



ORIGINAL ARTICLE

Numerical analysis of the explosion of gas tanks using computational fluid dynamics

Análise numérica da explosão de tanques de gás com o uso da fluidodinâmica computacional

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Abstract: Buildings are composed of several systems, each with specific designs and regulations to ensure that constructions are safe and viable. Many residential, commercial, and industrial buildings have systems with gas central storage, which must be subjected to strict safety criteria to avoid accidents. In addition to the safety mechanisms provided by manufacturers, designers of these gas central storage must consider other devices to reduce explosion risk and mitigate the damaging blast effects. Explosions are physical-chemical phenomena that are characterized by the sudden expansion of a material and, consequently, energy release. When an accidental explosion occurs, much damage is caused by the shock wave and fragments. In the case of pressure vessels, a mechanical explosion can occur. Studying this explosion is essential to developing a more reliable, safe design for surrounding buildings and its users. This work aims to study the effects of gas tank explosions. In this study, the Autodyn computational tool based on fluid dynamics (CFD) is used. This software allows the modeling of complex explosion scenarios and the evaluation of blast wave parameters. For each numerical model, the overpressure levels outdoors and indoors are evaluated. The results indicated how the wave overpressures are distributed in different scenarios, and from them, it was possible to analyze the damaging levels.

Keywords: explosion, LPG tank, shock wave, overpressure, damage.

Resumo: As edificações são compostas por vários sistemas, cada um com projetos e normas específicas para garantir que as construções sejam seguras e viáveis. Muitos edifícios residenciais, comerciais e industriais possuem sistemas com centrais de gás, as quais devem ser submetidas a rigorosos critérios de segurança para evitar acidentes. Além dos mecanismos de segurança fornecidos pelos fabricantes, os projetistas dessas centrais de gás devem considerar outros dispositivos para reduzir o risco de explosão e mitigar os efeitos danosos da explosão. As explosões são fenômenos físico-químicos que se caracterizam pela expansão súbita de um material e, conseqüentemente, liberação de energia. Quando ocorre uma explosão acidental, muitos danos são causados pela onda de choque e fragmentos. No caso de vasos sob pressão, pode ocorrer a explosão mecânica e a compreensão dos efeitos desse evento é essencial para o desenvolvimento de projetos mais confiáveis e seguro para as edificações e seus usuários. Este trabalho tem como objetivo o estudo dos efeitos da explosão de tanques de gás. Neste estudo, é utilizada uma ferramenta computacional baseada em fluidodinâmica computacional (CFD); o Autodyn. Esse software permite a modelagem de cenários complexos de explosão e a avaliação de parâmetros de ondas de choque. Para cada modelo numérico, são avaliados os níveis de sobrepressão no exterior e no interior. Os resultados indicaram como se deu a distribuição das sobrepressões da onda em diversos cenários e partir deles foi possível traçar estimativas de dano.

Palavras-chave: explosão, tanque de GLP, onda de choque, sobrepressão, danos.

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Data Availability: The data that support the findings of this study are available from the corresponding author, TRCM, upon reasonable request.



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1 INTRODUCTION

Residential and commercial buildings are composed of several systems, for example, structural, hydraulic, electrical, gas and others. In many constructions, there are gas supply systems, and, in some cases, this gas is stored in stationary tanks placed outside the building. These kinds of tanks are designed for high-pressure gas storage, the most common being LPG. There is an inherent risk of explosion when a gas tank is being used, and this risk can be related to manufacturing failures, careless maintenance, fire, incidents, and even criminal acts.

An explosion is a complex and non-linear phenomenon that results from a sudden energy release, and its magnitude is related to the amount of energy released [1]. The explosions can be originated from solid materials (plastic explosives, for example), liquids, or gas clouds, and they can be classified according to their nature as mechanical, chemical, or nuclear. Furthermore, there are also electrical explosions resulting from high-intensity electrical discharges. Chemical explosions occur through detonation (supersonic combustion process) or deflagration (subsonic combustion process).

The shock wave physics and its equations were studied by Zel'dovich and Raizer [2], who also explained the Lagrangian and Eulerian approaches applied to numerical analysis. An elementary and detailed explosion description and its effects can be found in the works of Kinney and Graham [1] and Needham [3].

This study focuses on mechanical explosion, which can be observed during the failure of a pressurized vessel. About this kind of explosion, Salzano et al. [4], Schleyer [5], and Ferradás et al. [6] presented a mathematical model to evaluate LPG tanks in a fire environment coupled with a risk analysis, an analysis of loading on structures and analysis the blast effects on buildings, respectively. The safety distance from a vapor cloud rapid deflagration was investigated by Li and Hao [7] using a numerical tool. In the context of a gas cloud, numerical simulations in environments with complex geometry were performed by Vianna and Cant [8], Ferreira and Vianna [9], [10], and Quaresma et al. [11]. These researchers used a computational tool with meshes based on Porosity Distributed Resistance (PDR). In the PDR approach, objects smaller than the computational grid occupy only part of each computational cell; thus, only part of the cell volume is available for flow [12]. According to Cain [13], the blast wave emanating from the bursting pressure vessel is somewhat similar to that caused by a high explosive detonation; however, the blast wave overpressure values may diverge at short standoff distances. Therefore, a suitable prediction of energy loss by dissipation process is needed in order to achieve accurate results when simulating stored energy using high explosives. Molkov and Kashkarov [14] compiled some methods in their research to predict mechanical energy stored in gas-pressurized tanks.

Gas explosion overpressures in confined spaces were numerically simulated by Wang et al. [15] and Li et al. [16]. In addition to these studies, using computational fluid dynamics, Cen et al. [17] and Pang et al. [18] performed gas tank explosion simulations in an apartment and in a kitchen, respectively. Numerical research about explosion overpressures in urban and residential environments and the use of obstacles to mitigate shock wave effects was carried out by Costa and Doz [19] and Vyazmina et al. [20].

Most recorded explosions involving gas tanks occur accidentally. Therefore, there is little data about overpressures and shock wave propagation from these explosions. Most information about these events is related to residual damage of damaged buildings. Despite this scenario, Stawczyk [21] and Tschirschwitz et al. [22] carried out experiments with exploding gas tanks, and a study about high-speed fragments from pressure vessel explosions was presented by Vaidogas [23].

Semi-empirical models are a reliable approach to studying explosion phenomena, and they can be used as an alternative to real-scale experiments that are expensive and dangerous to carry out. However, these models are unable to represent complex events such as shock wave reflections and channeling. Numerical methods are essential tools to overcome these limitations.

Currently, there are some numerical tools for explosion simulation, for example, Autodyn, FLACS, and STOKES (Shock Towards Kinetic Explosion Simulator). According to Quaresma et al. [11], the STOKES is a PDR-based code that can be used to modeling gas explosions in complex environments, the porous mesh generated by STOKES can evaluate the effects of small scale obstacles without the need of considerable mesh refinement. Autodyn is a tool that can simulate detonations, impacts and other severe loading problems, where the results can be remapped to other analysis systems within the Ansys® Workbench for further analysis. According to Tham [24], one unique feature of Autodyn is it allows different parts of a single problem to be modeled with their appropriate numerical formulation, allowing a user to couple different numerical solution techniques in a single problem.

This work aims the analysis of a gas tank blast effects in terms of overpressure data on close buildings. A correlation between the overpressure levels and the threshold parameters for buildings and its users is performed. The computational fluid dynamics (CFD) tool Autodyn from the Ansys® package is used for this research.

