Additional afterburning energy value to simulate fully confined trinitrotoluene explosions

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Abstract

Euler–Lagrange software packages are commonly employed in the analysis and design of chambers subjected to internal detonations of high explosives because they allow modeling the interaction between high-explosive gas products, air, liquid, and structures. In general, the expansion of high-explosive products is modeled by the Jones-Wilkinson and Lee equation of state, and additional extension methods such as the Miller or the additional energy release extensions are used to model the afterburning energy which is released after the detonation. These extension methods require that the additional energy by unit mass is predefined. Although the difference between the heat of combustion and the heat of detonation provides a specific value for the additional energy, for example, 10.01 MJ/kg TNT for trinitrotoluene charges detonated inside of chambers with rich oxygen, this value is generally inappropriate if high-explosive gas products and air are modeled separately, that is, by the Jones-Wilkinson and Lee equation of state and the ideal gas equation of state, respectively. This article explains how to determine an appropriate value for the specific additional energy value for use in the commercial software package AUTODYN for more reliable predictions of the quasi-static gas pressure in fully confined chambers subjected to trinitrotoluene explosion. The procedure detailed in this article can be applied to any kind of chamber geometries and chamber materials. A simplified chart for the afterburning energy as a function of the charge mass density is derived. The proposed approach in predicting the quasi-static gas pressure is validated with the quasi-static gas pressure described by the Unified Facilities Criteria's guideline and some experimental tests. A procedure to determine the additional afterburning energy that should be employed for highly deformable chambers is also explained.

Keywords

Additional energy, afterburning, high explosive, AUTODYN, equation of state, highly deformable chambers

Introduction

The pressure time-history observed on chamber walls due to fully or partially confined high-explosive (HE) explosions is commonly described by two components: (1) a train of shock waves and (2) the gas pressure component (Baker et al., 1983).

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The detonation of an HE is an almost instantaneous chemical reaction which causes the HE-condensed solid phase to rapidly expand and transform to highly pressurized gas products, generating a supersonic shock wave propagating through the explosive and air. This shock wave is consecutively reflected on the vessel's walls causing a train of reflected shock waves. The effect of the first shock wave is usually simplified by a triangular or an exponential function whose parameters are based on widely employed experimental curves available in different guidelines for spherical or hemispherical wave propagation modes (e.g. UFC-3-340-02, 2008). The temporal and spatial distribution of the re-reflected pressure pulses depends on the vessel geometry, the reflection pattern, and the HE position and shape, among others. That is, shock waves arrive generally at different times and the corresponding pressure profiles show different amplitudes and duration at different points of the chamber (as an exception, only spherical chambers with concentric spherical charges show axisymmetric pressure profiles). In fact, geometrical singularities such as corners, obstructions, or longitudinal sections cause significant amplifications or deamplifications (Beshara, 1994). Therefore, the prediction of the re-reflected shock waves is generally a difficult task because even small geometrical singularities can drastically change the temporal and spatial distribution of the pressure time-history. Three-dimensional (3D) analyses (such as computational fluid dynamics (CFD) software packages) are the most common tool to predict this complex phenomenon. On the other hand, the quasi-static (QS) gas pressure is not altered by the shock wave pattern because it is only related to the final residual state, that is, when the train of shock waves has been attenuated.

The gas pressure component is basically caused because the mixture of air and HE gas products is restrained to expand freely. The HE combustion (detonation and afterburning (AB) reactions) releases a substantial amount of chemical energy which is transformed into internal energy. The detonation and AB energies are gradually ceded to the enclosed gas and converted to internal energy, increasing its temperature and pressure and resulting in a residual QS gas pressure as soon as the gas mixture is quiescent inside the chamber. In the case of partially confined structures, the ventilation allows releasing pressurized gases, thus gradually reducing the total internal energy of the system (releasing mass) and decreasing the gas pressure and temperature until gases are at the same conditions as the external environment.

