Paper 6007

A NEW APPROACH FOR THE ANALYSIS OF A GAS EXPLOSION IN A TYPE B PACKAGE

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Abstract

DGDM is originally a type B package designed by the CEA to transport technological solid waste. This waste contains organic elements which are subject to flammable gas production by radiolysis and thermolysis.

This paper will present a new approach which is conducted in the safety analysis report of how the containment system (especially the bolted lid) withstand explosion. It has recently obtained a special arrangement for 18 months.

Different steps have been followed:

- Analytical calculation of conservative values of gas reached within the packaging during normal or accident conditions of transport (within limited time of transportation);
- Finite Element (FE) calculation in 3D model of the chemical reaction of detonation of the gas mixture;
- FE mechanical calculation of the structural response, with focus on the stresses on the lid and bolts and deformations (containment O-ring compression set; mechanical interferences with other components);
- Justification of the safety.

The modelling of the pressure vs time profiles in the cylindrical internal cavity of the package is innovative, taking into account the pressure wave progression, the multiple reflections with associated amplification factors. Different axial and radial locations for the ignition point are studied, focusing on their effect on the lid response. The potential reflection effect of the presence of a drum (containing the waste) in the cavity during the explosion is also analysed.

1 - Introduction

As a nuclear research institution, the CEA (the French Alternative Energies and Atomic Energy Commission), is working on many projects of cleaning up and dismantling nuclear facilities and managing radioactive waste. Among the variety of radioactive material to be taken care of, drums of solid organic waste mixed with nuclear matter are being shipped to storage areas in transportation packagings. One of the specific constraints of transporting this waste is the risk of the production of flammable gas by the decomposition of the organic matter due to the combined effects of radiations and temperature.

A CEA unit (CEA/STMR, Cadarache, France) is in charge of transport package construction, safety analysis and transport operations. The application for package approval (e.g. type B package) requires a complete and thorough safety demonstration in which flammable gas generation like radiolysis has become a major issue in the last few years. The main approach is to maintain the concentration of hydrogen under the Lower Flammability Limit but this is quite restrictive in terms of allowable thermal power. Another specific problem is that some waste that has not been reprocessed may contain, within an enclosed volume, a significant amount of dihydrogen produced during the storage phase, which could be released inside the container during shipment.

In 2000s, the CEA proposed an alternative solution: a cask designed to withstand dynamic pressure loads due to inner hydrogen/air mixture explosion, and a methodology to detect if such an event has happened and the subsequent measures to be taken. This is the case with the DGDM type B package. DGDM permits the creation of a vacuum and an inerting of the content with nitrogen before shipment. But as no guarantee could be made that the inerting would reach every void space inside the waste, despite the different preventive measures taken, the risk of an explosion is not zero. Even though such an explosion has never happened, the demonstration that DGDM could withstand such an explosion is crucial.

The first explosion evaluations which were conducted in the DGDM safety analysis report were initially based on 1D detonation pressure curves from the relevant literature. Many questions were raised about the representativeness of the models, or the accuracy of the results, especially as regards the treatment of wave reflection phenomenon. This paper will present the new methodology conducted in collaboration with ATR-Ingénierie ([1] and [2]), a specialist of rapid dynamic simulation with explosion expertise, for the reconduction of the special arrangement¹ of DGDM package [3]. The effects on the explosion results of the geometry and the location of the ignition point relative to the impact zone will be discussed.

¹ Licensed under special arrangement due to the non-satisfactory demonstration of the cumulation of an explosion with free drop tests.

2- DGDM transport package

A brief overview of DGDM transport package of solid waste in drums is presented hereafter. The original 1998 DGD concept (R66), from the collaboration between ROBATEL and CEA, was modified in 2003 to accommodate organic waste subject to radiolysis.

2.1 – Packaging description

DGDM is composed of a main cylindrical body, to which the lower shock absorber is welded (see **Figure 1**). The body is an enclosure made of stainless steel, containing lead and compound layers for radioprotection. An upper shock absorber encloses the upper part of the body. The overall dimensions are 1910 mm diameter and 1740 mm height. DGDM weighs 16424 kg loaded.

DGDM presents four compartments allocated for the waste drums. The effective diameter and height are respectively 399 mm and 641 mm. It can take 120 kg per compartment. Dedicated ducts create a communication path between the compartments. Each of the compartments is enclosed by a movable shielded plug. These plugs have been fitted with helicoidal grooves, whose purpose is to facilitate gas exchanges between the compartments and the volume under the lid. The DGDM also features an inerting system, which allows for the evacuation of the volumes and the injection of nitrogen up to the absolute pressure of 0.1 bar before shipment. A plug flange is bolted above, to retain the plugs under accident conditions. The flange and screw connection have been reinforced to withstand explosion.