2 EXPLOSION PARAMETERS

Several parameters can influence gas tank explosion analysis, such as the amount of stored energy, explosion standoff distance, tank geometry and overpressures distribution. In order to achieve reliable results these parameters must be correctly addressed by the predictive methods and numerical approach.

2.1 Method of predicting mechanical energy in pressure vessels

A reliable prediction of the stored energy in pressure vessels is an essential part of explosion analysis. Molkov and Kashkarov [14] presented a compilation of several methods to calculate the energy of a physical explosion, such as the Brode's equation, the isentropic expansion, the isothermal expansion and thermodynamic availability that are related with ideal gas model. The isothermal and thermodynamic availability models are restricted to cases where the temperature at the beginning and end of the process is the same. The energies obtained by the Brode models and isentropic expansion are similar and smaller than that obtained by previous two models, where, in this case, the Brode model is more realistic with less restricting assumptions. Molkov and Kashkarov [14] suggested also the Abel-Noble equation of state to non-ideal gas analysis, which improves the predictive capacity of energy stored in gas tanks, as it represents a more realistic situation of the problem. In a hermetically sealed vessel filled with pressurized gas, the mechanical energy can be calculated as the product of the mass of the gas, specific heat at constant volume, and temperature [14].

Introducing the Abel-Noble equation for energy calculation, we have Equation 1. Equation 2 is the gas co-volume expression [25], a parameter that represents the volume occupied by gas molecules per unit mass.

$$E = \left(\frac{P_g - P_0}{(R_u / M)T + b(P_g - P_0)} \right) V_g \left(\frac{C_v}{M} \right) T \quad (1)$$

$$b = \frac{RT_c}{8P_c} \quad (2)$$

Where E = stored mechanical energy (J); P_g = stored gas pressure (Pa); P_0 = ambient pressure (approximately equal to 101325,0 Pa at sea level); V_g = stored gas volume (m³); C_v is the specific heat at constant volume (J/mol·K); T = gas temperature (K); R_u = universal gas constant (equal to 8,314462618 J/mol·K); M = molar mass of gas (kg/mol); b = co-volume of gas (m³/kg); R = gas constant (J/kg·K), T_c = critical point temperature (K); and P_c = pressure of the critical point of the gas (Pa).

2.2 TNT-equivalent mass

Gas tank explosions can be analyzed using methodologies classified into three categories according to their nature: the TNT (trinitrotoluene) equivalence method, blast curve methods and numerical simulations [26]. Sochet [27] presents an overview of analytical models for explosion analysis and highlights their limitations.

TNT-equivalent method is an analytical model that uses the scaled distance and semi-empirical equations (detailed in the following item) to evaluate the overpressure peaks. Crowl and Louvar [28] mentioned that the main advantage of this method is the simple to use, this advantage was observed by Lopes and Melo [29] in the study on the explosion of hydrogen cylinders in nuclear power plants. As noted by Cain [13], the TNT-equivalent method can be used to estimate the gas tank explosion overpressure in the far field. In the nearby field, López et al. [30] observed that it is possible to use this method when the explosion yield is correctly adjusted to the model in order not to overestimate the overpressures.

The methodology adopted in this paper is a mixed process that involves analytical and numerical methods. The use of analytical models is related to predicting the mechanical energy stored in the tank, the TNT-equivalent mass, and the blast wave overpressure at validation points. TNT detonation and shock wave propagation analysis in complex scenarios are performed using numerical models.

In this study, only the mechanical energy of the explosion was considered since the contribution of the chemical portion only occurs if the gas mixture is ignited. Thus, the TNT-equivalent mass was obtained by the direct correlation between the mechanical energy stored in the gas tank and the specific energy released in a TNT explosion. This specific energy is approximately equal to 4.184 MJ/kg, Bolonkin [31]. The explosion yield in terms of the generated shock wave was estimated in an energy loss analysis detailed below in item 3.4.

2.3 Analytical equations for predicting explosion overpressures

Shock waves are disturbances that propagates through the air carrying a large amount of kinetic energy, the typical overpressures distribution of a shock wave is shown in Figure 1. Overpressure is an important parameter in a prior damage assessment, it is defined as the difference between the shock wave pressure and the ambient pressure.

Figure 1 also illustrates the shock wave phases. The positive phase of the shock wave shows a higher overpressure magnitude but a short duration when compared to the negative phase.

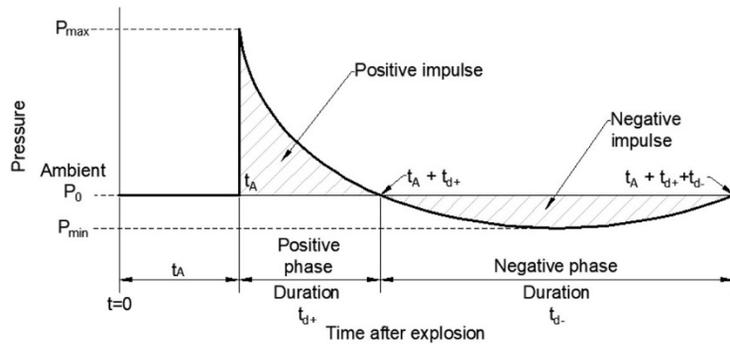


Figure 1. Typical scheme of a shock wave from an ideal explosion from a spherical source in an open environment [32] - adapted.

Semi-empirical methods can be used for a preliminary overpressure analysis, those methods are related with scaled distance (Equation 3) that measures the effects of the explosion in terms of energy dispersion by relating the standoff distance with explosive mass.

$$Z = \frac{R}{\sqrt[3]{W}} \tag{3}$$

Where Z = scaled distance ($m/kg^{1/3}$); R = distance from explosion center to analysis point (m); and W = TNT mass (kg).

The overpressures can be predicted with the semi-empirical models shown in Table 1, that are valid for open-air explosions from spherical explosive charges.

Table 1. Semi-empirical overpressure (ΔP) prediction equations [33].

Author	Prediction formulas	Requirement	Unit
Brode	$\Delta P = \frac{6,7}{Z^3} + 1$	(4) $\Delta P > 10$	Bar
	$\Delta P = \frac{0,975}{Z} + \frac{1,455}{Z^2} + \frac{5,85}{Z^3} - 0,019$	(5) $0,1 < \Delta P < 10$	Bar
Henrych	$\Delta P = \frac{14,072}{Z} + \frac{5,540}{Z^2} - \frac{0,357}{Z^3} + \frac{0,00625}{Z^4}$	(6) $0,05 \leq Z \leq 0,3$	Bar
	$\Delta P = \frac{6,194}{Z} - \frac{0,326}{Z^2} + \frac{2,132}{Z^3}$	(7) $0,3 \leq Z \leq 1$	Bar
	$\Delta P = \frac{0,662}{Z} + \frac{4,05}{Z^2} + \frac{3,288}{Z^3}$	(8) $1 \leq Z \leq 10$	Bar
Mill	$\Delta P = \frac{1772}{Z^3} - \frac{114}{Z^2} + \frac{108}{Z}$	(9) -	kPa
Kinney	$\frac{\Delta P}{P_0} = \frac{808 \left[1 + \left(\frac{Z}{4,5} \right)^2 \right]}{\sqrt{1 + \left(\frac{Z}{0,048} \right)^2} \sqrt{1 + \left(\frac{Z}{0,32} \right)^2} \sqrt{1 + \left(\frac{Z}{1,35} \right)^2}}$	(10) -	-
Newmark	$\Delta P = 6784 \frac{W}{R^3} + 93 \left(\frac{W}{R^3} \right)^{1/2}$	(11) -	Bar

2.4 Overpressure limits for damage to humans and structures

Overpressure levels can be directly related with building damage assessment, as shown in Table 2. According to Baker et al. [35] the damaging effects of explosions on building users can be direct and indirect. The direct effects are related to the shock wave overpressures (Table 3) and the indirect effects are related with debris at high speed from damaged materials.

