CHEMICAL ENGINEERING TRANSACTIONS
VOL. 36, 2014
A publication of AIDIC
The Italian Association of Chemical Engineering
www.aidic.it/cet
Guest Editors: Valerio Cozzani, Eddy de Rademaeker

ISBN 978-88-95608-27-3; **ISSN** 2283-9216
DOI: 10.3303/CET1436041

Numerical Simulation of Tanks Containing Pressurized Gas Exposed to Accidental Fires: Evaluation of the Transient Heat Up

Arianna D'Aulisa[a], Davide Simone[a], Gabriele Landucci*[b], Alessandro Tugnoli[a], Valerio Cozzani[a], Michael Birk[c]

[a] Dipartimento di Ingegneria Civile, Chimica, Ambientale e dei Materiali, Alma Mater Studiorum - Università di Bologna, via Terracini n.28, 40131 Bologna, Italy
[b] Dipartimento di Ingegneria Civile e Industriale, Università di Pisa, Largo Lucio Lazzarino, 56126 Pisa, Italy
[c] Department of Mechanical and Materials Engineering, McLaughlin Hall, Queen's University Kingston, ON. K7L 3N6 Canada
g.landucci@diccism.unipi.it

Fires may impact on process and storage equipment causing severe damages and potential accident escalation. In the present study, a Computational Fluid Dynamics (CFD) model was set up for pressurized vessels exposed to accidental fires, aimed at determining the transient behaviour of the stored fluid during the heat-up. The model was developed for vessels containing pressurized flammable gases, such as methane, propane and hydrogen. The ANSYS FLUENT software was used in order to implement a two-dimensional circular geometry considering a medium scale spherical tanker. The presence of a heat resistant coating was considered in the analysis. The model allowed predicting the velocity and temperature profiles, thus obtaining the pressurization rate in the vessel and providing key indications for the evaluation of the vessel resistance.

1. Introduction

Severe fires, mainly due to the ignition of accidental releases, may affect process equipment (Bi et al., 2011) or transport vessels (Lautkaski, 2009) leading to a catastrophic loss of containment. Hence, a key issue to enhance safety and to reduce the risks related to both fixed installations and hazardous materials transportation is the development and the application of specific protections able to reduce the loss of mechanical properties of the equipment exposed to fire. This measure is widely applied in fixed installations both onshore (Di Padova et al., 2011) and offshore (Tugnoli et al., 2012). On the contrary, several issues are still open concerning the possible implementation of effective fire protections, based on fireproofing coatings, for road and rail tankers in the specific European context (Paltrinieri et al., 2009). In the literature, several small and medium scale tests were carried out in order to investigate these issues and to provide indications on the effectiveness of fireproofing materials (Landucci et al., 2009a). Due to safety and economic reasons, a limited number of large scale tests is available, one performed in North America (Townsend et al., 1974) and one in Europe (Balke et al., 1999). Therefore, the use of advanced computer models able to reproduce the heat up of a vessel engulfed in flames may constitute a sound tool to design and verify the thermal protections (Birk, 1988).
In the present study, a Computational Fluid Dynamics (CFD) model was set up for pressurized vessels exposed to accidental fires, aimed at determining the transient behaviour of the stored fluid during the heat up. In particular, the model was preliminarily developed for vessels containing pressurized flammable gases, such as methane, propane and hydrogen.
As evidenced by experimental works (Birk and Cunningham, 1996), a key issue in modeling pressurized vessels exposed to fires is in the prediction of the stratification of the inner fluid during the heat up process. The stratification is due to a buoyancy driven flow, caused by the more rapid temperature increase of the vapour in contact with the vessel walls heated by the fire with respect to the bulk fluid. This process has a

Please cite this article as: D'Aulisa A., Simone D., Landucci G., Tugnoli A., Cozzani V., Birk M., 2014, Numerical simulation of tanks containing pressurized gas exposed to accidental fires: evaluation of the transient heat up, Chemical Engineering Transactions, 36, 241-246 DOI: 10.3303/CET1436041

direct influence on the pressurization rate of the vessel, and thus it affects the time to failure, e.g. the lapse of time between the fire start and the eventual vessel rupture (Birk, 1988).
The ANSYS FLUENT software (ANSYS Inc, 2011) was used in order to implement a two-dimensional circular geometry considering a medium scale spherical tanker. The model was first developed for unprotected vessels, then considering the presence of an external insulating coating layer.
The results of the simulations allowed predicting the pressurization rate in the vessel, thus obtaining key indications for the evaluation of the vessel resistance (e.g. the time to failure).

