Numerical predictions of the rollover phenomenon using computational fluid dynamics

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In the past six decades over 24 rollover incidents have occurred in the Liquefied Natural Gas (LNG) industry. During rollover, because of the heat losses at the tank walls, a stratified LNG may be naturally and suddenly homogenised while releasing a large amount of energy in the form of vapour. This rapid vaporisation can be dangerous due to the high pressure produced in the tank and because of the significant amount of LNG vapour that can be potentially released into the atmosphere, leading to possible explosions.

The current study is aimed at developing a predictive tool rolloverFoam, on the basis of open source Computational Fluid Dynamics (CFD) code, OpenFOAM, to reliably predict the occurrence of rollover. Such a predictive tool can be of assistance to safety study to prevent the occurrence of rollover through improved tank design, LNG handling procedures and storage. It may also be used by tank operators to monitor the conditions and take timely interventions to prevent the occurrence of rollover in some circumstances.

The modelling approach is based on the three-dimensional numerical study of a mixture consisting primarily of methane and some ethane to represent the minor constituents. The evaporation rate is calculated using the Hashemi-Wesson relation. The computational domain is initialized with a stratified liquid involving two layers with different thermophysical properties. The predictions of rolloverFoam were firstly validated with experimental data obtained from small scale experiments in the literature as well as with numerical results of previous researchers. Subsequently, the code is applied to analyse the La Spezia rollover accident which happened in 1973. The rollover time, the boil-off rate, the interface motion and the evolution of the strata' compositions and temperatures are monitored during the scenario. These predictions provided important insights into the underlying physics during LNG rollover process and the spontaneous mixing of the liquid layers. These will be discussed in detail in the full manuscript.

Keywords: LNG, Rollover, CFD, Double-diffusion, Safety, Buoyancy

Introduction

The Liquefied Natural Gas (LNG) industry is one of the fastest growing energy sector. Indeed, its world demand is supposed to double by 2025. As a result, it is necessary to develop more storage facilities as well as to optimise them in the available infrastructures. In some storage cases where LNG from different sources are added in the same tank, a rapid mixing called "rollover" occurs while releasing a high amount of vapour. In such a scenario, this sudden release, if not handled, could damage the tank structure and potential explosion hazard.

Rollover is a phenomenon known and studied since the 60s. In 1973, Sarsten [1] reported the rollover incident in La Spezia which happened after loading from below a denser liquid than the LNG initially present in the tank. Following this event, in the 70s -80s, in order to understand the rollover process, Chatterjee and Geist [2], Germeles [3] and Heestand [4] successively developed mathematical models based on a 1D approach. However, these do not take into account the spatial distribution of a rollover which is of prime interest when studying the phenomenon. Thus, the novelty of the presented work is to develop a Computational Fluid Dynamics (CFD) approach capable of predicting with good accuracy the spatial dynamics of the rollover phenomenon..