When a shock wave collides with a living being, part of its energy is reflected, and another fraction is absorbed and transmitted to body tissues. As a result, the absorbed kinetic energy causes stress waves, leading to rapid physical deformation that can result in a tissue rupture [32].

Table 2. Shock wave effects on structures [34].

Damage	Overpressure (ΔP)	
	Bar	psi
Glass breakage	0,01 – 0,015	0,15 – 0,22
Minimal damage to buildings	0,035 – 0,075	0,52 – 1,12
Damage to metal panels	0,075 – 0,125	1,12 – 1,87
Failure of wooden panels (buildings)	0,075 – 0,15	1,12 – 2,25
Failure in brick walls	0,125 – 0,2	1,87 – 3
Rupture of refinery tanks	0,2 – 0,3	3 – 4,5
Damage to buildings (metallic structures)	0,3 – 0,5	4,5 – 7,5
Damage to concrete structures	0,4 – 0,6	6,0 – 9,0
Probable total destruction of most buildings	0,7 – 0,8	10,5 - 12

Table 3. List of some damages caused to humans [34].

Damage	Overpressure (ΔP)	
	Bar	psi
Tolerable (does not cause damage)	up to 0,0001	up to 0,0015
Fall	0,07 – 0,1	1,05 – 1,5
Eardrum rupture	0,35 – 1,0	5,25 – 15
Lung injuries	2,0 – 5,0	30 – 75
Lethality	7,0 – 15,0	105 – 225

3 PRELIMINARY ANALYSIS

3.1 Gas tanks normative parameters

In this study, LPG tanks are considered static, that is, placed in fixed locations on the ground surface or underground. The design parameters established by ABNT [32] were considered in all modeled gas tanks, as summarized in Table 4.

Table 4. Types and characteristics of tanks according to ABNT [36].

Tank type	Tank volume	Distance from the tank to the building and openings	Model identification	
Aboveground	A	up to 0,5 m ³	next to the building and 3 m from the opening	model 1
	B	from 0,5 to 2,0 m ³	1,5 m from the building and 3 m from the opening	model 2
	C	from 2,0 to 5,5 m ³	3 m from the building	model 3
	D	from 5,5 to 8,0 m ³	7,5 m from the building	model 4
	E	from 8,0 to 120,0 m ³	15 m from the building	model 5
Underground	A	up to 8,0 m ³	3 m from the building	model 6
	B	from 8,0 to 120,0 m ³	15 m from the building	model 7

3.2 Tank manufacturing parameters

LPG tanks are hermetically sealed vessels resistant enough to withstand high internal pressures. Generally, these tanks have a rounded geometry to minimize the risk of rupture due to stress concentration.

In this work, the most common high-pressure design (2.0 MPa) was considered for all LPG tanks. These high pressures that keep the gas in a liquid state and vary as a function of the temperature and proportion of the hydrocarbon mixture.

3.3 Gas properties

Propane gas requires more pressure to liquefy than other hydrocarbons that compose LPG. Therefore, it represents a riskier situation when compared to other hydrocarbons. Table 5 presents the propane properties adopted in the energy prediction of all the tanks studied in this work.

Table 5. Physical and chemical propane gas properties adopted [25] – adapted.

Reference temperature (T)	15° C (288,2 K)
Specific mass in liquid state (ρ)	581 kg/m ³
Specific heat at constant pressure (C_p)	74,057 J/mol·K
Specific heat at constant volume (C_v)	65,744 J/mol·K
Specific heat ratio (γ)	1,126
Molar mass (M)	0,044097 kg/mol
Molar constant (R)	188,5 J/kg·K
Critical point temperature (T_c)	370 K
Critical point pressure (P_c)	4,26 MPa
Co-volume (b) – obtained by Equation 2	0,00205 m ³ /kg

3.4 Energy loss analysis

It should be pointed out that energy from an explosion is dissipated in several ways, such as shock waves, heat, sound, movement of fragments, and others. Therefore, not all the energy released in the explosion is carried by the shock wave, some part of this energy is lost. In a pressure vessel explosion, this energy loss is related with tank deformation and rupture process.

According to Lees [37], about 40% to 80% of the energy of the explosion is carried by the shock wave, it is possible to infer that the energy loss is a calibration factor. In order to calibrate the energy loss to the simulated models, a preliminary simulation based on the experiments of Tschirschwitz et al. [22] was made. The tank properties and the measured overpressures at gauges positions are shown in Table 6.

Table 6. Experimental data from Tschirschwitz et al. [22].

Tank		Moment of rupture		Overpressures (ΔP)		
Identification	Volume	Pressure in the tank	Gas temperature	(L = 5 m)	(L = 7 m)	(L = 9 m)
PC07 (experiment 1)	0,0272 m ³	82,1 bar	111,4 °C	0,15 bar	0,11 bar	0,09 bar
PC09 (experiment 2)	0,0272 m ³	86,9 bar	97,0 °C	0,15 bar	0,11 bar	0,10 bar

Note: L is the distance from the overpressure sensor to the center of the explosion.

The simulation results were compared with experimental and semi-empirical models, as shown in Figure 2. In this case, it is possible to see that the semi-empirical methods are not accurate enough for close range explosions because they do not account the shock wave reflection phenomena on the ground.

The estimated energy loss was initially recalculated through a model update process based on the experimental results. It was possible to define the value of energy loss at approximately 25%, which is within the values range exposed by Lees [37]. In this sense, the explosion yield concerning the portion of energy involved in the shock wave formation is 75%. This value was considered in subsequent simulations that share similar modeling.

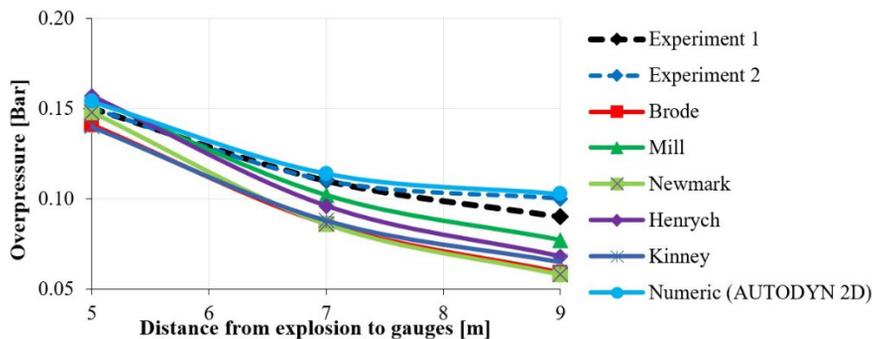


Figure 2. Overpressures as a function of the explosion distance of a propane gas tank with a volume of 27.2 liters.

3.5 TNT equivalent mass for each type of tank

The TNT equivalent mass was obtained considering the energy loss and the mechanical energy formulation from Equation 1, as shown in Table 7.

Table 7. Stored energy and TNT equivalent mass in each tank type.