The combustion of HE involves two processes: (1) the detonation and (2) the AB. The detonation is a super-fast chemical process which involves the reaction of only the own HE's components. In fact, the concentration of oxygen atoms in the HE indicates the oxidation potential during the detonation, and therefore, it is related to the amount of remaining oxygen and/or the still flammable products after the detonation. The oxygen balance (OB) index is commonly employed to categorize the oxidation potential, that is, it accounts for the fraction of molecules of oxygen (O_2) remaining after the oxidation of H, C, S, and so in the production of H_2O , CO_2 , and SO_2 . The OB index is negative (an oxygen deficient HE) if the amount of oxygen in the HE is limited and insufficient to attain the full oxidation. Then, the combustion is not finalized and some detonation products are still flammable (such as C, CO, H_2 , and CH_4). As a consequence, these still flammable HE products will interact with the surrounding oxygen inside the confined or partially confined structure, causing a secondary combustion or AB reaction (Edri et al., 2012). Therefore, the AB process is a set of relatively slow chemical reactions (deflagrations) that occurs just after the detonation reaction and is described by the turbulent oxidation of still flammable detonation products. For example, the trinitrotoluene (TNT, $C_7H_5N_3O_6$) is a very fuel-rich explosive and shows a negative OB index equal to -74% (Edri et al., 2012); therefore, a significant amount of still flammable detonation products will be burnt after the detonation of TNT.

The release of the detonation energy occurs on a time scale of microseconds, and the release of the AB energy occurs on a time scale of milliseconds. The AB is described by a variable rate that depends on the HE expansion, the local temperature, the pressure, and the turbulence, that

is, the interaction between the HE gas products and air (Kuhl, 2010). However, the AB reaction normally does not produce a shock wave, based on the fact that the interaction between the flammable HE gas product and air is generally described by a subsonic combustion, that is, a deflagration process.

The OB index does not provide information about exchange of energy during the explosion; thus, the energy release due to AB and detonation is commonly analyzed by thermo-chemical equilibriums. For example, Cheetah code predicts an energy release equal to 4495 kJ/kg_{TNT} during detonation process and the heat of combustion (detonation+AB energy) is equal to 14,500 kJ/kg_{TNT} in a chamber rich in oxygen, that is, the charge mass to volume ratio, or loading density (m_{TNT} / V_{vessel}) is less than 0.3871 kg TNT/m³ (Edri et al., 2013), where m_{TNT} is the TNT charge mass and V_{vessel} is the vessel volume. Thus, the AB released energy is 10,005 kJ/kg_{TNT}, which is equal to 223% of the detonation energy for chambers rich in oxygen subjected to internal TNT explosions. Note that the inclusion of metal particles (e.g. aluminum (Al) or ammonium perchlorate (AP)) in the HE can significantly enhance the heat release of some explosives due to intense burning of the metal particle during the AB stage; therefore, AB analyses are more important for this kind of thermobaric explosives.

Edri et al. (2013) have shown that the QS gas pressure, which is observed in fully confined vessels subjected to internal explosion of TNT, can be derived by assuming that HE products and air are modeled as a combined gas mixture and a thermodynamics model. That is, the QS gas pressure was obtained by assuming that the final mixture is described by a variable gamma (VG) ideal gas equation of state (EOS) and the combustion was modeled by a constant-volume process (or isochoric process). Then, the chemical balance was derived, concluding that the heat of combustion and detonation product concentrations are function of the loading density. The heat capacity ratio, the final temperature and the total energy release depend also on this ratio. Based on these assumptions, the QS gas pressure derived by the Edri's model has effectively matched the experimental QS gas pressure curve given in the Unified Facilities Criteria's guideline for fully confined chambers (UFC-3-340-02, 2008). Edri et al. (2013) also considered the chemical equilibrium so that the amount of oxygen available in the chamber limits the AB combustion, and a linear mass fraction coefficient was efficiently utilized to account for the AB energy release ratio.

