

# Risk Analysis of Pressurized Gas Release

Ibrahim A. Altuwair

*Faculty of Chemical Engineering, Northern Border University, Arar, Saudi Arabia.*

*Email: Ibrahim.Altuwair@nbu.edu.sa*

## Abstract

The study addressed one of the knowledge gaps in compressed gas safety, i.e., a predictive model to analyze explosive failure of natural gas (CNG) cylinder. The predictive model is a numerical model tested using experimental data. It accounts for the real gas effects, physical energy and combustion of the flammable gas. One of the concerns comes from pressurized gas cylinder is energy associated with compression. An unintentional rupture of a compressed cylinder filled with the natural gas would generate a rapid energy release in the form of the pressure energy. The result of release energy causes rapid mixing of released gas. The rapid mixing while may generate high overpressure, it may also cause flash fire. These effects are numerically simulated and validated using experimental data. This study identifies critical points for safer operation of complex CNG systems.

**Keywords:** compress, safety, cylinder, predictive, approach, model, energy, experiment, mechanical, rupture.

## Introduction

The use of alternative energies as fuel (i.e., hydrogen H<sub>2</sub>, liquefied petroleum gas LPG, and CNG) has become a controversial topic due to the safety issues associated with overpressure applications. According to the world statistics summary tabulated in table 1, there are more than twenty million natural gas vehicles NGVs on the roads worldwide. Given that the environmental and economic benefits attracted many industries to invest in it, and perform in more challenging environments, with higher energy densities and power efficiencies over longer lifetimes. These requirements are placing more pressures on these industries. However, most of the natural gas cars stored the fuel in a high-pressurized condition. Compared with vehicles used hydrogen as fuel, CNG has narrower flammability range, higher ignition energy, and lower burning rate. These

unique properties of CNG raise safety concerns and pose an essential question if whether the CNG cars are safe or not. The purpose of the study is to limit hazards associated with overpressure applications by adopting a safe approach. The following key aspects are addressed:

1. Developing methods to predict accidents using appropriate modeling techniques.
2. Developing an approach to evaluate the effects of resultant blast wave pressure versus the magnitude of the accident (consequence criteria).
3. Propose an alternative model for blast wave pressure .
4. Establishment of acceptable level (threshold value) for overpressure applications.

Therefore, considering the increased risk generated by overpressure, as previously described by prior literature, it is vital to develop a strategy to stop or mitigate an accident. The hazard approach found in this study given in figure 1.

### Compressed natural gas hazards

Alternative fuels including compressed natural gas (CNG), and hydrogen (H<sub>2</sub>) raises the controversial safety issues that require to discuss thoroughly. A blast wave is one of the problems that need to be measured when a high-pressure gas cylinder failed, in any fire or non-related fire accident occurred. Safety engineering for compressed gases is a new discipline underpinning the technological safety of emerging high-pressure systems and infrastructure. It encompasses previously acquired, and new knowledge generated by the international gas safety community published elsewhere [1]. The protection barrier is an ultimate mitigation measure against hazards and associated risks during an accident that involves, in particular, compressed natural gas storage. One of the technical features that make CNG systems different from others is very high-pressure storage up to 20-30 MPa. However, the

complexity to complete prediction and control of compressible gases is one of the scientist's challenges that may result in knowledge limitation. However, investigating the performance of such a CNG cylinder under different circumstances and configurations can be obtained by studying the underlying physico-chemical behavior model of CNG. Using that to design and optimize the CNG cylinder, fluid flow simulated concerning safety. CNG made of (CH<sub>4</sub>, C<sub>3</sub>H<sub>8</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>4</sub>H<sub>10</sub>, CO<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>S, N<sub>2</sub>, He, Ne, Xe), recommended by CCPS 2000. Regardless of the benefits of CNG [2], the safety concern of overpressure cylinder CNG considered as a problem. As a result of CNG operation, about 90% of emission reduction [3], also, noted that the potential for water pollution occurred with fossil fuels is at minimal [4]. The efficiency of any fuel indicated by its octane number; thus, CNG has a higher octane number ranged between (120- 130) [5].

### Worldwide NGV Statistics

<b>Natural Gas Vehicles:</b>	<b>27,414,984</b>
<b>Natural Gas Fueling Stations:</b>	<b>32,211</b>

### Regional Growth

	<b>NGVs</b>	<b>Stations</b>
ASIA-PACIFIC	19,766,181	19,492
EUROPE	2,005,744	5,060
NORTH AMERICA	224,500	1,857
LATIN AMERICA	5,150,210	5,592
AFRICA	268,349	210

Table 1: 'NGVs' is all land-based motor vehicles [1] April 2019

This paper tries to assess the safety and therefore,

reveal how the properties (pressure, velocity,

temperature, etc.) of compressed natural gas affect the risk, which results in overall consequence differences in a compressed natural gas vehicle in terms of hazard effect (dispersion energy) and accident consequences in typical accident events.

### **Past studies of accident modeling**

CNG fuel is stored onboard at high pressures. However, all vehicular high-pressure gaseous storage systems are required to be equipped with a safety device known as a thermally-activated pressure relief device (TPRD). For instance, when the temperature reading is more than 110 centigrade, the TPRD activated, and the contents of the storage will be released rapidly. This safety device significantly reduces the risk of the catastrophic ruptured vessel by venting the excess pressure outside. However, the released flammable gas could raise additional safety problems if it ignited. Therefore, the combustible gas release from TPRD can be considered as a typical incident example causing gas released. Then gas can be ignited immediately in the fire environment and causes jet fire impinging on the ground and spreading flame outwards. However, the lower flammability limit and combustion temperature are one of the CNG advantageous properties. Such as the light property of CNG in the air helps to reduce risks. However, high-pressurized condition and heavy weight of the CNG cylinder become a source of hazard [6]. The CNG cylinder storage parameters are selected, and details of parameters shown in Table 1. There is number of studies discussed the influence of overpressure. Janovsky [7] modeled pressure effects during the accidental explosion of gas. Olvera [8] analyzed the impact of buildings on gas diffusion for hydrogen using a fluid model, and as a result, the hazard of indoor gas release was more severe than that of indoor CNG release. Middha [9] carried out a CFD simulation study to

investigate the risk from hydrogen vehicles while Houf and his colleagues carried out CFD simulation on the gas release [10]. However, modeling gas flow considered one of a challenge in the field of simulation. Thus, there is no general flow model for all fluid flow situations. In traditional fluid flow modeling, all variables separate into mean values and fluid flow fluctuations. However, the influence of fluid flow on the CNG cylinder has not been systematically discussed. In the current study, a simulation study aims to investigate the influence of flow acceleration inside a CNG cylinder on the pressure drop. An early description of blast wave events given by Brinkley and Lewis [11], who also describe Karlovitz's theory [12]. The occurrence of overpressure blast most likely influenced by fluid flows.

