Numerical and experimental verification of physical blast thermodynamic model

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Abstract. Helium inventory in big cryogenic systems may be of the order of hundred tons. During the warm up of the machine the helium has to be stored in warm pressurized tanks. A potential rupture of the tank may create a danger to adjacent objects. In order to formulate recommendations concerning storage of compressed gases in close vicinity of nuclear installations, a thermodynamic model of physical blast has been formulated. The model has been experimentally verified in a laboratory scale test rig. To simulate rupture of compressed gas storage tanks, plastic tanks have been used. Scaling of the results to real cases like ITER compressed gas inventory requires good understanding of potential rupture of high volume gas storage tanks. Numerical model of tanks rupture have been elaborated and verified against experimental results. The model allows scaling of thermodynamic simplified description to real gas storage installations.

1. Introduction
Helium inventory in big cryogenic systems may exceed hundred tons. During normal operation of the machines helium is mostly located in cold masses, distribution system and refrigerators. During the machine warm up resulting e.g. from magnet resistive transitions or maintenance requirements the helium has to be stored outside the machine in liquid or gaseous form. The Large Hadron Collider helium storage system has a capacity of about 130 tons split between 45 tons in gaseous and 85 tons in liquid form. The gaseous helium is stored in 250 m$^3$ storage tanks which can be pressurized to 20 bar [1]. A total helium inventory of ITER tokamak, now under construction in Cadarache, is estimated as of about 25 tons. In case of the machine resistive transition or maintenance warm up, the helium at about 20 bar will be gathered in warm pressure tanks and in a cold quench tank precooled to 80 K. Additionally, compressed and liquid nitrogen will be gathered in the vicinity of helium tanks.

Rupture of any of the tanks filled with the gases will create a rapid energy release in the form of a physical blast. According to the present regulations the TNT equivalent approach is to be applied to evaluate the pressure wave following a potential gas storage tank rupture. The TNT evaluation method is based on the amount of energy stored in the pressurized gas container, expressed in equivalent of kilograms of TNT. The TNT equivalent pressure wave calculations make use of TNT-model proposed by Frazer-Nash for hydrogen explosions [2]. This approach seems to produce overestimated pressures compared to those obtained from alternative thermodynamic model as proposed in [1].

The aim of the present analysis is numerical verification of the thermodynamic model and analysis of different scenarios of the container rupture.
2. Pressure wave parameters

For evaluation purposes, the pressure wave is characterized by maximum pressure level $p$ at given distance $r$ from the centre of bursting container. Two models of maximum pressure distribution $p$ versus the distance $r$ of bursting container have been taken into account. In the first model pressure distribution is assumed to be the same as during explosion of TNT charge of mass equivalent to amount of energy stored in container. In the second model pressure distribution is calculated from static thermodynamic equations ruling gas expansion from some initial volume and pressure.

2.1. TNT-equivalent

For calculating stored energy of ideal gases the Brode formula is applied [2], similarly to the calculation done for ITER [1], as recommended by the Center of Chemical Process Safety (1994/15). The formula for energy stored in a container of volume $V$ and under pressure $p$ is as follows

$$E(p, V) = \frac{V(p-p_{amb})}{\kappa-1}$$

where $\kappa$ is the gas specific heat ratio and $p_{amb}$ is the ambient pressure.

When the equivalent mass of TNT is calculated, the model proposed by Frazer-Nash for hydrogen explosion is used to calculate maximum pressure $p(r)$ distribution versus distance from the bursting container – details are given in [3].

2.2. Thermodynamic model

In the thermodynamic model it is assumed that an ideal gas occupies some space of volume $V_{con}$ under pressure $p_{con}$, restricted by rigid walls. At a specified time, the walls are fully and suddenly removed, which results in gas expansion in the form of a sphere with volume $V_{sph}$. The pressure in the space occupied by the expanding gas is assumed to be uniform as speed of sound is much higher than gas particle velocity. Also, the expansion process is assumed to be isentropic, because of its rapidity, which prevents heat exchange between gas and environment. Using these assumptions the distribution of maximum pressure $p(r)$ versus distance $r$ can be evaluated from the equation [4]:

$$p(r) = p_{con} \left(\frac{V_{con}}{V_{sph}(r)}\right)^{\kappa}$$

3. Experiment

A laboratory scale experimental test rig has been designed, built and commissioned to explore the physical explosion phenomenon. The experimental gas tank is a 5 liter plastic bottle (PET container). The bottle can be filled with different gases and pressurized up to 5 bar. The bursting is triggered by cutting the sidewall of the PET container by a heated resistive wire (fig. 1). The first pressure sensor P1 was located 148 mm from the centre of container. The details of the experiment layout and preliminary results of experiment were presented in [3].