Similarly, Donahue et al. (2013) have studied fully confined TNT explosions using CFD models; they employed a new EOS for the gas products denoted as the AB EOS. This EOS uses a combination of methods, that is, using the classical Jones-Wilkinson and Lee (JWL) EOS in the high-pressure regime and transitioning to a VG EOS at low-pressure range. The authors concluded that a better agreement was obtained for the transient pressure time-history and the QS gas pressure through the utilization of the AB EOS in combination with the VG EOS for air with a simplified mixing model (Donahue et al., 2013). Kuhl (2010) have employed a separate EOS for the detonation products, that is, before AB a JWL EOS is employed, and the combustion products with an ideal gas EOS is used after AB according to an appropriate temperature value based on the thermodynamic state as function of the gas internal energy. Kuhl's model has considered the following: (1) a multi-component gasdynamic conservation law, (2) a fast chemistry model for TNT-air combustion, (3) a thermodynamics model for frozen reactants and equilibrium products, (4) a high-order Godunov method, and (5) implicit large eddy simulation (ILES) approach to capture the energy-bearing scales of the turbulence. In summary, these articles show that a more accurate prediction of the QS gas pressure can be achieved if the final gas mixture (HE products, HE sub-products and air) is simulated according to an appropriate EOS with consideration of the thermodynamic state and the chemical equilibrium for the entire volume or by individual cells according to a combined ideal gas EOS in agreement with the heat capacity ratio associated with the residual mixture.

Despite that these methods give more accurate results based on the fact that they describe the AB according to a physical model, they involve significant computational efforts and are not available in commercial software yet. The simulation of AB reactions involves complex turbulence interaction sub-models which have not been calibrated for all situations and also contain a significant uncertainty. In fact, turbulent combustion models require a deep knowledge on fluid dynamics and chemical reactions which increase the complexity on the utilization of these tools. On the other hand, commercial software packages provide simplified AB methods which can be used with an acceptable certainty and accuracy if they are properly used. Using these commercial packages involves relatively simple mathematics and an affordable calculation time, that is, they can be used more efficiently. The AB energy release modifies the arrival time of the re-reflected pulses and slightly their magnitudes, and also the gas pressure component which is amplified as soon as the AB energy is released. The degree that AB modifies the secondary pulses is related to the AB energy release rate which can be controlled by assuming different reasonable values for design rather than relies on complex turbulent combustion models which also involve uncertainty. The gas pressure component can be appropriately simulated if a correct AB energy value is used in combination with a reasonable AB energy release rate. In other words, simplified AB methods can be used to predict blast loading with a similar accuracy as sophisticated methods provide.

Commercial CFD software packages such as AUTODYN still uses the traditional JWL EOS to simulate detonation of condensed phase explosives; likewise, air is separately modeled by the ideal gas EOS. However, The JWL EOS is not a fundamental equation of thermodynamics, and therefore gives an incomplete specification of states (Kuhl, 2010). For example, the JWL function does not provide information on the product's states when non-isentropic reflections or AB occurs (Kuhl, 2010). On the other hand, AUTODYN provides some simplified approaches such as the Miller Extension (Miller, 1996) or the Additional Energy method which allow increasing gradually the internal energy of the HE gas products in order to include a simplified AB energy release model. Based on these methods, this study establishes an appropriate additional energy value that simulations through AUTODYN software package should employ in order that the QS gas pressure can be accurately simulated. In derivation, the air is assumed to behave isentropically after that the train of shock waves is relatively attenuated. Based on this assumption, the QS gas pressure can be determined from the internal energy equilibrium of "advanced steps," that is, when the kinetic energy is less than 1% of the total energy. Similarly, the additional AB energy can be also related to isentropic work based on the fact that this combustion is described by deflagrative processes; then, the additional energy value can be obtained by the QS equilibrium from simulations without extension methods (or without AB), that is, results for simulation without AB are employed to predict the AB energy value required to derive a reliable QS gas pressure value. The accuracy of the proposed approach in simulating QS gas pressure is verified through comparisons with those defined by UFC's charts and available experimental results.

QS gas pressure

AUTODYN's simulations of HE detonations inside fully confined chambers involve generally two gases, which are separately modeled. They are the medium of propagation, which is usually modeled by the ideal gas EOS (e.g. air), and the gas associated with HE detonation products (e.g. TNT), which is generally described by the JWL EOS.

In a fully confined TNT explosion, the energy of enclosed gases inside a rigid vessel remains constant according to the first law of thermodynamics. That is, gases behave adiabatically without ceding heat to the chamber or surroundings and a negligible volume variation occurs if the chamber behaves as a rigid structure. Therefore, the sum of the internal energy and the kinetic energy of TNT gas products and air is a constant value.