Furthermore, this was experimentally studied by several scholars as Oppenheim and Urtiew [13]. Lee and Moen who have given useful reviews of mechanisms of the effects flow on overpressure explosion events [14]. Also, Lewis and Von Elbe published their investigations of explosion mechanisms and the speed of fluid [15]. Furthermore, Kuo studied the principle of combustion [16], and different mechanisms of the blast investigated, each including the fluid flow and formation of shocks [17] given an explanation of the explosion due to the velocity of the shock wave. Cheng et al. [18] investigate the propagation process of the methane explosion. Using the theoretical calculation, numerical simulation and physical experiments, obtaining the initial blasting stress, displacement, and overpressure of the fluid blast are much better than that of ordinary blasting. Furthermore, the probit analysis is a method of analyzing the dose-effect relation, thermal radiation, and overpressure, however, can also be a useful analysis method to determine equipment damages subjected to blast wave [19, 31]. It is

studied and confirmed by many researchers [20, 23, and 31]. Eisenberg [23] presented a model based on experimental analysis of storage tank deformation, restricted by rigid walls. Then, the probability of failure derived from the cumulative expression for a normal Gaussian probability distribution [20]. Also, Khan and Abbasi [32], who proposed a probit function similar to the Eisenberg expression, and gave the same probit constants of Eisenberg model [23]. Thus, the model proposed by Eisenberg has been used in this study.

**Hazard Assessment**

In the framework of the study, particularly hazard assessment, for the overpressure storage damage applied. In the following expression model, the calculation of damage obtained in terms of Probit

Equation (PE). It is given in probit analysis [20], it is one of the major analysis application of the method to hazard assessment in the process industries has been performed by Eisenberg 1975. It is another way for expressing the probability P of damage. It is given in the following equation:

$$The\ distribution\ function\ (df) = \int_{-\infty}^x F(x) dx \quad 1.0$$

Then, the probability P of damage, therefore, obtained as:

$$P = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{Y-5} e^{-\frac{u^2}{2}} du \quad 1.1$$

Similarly, for log-normal distribution

$$Y = a + b \ln x, \quad 1.2$$

%	0	1	2	3	4	5	6	7	8	9
0	-	2.67	2.95	3.12	3.25	3.36	3.45	3.52	3.59	3.66
10	3.72	3.77	3.82	3.87	3.92	3.96	4.01	4.05	4.08	4.12
20	4.16	4.19	4.23	4.26	4.29	4.33	4.36	4.39	4.42	4.45
30	4.48	4.5	4.53	4.56	4.59	4.61	4.64	4.67	4.69	4.72
40	4.75	4.77	4.8	4.82	4.85	4.87	4.9	4.92	4.95	4.97
50	5	5.03	5.05	5.08	5.1	5.13	5.15	5.18	5.2	5.23
60	5.25	5.28	5.31	5.33	5.36	5.39	5.41	5.44	5.47	5.5
70	5.52	5.55	5.58	5.61	5.64	5.67	5.71	5.74	5.77	5.81
80	5.84	5.88	5.92	5.95	5.99	6.04	6.08	6.13	6.18	6.23
90	6.28	6.34	6.41	6.48	6.55	6.64	6.75	6.88	7.05	7.33
-	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
99	7.33	7.37	7.41	7.46	7.51	7.58	7.65	7.75	7.88	8.09

Table 2: Transformation of Percentages to Probit, Ref. Source, ref.[20]

The probit is a random variable with a mean of 5 and variable 1. The probability replaced in probit work by a range of (0 to 100 %) is tabulated in Table 2 [20]. The author defined the probability function as (Y) called “Probit Function” to create a relationship between (E) represents equipment damage and (P<sub>o</sub>) represents the maximum pressure. (Y) represents probit function; (P<sub>o</sub>)

represents peak pressure, P<sub>a</sub>, a and b are constants (i.e. 23.8 and -2.92) [23]. It is an alternative way of expressing the probability P of damage. Also, the estimation of damage can be measured by Eisenberg expression as:

$$P_0(Pr) = e^{(Pr-a)/b}, \quad 1.3$$

Thus, knowing the characteristics of the blasting wave helps to illustrate a relationship between the overpressure and damage probabilities. The data given in following table 3 based on transformation percentage to probit tabulated in table 2. The data shows a proportional relationship between the probability and overpressure. There are a sudden pressure increase at the range of the points (0.4,17) and (0.9,29.8) Table 3.

Probability of failure	$P_r$	$P_0$ (MPa)
0.05	3.36	10.9
0.4	4.75	17.6
0.9	6.28	29.8

Table 3: The shock wave and the damage probability

Furthermore, thesis research [20] described the fluctuation of flow as a significant contributor to flow acceleration and increase the flow surface. Knut [20], however, mathematically determined the influence of the fluid flow on reaction rates. Gas flow may deform the surface area resulting in which a series of explosion occurs [21]. Also,

the mechanism study of Zeldovich explained the influence of the fluid flow and induction time. He mentioned, in most cases, the intrinsic mechanism triggering a detonation is the explosion of a non-uniformly preconditioned region of fuel in which a spatial gradient of induction time has been created by fluid flow, shock heating, or both [22]. Wagner and coworkers [24] have studied the mesh size by developing experiments in which deflagrations were passing through screens of specified mesh sizes. Some analysts suggested that to create turbulence of the required scale and intensity; a deflagration could make the transition to detonation. Therefore, the importance of fluid flow inside CNG cylinder and controlling the internal energy may become an essential factor and key for advanced fueling systems. An alternative model presented by Pitblado [35], defining the separation distance but the probability of failure showed some uncertainties. In the current study, we try to adopt a hazard method to get guidance for safe CNG cylinder design, figure 1. Also, simulation design approach using highly computational simulation, COMSOL.