2. Behaviour of vessel exposed to external fire

Figure 1 shows the schematization of the phenomena involved during the heat up of a pressurized gas vessel exposed to fire heat radiation.

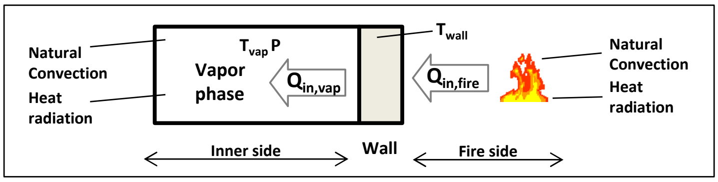

Figure 1: Physical phenomena involved during fire heat-up of a pressurized gas vessel

As shown in the figure, the vessel is heated up by the flames due to radiation and convection receiving the heat load $Q_{in,fire}$. Heat is then transferred by conduction through the vessel wall, which can be protected by a layer of insulating coating, resulting in heat flux towards the vapour phase ($Q_{in,vap}$). This phenomenon causes the vapour temperature (T_{vap}) and pressure (P) increase. Heat is transferred by convection and also by radiation when wall temperature grows due to the fire heat load. Vapour presents a significant thermal inertia, e.g. low convective heat transfer coefficients, due to low thermal conductivity and low velocities.
The convective heat transfer joined with a buoyancy driven flow results in thermal stratification of the vapour (Heymes et al., 2013). In fact, the temperature of the upper vapour layer exceeds the average fluid temperature value. The temperature rise in the fire engulfed vessel leads the pressure growth: the tank pressure is driven up by the warmest vapour layer, increasing the stress intensity on the vessel. On the same time, the vessel wall temperature rise results in the weakening the wall construction material resistance properties of the tanker wall. When the vessel resistance equals the stress intensity, the vessel integrity is jeopardized with severe deformations on the vessel shell and possible rupture (Landucci et al., 2009b).
In case of severe vessel heat up, the failure may also occur before the opening of the pressure relief valve (PRV), due to severe weakening of construction material. Hence, the installation of a heat resistant coating, able to mitigate the heat up and reducing the vessels wall temperature, is a key strategy to avoid the vessel rupture.

3. Modeling vessels exposed to external fire

3.1 Set up of CFD simulations

In the present study, spherical vessels containing only a gas phase are considered. These can be representative of a pressurized gas storage buffers or of a liquefied pressurized gas storage with a low value of the filling level.
The aim of the present study is to develop a model able to reproduce the vessel heat-up, as described in Section 2.1, and the behaviour of the inner gas, accounting for the buoyancy-driven flow and the temperature stratification resulting from the external fire heat load, including the effect of heat transfer by radiation from the vessel wall to the vapour.
In the present study the simulation of the vessel behaviour after the pressure relief valve (PRV) opening, thus considering gas outflow and strong mixing effects, is not taken into account, as it will be addressed in the further development of the present activity.
A commercial CFD (Computational Fluid Dynamic) tool, ANSYS FLUENT (ANSYS Inc, 2011), is used to set up the fluid dynamic model. The main equations considered are: 1) Continuity equation; 2) Energy equation; 3) Momentum equation; 4) Radiative Heat Transfer equation.
Since gas physical properties are strongly affected by the temperature rise, in the model developed the continuity and the momentum equation are coupled to the energy equation, and the solution of the energy

equation provides the temperature distribution in the flow field. The vapour phase participation to the radiative heat transfer is not considered. A standard k-ε model is used to account for the turbulence (Ferziger and Peric, 2002).
Table 1 summarizes the features of the model developed and the geometry of the reference tank considered in the simulations. Figure 2 shows the computational grid used for the calculations. As shown in the figure, the domain is axisymmetric and a spherical coordinates system is set up, thus reducing the number of cells needed for the study (see Table 1).