![Fig. 1. The experiment setup, location of the pressure sensors along the experimental test rig [3].](image-url)

An example of recorded pressures history is shown in figure 2. The pressures exhibit two peak values, reflecting the effect of pressure wave perturbation caused by the dynamics of the container rupture. The first peak is a short distance jet effect and the second one is a results of blast wave due to
rupture of a whole container. The comparison of maximum recorded pressure levels with pressure calculated with the TNT model and thermodynamic model is presented in figure 3.

![Fig. 2. Example of pressures history recorded by transducers numbered as in fig 1. The maximum initial pressure equal to 4 bara.](image)

![Fig. 3. Comparison of blast pressures calculated by thermodynamic model, TNT model and experiment.](image)

The experiments show various modes of destroying of the container. It can be destroyed by a heavy fragmentation (separation of the bottle shell into multiple fragments), by division of the shell into two parts, or by only opening a hole in the container surface. For deeper insight into the process of pressure wave propagation, a numerical model is used.

4. Simulation

4.1. Numerical model

Simulation of the bottle rupture is carried out with the use of Finite Element Method in Ls-DYNA, code developed for dynamic simulation with explicit integration scheme. The simulation model is divided in two parts. A surrounding and gas inside the bottle is modeled as a volume with Multi Material Arbitrary Lagrangian-Eulerian technique (MM-ALE), commonly used for estimation of the blast wave interaction with structures [5, 6].

The air volume is discretized into 2 millions of solid elements. During simulation, each solid element, can contain a mixture of different gases whose composition can be observed. In simulations both gases – surrounding air and the gas pumped into the bottle is the same, but due to the Multi-Material technique, one can observe movement of both gases separately.
The second part of model is a bottle, modeled as Lagrangian area. The geometry of the bottle is modeled and discretized with Belytschko-Tsay shell elements [7]. In simulation, nonlinear elastic-plastic material model is applied. The mechanical characteristic of the material of the bottle shell was measured in an uniaxial tensile test. The strain-rate sensitivity of the material is neglected due to relatively low rate of deformation and low influence on dynamic pressure distribution after the breaking of bottle.

In the material model, the possibility of damage of the bottle shell is included, the equivalent strain is applied as a damage criterion. After reaching maximum strain, the shell element is removed from analysis and the bottle can be progressively destroyed by accumulated internal pressure. Both parts of the model MM-ALE and structural are mechanically coupled by pressures. The fluid-structure interaction (FSI) algorithm transfers the pressure from MM-ALE region to the container, and simultaneously the gas is confined by the shell.

In the experiment, the breaking of bottle was initiated by the hot wire touching the bottle surface. To resemble the experimental layout, in the small area of bottle is made out of weaker material in order to initiate the breaking process at given point and internal pressure. The view of simulation model is presented in figure 4. In the air region, 10 virtual pressure sensors are located to observe the pressure changes.

4.2. Results and discussion

In the first stage of simulation, the various rupture modes are investigated. All simulation are carried out with identical parameters except to small changes in ultimate strain for material of the container shell. In figure 5 the characteristic modes of rupture are presented.

After burst of container the pressure wave is expanding in general spherically. The thermodynamic and TNT models of the wave propagation both assume that pressure is the function of distance \( r \) and time. In the case of non-spherical containers it is not true, because the shape of container influences of the amplitude of pressure. Even for the rupture mode most similar to instantaneous disintegrating of the container shell (fig. 5a), the pressure wave shape is spherical, but the shape of container influences the pressure distribution of the sphere surface. The pressure is lower along axis of container, and higher in the plane perpendicular to the container axis. This effect is presented in figure 6.
Fig. 5. Various modes of the container rupture:

a) fragmentation of the container shell into multiple parts,
b) rupture of the container without fragmentation,
c) division of container into two parts,
d) evacuation of internal gas through single hole.

Non-symmetrical rupture of the container influences the shape of the pressure wave front. The rupture modes presented in figures 5b, 5c and 5d produce directional waves with pressures much higher on side of the rupture. An example of non-symmetrical rupture process (rupture mode fig. 5c) is presented in figure 7. The pressure wave is focused in one direction and the pressure amplitude is significantly higher than in symmetrical rupture case.

Fig. 6. Symmetrical rupture of axisymmetric container, spatial pressure field [Pa].

In order to visualise the process of interaction of wave and the object loaded by pressure, in part of simulations, the obstacle is placed on the way of traveling of pressure wave. It is located at distance 600mm from the bottle axis. When the traveling wave interacts with the obstacle, the incident pressure amplitude is amplified to reflected pressure value. The amplification ratio strongly depends on the
incident pressure level. For the incident wave overpressure below 0.25 bar, amplification ratio is equal to 2, but for higher overpressures the value of the amplification ratio can exceed 10 [8]. For this reason, the scaling possibility of the pressure wave effect is limited.