Rollover

LNG is stored at -160°C at around the atmospheric pressure in heavily insulated tanks so as to keep it under its liquefied form. However, despite this insulation, the liquid is heated at the walls and because of buoyancy, it rises along the wall. Once the liquid reaches the surface, part of it evaporates and the remaining part cools down and sinks. These motions form convection cells in the tank while releasing normal amounts of boil-off gases (BOG). This case is illustrated in Figure 1a) for a homogeneous LNG. LNG is a multicomponent fluid. As illustrated in Table 1 below, its composition depends on its source of production. Different LNG from several sources often have different densities. When adding them in the same tank, it may lead to stratification especially if a denser LNG is injected at the bottom of a lighter LNG or a lighter LNG is added at the top of a denser LNG.
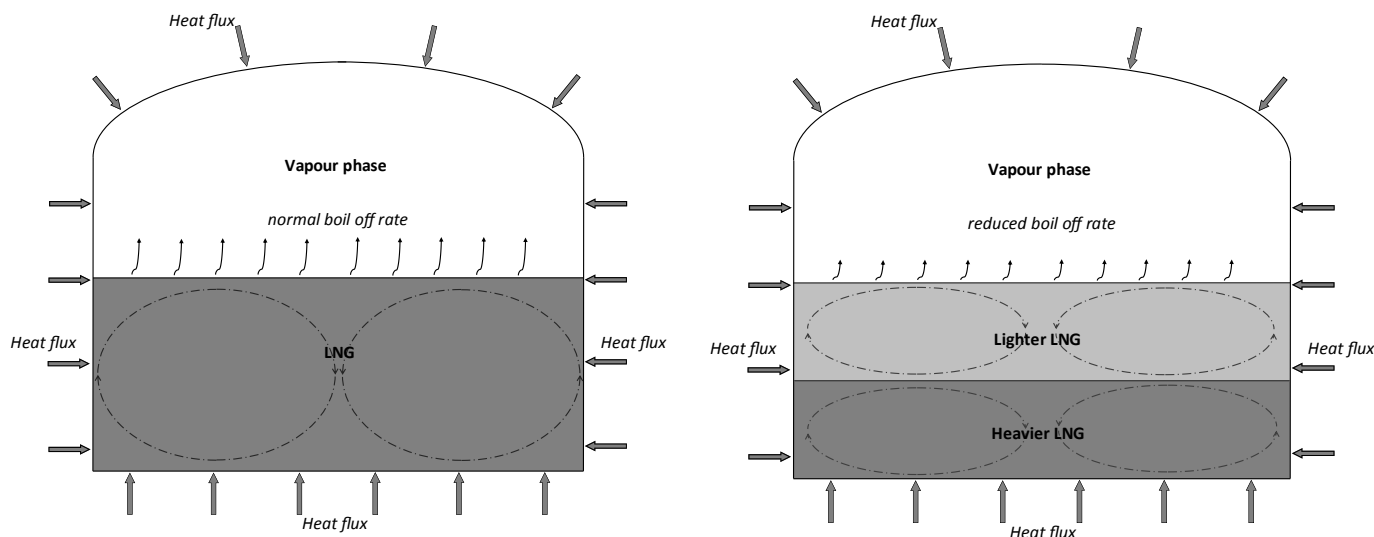
Figure 1a) and b): Schematic representations of the natural convection current in a homogeneous LNG on the left and a stratified LNG on the right

The stratified flow is composed of a lighter layer on a heavier one as illustrated in Figure 1 b). Buoyant convective currents are set up in both layers, but due to the head pressure of the upper layer, the boil off rate is reduced. The heat losses at the walls are disrupting this apparently stable equilibrium. Indeed, while the lower layer gets lighter due to the heat coming mainly from the bottom wall, the upper layer gets denser because of evaporation. When the densities equalise between the two layers, a rapid mixing occurs, and the saturated vapour "trapped" in the lower layer is suddenly released.

If this boil off is not handled in time, it can lead to an over-pressurization in the tank which can damage the reservoir structure, and release in the atmosphere large amounts of LNG potentially flammable and explosive.

Source	LNG molar composition in %						LNG density kg/m³
	Nitrogen	*Methane*	*Ethane*	*Propane*	*Others*	*Total*	
Australia	0.04	87.33	8.33	3.33	0.97	100	467.35
Algeria	0.63	91.40	7.45	0.57	0.05	100	446.65
Libya	0.59	82.57	12.62	3.56	0.65	100	478.72
Qatar	0.27	90.91	6.43	1.66	0.74	100	453.46
USA	0.17	99.71	0.09	0.03	0.01	100	421.39

Table 1: Composition of LNG with different origins (source GIIGNL [5])

Rollover prediction models

Past works

In 1973, Chatterjee and Geist [2] paved the way for modelling rollover. They implemented a lumped parameter model in a unidimensional model. Following this study, many works used the same fundamental concepts, such as Heedstand and Shipman [4], Bates and Morrison [6] and Deshpande et al. [7]. Nowadays, these models are largely used in industry. However, in spite of their acceptable accuracies, these models do not provide a spatial representation of rollover and cannot explain its complex mechanism other than an equalisation of the average densities inside the two strata.