Table 1: Summary of the features of the CFD model developed for pressurized vessels engulfed by fires

Item	Description or selected value
Vessel geometry:	Spherical Vessel; external diameter = 1,700 mm; Wall thickness = 10 mm
Boundary conditions	Constant heat radiation temperature
Initial conditions required	Initial pressure and temperature
Mathematical models	Turbulent Flow: Standard k-ε Model Scalable Wall Function (ANSYS Inc, 2011) Radiation: S2S Model (ANSYS Inc, 2011)
Convergence criterion	10^{-6} for all the equations
Type of mesh	Structured mesh
Number of elements	18,600 cells

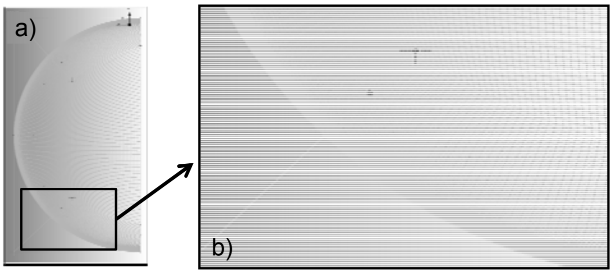

Figure 2: Mesh adopted in the present study for the analysis of pressurized gas spheres engulfed by fires: a) overview: b) detail

3.2 Definition of case studies

Table 2 summarizes the four case studies considered in the present analysis. The same heat load conditions are imposed, assuming a full engulfment in a large scale fire with constant radiating temperature (T_f). The influence of the stored gas on the temperature and pressure behaviour of the pressurized vessel is investigated in case studies 1, 2 and 3, respectively considering hydrogen, methane and propane as stored substances. No thermal protections (unprotected vessels) were considered.

Table 2: Summary of the case studies analysed with the CFD tool. P_0 = initial pressure; T_0 = initial temperature; T_f = effective fire radiation temperature

ID	Stored gas	Insulating coating	Boundary conditions	Initial conditions
1	Hydrogen	NO	Full engulfment in fire	T_0 = 300 K
2	Methane	NO	T_f = 1,144.15 K	P_0 = 5 barg
3	Propane	NO		
4	Methane	YES		

In case study 4, an insulating coating layer is implemented on the outer surface of the vessel in order to evaluate the effect of passive fire protection on the vessel heat up. An inorganic formulation with constant thermal conductivity (set equal to 0.1 W/(mK)) and 10mm thickness is considered as heat resistant coating. In order to obtain conservative results, the thickness of the vessel wall is neglected, assuming an uniform temperature in the steel due to the high thermal conductivity. In all the considered case studies, the presence of the PRV is taken into consideration. In fact, the simulation end is fixed at the PRV opening time. The PRV opening pressure is set to 1.6 MPa.

4. Results and discussion

4.1 Simulation of unprotected vessels

The present Section discusses the CFD results obtained for pressurized spheres containing different gases simulated in absence of thermal protection. Table 3 summarizes the PRV opening time for each case study. As expected, increasing the thermal inertia of the gas allows delaying the pressure and temperature rise due to the heat up.

Table 3: Summary of PRV opening time for the unprotected case studies.

ID	Stored gas	PRV opening time (s)
1	Hydrogen	38
2	Methane	72
3	Propane	99

The advantage of CFD modelling of pressurized vessels engulfed by fires is related to the possibility of obtaining local predictions of temperature and fluid velocities, thus supporting a more accurate evaluation of the inner pressure growth. This allows having a more precise evaluation of vessel resistance respect to lumped parameters models (Landucci et al., 2009b).
In order to show examples of the possible results obtained by CFD, Figure 3 and 4 report temperature and axial velocity maps obtained for the methane simulation (case study 2). In both figures, the CFD results are obtained at different times.