An example of interaction of the pressure wave with obstacle is shown in figure 7. It resembles the small-scale experimental setup. For this case, the overpressure value at the obstacle is low and reflected pressure is only twice higher than incident pressure. One can observe a negative pressure areas developed behind the wave front and behind an obstacle. These negative pressure regions are typical for the high-explosive blasts and are potentially dangerous too. The values of local pressures highly depends on the geometry of the obstacle.

For comparison, the pressure wave history was calculated for the energy-equivalent TNT detonation. The pressures was calculated with Kingery-Bulmash empirical equation [9] implemented in CONWEP military code, widely used for evaluation of the effects of TNT detonation [5, 6]. The TNT pressures are overestimating the pressures produced by the damaged container, it confirms the conclusion from preliminary analysis [3]. Nevertheless the shapes of the pressure profile is different. The TNT pressure pulse is much shorter. Direct comparison of the pressures obtained from MM-ALE simulation and from TNT model for pressure sensors p2 (located close to the container) and p10 (the most distant one) is presented in figure 8.

The pressures in function of the distance \( r \) from the container axis are presented in figure 9. The pressures obtained from TNT-equivalent calculations overestimates pressures for all distances. On the other side, the thermodynamic model underestimates pressures for all distances. The pressures from MM-ALE simulation are located between TNT model and thermodynamic model.
Results are lower than experimental results at close range. In that area the depressurisation process is highly unstable and strongly depends on local damage of the container shell. At higher distances MM-ALE simulation results slightly overestimate measured values, nevertheless the estimation is better than TNT equivalency.

![Fig. 9. Maximum pressures as a function of distance $r$ from the centre of container. Results from experiment, thermodynamic model, numerical simulations and energy-equivalent TNT model.](image)

In the estimation of risk of the damage caused by blast wave, the maximum pressure level is not the only parameter taken into consideration. The second important parameter is the pressure impulse \([9]\) defined by equation:

$$i_s = \int_{t_a}^{t_a+T_s} p(t) dt$$ \hspace{1cm} (3)

where:

t\(_a\) - time of a wave arrival

\(T_s\) – duration of an overpressure phase

The TNT model and MM-ALE simulation are able to provide the estimations of the pressure impulse values. In figure 10 the incident pressure impulse as a function of distance $r$ is presented for both models.

The difference between impulses is very significant. While the TNT model overestimate the peak pressures, the values of pressure impulse are severely underestimated by this model. This is result of different shape of the pressure waves shown in figure 9. Second reason is the directional character of the simulated rupture of container, which cannot be considered in TNT model.

5. Conclusion

In the paper, the numerical simulations of the pressurized container rupture were presented. The FEM numerical model was prepared as a small-scale one in order to validate the results by an experimental bursting of pressurized PET containers. The experimental investigation of the rupture process reveals significant dispertion of results, because of various modes of the container rupture, obtained as well in simulations.

The results of simulations were compared to previously examined simplified methods of evaluation: TNT energy-equivalent method and thermodynamic method. The numerical simulation is
able to capture two important phenomena neglected by the simplified methods. The first one is the pressure distribution on the wave front due to initial shape of the container. A deviation of the container shape from sphere results in non-uniform distribution of the pressure on the wave front. In case of an axisymmetric container, the pressure reaches highest value in the plane perpendicular to the container axis.

The second effect captured by simulations is a possibility of non-symmetric rupture of the container. For the analysed material, slight changes of the material ultimate strength result in completely different patterns of the container rupture. A directional rupture, similar to the one observed in the experiment, produces a directional pressure wave, which cannot be correctly predicted by analytical methods assuming spherical propagation of the wave.

The maximum pressures at sensor points predicted by simulation are located between the TNT model overestimating the experimental results and the thermodynamic model underestimating it.

In addition to the analysis of maximum pressure levels, the pressure profile and total pressure impulse was evaluated. The TNT model generates a high amplitude but short pressure pulse. The MM_ALE simulation model predicts lower amplitude but longer pulses, similar to ones recorded in experiment. Due to the significant dispersion in experimental results, more experimental data is required to evaluate MM-ALE simulations.

The presented MM-ALE simulation of the pressure wave propagation process is able to take into account more details of the process of the pressurized container rupture than simplified TNT energy-equivalent and thermodynamic models. The method requires high computing power, nevertheless takes under consideration the shape of container, the mode of a container rupture and the worst case of directional gas release. In the connection with the model of an obstacle, it is possible to predict values of the reflected pressure and reflected pressure impulse values.

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