$\Delta P^*$ (kPa)	Damage	Reference	$\Delta P^*$ (kPa)	Damage	Reference
37.42	Catastrophic failure, pipe supports	[34]	14.00	Minor damage of the atmospheric tank	[40]
18.70	Minor damage, floating roof tank, cracking(50% filled)		20.00	Deformation of atmospheric tank	
5.17	Minor damage, cone roof tank		25.00	Atmospheric tank destruction	
25.30	Minor damage, reactor chemical		38.00	Deform of non-pressure equipment	
22.10	Catastrophic failure, cooling tower		42.00	Pressure vessel deformation	
39.12	Minor damage, pressure vessel horizontal		53.00	Pressure vessel failure	
42.51	Catastrophic failure, cone		70.00	Failure of spherical pressure vessel	
61.22			95.30		
81.63			108.90		
88.44					
108.84					
136.05					

	roof tank (100% filled) Catastrophic failure, pressure vessel horizontal Minor damage, pressure vessel vertical Catastrophic failure, pressure vessel vertical Catastrophic failure, tank sphere Catastrophic failure, floating roof tank (100% filled)			Deformation of steel structures 99% structural damage of vertical, steel pressure vessel 99% structural damage of spherical, pressure steel vessel	
35.50	Structural damage of equipment	[35]	17.00 29.00	Minor damage, tower Distillation tower and cylindrical steel vertical structure	[41]
6.10 20.40 34.00	1% structural damage to equipment 50% structural damage to equipment 99% structural damage to equipment	[23]	20.00 27.00	Displacement of steel supports Failure of the steel vessel	[42]
10.00 20.00 10.00	5% damage of process plant 100% damage, Atmospheric Tank 50% damage of tank	[39]	39.00 136.00	Structural damage to pressure vessel Structural damage, low pressure vessel	[43]
9.90	Failure of equipment	[37]	70.00	Structural damage of equipment	[36]
10.00 30.00	Failure of atmosphere equipment Failure of pressure vessel	[38]	39.00 136.00	Structural damage to pressure vessel Structural damage, low pressure vessel	[43]
7.00	Failure of connection	[44]			

Table 4: Data reported in the literature for damage caused by overpressure (kPa) Damage Reference.

### The Methodology of the Study

Figure 1, illustrates the study framework in several steps, this approach for implementation of the risk model. In this study, as a central part. The first step, it aims to identify the hazard related to

the system for fire-related or non-fire related to the internal pressure elevated inside a CNG cylinder. The identification of hazards relevant to the accident scenario with overpressure vessel in a fire. Those were identified based on prior studies as physical (overpressure) and thermal

(fire) effects.

The second step is to determine the consequence of CNG cylinder failure or rupture by presenting the research method compared with experimental and theoretical modeling schemes. In the consequence analysis, an alternative model adopted [33] for non-related fire. The prior selected model designed based on a baker method. It allows the estimation of hazard distances in which the pressure and thermal effects cause death, serious and slight injuries from fire and explosion calculated by best fit-engineering model. The earlier models mentioned, including [23], were tested for estimation of initiating event (overpressure) frequency, and calculation of the probability failure resulting in tank rupture. However, the

limitation of physical parameters may be a source of error in many of those models. In this study, an appropriate technical method used (i.e., event tree). The estimation of the effect of pressure on the surface of the CNG cylinder using cost-effective model COMSOL. The analyses take into account the correlations between evolutionary parameters at high-pressure assuming that the system is a single phase thermodynamically closed. Finally, therefore, risk can be obtained as a function of the tank rupture probability. The study provides a systematic engineering model to identify the effect of the blast wave. It is based on pressure and potential energy. More details of the study approach given in the following sections.

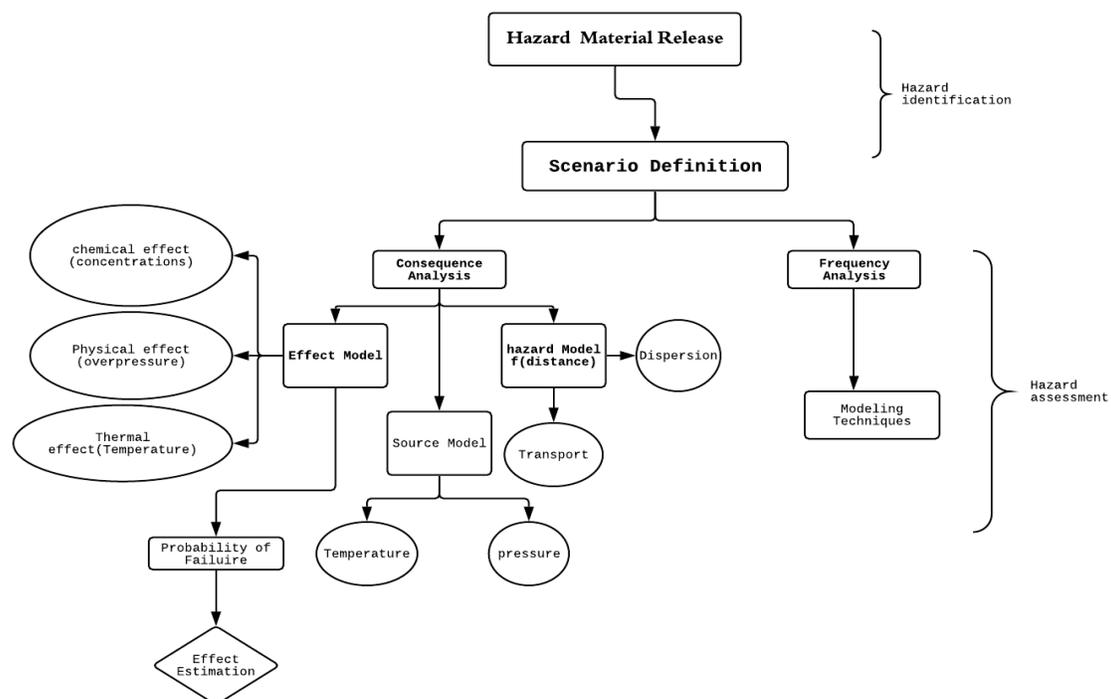


Figure 1: Hazard Assessment of Compressed gas on-Board Vehicle

The proposed methods for calculating stored energy of ideal gas presented theoretically and

experimentally. Arrhenius model is well-known equation used [21] to determine the thermal

explosion while physical strength [19] obtained using empirical methods as Brode model, Baker model, and kinetic energy model which are recommended by the center of Chemical Process Safety (CCPS) (1994/15). Also, a model studied by Eisenberg [23] was used and observed by many scholars.

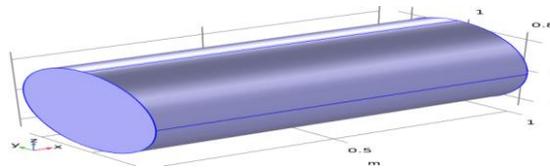
A numerical simulation approach performed as a result of a fully wrapped aluminum [solid, bulk] composite cylinder. The cylinder filled with CH<sub>4</sub> (2500-3000 psi) with a single-phase fluid in 3D Cartesian coordinates (spatial). The CNG cylinder assembly as specified in global technical regulation (GTR) on fuel vehicle consists of the compressed storage system and material specification. Furthermore, the geometry and domain of the cylinder illustrated Plot 1. It describes the mesh designed on the cylinder along the geometric of cylinder maximum element 0.0795, minimum element size 4.5E-04, and maximum element rate. The flow reaches its maximum with an increase in velocity possibly

occurring near the wall Plot 2.