If the chamber is flexible and experiences deformation, the energy conservation is still maintained, but the internal and kinetic energies of the gases should be corrected by taking into consideration the energy associated with the chamber deformation. This will be discussed in section “Highly deformable chambers” of this article. Chambers that will be analyzed from this section to section “Simplified AB energy approach” show that their total energies (internal and kinetic) are two orders of magnitude lower than the energy exhibited by internal gases; thus, these chambers can be considered as rigid in terms of the gas energy conservation analysis, that is, no correction is required. Hence, the following results are applicable to only rigid chambers or chambers with relatively small deformation only. For chambers with relatively large deformations, the results are presented and discussed in section “Highly deformable chambers.”

Based on the gas energy conservation assumption, the total gas energy at any particular time is a constant, that is, it can be calculated from the initial state where only internal energy is assigned to each gas

$$U_{total} = E_0^{TNT} \cdot m_{TNT} + E_0^{air} \cdot \rho_0^{air} \cdot (V_{vessel} - V_0^{TNT}) \quad (1)$$

where U_{total} is the total internal gas energy (kJ), E_0^{TNT} is the initial specific internal energy of TNT products (kJ/kg), m_{TNT} is the TNT charge mass (kg), E_0^{air} is the initial specific internal energy of air (e.g. 2.068E5 J/kg for air at standard temperature and pressure (stp), that is, 298 K and 1 atm), ρ_0^{air} is initial air density (e.g. 0.001225 g/cm³ at stp), V_{vessel} is internal gas volume according to the model (m³), $V_0^{TNT} = m_{TNT} / \rho_0^{TNT}$ is the initial TNT volume (m³), and $\rho_0^{TNT} = 1.63$ g/cm³. Then, the air mass is equal to $m_{air} = \rho_0^{air} \cdot (V_{vessel} - V_0^{TNT})$ (kg).

Note that AUTODYN assumes a default E_0^{TNT} value equal to 3.680982E6 J/kg, which is computed as the ratio between the Chapman–Jouguet (CJ) chemical energy of the explosive ($\varepsilon_{0-CJ}^{JWL} = 6.0E6$ kPa according to the default AUTODYN’s TNT model) and the initial TNT density (ρ_0^{TNT}). Also note that the JWL EOS theory states that ε_{0-CJ}^{JWL} (referenced to the CJ point) is the maximum chemical energy released when HE gas products are expanded to an infinite volume; thus, ε_{0-CJ}^{JWL} is not necessarily equal to the initial internal energy allocated in the TNT gas products (referenced to the initial density, ρ_0^{TNT}). In fact, the initial specific TNT mass energy (E_0^{TNT}) based on the CJ isentropy and the JWL EOS (and AUTODYN parameters) is equal to 3.1961E6 J/kg, which is different from the default TNT parameter proposed in AUTODYN. However, in the course of this research, the default AUTODYN value (i.e. $E_0^{TNT} = 3.680982E6$ J/kg) is used for all the following analyses and simulations. According to Price and Ghee (2009), the detonation energy from AUTODYN models is calculated as $E_{det} = -\Delta E^{TNT} = E_0^{TNT} - E^{TNT}$; therefore, the detonation energy is in agreement with the hydrodynamics method after expansion to standard atmosphere. In that case, the detonation energy tends to the initial TNT internal energy ($E_0^{TNT} = 3.68$ MJ/kg) which disagrees with the heat of detonation according the chemical equilibrium (e.g. 4.495 MJ/kg according to Cheetah code).

Based on the energy and volume conservation assumptions described above, it is concluded that the variation of the internal energy of the two gases during the wave propagation process is opposite (opposite sign) but equal in magnitude. That is, the variation of volume along the interface of these gases is the same and therefore the work done by each gas is the same in magnitude but opposite in sign. That is

$$\Delta U_{TNT} = \Delta W_{TNT} = - \int P dV_{TNT} \quad (2)$$

$$\Delta U_{air} = \Delta W_{air} = -\int PdV_{air} = \int PdV_{TNT} = -\Delta U_{TNT} \quad (3)$$

The work done by gases during a detonation process involves a fast interface contact due to the high particle velocity pattern observed during the train of shock waves; therefore, the work done by gases through their interface is not reversible (i.e. non-isentropic). For this reason, isentropic gas equations are not valid during the time that the trains of shock waves and/or dynamic pressures are predominant. In general, the prediction of the non-isentropic work along the interface is a complex task because of the variable distribution of gases inside the vessel and the reflection process; thus, 3D models such as CFD simulations are generally needed to capture these complex phenomena.