Tank type		Mechanical energy stored in the tank [J]	Energy loss rate	Specific energy of the TNT explosion [J/g]	TNT equivalent mass [kg]
Aboveground	A	7.005.291,9	25,0%	4184,0	1,256
	B	28.021.167,7	25,0%	4184,0	5,023
	C	77.058.211,2	25,0%	4184,0	13,813
	D	112.084.670,8	25,0%	4184,0	20,092
	E	1.681.270.061,9	25,0%	4184,0	301,375
Underground	A	112.084.670,8	25,0%	4184,0	20,092
	B	1.681.270.061,9	25,0%	4184,0	301,375

4 NUMERIC SIMULATIONS

The simulations were performed using Autodyn from Ansys® Workbench, this software uses explicit time integration to solve the fundamental equations of fluid dynamics: the equation of continuity, momentum, and energy. Several materials and problems can be modelled in Autodyn, where the mathematical relationships between internal energy, density, pressure, stresses, and strains are summarized in an Equation of State (EOS), strength constitutive model and failure criteria, also cell erosion conditions can be enabled.

Autodyn is suited to modelling severe and fast loading problems such that involving impacts, explosions, and fragmentation.

Previous numerical simulations showed that mesh size influences the numerical accuracy and the computation time consumption as well. The influence of mesh size for all simulated models results was investigated.

4.1 Problems modelling

Two environments that represents common situations in typical urban buildings were simulated (Figures 3 and 4). These models were built to meet the standoff specifications described by the ABNT [36], as presented in Table 4.

The walls and slabs' thickness are 100 mm in all models, and the height between the floor and slab is 2900 mm. Walls and slabs are made of 35 MPa concrete, and the ground is composed of sand. All materials used are present in the Autodyn library.

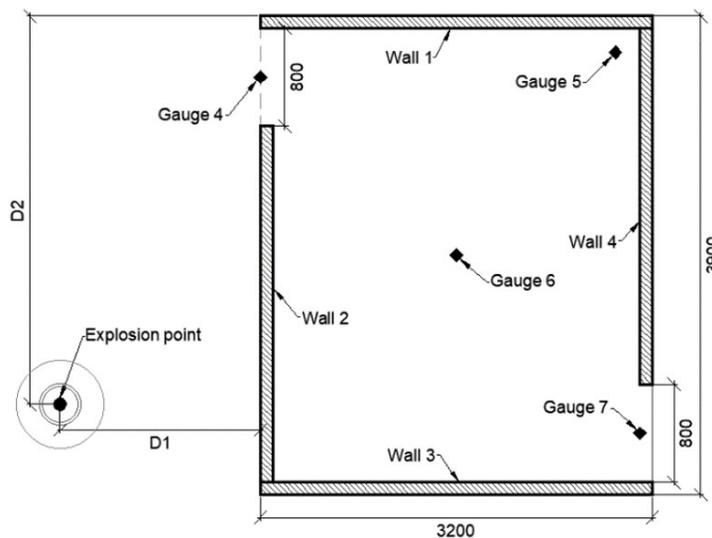


Figure 3. Floor plan for models 1 and 2 (All dimensions are in millimeters)

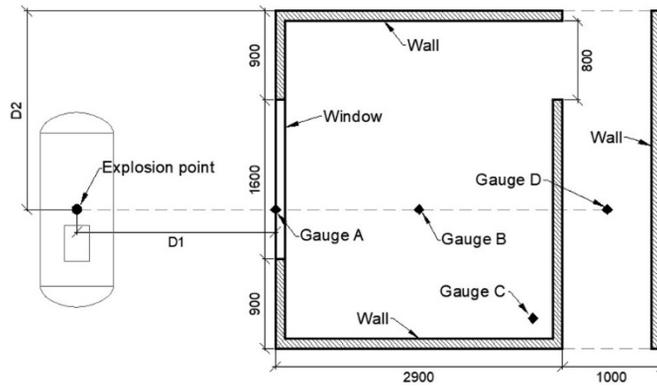


Figure 4. Floor plan for models 3 to 7 (All dimensions are in millimeters)

The main objective of the simulations was to measure the overpressure peaks around and inside the building in the first few milliseconds after detonation (between 20 ms and 40 ms). The simulation of large deformations, strain, and fragmentation may lead to an increased simulation time. To avoid this nuisance, rigid solid elements were used as boundary conditions, this consideration had a minor impact on overpressure final peak results. This consideration was also adopted in the simulations carried out by Luccioni, Ambrosini, and Danesi [38]. The solid elements were discretized with a Lagrangian mesh and the air with a Eulerian mesh. The boundary condition imposed on the faces of the air domain was “flow out” to not reflect the shock wave.

Table 8 shows the tank details for each model, where distance D1 is equal to half of the tank diameter added to the minimum distance provided in Table 4.

Table 8. Detailing of the tanks in each model.

Model	Tank situation	Tank diameter [mm]	Distances of the explosion in relation to the building		Explosion point height from ground level [mm]
			D1 [mm]	D2 [mm]	
1	aboveground	1000	500	3900	+ 1200
2	aboveground	1200	2100	3050	+ 1200
3	aboveground	2000	4000	2000	+ 1200
4	aboveground	2200	8600	2000	+ 1200
5	aboveground	2400	16200	2000	+ 1300
6	underground	2000	4000	2000	- 1500
7	underground	2400	16200	2000	- 1700

Note: the plus sign (+) indicates the explosion point is above ground level and the minus sign (-) indicates the point is below ground level.

Before discretizing the entire models in the Autodyn 3D environment, the TNT explosives were simulated as wedge elements. The wedge element is one-dimensional, so the processing time is faster. Figure 5 presents the wedge concept of spherical geometry and the discretization in Autodyn. After this first approach for detonation, the explosion data was remapped to the three-dimensional models.

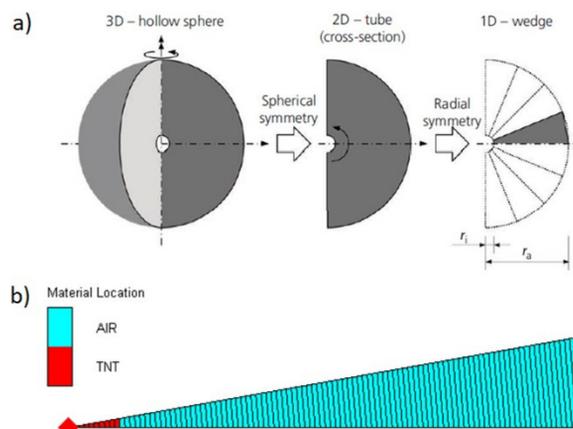


Figure 5. a) Wedge model for spherically symmetric problems [39]; b) Discretized wedge with air and TNT on Autodyn.

4.2 Aboveground stationary tank simulations

Aboveground stationary tanks are placed outside the building. The overpressure gauges were placed at the corners (200 mm from building wall surface), the middle of the door, room center, and windows.

In larger models, some gauges were placed in the external space next to the explosion. Gauges 1, 2, and 3 are placed in positions where there was no effect of shock wave reflection influence on initial results. The data obtained from these three overpressure gauges were compared with the results of the semi-empirical methods.

Table 9. Discretization data for models 1 and 2 with 25 mm mesh.