Description	Value
Maximum element size	0.0795
Minimum element size	4.5E-04
Curvature factor	0.3
Predefined size	Fine
Minimum element quality	0.8661
Average elements	0.964
Triangular elements	264
Width (m)	1.5
Height (m)	0.4

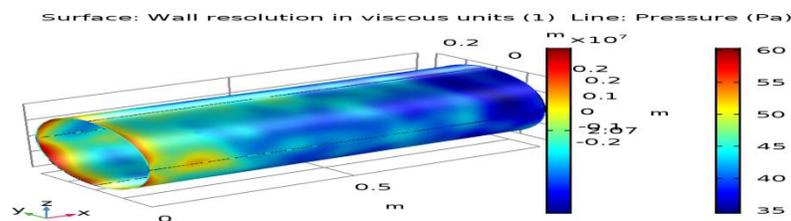
Table 5: Geometry statistics of CNG cylinder

However, the capture of all physical features, such as shock waves is a challenge. The aim of numerical study of CNG onboard is to broaden knowledge of compressible gas flow in non-uniform regions with emphasis on the development of shock waves. We plan to use COMSOL to design overpressure (CNG) cylinder rupture.



Plot 1: The 3-D CNG cylinder

The simulation results show the effects on the wall cylinder filled out with CNG Plot 2.



Plot 2: The result of the simulation study for CNG Cylinder

In the simulation, plot 2 illustrates the characterization of the impact of the mechanical energy on the CNG demonstrated, and the

probability of failure as a function of internal pressure can be provided by equation 1.3.

The hazard of Thermal and Physical Energy

The hazard has been theoretically and experimentally determined includes physical energy. Molkov has suggested an alternative method by adding chemical energy to its model. In this study, the proposed model provided. Arrhenius equation, for instance, is one of the models that can be used to determine the effect of thermal radiation. However, in the previous methods, it is denied. However, this study, determine the effect of the thermal radiation on people and structure by adopted probability model, where  $x = (t.q^{4/3})$ , where  $t$  represents the time, and the  $q$  is the heat. A model [33] given as of mechanical energy of physical explosion written as  $(E_{\text{physical}}) = (E_{\text{thermal}}/0.052)$ . The modeling material described through structural changes due to temperature distribution, causing structure change and thermal expansion. This thermal stress contributes unstable behaviour of fluid affecting the thermodynamic states of the flow. Zel'dovich and Knut [23,21] have profoundly discussed the fire and explosion modeling and risk assessment for determining the thermal distribution from point to point between simultaneous heat release and energy transport.

He adopted a mathematical model in his final thesis for thermal evolution of gas explosion. The author believes that the thermal explosion initiated by a sudden increase in temperature results from mechanical effects (such as, compression) that trigger the temperature.

Furthermore, also discussion of the process occurring over significant different time scales. The time from the gas heated to the exothermal rate start is called the induction time [26]. Schultz and Shepherd compiled theoretical and experimental data on induction times for a large variety of gases [27]. Shen [49] proposed an engineering model based on the assumption of the energy of combustion of gas released into atmosphere added to the mechanical energy of CNG. The model created the relationship between the overpressure in blast wave and distance. Isothermal expansion model, also modeling of Kinetick Energy (MKE) used for the evaluation of the physical effects caused by fragment. Thus, the affected area and the magnitude of the consequences of the accident can be measured.

$P_1$ (Pa)	$P_a$ (Pa)	$V_g$ $= (nRT/P)$ ( $m^3$ )	$Y$	$Mc$ (kg)	$Mv$ (kg)
200E05	101.3E03	0.047	1.3	0.65	83.4

Table 6: cylinder physical parameters

Thus, the parameters obtained as tabulated in the following table 7.

Parameters	Empirical Models	Simulation Model
Velocity (m/s)	Energy model 172.28  Moore model 179.65	171.1
Energy (j)	2.281E06	2.067E06

Table 7: The outcomes of studied models, Appendix A

The changes in energy determined. However, an agreement in the results of both simulation the empirical models observed, see Table 7. It is vital to notice, however, existing methods for determining a blast wave affected by the coefficient value of the mechanical energy ( $\alpha$ ) [33]. The uncertainty of the source of energy stimulating the blast wave as it propagates outwards. Also, empirical methods in previous sections were not sufficient to obtain precise outcomes. The study tried to adopt a reliable methodology leading to accurate prediction for a physical explosion of CNG cylinder. The model proposed by Molkov [33] valid for all compressed gases and compared to data generated experimentally. Therefore, a model application, in this study, to determine the overpressure storage CNG in blast wave ( $\bar{r}_p$ ) used, as shown in equation 1.5.

$$\bar{r}_p = \sqrt[3]{r \left( \frac{P_s}{\alpha E_1 + \beta E_2} \right)} \tag{1.5}$$

$E_1$  and  $E_2$  are mechanical energy and chemical energy,  $\beta$ , and  $\alpha$  coefficients (0.09 & 0.12 respectively [33]). Molkov has mentioned that the blast wave subject to energy release rate more than on the amount of energy, therefore he added the energy of combustion of gas released into atmosphere to the mechanical energy of compressed gas [33]. In case of CNG if burns in the presence of oxygen, carbon dioxide and water produced. This process of combustion releases energy. If the energy released during a chemical reaction, an exothermic reaction produced. The combustion of CNG gas releases ( $CH_4$ -50.1 kJ/g). It is an equivalent of 802.3 kJ/mol CNG, Appendix A.

Mass of CNG	No. of mole	No. of mole (O <sub>2</sub> )	The total amount of mixture F/A
1.85kg	115.63	275.19	3.38

Table 8: The calculation results of mass, mole, and total mixture

CNG (kJ/mol) = 802.3

$v_b \frac{2}{3}\pi r_b^3 = 62.25$

CNG (m<sup>3</sup>) = 2.59

The total mechanical energy  $E_m = 5.30$  MJ, chemical energy  $E_{ch} = 92.5$  MJ,  $v_u$  =unburn volume ( $\frac{2}{3}\pi r_u^3$ ), and  $v_b$  =burned volume ( $\frac{2}{3}\pi r_b^3$ ).