The containment is guaranteed by a containment lid, bolted to the body flange. The lid and screw connections have also been redesigned to withstand internal explosion.



Figure 1 - DGDM cross-section view

2.2 - Type of waste description

Currently, four types of contents transported in DGDM may produce inflammable gas. These are Medium Level Waste, activated or contaminated by radioactive matter, which can be:

- either radiolysable or thermolysable themselves,
- or contained in radiolysable/thermolysable packaging.

The objects (metallic waste, glass, filter, soil, rubble, etc.) are of small dimensions.

One type of content is preconditioned before the storage phase in a radiolysable drum which is leak tight up to a specific pressure (see **Figure 2**). Hence, the free volume of the drum can be considered as a gas pocket, which is specific to this content. In this case, in a very conservative approach, one must consider that the totality of the pressurized gas is dihydrogen.



Figure 2 – Preconditionning leak tight drum

Before being loaded into the DGDM, the wastes is put into 50 L or 60 L steel drums and overdrums in order to ease the handling and to preserve the DGDM compartments from contamination. A [®]Poral valve (or equivalent) is fitted to these drums to allow the passage of gas. One drum (or overdrum) fits in one DGDM compartment.

The allowed thermal power differs from one content to another but the maximum value is obtained in the following configuration: 1.6 W per drum for a content of 3 drums, one compartment being empty. The smallest allowed thermal power is 0.27 W per drum.

3 – Analytical calculation of conservative values for the gas prior to explosion

The object of this intermediary calculation is to determine the input data for the explosion calculations. It consists of establishing:

1) The maximum temperature during transportation (in Normal Conditions of Transport (NCT) and Accident Conditions of Transport (ACT)),

- 2) The number of moles of the mixture of combustible, combustive and non combustible gases (based on the gas present in the waste before shipment, the temperature, the gas production during transportation),
- 3) The maximum internal pressure (based on the number of moles of total gas before shipment, the temperature, the total gas production during transportation, the free volumes of the compartments and the area under the lid),

<u>3.1 – Maximum temperature</u>

The determination of these values is made by finite element calculations, with respect to the IAEA SSR-6 requirements on thermal matter in NCT and ACT. The inner thermal power contribution is negligible.

The temperature, spacially averaged, reached in a compartment in NCT is 50°C.

 \rightarrow As for ACT, the selected temperature for the compartment is 102°C.

3.2 - Number of moles evaluation

The rate of radiolytic and thermolytic gas production is based on classic literature G_{α} value and thermal decomposition rates for PE, PVC, cellulose and cotton. 100% of the thermal power and the organic weight are considered to participate in the gas production.

The number of moles is processed over a period of 19 days of shipment, including:

- 5 days allowed for shipment,
- Plus an additional 7 days in case of an NCT event (in application of ASN requirements)
- Plus an additional 7 days in case of an ACT event.
- \rightarrow The maximum number of moles of H₂ and N₂ is calculated at 4.6 mol and 4.3 mol.

 \rightarrow The number of moles of O₂ is set at the stoechiometric value: 2.3 mol.

3.3 - Pressure evaluation

The free volumes are worked out from the volumes of the empty container (see **Figure 1**) minus the volume occupied by the drums. Basically, the drums are considered 100% full, except in the case of the preconditioned waste in a leak tight drum. In that specific case, in order to maximize the gas addendum during shipment, a free volume of 50% of pressurized gas is taken into account. The pressure of the gas has been established at 2.8 bar abs, on the basis of tests carried out on a significant amount of drums.

 \rightarrow The calculated maximum pressure inside the DGDM cavity is rounded up to 1.65 bar.

<u>3-4 – Input Data and margins summary</u>

The input data for the reactive initial mix is derived from calculations contained in the previous section: n_{H2} =4.6 mol; n_{O2} =2.3 mol; n_{N2} =4,3 mol, i.e. n_{total} =11.2 mol with the following initial conditions: T= 375 K; P = 1.65 bar; which corresponds to a gaseous volume of V = 212 L.

The main margins allowed for in the input data calculations are as follows:

- A maximized number of O2 moles,
- 100% thermal power and organic weight considered to contribute to gas production,
- α -radiolysis only (no γ -radiolysis),
- 100% full drums (no void rate),
- A preconditioned drum filled with 100% H2 gas,
- The additional time allowed for NCT events.

4 – Chemical reaction of detonation

The software used by ATR Ingénierie is COM3D v3.9. COM3D is a Computational Fluid Dynamics (CFD) code developed by Forschungszentrum Karlsruhe (FZK) to model turbulent combustion phenomena in complex geometries [4].