Part	Origin point coordinates			Dimensions in each direction [mm]			Number of mesh elements in each direction		
	x	y	z	Dx	Dy	Dz	Nx	Ny	Nz
Air	0	0	0	5800	3100	3900	232	124	156
Ground	0	0	0	5800	100	3900	232	4	156
Wall 1	2600	100	0	3200	2900	100	128	116	4
Wall 2	2600	100	900	100	2900	2900	4	116	116
Wall 3	2600	100	3800	3200	2900	100	128	116	4
Wall 4	5700	100	100	100	2900	2900	4	116	116
Slab	2600	3000	0	3200	100	3900	128	4	156

Models 1, 2, 3, and 4 were discretized with 100, 50, and 25 mm meshes. The model 5 was discretized with 100 and 50 mm meshes only, due its large geometric dimensions. Table 9 presents the discretization data of models 1 and 2, and Figure 6 shows them already discretized in Autodyn. All other models followed the same discretization procedure.

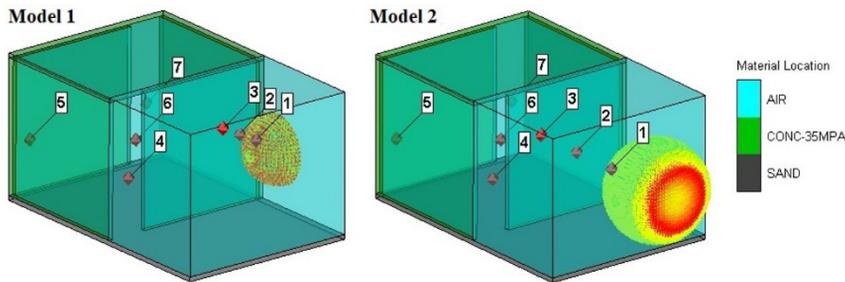


Figure 6. Models 1 and 2 discretized in Autodyn.

The modelled space of models 3 to 7 were wider because the tanks are bigger in size, as presented in Figure 4. Figure 7 presents the models 3, 4 and 5 in Autodyn interface. The external gauges are identified with numbers and the internal ones with letters. The internal gauges are arranged in the same positions for all models.

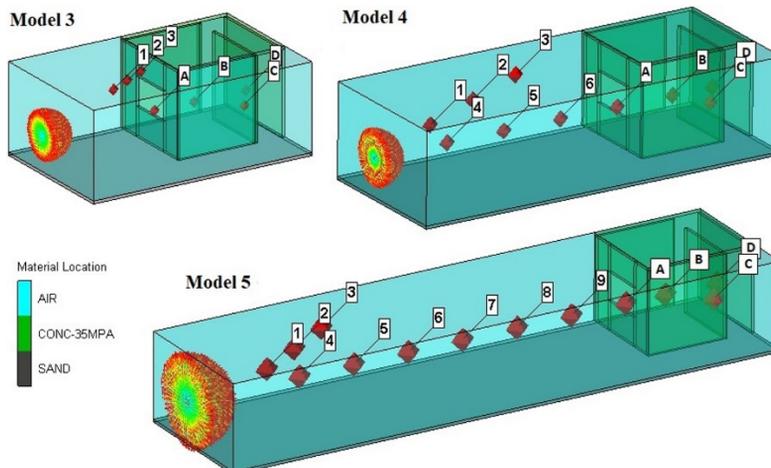


Figure 7. Models 3, 4 and 5 discretized on Autodyn.

The distances of the external gauges to the explosion center are detailed in Table 10.

Table 10. Distance in meters from the external gauges to the explosion center.

Gauge	1	2	3	4	5	6	7	8	9
Model 1	1,594	2,790	3,986	-	-	-	-	-	-
Model 2	1,368	2,438	3,509	-	-	-	-	-	-
Model 3	2,689	3,087	3,735	-	-	-	-	-	-
Model 4	2,112	3,697	5,281	2,600	4,600	6,600	-	-	-
Model 5	3,040	4,050	5,070	4,200	6,200	8,200	10,200	12,200	14,200

4.3 Underground stationary tank simulations

The tank's arrangement is underground because they are inserted in reinforced concrete shelters below ground level as shown in Figure 8. The simulated models 6 and 7 share the same building design as presented in Figure 4 as well the minimum safety distances according to ABNT [36] recommendations summarized in Table 4. Figure 9 presents models 6 and 7 discretized in Autodyn.

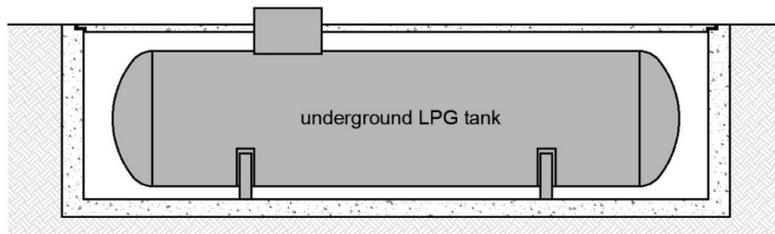


Figure 8. Sectional diagram of the concrete shelter for the underground tanks.

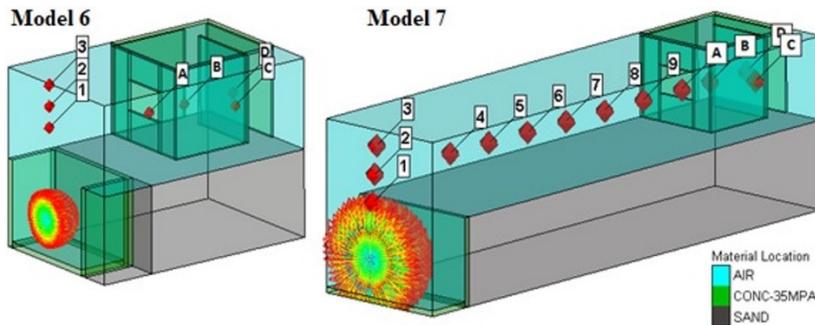


Figure 9. Models 6 and 7 discretized in Autodyn.

The sealing of the upper part of the shelter (the cover) was disregarded to analyze a critical situation for all models. Table 11 presents the distances of the external gauges to the explosion center.

The models 6 was discretized with 100, 50, and 25 mm meshes and the model 7 was discretized with 100 and 50 mm meshes only.

Table 11. Distance in meters from the external gauges to the explosion center.

Gauge	1	2	3	4	5	6	7	8	9
Model 6	3,000	3,700	4,400	-	-	-	-	-	-
Model 7	2,009	3,015	4,020	4,200	6,200	8,200	10,200	12,200	14,200

Note: the distances from gauges 4 to 9 refer to the horizontal components for model 7. The explosion point is below ground level.

4.4 Numerical models validation

Figures 10, 11, and 12 present the overpressure results for gauges 1, 2, and 3 of all models. It is possible to observe a good convergence between the numerical and semi-empirical results.

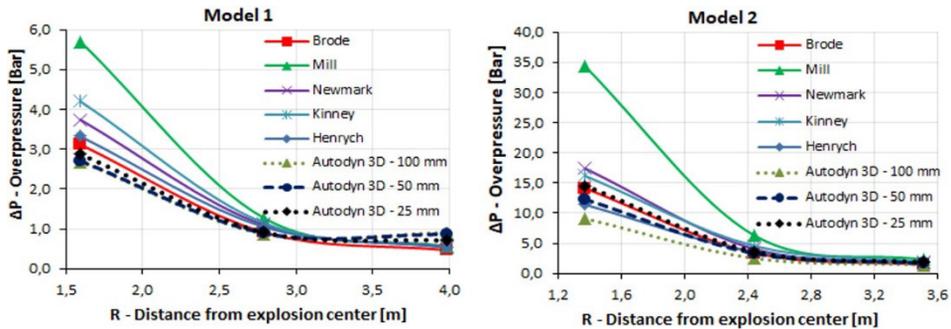


Figure 10. Overpressure peaks on gauges 1, 2, and 3 for models 1 and 2.

