build up.
6. Conclusion

A CFD multi-phase model was developed to investigate the self-pressurization of LNG tanks for heavy-duty truck refueling service. Key aspects of the heat transfer from the external environment to the tank lading have been identified and simulated. The study may represent a base to extend the knowledge on large scale cryogenic storage tanks. The accidental loss of vacuum in the insulation system has shown to considerably affect the pressure build-up, pointing out the major role of the thermal coating in the self-pressurization phenomenon. The model represents a useful tool predicting the dynamic behavior of the LNG tanks during the heat-up, and it may help supporting the insulation design or to provide relevant information for the emergency response in case of insulation failure.

References

Kassemi M., Kartuzova O., 2016, Effect of interfacial turbulence and accommodation coefficient on CFD predictions of pressurization and pressure control in cryogenic storage tank, Cryogenics, 74, 138–153.