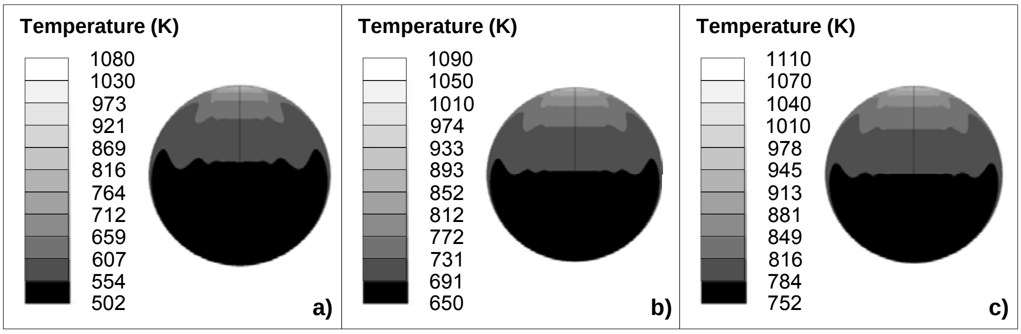

Figure 3: Example of temperature profiles obtained for methane (case study 2) at different time steps: a) 24 s; b) 48 s; c) 72 s

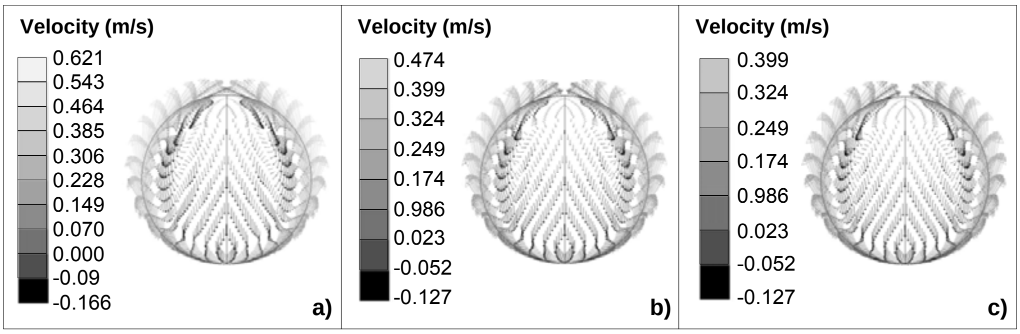

Figure 4: Example of axial velocity profiles obtained for methane (case study 2) at different time steps: a) 24 s; b) 48 s; c) 72 s

Figure 3 shows that gas temperature stratification occurs during the heat up process. This is due to a buoyancy driven flow, which causes the rise of hotter gas layers. This is confirmed by the analysis of Figure 4 in which the axial velocity profiles (plotted in form of vectors) are represented at the time step of the correspondent temperature map. In fact, Figure 4 clearly shows that the flow induced by buoyancy forces leads to the stratification of hot gas layers. It can also be seen that at the beginning of the heat

exposure (Figure 4a) the maximum velocity is higher than the one predicted in the last step (Figure 4c), since the fluid is approaching a quasi-steady state.
In order to analyze the behavior of the vessel during fire exposure, charts representing the dynamic temperature and pressure rise can be obtained by the software. Figure 5 shows an example of charts obtained for the three gases, reporting pressure and average gas temperature as a function of time. The figure shows that increasing the thermal inertia of the gas allows reducing the severity of the heat up. In fact, the highest average gas temperature is predicted for hydrogen (Figure 5a), while lower values are obtained for methane (Figure 5b) and propane (Figure 5c).