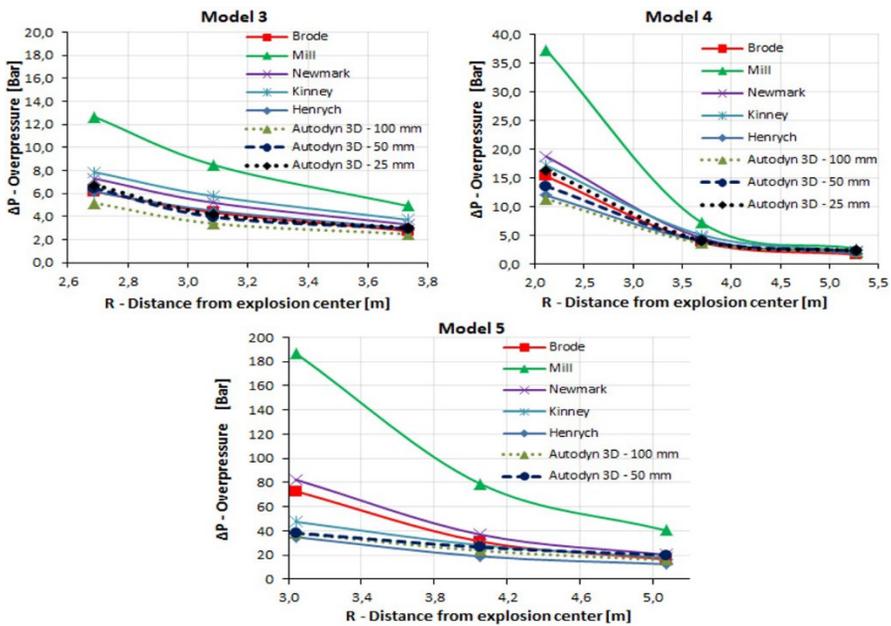


Figure 11. Overpressure peaks in gauges 1, 2, and 3 for models 3 to 5.

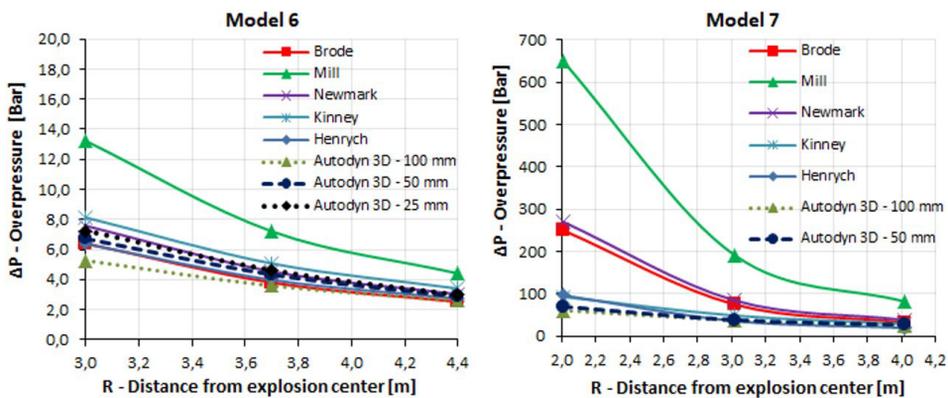


Figure 12. Overpressure peaks in gauges 1, 2, and 3 for models 6 and 7.

5 RESULTS AND DISCUSSIONS

Figures 13, 14, and 15 presents the overpressure results of all models. It is possible to see that more refined mesh tends to show higher overpressure values, this can be related with the more accurate interaction of the shock wave reflections.

The aboveground tank explosion simulation results showed that peak overpressure decreases as the explosion distance increases.

It is possible to notice the effect of the shock wave reflection in gauge 5 when comparing models 1 and 2. In quantitative terms, considering the models 1 and 2 of 25 mm mesh size, the overpressure increased 87,6% at gauge 5.

The channeling effect caused by shock wave confinement was noticed in models 3, 4, and 5, which can be identified by the overpressure levels in gauge D.

Considering the underground tank explosion, the results showed a substantial reduction in overpressure levels when compared to aboveground tanks. In model 6, for example, which is based on an underground tank, the overpressure peaks of most gauges are lower than the measured values of the model 3 aboveground tank, which has a smaller volume.

When comparing models 5 and 7, it is clear that the underground tank model showed many advantages in terms of safety over the stationary open-air models.

Considering the damage assessment, it is clear that all accidental explosions simulated in this paper may represent some risk level for both the building and its users. These risks can be identified by correlating the simulation results with the parameters of Tables 2 and 3. It was noted that there is no risk of death in the indoor environments of all analyzed models; however, several injuries can occur, such as eardrum rupture and lung damage.

The observed overpressure levels can result in glass breakage, brick wall failure, and even possible minor damage to structural components.

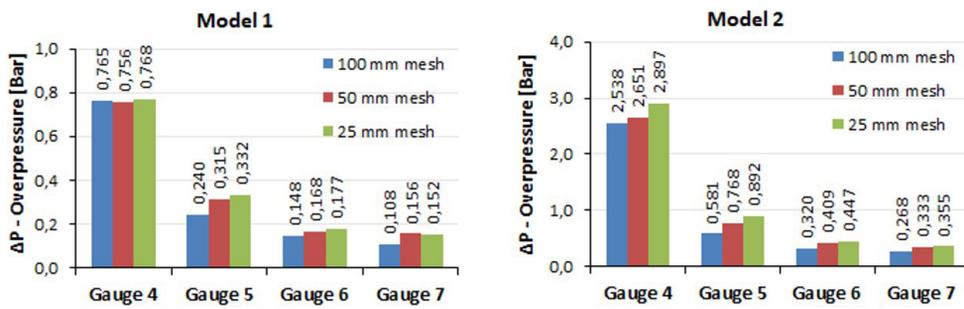


Figure 13. Overpressure peaks in gauges 4 to 7 of models 1 and 2 (explosions of aboveground tanks with volumes of 0,5 m³ and 2,0 m³).

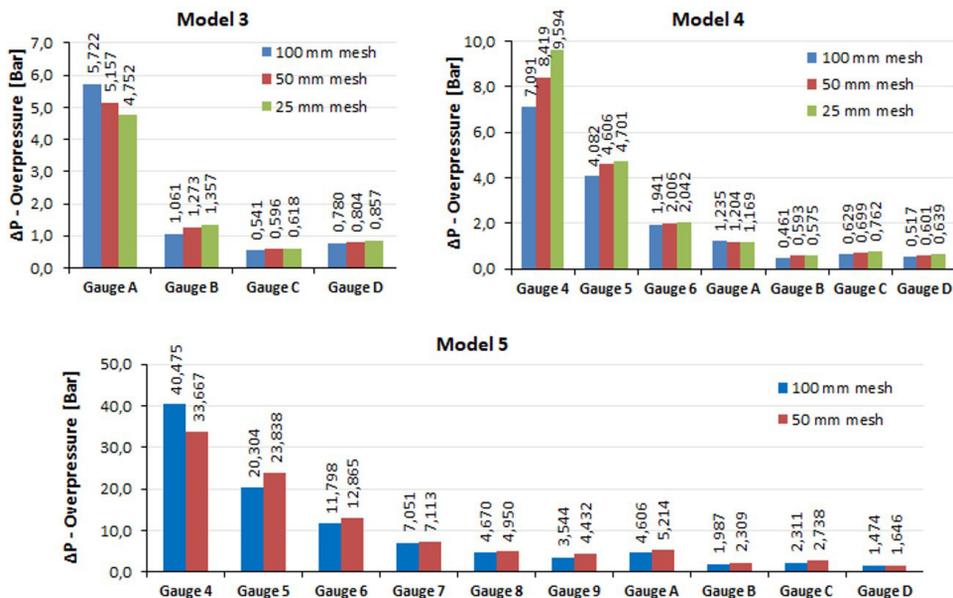


Figure 14. Overpressure peaks in gauges of models 3, 4, and 5 (explosions of aboveground tanks with volumes of 5,5 m³, 8,0 m³, and 120 m³).