The shock waves are gradually attenuated due to viscous dissipation (non-isentropic work) which transforms the kinetic gas energy to internal gas energy. In other words, the QS gas pressure appears as soon as the kinetic energy (shock waves) is transformed into internal energy, that is, the QS gas pressure is observed once the final gas mixture is quiescent inside the chamber. The non-isentropic work occurs when the shock waves propagate inside the vessel, that is, the dynamic pressure is significant and/or the kinetic gas energy is still important. Therefore, gases can be only modeled according to isentropic equations if the train of main shock waves is considerably attenuated. Therefore, the residual QS gas pressure can be estimated by isentropic equations and AUTODYN results associated with the “advanced time-steps” only. These “advanced time-steps” should satisfy the following two conditions:

1. Time-steps after six shock waves (this condition has been arbitrarily selected and it is not strictly mandatory, that is, it can be ignored as soon as the second condition is satisfied);
2. Time-steps when the total kinetic energy is less than 1% of the total internal energy (this condition is mandatory).

To summarize, the QS gas pressure is calculated according to the following assumptions:

1. Air will behave isentropically after the kinetic gas energy is substantially attenuated, that is, any time which satisfies the “advanced time-steps” conditions can be used to predict the QS gas pressure.
2. The work done by air and TNT gas products should show the same magnitude but opposite sign (conservation of energy).
3. Both gases are subjected to the same QS gas pressure.
4. Gases are described by their respective EOS.

In this study, the JWL EOS for the TNT gas products is employed according to the AUTODYN's default parameters, that is

$$P_{TNT}^{JWL}(v, E^{TNT}) = A \cdot e^{-R_1 v} \cdot \left[1 - \frac{\omega}{v \cdot R_1} \right] + B \cdot e^{-R_2 v} \cdot \left[1 - \frac{\omega}{v \cdot R_2} \right] + \frac{\omega \cdot \rho_0^{TNT} \cdot E^{TNT}}{v}; \quad v = \frac{\rho_0^{TNT}}{\rho^{TNT}} \quad (4)$$

where $A = 3.7377 \cdot 10^8$ kPa, $B = 3.7471 \cdot 10^6$ kPa, $R_1 = 4.15$, $R_2 = 0.9$, and $\omega = 0.35$.

Similarly, the default AUTODYN ideal gas EOS is used for air (with $\gamma_{air} = 1.4$)

$$P_{air}^{ideal}(\rho_{air}, E_{air}) = \rho_{air} \cdot (\gamma_{air} - 1) \cdot E_{air} \quad (5)$$

Figure 1. AUTODYN 3D model, one-eighth fully confined spherical chamber.

As an example, the analysis of a spherical monobloc chamber with a mean radius equal to 1500mm and a thickness of 5.23 mm, made of steel BHW35 and subjected to a spherical TNT charge mass equal to 7.06kg and detonated at its center (Figure 1), is presented. The system is simulated in ANSYS AUTODYN x64 v14.0 (+Beta options). Details about the Finite Element model can be summarized as follows:

1. A bilinear isotropic hardening material is employed (perfect elastic–plastic material) with properties of steel BHW35 (density $\rho_s = 7800 \text{ kgf/m}^3$, bulk modulus $K = 1.644 \cdot 10^8 \text{ kPa}$, shear modulus $G = 8.476 \cdot 10^7 \text{ kPa}$, and yielding strength $\sigma_y = 3.9 \cdot 10^5 \text{ kPa}$).
2. 3D analyses with triple symmetry being employed, that is, only one-eighth of the spherical chamber is analyzed.
3. Cubical multi-material Euler-3D elements of 13.3 mm edge sizes and a total of 1,728,000 elements in the model are employed to simulate gases (note that the simulated QS results are not greatly modified when the mesh has been halved in mesh convergence analysis); the Euler domain size is $1.6 \text{ m} \times 1.6 \text{ m} \times 1.6 \text{ m} = 4.096 \text{ m}^3$.
4. Remapping techniques have been used, that is, an initial one-dimensional (1D) Euler multi-material simulation with a finer mesh (0.2 mm size) has been employed to simulate the initial radial propagation of shock wave, that is, until the first shock wave almost reaches the chamber wall at 0.55 ms after detonation.
5. Shell Lagrange elements are utilized for the chamber (1300 elements).
6. Fully coupled Euler/Lagrange interaction is employed, and the shell thickness was artificially increased to be equal to twice of the Euler element size (i.e. 27 mm) in order to ensure the proper Euler/Lagrange interaction. (Note that the dynamic chamber response is defined according to the original shell thickness, that is, 5.23 mm.)