No. of O<sub>2</sub> (mol) = 275.19

$v_u$  (m<sup>3</sup>) = 8.75

Application	H2	H2	H2	CNG
	<u>170 L,</u> <u>35 MPa</u>	<u>33 L,</u> <u>70 MPa</u>	<u>12 L,</u> <u>70 MPa</u>	<u>84 L, 30</u> <u>MPa</u>
P <sup>-</sup> st (-)	54	80	80	46
r <sup>-</sup> v (-)	0.069	0.058	0.058	0.0041
rv (m)	0.34	0.2	0.14	0.15
rb (m)	7.91	5.46	3.89	3.08

Table 9: Overpressure  $P^-$  as a function of distance  $r^-$

For comparison, mechanical energy coefficient  $\alpha = 0.14$  used to find out the blast wave overpressures at different ranges, the maximum pressures onboard vehicle tank test are as follows: 140 KPa at a distance 1.22 m and 80 KPa

at a distance 2.44 m. The determined value of overpressure used with the radius equivalent volume spherical vessel given in the following table.

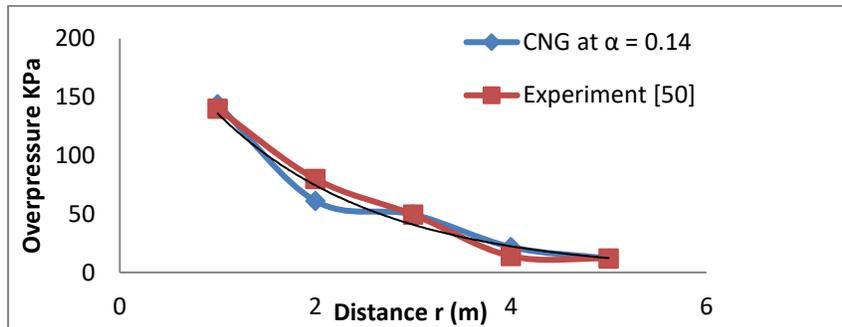


Figure 2: Experimental data and CNG pressure with  $\alpha = 0.14$

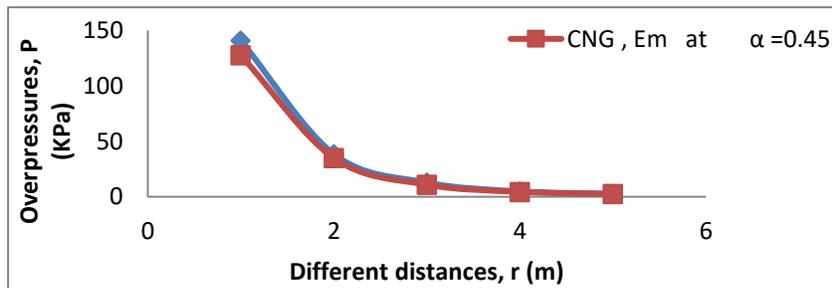


Figure 3: Experimental data on the blast wave [33] and CNG with  $\alpha = 0.45$

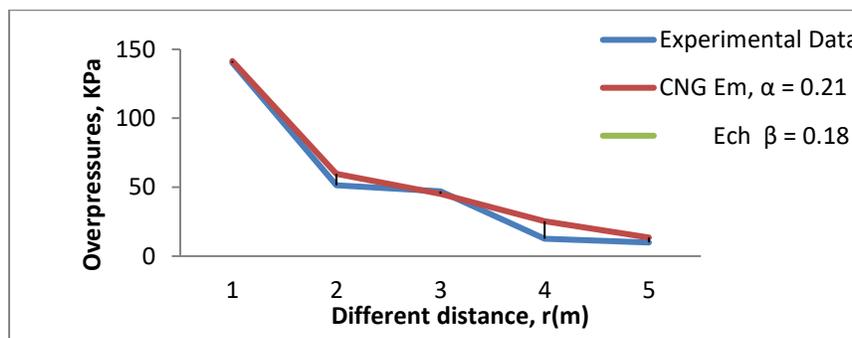


Figure 4: Experimental data on the blast wave and CNG with ( $\alpha = 0.45$  &  $\beta = 0.18$ )

Reference	Overpressure, P (kPa), at different distance r (m)				
	r=1.22	r=2.44	r=4.8 8	r=9.7 5	r=15.24
Scaling $E_m, \alpha = 0.12$ $E_{ch} \beta = 0.09$	143.9	61.2	49.65	21.8	11.96
Experiment [50],	140	56-80	30-69	14	12
[33] $E_m$ at $\alpha = 0.14$	140.84	38.5	12.77	4.86	2.68
CNG, $E_m$ at $\alpha = 1.8$	518.25	98.42	40.73	10.18	6.02
CNG, $E_m$ at $\alpha = 0.14$	127.60	34.88	10.87	4.40	2.43
CNG $E_m, \alpha = 0.19$	140.34	51.3	47.1	12.63	9.89
CNG $E_m, \alpha = 0.21$ $E_{ch} \beta = 0.18$	141.5	59.62	45.12	25.42	13.50

Table 10: Comparison of CNG model calculations and experimental data [33]

The analysis shown in figures 2, 3, and 4, observed the use of methodology of non-related fire for tank rupture which partially matches the experimental data in figure 2. The prediction of energy coefficient ( $\alpha$ ) for the designated distance to match the experimental data was defined. Molkov [33] proposed a methodology to determine the total energy. The mechanical energy with the fraction of  $\alpha = 0.45$  illustrated and

the amount of mechanical energy contributing to the blast wave estimated as  $\alpha E_m = 0.84$  MJ. The fraction stored in mechanical energy and chemical energy contribute to the blast wave can be estimated as  $\alpha E_m = 0.4$  MJ. The total amount of chemical energy strengthen the blast wave is  $\beta E_{ch} = 19.35$  MJ. For best results for both ( $\alpha = 0.21$  and  $\beta = 0.18$ ) fits the experimental data given in Table 14. Figure 4 provides the best

curve that matches the experimental results with mechanical energy coefficients of ( $\alpha=0.45$ ) and chemical energy coefficient of ( $\beta=0.21$ ).

### The Study Energy Model

Due to the limitation of previous methods and do not provide detailed information about the contribution of all elements to blast wave. However, a blastwave approach proposed. In this study, the integration of total energy of compressed gas (CNG) described as follows:

$$f(a) = \int_0^r E_t dr \quad 1.6$$

$E_t$  represents the total energy includes internal energy and kinetics energy equation 1.7. therefore,

$$E_t = \left( \frac{p}{\gamma-1} - \frac{\rho u}{2} \right) \quad 1.7$$

$\gamma$  represents the ratio of specific heats,  $p$  represents pressure,  $\rho$  represents density, and  $u$  represents the velocity. In the proposed model, the correlation between energy and pressure can be used to define the total energy. The advantage of proposed model is that it depends on the type of application. It represents essential parameters when blasting occurred.