4.1 - COM3D modelling

As the volumes in the compartments and under the lid are almost separated because of the shielded plug shape, two different models must be implemented (see **Figure 3**):

- for the compartment,
- for the volume under the lid.



Figure 3 – Geometry of COM3D models

The reactive initial mix volumes (in blue on **Figure 3**) are modelled with 6 mm hexaedric cells. The walls (in grey on **Figure 3**) are unyielding. The ignition point is modelled by a sphere at a temperature of 3000 K and 100 bar. Two alternative locations (central and peripheric) are studied for the lid and one for the compartment.

Several pressure sensors (green points on **Figure 4**) are positioned on the wall where the pressure history has to be recorded, but also on the fictive line from the ignition point to the impacted wall. The pressure profiles on the wall are defined as followed: $P_{Zi}=(P_{sensor(i-1)}+P_{sensor i})/2$ in an axisymmetric configuration or $P_{Zi}=(P_{sensor-X(i-1)}+P_{sensor-Xi}+P_{sensor-Y(i-1)}+P_{sensor-Yi})/4$ otherwise. The profile of the zones for the sidal ignition point (location 1) mimicks the flame wave shape in its progression over time.



Figure 4 –COM3D model instrumentation 4.2 – COM3D results

In the compartment:

From **Figure 5**, the following observations can be made: the flame front speed of 2009 m/s is typical of a detonation process. A reflection on the shielded plug wall happens at a time of 0.21 ms when the majority of the gas is burnt. The reflection coefficient can be assessed at 3.4. The pressure on the wall varies from 51 bar to 160 bar (peak with low energy). At the end, the residual pressure tends to P_{AICC} (for Adiabatic Isochoric Complete Combustion Pressure), which is 13.9 bar.



Figure 5 – Pressure curve in the compartment along the central axis

Figure 6 shows that the first reflection impacts both the center (zone 1) and the side (zone 3) in terms of maximum pressure, with zone averaged pressure up to 80 bar, then the pressure wave maximum remains central (in zone 1; up to 95 bar for a short period of time). Due to the spatial average, the maximum pressure of 160 bar found in one point (fig.5) decreases to 95 bar in zone 1.



Figure 6 – Pressure curves of the 3 zones on the bottom wall of the shielded plug

In the volume under the lid:

The flame front speeds are also about 2000 m/s in the 2 alternative configurations (see **Figure 7**). The maximum pressure in the zone is about 70-80 bar in both configurations.



Figure 7 – Pressure curves in the 8 zones of the lid – Centered and sidal ignition point

5 – Mechanical calculation

5.1 - RADIOSS modelling

The software used by ATR Ingénierie is RADIOSS v11. It deals with highly non-linear problems under dynamic loadings. The meshing is performed on a quarter of the container model (configuration "compartment" and "under the lid" with a central ignition point; see **Figure 8**), and with half of the container (configuration "under the lid" with a sidal ignition point). The use of a quarter model for the compartment implies that 4 simultaneous explosions are actually taken into account for the structure dimensioning, which is very conservative.



Figure 8 – Compartment and lid meshing

The 5 mm mesh size in the containment gasket zone allows for the deduction of the relative vertical displacements, especially for the central gasket (see **Figure 9**).



Figure 9 – Principles for modelling the gasket aperture

Screws are modelled with pretightening (like a spring with a defined stiffness between 2 rigid bodies). The effect of torsion is added in post-treatment.

Concerning the loads distribution, the same zoning as in COM3D is applied on the surfaces. It is also considered that after 3 ms, the pressure has flattened at P_{AICC} up to 1 s.

5.2 - RADIOSS results

Results for the compartment

The flange suffers small plastic strain (< 3%; see **Figure 10**). The maximum residual deflection on the flange is 4.4 mm, located on the rim, which remains inferior to the gap between the flange and the lid (31 mm).





Figure 10 – Plastic deformation and uplift of the flange

According to **Figure 11**, the ultimate strength at 100°C of the central screw is exceeded on the first dynamic loading, the other eight screws remaining under the yield strength at 100°C. Considering that, due to the model, the central screw experiences four explosions in the four compartments (see §5.1), it is certain that this screw stress is vastly overestimated. An assessment of the impact of only one explosion would be a stress of 480 MPa, which is under the yield strength at 100°C.



Figure 11 – Von Mises stresses in flange screws

Results for the lid:

Between the two configurations, it is the second which leads to the maximum damages. Hence, only the configuration 2 results are presented hereafter in **Figure 12** and **Figure 13**. The integrity of the lid is guaranteed with large margins. For information, the calculated displacement of 0.719 mm for the 12 mm o-ring gasket in a 9.2 mm depth groove reduces the compression set from 23.3 % to 17.4%, which is still acceptable as a single influencing factor.