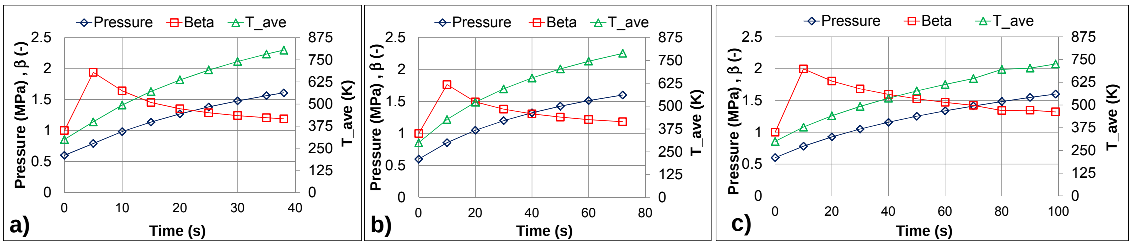

Figure 5: Average gas temperature, pressure profiles and dynamic stratification index behavior for: a)hydrogen, b) methane, c) propane

In order to quantify the level of stratification in the fluid, a dynamic stratification index (namely, β) was defined as follows:

$$\beta = T_{max} / T_{avg} \tag{1}$$

in which T_{max} is the maximum gas temperature and T_{avg} is bulk gas average temperature of the gas, both evaluated by the CFD tool at the same time. Quite clearly, this parameter at unitary at the simulation start. Then, its behaviour is strongly affected by the type of gas and fire exposure conditions.
In the charts shown in Figure 5, the β index is also reported as a function of time for the considered case studies. In all the simulated cases, the index features a rapid growth after which a maximum value is reached. The maximum predicted β value is about 2 for all the simulated gases, thus evidencing that the hottest gas layer, close to the vessel wall, reaches temperatures which are double with respect to the ones of the gas bulk at the beginning of the fire exposure. Then, while the heat is transferred into the lading and the inner fluid reaches the quasi-steady state, as evidenced by the velocity profile, a decrement of β is evaluated, and a plateau is reached. The value of β at the plateau is strongly affected by the type of gas, and is higher for gases having higher thermal inertia. In other words, for high values of gas thermal inertia (e.g., heat capacity and/or gas density), the temperature stratification is more pronounced.

4.2 Simulation of vessels in presence of passive fire protection

In case study 4 (see Table 3) the presence of an insulating coating layer is implemented in the simulations of the sphere containing methane. A comparison with the correspondent non-protected case (e.g., case study 2) is carried out.

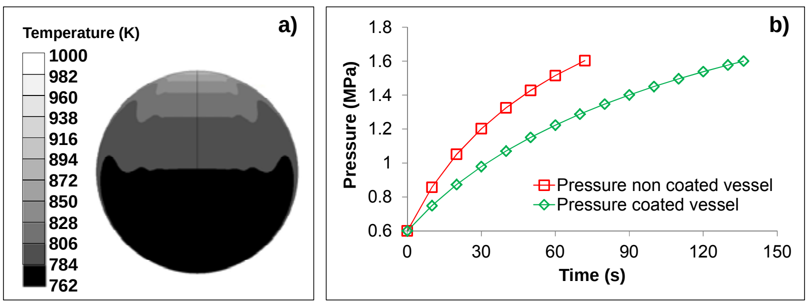

Figure 6: a) Average gas temperature for coated vessel at PRV opening time (136s), b) pressure profiles comparison between uncoated and coated vessel (case studies 2 and 4).

It is worth to mention that complicating phenomena concerning the PFP behaviour (e.g., devolatilization, degradation, swelling, etc.) described in several works (Gomez-Mares et al., 2012a,b) are neglected in order to limit the complexity of the simulation. Figure 6a shows the temperature map of the vapour at the PRV opening time (136 s). As shown in the figure, the gas stratification is still significant even if lower temperatures are predicted with respect to the unprotected case. Moreover, the PRV opening time is more than doubled with respect to the previous case as a consequence of the less severe tank heat up. This is evidenced by Figure 6b, in which the pressure rise curve is compared for the protected and unprotected cases. Hence, the effect of the PFP on the heat up of the vessel is assessed in detail.