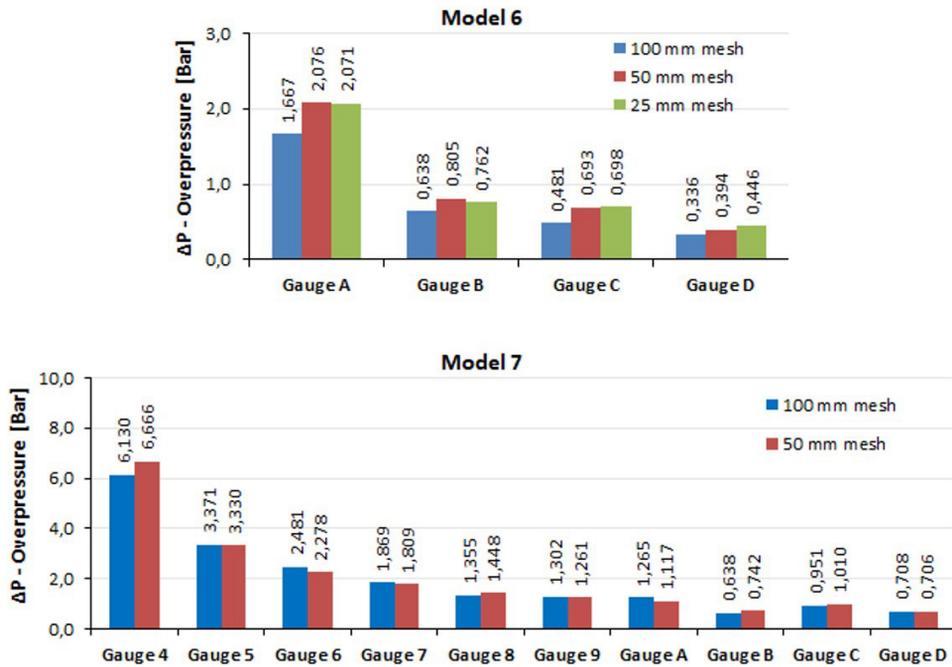


Figure 15. Overpressure peaks in the indicated gauges of models 6 and 7 (explosions from underground tanks with volumes of 8,0 m³ and 120 m³).

6 CONCLUSION

In this work, numerical simulations were performed with TNT-equivalent mass to represent the propane tanks explosion.

It was observed in the numerical simulations that there is an overpressure increase in models with refined meshes, this can be related with the more precise interaction of the shock wave with solid surfaces that leads to a more accurate shock wave reflection modeling.

The results also showed that the shock wave reflection and channeling phenomena directly influenced the overpressure results. Reflection phenomenon occurred mainly in the building internal environments and its effects were more evident in the corners. Shock wave channeling occurred in the models with narrow corridors.

The underground tanks simulations results showed a different shock wave behavior around the explosion. In this case, there is predominantly a redistribution of the blast energy through the medium since the dispersions by the tank sides tend to be contained by the ditch and redirected upwards. Therefore, the energy that reaches the building represents a small portion of what was released by the explosion. It is possible to conclude that underground tanks represent a very efficient technique to mitigate the accidental explosion effects, which justifies its use in urban environments.

Numerical simulations validated by experimental data can be a useful tool to provide a reliable data about the overpressure distributions in close range standoffs that can aid building designers to a safer placement of gas tanks considering distances from buildings and pedestrian walkways.

REFERENCES

- [1] G. F. Kinney and K. J. Graham, *Explosive Shocks in Air*, 2nd ed. New York: Springer Science+Business Media, 1985.
- [2] Y. B. Zel'dovich and Y. P. Raizer, *Physics of Shock Waves and High-Temperature Hydrodynamic Phenomena*. New York: Academic Press, 1966.
- [3] C. E. Needham, *Blast Waves*, 2nd ed. Berlin: Springer, 2010.
- [4] E. Salzano, B. Picozzi, S. Vaccaro, and P. Ciambelli, "Hazard of pressurized tanks involved in fires," *Ind. Eng. Chem. Res.*, vol. 42, no. 8, pp. 1804–1812, 2003, <http://dx.doi.org/10.1021/ie020606r>.
- [5] G. K. Schleyer, "Predicting the effects of blast loading arising from a pressure vessel failure: a review," *Proc. Inst. Mech. Eng., E J. Process Mech. Eng.*, vol. 218, no. 4, pp. 181–190, 2004, <http://dx.doi.org/10.1243/0954408042466936>.
- [6] E. G. Ferradás, F. D. Alonso, J. F. S. Pérez, M. D. Miñarro, A. M. Aznar, and J. R. Gimeno, "Consequence analysis to buildings from bursting cylindrical vessels," *Process Saf. Prog.*, vol. 28, no. 2, pp. 179–189, Jun 2009, <http://dx.doi.org/10.1002/prs.10311>.