However, it is worthy of mentioning that the temperature effect on stored energy is a source of pressurizing a CNG system due to thermal expansion and can be added to the maximum pressure. The following graph describes the threshold for the CNG cylinder corresponding to the maximum pressure during the simulation and its corresponding time (251 atm and 9-10 minutes). In case if malfunctioned, the time can be the critical factor to avoid sudden or unintentional events (i.e, a burst).

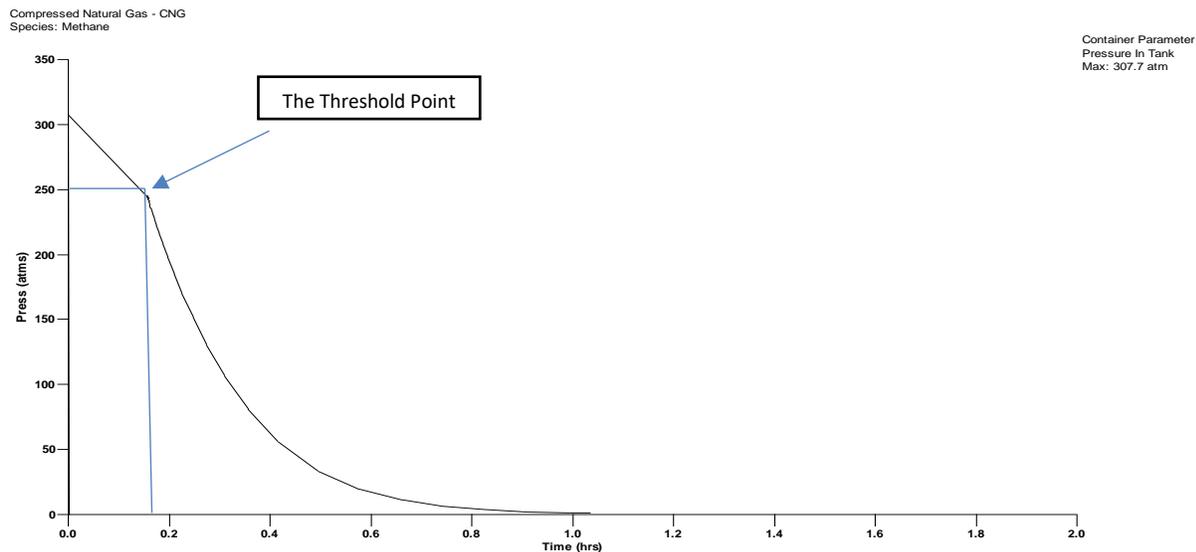


Figure 5: The simulation outcome of resistance time of the CNG cylinder

In figure 5, the prediction of the resistance time of CNG cylinder investigated. On the other hand, a steep gradient generated by compression may affect temperature gradient resulted in a hot spotty. This helps to predict failure, i.e. burst or leak of cylinder occurs. It noticed that model

gives the possible consequences and the time required for safe operation. The generated time indicated that at pressure 251 atmosphere and 0.16 hrs, a pressure fluctuation triggers sudden onset event is possible. The time and exposure curve in the following figure gives a possible

incident scenario for CNG cylinder based on the given fault tree. It showed the potential damage initiated at level 2.5 to the maximum damage

level depend on the parameters of the fuel when an accident occurred i.e., physical and chemical energies.

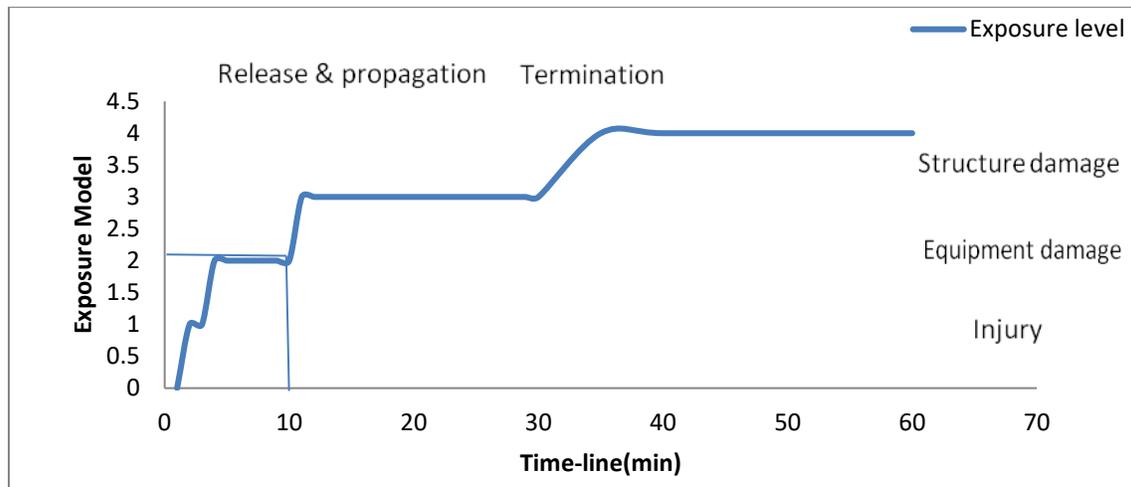
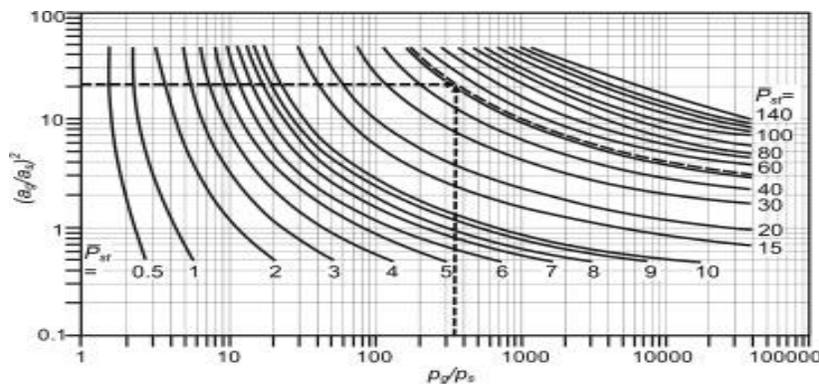


Figure 6: The outcomes of exposure model for a blasting wave of CNG cylinder

The above curve, Figure 6, developed as a result of the simulated outcome described previously in figure 5. It is important to notice that the transformation from phases to phase is changed as discrete function. The shorter time-line can be

observed at the initiated event than propagation at range (2.0-2.5) given a possible minimum equipment damage and a maximum as minimum structural damage.