5. Conclusions

In the present study the CFD modeling of pressurized vessels engulfed by fires is presented. The model was developed for pressurized gas spheres, thus considering only one phase in the domain. The case studies analyzed demonstrate the potentialities of the modeling tool in providing detailed pressure, velocity and temperature predictions. The study demonstrated the influence of gas thermal inertia, e.g. heat capacity and/or density, on the thermal stratification during fire exposure. A future development of the activity will be the modeling of cylindrical vessels containing pressurized liquids in order to assess the influence of liquid temperature stratification on the pressure growth and thus determining key information for the evaluation of vessel resistance. Moreover, the implementation of the fluid dynamic behavior of the stored fluid in structural analysis by FEM and the implementation of sub-models able to reproduce fire protection thermal behavior will be critical issues to be addressed.

References

ANSYS Inc, 2011, ANSYS FLUENT User's Guide. ANSYS Inc, Canonsburg, PA, USA.

Balke C., Heller W., Konersmann R., Ludwig J., 1999, Study of the Failure Limits of a Tank Car Filled with Liquefied Petroleum Gas Subjected to an Open Pool Fire Test. Federal Institute for Materials Research and Testing (BAM), Berlin, Germany.

Bi M.-S., Ren J.-J., Zhao B., Che W., 2011, Effect of fire engulfment on thermal response of LPG tanks, J. Hazard. Mat., 192, 874– 879.

Birk A.M., 1988, Modelling the response of tankers exposed to external fire impingement, J. Hazard. Mater. 20, 197-225.

Birk A.M., Cunningham M.H., 1996, Liquid temperature stratification and its effect on BLEVEs and their hazard. J. Hazard. Mater. 48(1–3), 219–237.

Di Padova A., Tugnoli A., Cozzani V., Barbaresi T., Tallone F., 2011, Identification of fireproofing zones in Oil&Gas facilities by a risk-based procedure, J. Hazard. Mater. 191(1-3), 83-93.

Ferziger J.H., Peric M., 2002, Computational Methods for Fluid Dynamics. Springer-Verlag, Berlin, Germany.

Gomez-Mares M., Tugnoli A., Landucci G., Barontini F., Cozzani V., 2012a, Behaviour of intumescent epoxy resins in fireproofing applications, J. Anal. Appl. Pyrol. 97, 99-108.

Gomez-Mares M., Tugnoli A., Landucci G., Cozzani V., 2012b, Performance assessment of passive fire protection materials, Ind. Eng. Chem. Res. 51 (22), 7679–7689.

Heymes F., Aprin L., Birk A.M., Slangen P., Jarry J.B., François H., Dusserre G., 2013, An experimental study of an LPG tank at low filling level heated by a remote wall fire, J. Loss Prev. Proc. Ind., 26, 1484-1491.

Landucci G., Molag M., Reinders J., Cozzani V., 2009a, Experimental and analytical investigation of thermal coating effectiveness for 3 m^3 LPG tanks engulfed by fire, J. Hazard. Mater. 161, 1182-1192.

Landucci G., Gubinelli G., Antonioni G., Cozzani V., 2009b, The assessment of the damage probability of storage tanks in domino events triggered by fire, Acc. Anal. Prev. 41(6), 1206-1215.

Lautkaski R., 2009, Evaluation of BLEVE risks of tank wagons carrying flammable liquids, J. Loss Prev. Proc. Ind., 22, 117–123.

Paltrinieri N., Landucci G., Molag M., Bonvicini S., Spadoni G., Cozzani, V., 2009, Risk reduction in road and rail LPG transportation by passive fire protection, J. Hazard. Mater. 167, 332-344.

Townsend W., Anderson C.E., Zook J., Cowgill G., 1974, Comparison of Thermally Coated and Uninsulated Rail Tank-Cars Filled with LPG Subjected to a Fire Environment, report FRA-OR&D 75-32. US Department of Transportation DOT, Washington, DC.

Tugnoli A., Cozzani V., Di Padova A., Barbaresi T., Tallone F., 2012, Mitigation of fire damage and escalation by fireproofing: A risk based strategy, Rel. Eng. and Syst. Saf. 105, 25-35.