To fill this gap, some researchers such as Shi et al. [8], Seveleder [9] and Lemembre [10] implemented 2D codes which were assuming rollovers as being double-diffusive processes. Their codes could reproduce the rollover phenomena well but only qualitatively. The main novelty of the present work is to develop an accurate rollover prediction model, rolloverFoam, within the frame of the open source CFD toolbox OpenFOAM.

Model and Equations

During LNG rollover, the dominant phenomena are the buoyancy-induced flow and the boil off release. The present study is focused on the hydrodynamics of the rollover and the double-diffusive convection.

The LNG solution is assumed to be a binary solution made of ethane diluted in methane. Indeed, as it can be observed in Table 1, usually 90% of LNG is made of methane and the rest is essentially ethane with fewer amounts of heavier hydrocarbons and nitrogen.

The variation of density with dilute concentration and temperature is small compared to the density of the fluid, and the latter is assumed to be incompressible which justifies the use of the Boussinesq approximation. The density can then be expressed as:

$$\rho = \rho_0\big(1 + \beta_C(C - C_0) - \beta_T(T - T_0)\big) \tag{1}$$

with ρ_0 the reference density, β_C the solutal expansion coefficient, β_T the thermal expansion coefficient, C the solute concentration, C_0 the reference solute concentration, T the temperature and T_0 the reference temperature.

The equations governing the problem are, in the order, the mass continuity, the momentum, the mass transport and the energy transport equations and are as follows:

$$\nabla.\vec{u} = 0 \tag{2}$$

$$\rho_0 \frac{D\vec{u}}{Dt} = -\overrightarrow{\nabla p} + \mu\nabla^2\vec{u} + \rho_0\vec{g}[\beta_C(C - C_0) - \beta_T(T - T_0)] \tag{3}$$

$$\frac{DC}{Dt} = \alpha_C\nabla^2 C \tag{4}$$

$$\frac{DT}{Dt} = \alpha_T\nabla^2 T \tag{5}$$

where $\vec{u}$ stands for the velocity vector, $\overrightarrow{\nabla p}$ the pressure gradient, μ the dynamic viscosity, $\vec{g}$ the gravity vector, α_C the solutal diffusivity and α_T the thermal diffusivity.

In this model, heat conduction and molecular diffusion are dominating the rollover. As a result, the transport of concentration due to gradients of temperature (Soret effect) is neglected as well as the transport of temperature due to gradients of concentration (Dufour effect).

An important aspect in simulating rollover is modelling the evaporation at the liquid surface in contact with the vapour of LNG. Hashemi-Wesson's relation [11] is commonly used when dealing with evaporation. The boil off rate is then defined as:

$$\dot{m} = C \frac{\lambda}{L}\left(\frac{\beta_T g}{\alpha v}\right)^{1/3}\Delta T^{4/3}$$

Where $\dot{m}$ stands for the boil off rate, C is a constant equal to 0.328 defined by Hashemi and Wesson [11], v is the kinematic viscosity and ΔT is the difference in temperature between the surface and the bulk.

Evaporation has a critical role during rollover because while the liquid gets lighter at the walls due to buoyancy and rises, it gets heavier in the vicinity of the free surface sinks and stirs the interface to some extent. This phenomenon is also accelerated because the evaporation of methane which is lighter than ethane makes the liquid even more denser.

Results and Discussion

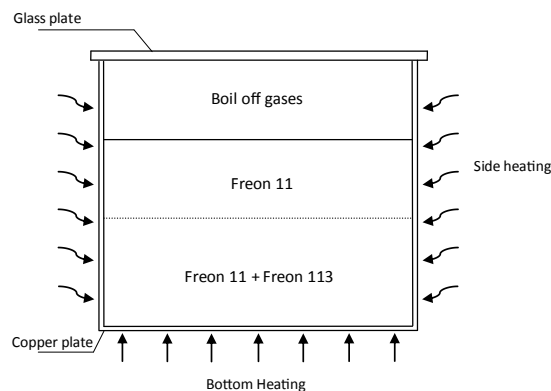### Simulation of an experimental scenario for model validation

Figure 2:Experimental Set up (adapted from [12])

Instead of using LNG, Nakano and Sugawara [12] in their rollover experiments used Freon because it remains liquid under standard conditions for temperature and pressure. Besides, its saturation temperature is 22.8 ^{0}C which enabled them to experiment the boil off during the rollover.