Figure 12 – Plastic deformation and uplift of the lid – focus on gasket zone



Figure 13 – Von Mises stresses in lid screws

6 – Impact of the ignition point location inside a compartment

An additional analysis studies the effect of the ignition point location, relatively to the flange wall. Two configurations were chosen (see **Figure 14**):

the first similar to §4.1 geometry. The distance between the ignition point and the flange has been reduced from 419 mm to 368 mm in order to maximize the loading surface under the flange (R= 189 mm to R= 201.5 mm which is the radius of the compartment). As seen in Figure 5, the pressure wave has time to flatten sufficiently to produce maximum impact. Point 1 compares directly with §4.1. Points 2 and 3 are distributed equally between center and side.

- The second which introduces an object inside the cavity (a drum). The drum geometry reduces even more the distance to the plug (318 mm compared to 368 mm), except for point 4 which is now 640 mm from the flange. Point 5 is the reference for comparison with configuration 1. Point 4 allows for the study of the effect of a confined space on wave amplification. Point 6 was chosen to test the edge effect on the pressure wave.



Figure 14 – New geometry of COM3D models

In order to sort out the six configurations and select the most severe pressure curves to input in Radioss, the impulse² and maximum peaks (though temporally and spatially limited) were analysed (see **Figure 15**). As a result, the mechanical calculations were pursued with point 1 curve which maximizes the impulse and point 4 curve which maximizes pressure (9 sensors over 80 bar, with one at 160 bar).



Nota: due to numerical convergence failure, the impulse curve for point 4 has been remeshed

Figure 15 – Average impulse curves of the 6 ignition points - Point 4 pressure curves

² The impulse I delivered by a blast is the cumulative integral of the pressure profile plotted against time: $I=\int_{t}^{t+t_0} P(t)dt$. The greatest effect on the structure is usually obtained from the highest impulse value.

The alternative scenarii studied in this paragraph have impacted very slightly on the flange strain (see **Table 1**: 3.4 % compared to 2.9%) and on screw stresses (757 MPa compared to 744 MPa) without changing the conclusion of paragraph 5.2. Two tendencies may be noticed, but it will be difficult to draw solid conclusions due to the limitation of the effects detected:

- As soon as the wave has sufficient distance to flatten, the greater loading surface is the more impact the pressure will have (point 1 (d=368 mm; r=201.5 mm) compared to the point in §4.1 (d=419 mm; r=189 mm) on one hand, and to point 5 (d=318 mm; r = 201.5 mm) on the other hand),
- Confined spaces with a greater reflection coefficient may increase the loading (point 4 with a coefficient of 3.8).

		Blast calculation COM3D				Structural calculation RADIOSS		
		Flame front pressure 1st reflection	1st reflection coefficient	Flame front speed	Theorical PAICC	Flange rupture limit	σVM Flange screw (dyn. /rés.)	Flange residual deflection
		(bar)	(-)	(m/s)	(bar)	(%)	(MPa)	(mm)
						< 37%	< 737 MPa	
Compartment blast (2013)	(r 189mm)	51,3	3,4	2009	13,9	2,9	744 / 389	4,4
Compartment blast (2015)	Point 1	82,4	2,4	1115	13,9	3,2	751 / 393	4,6
	Point 4	70,4	3,8	1630	13,9	3,4	757 / 393	4,2

Table 1 – Results table for all the ignition point configurations in compartment

7 - Conclusion and perspectives

This new approach for the analysis of a gas explosion in DGDM opens up possibilities for the conception of CEA packages designed to withstand an explosion, such as TIRADE (R76) package [6]. The 3D modelling of the chemical explosion and its interfacing with 3D dynamic structural calculation software leads to more accurate results, because of its ability to take into account reflection phenomena on the container walls, or on small elements such as bolts or spaces between drums and walls.

The demonstrations for TIRADE (R76) package rely on a series of explosion tests [6], which was enabled by a preliminary CEA experimental program [5], in particular for the definition of the detonation chamber and other specific experimental accessories.

As a future prospect, a first step would consist of matching COM3D results to existing field data ([5] and [6]) in order to improve the accuracy of the software in the specific area of transport packages and not only rely on feedbacks from other field. Thus, the software will permit the study of specific configurations without the need of performing other experimental investigations.

The objective remains to make more accurate safety calculations, to design, if necessary, primary waste containers or fuel canisters, or in very specific cases, transport packages that can withstand high pressure loads arising from inner cavity hydrogen explosion.

References

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- [4] Analysis methodology for hydrogen behavior in accident scenarios, W. Breitung, FZK
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