The numerical results indicate that although the chamber's material is modeled as a perfect elastic–plastic material, it behaved rigidly owing to the large stiffness associated with the breathing mode of the spherical chamber. As a result, the kinetic energy and internal energy associated with the chamber deformation are two orders of magnitude lower than the energy observed for air and TNT gas products; thus, the total gas energy is a constant during each time-step along the simulation. Likewise, the volume variation due to chamber deformation is insignificant in comparison with the initial chamber volume.

Table 1. AUTODYN results for TNT and air gases for an advanced time-step (16.55 ms after ignition).

	Mass (kg)	Volume (m ³)	ρ (kg/m ³)	E (kJ/kg)	P (kPa)	ΔW (kJ)
TNT	7.056	3.861	1.828	1553.3	993.6	-15,013
Air	16.848	9.898	1.702	1173.8	799.2	16,292

TNT: trinitrotoluene.

Figure 2. AUTODYN simulation without afterburning (spherical chamber 7 kg TNT).

Table 1 shows the results obtained from the simulation at 16.55 ms after ignition (Figure 2, without AB), where the average gas densities (ρ) are calculated from the simulated masses and volumes, the average specific internal energies (E) are derived from the ratio between their total internal energies and their respective masses, the pressures are calculated from their respective EOSs (equations (4) and (5)), and the work done by the TNT gas products and the air are calculated, respectively, by

$$\begin{aligned}\Delta W_{TNT} &= \Delta E^{TNT} \cdot m_{TNT} = (E^{TNT} - E_0^{TNT}) \cdot m_{TNT} \\ \Delta W_{air} &= (E_{air} - E_0^{air}) \cdot m_{air} = \frac{P \cdot V_{air} - P_0 \cdot (V_{vessel} - V_0^{TNT})}{\gamma_{air} - 1}\end{aligned}\quad (6)$$

From the results in Table 1, we can conclude that at 16.55 ms after the ignition, gases have not reached the residual QS state yet, that is, works and pressures obtained individually for air and TNT gas products are not the same. On the other hand, we can assume that air will behave isentropically from this “advanced time-step” (i.e. it satisfies the two conditions detailed above); therefore, the QS air volume (V_{air}^{QS}) can be expressed as a function of the absolute QS gas pressure (P_{QS}) and the air absolute pressure and volume obtained for the advanced time-step (AD) ($V_{air}^{AD} = 9.898 \text{ m}^3$ and $P_{air}^{AD} = 799.2 \text{ kPa}$)

$$V_{air}^{QS} = V_{air}^{AD} \cdot \left(\frac{P_{air}^{AD}}{P_{QS}} \right)^{1/\gamma_{air}} \quad (7)$$

Based on this isentropic relationship (equation (7)), a simple iterative procedure is proposed to obtain the QS gas pressure, which is described by the following steps:

1. An arbitrary QS gas pressure value (P_{QS}) is selected (similar to the air pressure value at the selected “advanced step”).
2. The QS air volume (V_{air}^{QS}) is obtained from equation (7).
3. The QS TNT gas product volume (V_{TNT}^{QS}) is obtained from conservation of volume, that is, $V_{TNT}^{QS} = V_{vessel} - V_{air}^{QS}$ (note that chamber behaved as a rigid structure).
4. Gas densities are calculated from masses and QS volumes, that is, $\rho_{TNT}^{QS} = m_{TNT} / V_{TNT}^{QS}$ and $\rho_{air}^{QS} = m_{air} / V_{air}^{QS}$ (air and TNT masses are constant for fully confined vessels).
5. The EOS equations (equations (4) and (5)) are used to determine the specific mass energies (and E_{air}^{QS}) based on the assumed QS pressure and gas densities.
6. Gas works are computed according to equation (6).
7. Gas works should show the same absolute value with opposite sign, otherwise select another QS gas pressure and return to step 1.