The liquid used in this experiment was a mixture of Freon 11 and Freon 113. It is placed in an enclosure which is 490 mm wide, 390 mm high and 200 mm deep. Stratification was then obtained after a slow injection of a denser mixture at the bottom of a lighter one. In these experiments, the interface between the two liquids is located at around 2/3 of the liquid height.

The stratified liquid could then be heated from the sides and the bottom as shown in Figure 2 via copper plates heated electrically.

Table 2 shows the different parameters used in the different experiments. Numerical simulations have been carried out and compared to the test results. During these simulations, the Reynolds number is around 2.10^4 but the flow is supposed to be laminar because the Rayleigh number does not exceed 10^{13} which is the limit for fully turbulent flow [10]. A mesh sensitivity study was done on this case and also 2D and 3D models were compared. The results were showing no difference which enabled us to study for this validation test case 2D models and the mesh was made of 4000 cells.

Experiment Conditions								Experimental Results		CFD Simulation Results		Comparison Experiments/Simulation	
Heating Condition	Run No	Freon 113 Concentration [wt%]		Heat Flux [W]		Initial Height [mm]		Time until mixing started [min]	Mixing time [min]	Time until mixing started [min]	Mixing time [min]	Relative difference in time until mixing started [%]	Relative difference in mixing time [%]
		Upper Layer	*Lower Layer*	*Side*	*Bottom*	*Upper Layer*	*Lower Layer*						
Side Heating	*6*	0.3	6.6	30	0	114	216	160	55	150	50	**6.25**	**9.09**
Side and Bottom Heating	*8*	0.6	8.4	30	12	139	206	150	20	160	20	**-6.6**	**0**
	14	1.1	17.4	30	30	128	216	125	5	120	5	**4**	**0**
	15	0.6	22.1	30	20	131	211	176	24	174	21	**1.13**	**14**

Table 2: Experimental and numerical results

The time until mixing started obtained numerically is compared to the one obtained experimentally for different cases (numbers 6,8,14 and 15) as depicted in Table 2. In all the four cases simulated, the time before the strata start mixing is less than 7% different from the experimental ones and the mixing times are less than 14%.

Quantitatively, the evolutions in densities, concentrations and temperatures are compared with the ones obtained during the test 15 and shown in Figure 3. During this test, the heat input at the bottom is around 20 W and on the sides it is around 30 W. Also, Freon 113 is 0.6% of the weight of the top layer while it represents 22.1% of the bottom one.
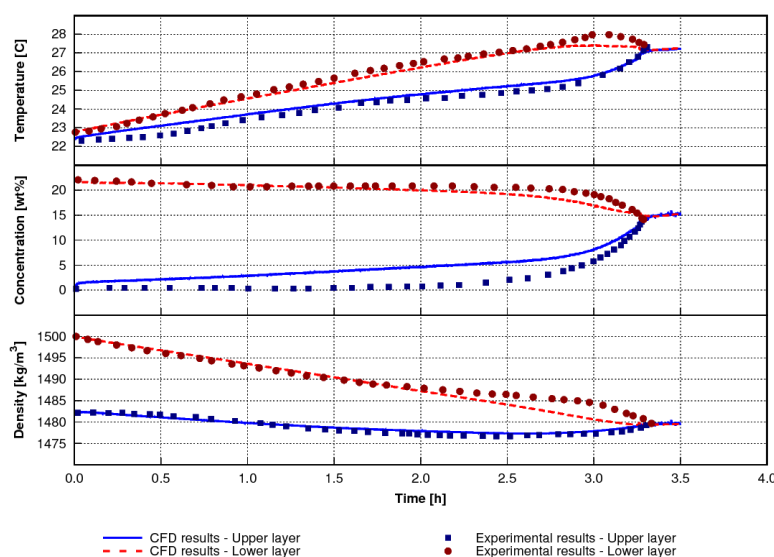