- [7] J. D. Li and H. Hao, "Investigation of safety distance effect on gas storage tanks subjected to vapor cloud fast deflagration by using flacs," in *EASEC16 (Lecture Notes in Civil Engineering 101)*, C. M. Wang, V. Dao and S. Kitipornchai, Eds., Singapore: Springer Nature Singapore Pte Ltd., 2021, pp. 667–676.
- [8] S. S. V. Vianna and R. S. Cant, "Modified porosity approach and laminar flamelet modelling for advanced simulation of accidental explosions," *J. Loss Prev. Process Ind.*, vol. 23, no. 1, pp. 3–14, Jan 2010, <http://dx.doi.org/10.1016/j.jlp.2009.08.002>.
- [9] T. D. Ferreira and S. S. V. Vianna, "The Gilbert Johnson Keerthi distance algorithm coupled with computational fluid dynamics applied to gas explosion simulation," *Process Saf. Environ. Prot.*, vol. 130, pp. 209–220, Oct 2019, <http://dx.doi.org/10.1016/j.psep.2019.08.010>.
- [10] T. D. Ferreira and S. S. V. Vianna, "Collision of convex objects for calculation of porous mesh in gas explosion simulation," *J. Loss Prev. Process Ind.*, vol. 69, pp. 104347, Mar 2021, <http://dx.doi.org/10.1016/j.jlp.2020.104347>.
- [11] T. L. S. Quaresma, T. D. Ferreira, and S. S. V. Vianna, "A hybrid BML-fractal approach for the mean reaction rate modelling of accidental gas explosions in partially confined obstructed geometries," *Process Saf. Environ. Prot.*, vol. 152, pp. 414–426, Aug 2021, <http://dx.doi.org/10.1016/j.psep.2021.06.008>.
- [12] T. D. Ferreira, S. S. V. Vianna, and R. G. Santos, "PFS - Porosity Flow Solver: an alternative computational tool for complex flow modelling," in *An. Cong. Bras. Eng. Quím.*, Fortaleza, 2016.
- [13] M. R. Cain, *Pressure Vessel Burst Test Study*. Titusville, 1996. [Online]. Available: <https://apps.dtic.mil/sti/pdfs/ADA322032.pdf>
- [14] V. Molkov and S. Kashkarov, "Blast wave from a high-pressure gas tank rupture in a fire: Stand-alone and under-vehicle hydrogen tanks," *Int. J. Hydrogen Energy*, vol. 40, no. 36, pp. 12581–12603, 2015, <http://dx.doi.org/10.1016/j.ijhydene.2015.07.001>.
- [15] D. Wang, X. Qian, M. Yuan, T. Ji, W. Xu, and S. Liu, "Numerical simulation analysis of explosion process and destructive effect by gas explosion accident in buildings," *J. Loss Prev. Process Ind.*, vol. 49, pp. 215–227, 2017, <http://dx.doi.org/10.1016/j.jlp.2017.07.002>.
- [16] Z. Li, J. Wu, M. Liu, Y. Li, and Q. Ma, "Numerical analysis of the characteristics of gas explosion process in natural gas compartment of utility tunnel using FLACS," *Sustainability*, vol. 12, no. 1, pp. 153, 2019, <http://dx.doi.org/10.3390/su12010153>.
- [17] K. Cen, B. Song, R. Shen, Y. Zhang, W. Yu, and Q. Wang, "Dynamic characteristics of gas explosion and its mitigation measures inside residential buildings," *Math. Probl. Eng.*, vol. 2019, pp. 1–15, 2019, <http://dx.doi.org/10.1155/2019/2068958>.
- [18] L. Pang, Q. Hu, M. Jin, and K. Yang, "Effect of congestion on flow field of vented natural gas explosion in a kitchen," *Adv. Civ. Eng.*, vol. 2021, pp. 1–22, 2021, <http://dx.doi.org/10.1155/2021/6671875>.
- [19] M. L. Costa No. and G. N. Doz, "Study of blast wave overpressures using the computational fluid dynamics," *Rev. IBRACON Estrut. Mater.*, vol. 10, no. 3, pp. 669–686, Jun. 2017, <http://dx.doi.org/10.1590/s1983-41952017000300007>.
- [20] E. Vyazmina, S. Jallais, A. Beccantini, and S. Trélat, "Protective walls against effects of vapor cloud fast deflagration: CFD recommendations for design," *Process Saf. Prog.*, vol. 37, no. 1, pp. 56–66, 2018, <http://dx.doi.org/10.1002/prs.11930>.
- [21] J. Stawczyk, "Experimental evaluation of LPG tank explosion hazards," *J. Hazard. Mater.*, vol. 96, no. 2–3, pp. 189–200, 2003, [http://dx.doi.org/10.1016/S0304-3894\(02\)00198-X](http://dx.doi.org/10.1016/S0304-3894(02)00198-X).
- [22] R. Tschirschwitz et al., "Mobile gas cylinders in fire: consequences in case of failure," *Fire Saf. J.*, vol. 91, pp. 989–996, 2017, <http://dx.doi.org/10.1016/j.firesaf.2017.05.006>.
- [23] E. R. Vaidogas, "Predicting the ejection velocities of fragments from explosions cylindrical pressure vessels: uncertainty and sensitivity analysis," *J. Loss Prev. Process Ind.*, vol. 71, pp. 104450, 2021, <http://dx.doi.org/10.1016/j.jlp.2021.104450>.
- [24] C. Y. Tham, "Numerical simulation on the interaction of blast waves with a series of aluminum cylinders at near-field," *Int. J. Impact Eng.*, vol. 36, no. 1, pp. 122–131, Jan 2009, <http://dx.doi.org/10.1016/j.ijimpeng.2007.12.011>.
- [25] Y. A. Çengel and M. A. Boles, *Thermodynamics: An Engineering Approach*, 8th ed. New York: McGraw-Hill, 2014.
- [26] Center for Chemical Process Safety, *Guidelines for Vapor Cloud, Explosion, Pressure Vessel Burst, BLEVE and Flash Fire Hazards*, 2nd ed. New York: Wiley, 2010.
- [27] I. Sochet, "Blast effects of external explosions," in *Proc. Eighth Int. Symp. Hazards, Prev. Mitig. Ind. Explos.*, Yokohama, Japan, 2010.
- [28] D. A. Crowl and J. F. Louvar, *Chemical Process Safety: Fundamentals with Applications*, 4th ed. New Jersey: Pearson Prentice Hall, 2020.
- [29] K. B. Lopes and P. F. F. F. Melo, "Analysis of the effects of explosion of a hydrogen cylinder on the transfer of radioactive liquid wastes at nuclear power stations," in *Proc. 2011 Int. Nucl. Atl. Conf. – INAC 2011*, 2011.
- [30] E. López, R. Rengel, G. W. Mair, and F. Isorna, "Analysis of high-pressure hydrogen and natural gas cylinders explosions through TNT equivalent method," *V Iber. Symp. Hydrog. Fuel Cells Adv. Batter.*, 2015, <http://dx.doi.org/10.13140/RG.2.1.2336.8401>.
- [31] A. Bolonkin, "Cumulative thermonuclear inertial reactor," *Energy Sustain. Soc.*, vol. 6, no. 1, pp. 8, 2016, <http://dx.doi.org/10.1186/s13705-016-0074-z>.
- [32] I. Cernak, "Animal models for concussion: molecular and cognitive assessment - relevance to sport and military concussions," in *Brain Neurotrauma*, 1st ed., F. H. Kobeissy, Ed., Gainesville: CRC Press, 2015, pp. 674–687.
- [33] M. L. Costa No. and G. N. Doz, "Estudo numérico das pressões de onda de choque em diferentes meios e sua transmissão," *Rev. Sul-americana Eng. Estrut.*, vol. 14, no. 2, pp. 55–76, 2017, <http://dx.doi.org/10.5335/rsae.v14i2.7219>.

- [34] W. C. L. Silva, "Blast – efeitos da onda de choque no ser humano e nas estruturas," M.S. thesis, Ins. Tecnol. Aeronaut., São José dos Campos, 2007.
- [35] W. E. Baker, P. A. Cox, P. S. Westine, J. J. Kulesz, and R. A. Strehlow, *Explosion Hazards and Evaluation*. Amsterdam: Elsevier Science, 1983.
- [36] Associação Brasileira de Normas Técnicas, *Liquefied Petroleum Gas Central Storage – LPG*, ABNT NBR 13523, 2019.
- [37] F. P. Lees, *Loss Prevention in the Process Industries: Hazard Identification, Assessment and Control*, 2nd ed. Oxford: Butterworth-Heinemann, 1996.
- [38] B. Luccioni, D. Ambrosini, and R. Danesi, "Blast load assessment using hydrocodes," *Eng. Struct.*, vol. 28, no. 12, pp. 1736–1744, Oct 2006, <http://dx.doi.org/10.1016/j.engstruct.2006.02.016>.
- [39] J. Zimbelmann and C. Boley, "Underground explosions: Estimating the safe distance," *Geotech. Res.*, vol. 3, no. 3, pp. 67–89, 2016, <http://dx.doi.org/10.1680/jgere.16.00005>.

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