Following the example detailed in the course of this section ($m_{TNT} / V_{vessel} = 0.51 \text{ kg/m}^3$), the absolute QS gas pressure (P_{QS}) calculated according to this procedure is equal to 821.8 kPa, the QS air volume (V_{air}^{QS}) is 9.703 m^3 , the QS TNT volume (V_{TNT}^{QS}) is 4.056 m^3 and the interface gas work ($\Delta W_{air} = -\Delta W_{TNT}$) is 16450 kJ (i.e. $\Delta E^{TNT} = 2331 \text{ kJ/kg}_{TNT}$). Note that results obtained by simulations with longer time analysis (e.g. 50 ms) have shown that the QS gas pressure approaches to the value determined through this procedure, that is, results based on the “advanced time-step” at 16.55 ms (Figure 2).

The QS gas pressure is also obtained through the same procedure for the following groups of simulations:

1. Spherical chambers with the same radius ($R = 1500 \text{ mm}$) and different spherical TNT charge masses (7.06, 15.15, 30.05, and 120.08 kg);
2. Spherical chambers with a different radius ($R = 750 \text{ mm}$) and different charge values (0.14, 0.57, 1.14, 2.81, 6.93, and 10.92 kg);
3. Cubical rigid chambers with an edge length equal to 3000 mm and the same group of charges analyzed for chamber with $R = 1500 \text{ mm}$ (7, 15, 30, and 120 kg) (Figure 3).

Table 2 summarizes the results, where t is the actual chamber shell thickness, t_a is the thickness employed for the fully coupled Euler/Lagrange interaction, P_{QS} is the absolute QS gas pressure derived by simulation without AB (i.e. from the advanced time-steps analyses) (Figure 4), $\Delta E^{TNT} = E_{QS}^{TNT} - E_0^{TNT}$ is the TNT release energy at the QS state for simulations without AB (Figure 5), P_{UFC} is the absolute QS gas pressure according to the UFC’s chart (Figure 4), and ΔE_{ad} is the additional AB energy by TNT mass to match the UFC QS gas pressure (Figure 7). The procedure to determine ΔE_{ad} is described in the following section.

Figure 3. AUTODYN 3D model, one-eighth fully confined cubical chamber.

Table 2. Summary of AUTODYN Results and Additional AB energy for Spherical and Cubical Chambers.

m_{TNT} (kg)	t (mm)	t_a (mm)	V_{vessel} (m ³)	m_{TNT} / V_{vessel} (kg/m ³)	P_{QS} (kPa)	ΔE^{TNT} (kJ/kg _{TNT})	P_{UFC} (kPa)	E_{ad} (kJ/kg)
<i>Spherical chambers R=1500 mm</i>								
7.06	5.23	27	13.76	0.51	822	2331	1570	4085
15.15	9.62	27	13.76	1.10	1617	1887	2165	1407
30.05	16.84	27	13.76	2.18	3069	1430	3544	744.3
120.1	54.93	54.93	13.37	8.98	12028	816	11337	—
<i>Spherical chambers R=750 mm</i>								
0.14	0.70	13.40	1.72	0.08	222	3287	461	7974
0.57	1.99	13.40	1.72	0.33	574	2688	1206	5330
1.14	3.44	13.40	1.72	0.66	1027	2167	1693	2816
2.81	7.10	13.40	1.72	1.64	2340	1606	2828	839
6.93	15.35	15.35	1.71	4.04	5541	1140	5975	303
10.92	23.11	23.11	1.69	6.47	8749	948	8732	—
<i>Rigid cubical chambers L=3000 mm</i>								
7.77	—	27	26.28	0.30	526	2987	1134	5738
15.15	—	27	26.28	0.58	918	2573	1652	3559
30.05	—	27	26.28	1.14	1693	2069	2227	1308
120.08	—	27	26.28	4.57	6277	1262	6621	213

All cases have shown that the QS gas pressure is properly obtained from the “advanced time-steps” (kinetic energy is less than 1% of the internal energy). That is, prolonged time simulations have always approached to the value computed by the above procedure.