Figure 3: Comparison of numerical results for the evolution of temperatures, concentrations and densities for both strata with experimental results (test 15)
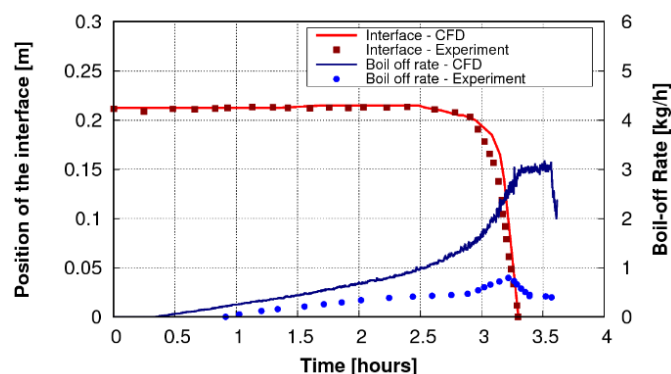
Figure 4: Comparison of numerical results of the evolution of the interface and the boil off rate during rollover with experimental data (test 15)

As shown in Figure 3, the predictions are in good agreements with the measurements. However, the results for concentration show a difference less than 20% but this difference may be due to the fact that the collected data are averaged over the top and bottom layers in the simulated case while in the experiment it is evaluated locally with probes but whose coordinates are unknown. Also, while "mixing patterns after stirring the interface" have been observed by Nakano and Sugawara [12], this was not the case in the experimental results but has been revealed in the present predictions. This explains why the averaged concentration of the lower layer increases before the rollover while it does not according to the experimental data reported.

Also, the boil off rate and the interface position are compared on Figure 4. As shown, the interface moves downward rapidly. Indeed, in less than 5 min time, the interface disappears and the liquid is homogenised. As far as boil off rates are concerned, the one calculated is 3 times higher than the experimented one. The model has to be improved but the trends are similar and it highlights the sudden evaporation of Freon 11 during the sudden mixing which happens when the interface starts moving downwards.
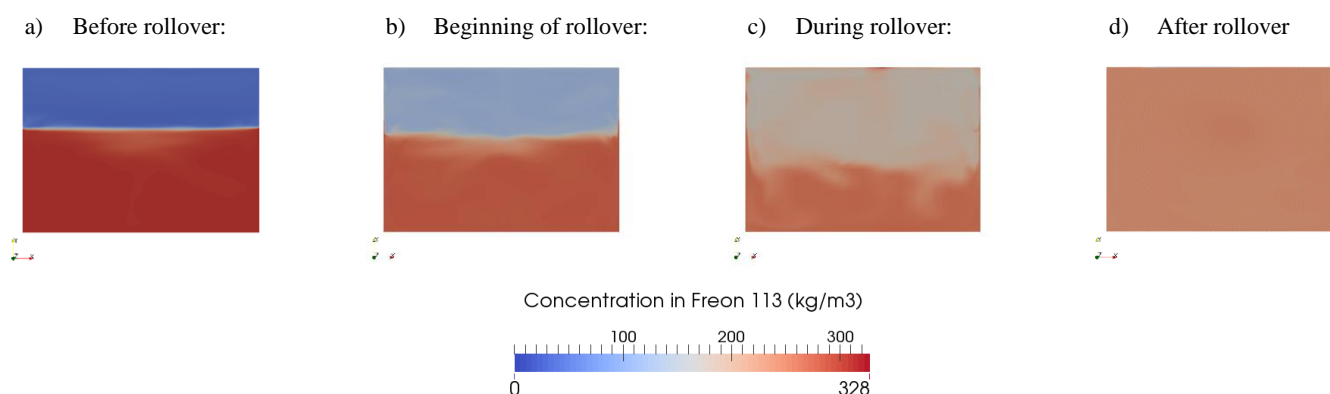
| a) Before rollover: | b) Beginning of rollover: | c) During rollover: | d) After rollover |

Concentration in Freon 113 (kg/m3)