Appendix A-1: Determination of overpressure by the squared ratio of the speed of sound and the the ratio of the initial pressures

Harmful effect	Overpressure, kPa	Impulse, kPa s
Threshold for skin laceration from flying glass	6.9–13.8	0.512
Threshold for serious wound from flying glass	13.8–20.7	1.024
1% eardrum rupture probability*	16.5	–
50% serious wound from flying glass	27.6–34.5	1.877
50% probability of eardrum rupture	43.5	–
Near 100% serious wound from flying glass	48.3–55.16	3.071
90% probability of eardrum rupture	84	–
1% probability of fatality due to lung haemorrhage**	100	–
50% probability of fatality due to lung haemorrhage	140	–
99% probability of fatality due to lung haemorrhage	200	–

#### Appendix A-2: Threshold of harmful pressure effects on people [50]

Element	Damage	Overpressure, kPa
Window frame	5% broken <a href="#">[20]</a>	0.69–1.0
	50% broken <a href="#">[20]</a>	1.45–2.5
	90% broken <a href="#">[20]</a>	3.7–6.0
House	Minor damage to house structures <a href="#">[20]</a> *	4.8
	Failure of doors and window frames <a href="#">[20]</a>	5.3–8.9

Element	Damage	Overpressure, kPa
	Partial demolition of the house turns inhabitable [20]**	6.9
	A partial collapse of walls and roof of the house [20]	13.8
	50% destruction of brickwork of house [20]	17.3
	Almost total destruction of the house [20]***	34.5–48.3
Other	Possible total destruction of building [20]	69
Industrial building	Break of the cladding of light industrial building [20]	27.6
Heavy steel frame industrial building, single level, low strength wall [25]	Blowing-in of windows and doors, ripping off of the light siding	7
	Distortion of the frame (minor to major)	49.2
	Severe distortion/collapse of the frame	61.5

Element	Damage	Overpressure, kPa
Reinforced concrete frame office building, 3–10 levels, low strength walls [25]	Blowing-in of doors and windows, ripping of light siding, cracking of interior partitions	7
	Moderate distortion of the frame, blow-down of interior partitions, spalling of concrete	55.4–61.5
	Severe distortion of the frame, incipient collapse	68.8–76

Appendix A-3: Threshold of harmful pressure effects on the structure [50]

Object	Criterion for separation	Deterministic separation distance, m			
		Stand-alone:	On-board:		
		10 m <sup>3</sup> , 100 MPa	170 L, 35 MPa	33 L, 70 MPa	12 L, 70 MPa
Humans	No-harm [10]	470	90	57	35
	Injury [20]	78	16	11	7.5
	Fatality [20]	23	2	1.4	1
Buildings [17]	Minor damage [20]	190	36.5	25.5	18

Object	Criterion for separation	Deterministic separation distance, m			
		Stand-alone:	On-board:		
		10 m <sup>3</sup> , 100 MPa	170 L, 35 MPa	33 L, 70 MPa	12 L, 70 MPa
	Partial demolition [20]	136	29	20.6	14.5
	Almost total destruction [20]	49	9.7	6.7	4.8
Buildings [8]	Minor damage [10]	115	–	–	–
	Major damage [10]	42	–	–	–
	Partial demolition [10]	25	–	–	–

Appendix A-4: Separation distances for selected typical compressed gas storage applications [50].

## Conclusion

Various methods for obtaining solutions for blast wave were studied however, the inapplicability of those methods defined. A solution of the compressed gas model inside a cylinder satisfying the experimental results obtained.

The primary instances those stimuli an overpressure event are exceeding the design failure pressure or material imperfection failure at the operating pressure. A comparison of the performance of the proposed models of mechanical energy for the CNG cylinder obtained with regards to experimental data. The pressures

used for determining the internal energy in the overpressure system (i.e. CNG) defined as follows:

- Possible maximum pressure
- Burst pressure (worst case scenario, i.e., even tree)

The problem of the propagation of blast waves in a compressed gas mixture has been studied, both theoretically and experimentally. The theoretical investigation primarily concerned on the development of analytical solutions while in the experimental studies including simulation and prior studies, focus on gaining a comprehensive

understanding of the process of blast wave inside the cylinder.

## References

- [1] Global natural gas vehicle statistics, NGV. December 28, 2018, [http://www.iangv.org/stats/NGV\\_Global\\_Stats1.htm](http://www.iangv.org/stats/NGV_Global_Stats1.htm)
- [2] Hill, P.L., Mtui, P. G., "Natural Gas Fueling of Diesel Engines," *Automotive Engineering*, November 1996, pp. 87-90
- [3] A Practical Guide to Natural Gas Vehicles, RP Publishing, CO, 1996
- [4] Acker, G., "Experience Using LNG as a Marine Engine Fuel," *MARINE TECHNOLOGY*; Vol. 23, No. 2, June 1989, pp. 33-39.
- [5] Butler, C. A., and Casarella, R. P., the Safe Guide to Natural Gas Vehicles. RP Publishing, Inc., CO, 1996.
- [6] Wilcox, M Burrows, S Ghosh, BM Ayyub: Risk-based technology method for the safety of marine compressed natural gas fuel system; *Marine Technology*, 2001.
- [7] Janovsky, B., Selesovsky, P., Horkel, J., Vejs, L. " Vented confined explosion in Stramberk experimental mine and Auto Rea Gas simulation" *Loss Prevention in The Industries*, 19, pp.280-287.
- [8] Olvera, A.H., Choudhuri, A.H.: Numerical simulation of hydrogen dispersion in the vicinity of a cubical building in stably stratified atmospheres; *International Journal Hydrogen Energy*, 31 (15) (2006), pp. 2356-2369
- [9] Middha, P., Hansen, O.R.; CFD simulation study to investigate the risk from hydrogen vehicles in tunnels; *International journal of Hydrogen Energy*, 34 (14) (2009), pp. 5875-5886
- [10] Houf, W.G., Evans, G.H., Merilo, E., Goethe, M., James, S.C.: Releases from hydrogen fuel-cell vehicles in tunnels *Int. J Hydrogen Energy*, 37 (1) (2012), pp. 715-719
- [11] Brinkley, S.R, Jr., and Lewis, B., *Seventh Symposium (International) on Combustion*, the Combustion Institute, Pittsburgh, pp. 807–811, 1959
- [12] Karlovitz, B., *Selected Combustion Problems*, p. 176, London, Butterworths, 1954
- [13] Urtiew, P. and Oppenheim, A.K., *Proc. Roy. Soc. Lond. A*, 295:13–28 (1966), & Oppenheim, A.K., Laderman, A.J., and Urtiew, P.A., *Combust. Flame*, 6:193–197 (1962)
- [14] Lee, J.H.S. and Moen, I.O., *Program Energy Combustion Science*, 6:359–389 (1980).
- [15] Lewis, B. And von Elbe, G., *Combustion, Flame, and Explosion of Gases*, Academic, 1987. 3rd edition, pp. 566-573.
- [16] Kuo, K.K., *Principles of Combustion*, Wiley, New York, 1986
- [17] Alexander N. Kravtsov<sup>1,\*</sup>, Jacob Zdebski, Pavel Svoboda, Vaclav Pospichal: *Numerical Analysis of Explosion to Deflagration Process due to Methane Gas Explosion in Underground Structures*. Czech Technical University, Faculty of Civil Engineering, Prague, Czech Republic, Czech Republic
- [18] Cheng, V., Wenhui, H., Jianguo, N., Yuanyuan, Y. "High-resolution numerical simulation of a methane explosion in bend ducts," *Safety Science* 50, pp. 709–717, 2012
- [19] CCPS, *Guidelines for Chemical Process Quantitative Risk Analysis*, second ed.,