Figure 5a),b), c) and d): Concentration fields at different stages of rollover

One of the main advantages of the proposed CFD approach is that it gives a spatial representation of rollover unlike the 1D models mentioned earlier. For this validation test case, it confirms the observation made by Morioka [13], Nakano and Sugawara [12] that rollover happens when a layer from the bottom breaks the interface and penetrates inside the top layer as it can be observed close to the side walls on Figure 5 b). This interface breaking is then possible, because previous convective motions in the top layer have swept some particles of Freon 113 from the interface towards the top layer, making it denser while making at the same time the bottom one lighter because poorer in Freon 113. After, this interface breaking, because of buoyancy, the liquid from the bottom layer rises next to the side walls and enters inside the top layer while the interface is pushed downwards.

Having validated the predictions of rolloverFoam with this small scale experiment, the code has then been used to reproduce the rollover in the Le Spezia accident.

CFD simulation of La Spezia accident:

On the 21st of August 1971, a rollover happened after bottom filling a tank with a heavier LNG than the one already in the 50 000 m^3 tank. Thirty six hours after the filling started, a sudden overpressure is observed in the tank as well as a sudden release of LNG vapour. Indeed, almost 186 tons of Natural Gas were released in the atmosphere in less than 16 hours. This was the La Spezia accident, one of the most known rollover incidents in history and documented in detail [1].

No damages were observed during this incident because measures were taken in time by the operators. However, it would be interesting to understand the rollover process in order to predict it and help to avoid its occurrence.

As illustrated in Table 1, LNG is a mixture mainly made of methane (around 90%) and ethane (slightly less than 10%). As a result, it is assumed to be a binary mixture and previous model can be applied to this case. A preliminary laminar and 3D model is demonstrated in this article. The model is initialized as shown on Figure 6.
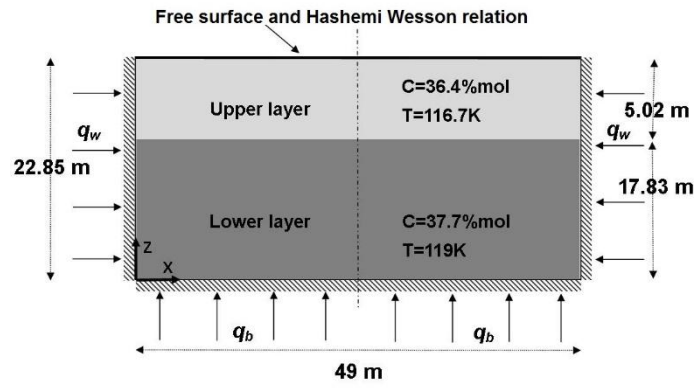
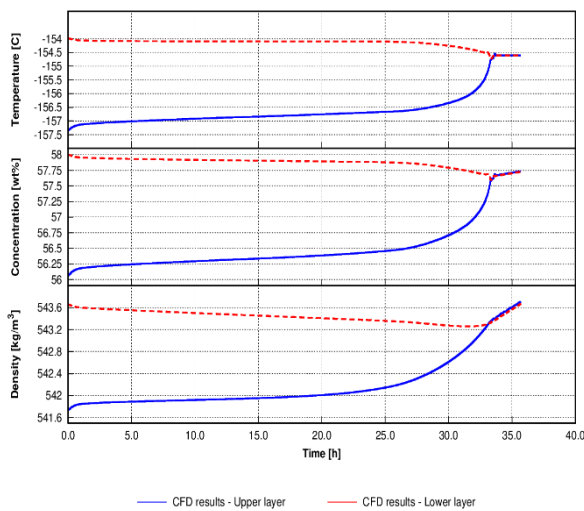*Figure 6: Initial conditions for La Spezia case*