- AICHe, New York, 2000.
- [20] Finney D.J., "Probit Analysis," Cambridge University Press, 1971.
- [21] Knut Vagsæther; "Modelling of gas explosions," Faculty of Technology Telemark University College Norway, October 2010
- [22] Alexei M. Khokhlov, Elaine S. Oran, J. Craig Wheeler: A Theory of DDT in Unconfined Flames, Department of the Astronomy University of Texas. Washington
- [23] Zel'dovich, Ya.B., Librovich, V.B., Makhviladze, G.M. and Sivashinsky, G.I., in 2nd International Colloquium on Explosion and Reacting Systems Gas dynamics, 1969, Aug. 24–29., p.10
- [24] Eisenberg N.A., Lynch C.J., Breeding R.J., "Vulnerability Model: A Simulation System for Assessing Damage Resulting from Marine Spills," Rep. CG-D-136-75, Enviro Control Inc., Rockville, MD, 1975.
- [25] Wagner, H.Gg., in Proc. Int. Specialist Conf. Fuel-Air Explosions, U. Waterloo Press, 77–99 (1981).
- [26] Pasquill-Gifford vertical dispersion parameter as defined in the Industrial Source Code (ISC) model of EPA (Bowers, 1979).
- [27] Shepherd, J. "Detonation in gases, Proceedings of the Combustion Institute, 32(1), (2008), 83-98.
- [28] Schultz, E. and Shepherd, J. Validation of Detailed Reaction Mechanisms for Detonation Simulation Explosion Dynamics Laboratory Report FM99-5, 2000.
- [29] Brode, H. L. (1959). Blast Wave from a Spherical Charge. *Physics of Fluids* (1958-1988) 2, 217.
- [30] Lee, J., and Moen, I "THE MECHANISM OF TRANSITION FROM TO DETONATION IN VAPOR CLOUD," *Prog.Energy Combust.Sci.*, Vol.6, pp. 359-389, 1980. McGill University, Montreal, Canada
- [31] Paulsen. S.S. (2009). "Pressure Systems Stored-Energy Threshold Risk Analysis" PNNL-18696. August 2009.
- [32] Lees F.P., "Loss Prevention in the Process Industries," second ed., Butterworth-Heinemann, Oxford, UK, 1996
- [33] Khan I.F., Abbasi S.A., J. Loss Prevent. Process Ind., 14 (2001), p. 43.
- [34] Molkov, V., Kashkarov, S. "BLAST WAVE FROM A HIGH-PRESSURE GAS TANK RUPTURE IN A FIRE: STANDALONE AND UNDER-VEHICLE HYDROGEN TANKS," Hydrogen Safety Engineering University of Ulster, Newtownabbey, UK
- [35] Nelson, R. W. *Hydrocarbon Process.* August (1977,) 103.
- [36] Bagster, D. F., Pitblado, R. M. *Proc. Safety Environ. Protect.* 69 (1991) 196
- [37] Henrych, J. *The Dynamics Of Explosion and Its Use*, Developments in Civil Engineering, vol. 1, Elsevier Scientific Publishing Company, Amsterdam, 1979.
- [38] HSE, Health, and Safety Executive, *Canvey: An Investigation of Potential Hazards from Operations in the Canvey Island/Thurrock Area*, London, UK, 1978.
- [39] Bottelberghs, P.H., Ale, B.J.M.: *European Seminar on "Domino Effects,"* Leuven, 1996.
- [40] Barton, R.F.: *Fuel gas explosion guidelines—practical application*, IChemE Symposium Series no.139, Sedgwick, 1995, pp. 285–286.
- [41] Gugan, K. *Unconfined Vapour Cloud*

- Explosions, the Institutions of Chemical Engineers, Rugby, 1979.
- [42] Schneider, P., Loss, J. Prevent. Process Ind. 10 (3) (1997) 185.
- [43] Clancey, V.J. in 6th Int. Meeting of Forensic Sciences, Edinburgh, 1972.
- [44] Wells, G.L., Safety in Process Plant Design, Wiley, Chichester, 1980
- [45] NFPA standard 72, National Fire Protection Association Quincy, MA
- [46] Fire System Integrity Assurance, Report No. 6.85/304, 2000. The international Association of Oil&Gas Producers.
- [47] Centre for Chemical Process Safety, Guidelines for Process Quantitative Risk Analysis. American Institute of Chemical Engineer in NY, 1989.
- [48] The SFPE Handbook of fire protection engineering sccond edition, DiNenno, P.J., Editor, Published by the society of Fire Protection Engineer, 1995.
- [49] Guidelines of Chemical Hazard Analysis Procedure, U.S. Department of Transportation Washington, D.C. 1989.
- [50] Chuanchuan S., Li M., Gai H., Yingzhe W., Jinyang Z., Yan L., Jun H.”Consequence Assessment of High-Pressure Hydrogen Storage Tank Rupture during Fire Test”, Institute of Process Equipment, Zhejiang University, Hangzhou, 310027, China institute of Solid Mechanics, Zhejiang University of Technology, Hangzhou, 310014, China cInspection and Research Institute of Boiler and Pressure Vessel, Dalian, 116000, Chin
- [51] Weyandt, N. “Analysis of Induced Catastrophic Failure Of A 5000 psig Type IV Hydrogen Cylinder,” Southwest Research Institute report for the Motor Vehicle Fire Research Institute, 01.06939.01.001, 2005.