Figure 7: Evolution of densities, concentrations and temperatures during the simulation of La Spezia accident
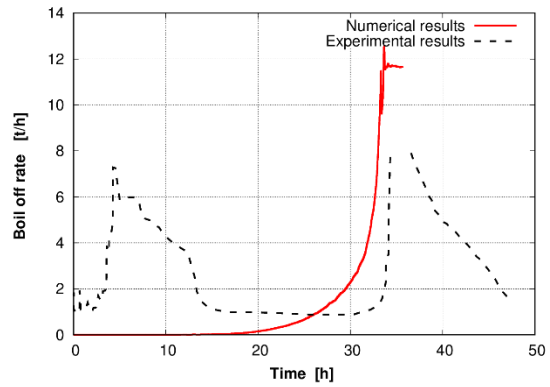
Figure 8: Evolution of the boil-off rate during the simulation of La Spezia accident

Figure 7 shows the evolution of the densities, temperatures and concentrations in the upper and lower layers during the rollover. Figure 8 compares the predicted and recorded evolution of the boil-off rate, which was the only quantified recordings from the accidents which could be used for comparison. The predictions demonstrate similar pattern as the experiments, showing a drastic surge around 30 hours which was the moment the rollover started. The intensities of this boil-off peak are also similar. Some differences are found with the experimental boil off rate but these could be caused by the neglecting of the reduced boil-off rate explained in Figure 1b). Also, while the LNG is added to the tank, during the first 16 hours, the LNG already available is stirred which generates a higher amount of LNG vapour. This latter has also been neglected in the numerical model where the liquid is assumed to be initially stratified and at rest.
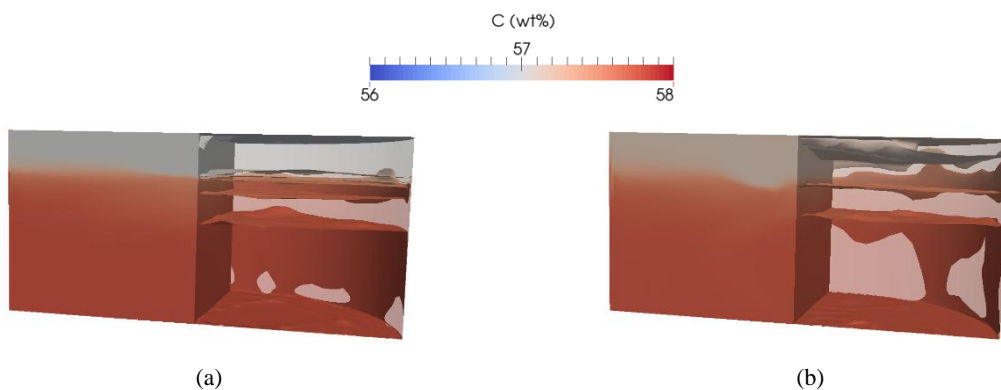

Figure 9: Concentration fields and isodensity lines in half of the tank before rollover (a) and at the beginning of rollover (b)

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The developed CFD tool shows a similar behaviour for the rollover than in the experimental case. Indeed, as it can be observed in Figure 9 with the isodensity lines which rise close to the walls and to the interface, it turns out that the rollover is also due to a layer from the bottom which penetrates inside the top layer while breaking the interface.

However, because of the lack of data more simulations are needed. Besides, the Rayleigh number is around 10^{18} which means the flow is fully turbulent. As a results, the model needs to be improved in order to take into account the turbulence in large tanks.

Conclusion

A predictive tool for rollover, rolloverFoam, has been developed with the frame of open source CFD code OpenFOAM. The validation study with small scale experimental data has shown relatively good agreements between the predictions and measurements. In addition, the three-dimensional results have provided good insight of the rollover phenomenon. The code has also been applied to simulate the large case scenario in the La Spezia accident and shown promising results. Indeed, in this case, the amount of boil-off gases when the rollover started and the mixing time are close to the ones observed during the accident. The code can potentially be of interest to predict the occurrence of rollover and assist the understanding the influence of boil-off rate of many parameters such as the size of the layers, the difference in concentration of ethane as well as the difference in temperature between the layers. It could also help to optimize the use of fans to mix the layers once a stratification is noticed and as a result save considerable amount of energy. More validation studies will, however, be beneficial, to further demonstrate the robustness and potential applications of the code.

Acknowledgments

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