It should be noted in Table 2 that different chamber wall thicknesses were considered in the analysis; therefore, different chamber deformations are expected. However, these deformations did not affect the gas energy conservation in all the studied spherical chambers indicated in Table 2, implying the spherical chambers have behaved as rigid structures with negligible deformations. Therefore, results associated with chamber structural responses are not shown in the table. In contrast, results of cubical chambers have shown significant deformations when flexible chamber

Figure 4. Quasi-static gas pressure based on AUTODYN simulations.

Figure 5. Detonation energy released by TNT gas products during detonation expansion.

walls were used, which affected the gas energy conservation derived above with rigid chamber wall assumption. Therefore, cubical chamber simulations were performed here with rigid structure assumption for comparison. The results displayed are hence applicable to rigid or almost rigid chamber structures only. The results corresponding to deformable chambers will be presented in section “Highly deformable chambers”.

Figure 4 shows the QS gas pressure obtained through the proposed procedure (in kPa) for all cases mentioned above (spherical and cubical chambers). From Figure 4, it is observed that the QS gas pressure has an almost linear relationship with the charge mass density with a correlation coefficient of $r = 0.99998$.

Figure 4 also shows the QS gas pressure from the UFC guidelines (UFC-3-340-02, 2008) (red curve). The red curve is the Figure 2-152 “Peak Gas pressure by a TNT Detonation in a Partially Contained Chamber” (UFC-3-340-02). Note that the red curve is not shown in logarithmic scale as UFC does, and it is also expressed as an absolute pressure (we have added the atmospheric pressure at sea level, 101.3 kPa, to the overpressure given in UFC). The UFC curve defines the peak gas pressure for the general vented case, associated with QS pressure before venting occurs. This QS gas pressure is also valid when very small ventilation occurs. Therefore, the maximum gas pressure given in UFC is the QS gas pressure corresponding to the fully confined case. Edri et al. (2013) compared the UFC curve with experimental results of TNT confined explosions published by Weibull (1968) and also with the chemical equilibrium approach. They concluded that “it can be seen that a very good agreement is obtained between the results, the UFC curve and the thermodynamic model result for the gas pressure through all range of W/V .” Therefore, it can be concluded that the UFC curve, which is experimentally fitted based on test results of partially vented chambers with small venting areas where the vent properties ranged from $0 \leq A_f/V^{2/3} \leq 0.022$ (UFC-3-340-02, 2008), has been validated against experimental data and theoretical derivations for the fully confined case also.

Differences between AUTODYN (without AB) and UFC predictions could be theoretically corrected using additional energy methods, which should be associated with the AB reaction. As shown in Table 2, AUTODYN simulations without AB underpredict the QS pressure as compared to the UFC values when the mass density is small; therefore, the additional AB energy can be used to correct the QS gas pressure. Nevertheless, the QS pressure is overestimated when $m_{TNT}/V_{vessel} \geq 6.5 \text{ kg/m}^3$, indicating that the additional energy methods are not applicable when charge mass density is higher than this value.

Edri et al. (2013) have determined the QS gas pressure based on the chemical equilibrium of the final mixture, assuming a constant-volume combustion process and a VG ideal gas EOS. Similarly, Edri et al. (2012) have derived a simplified equation for the QS gas pressure based on the energy per unit mass release value (ΔE^{TNT}) and a constant gamma value for the final mixture. In general, authors stated that

the adiabatic index of the detonation products [mixture], γ , was taken as equal to 1.4 which is more suitable for low pressure range [heat of combustion domain or rich oxygen chambers], while for the second range $\gamma = 1.25$ was taken, which is more suitable for high pressure levels [heat of detonation domain or deficient oxygen chambers]. (Edri et al., 2012)

The variation of ΔE^{TNT} and γ depends on the ratio m_{TNT}/V_{vessel} , and it was detailed through the chemical equilibrium analysis (Edri et al., 2013). Figure 4 shows the simplified curve based on the simplified approach derived by Edri et al. (2012) for the QS gas pressure associated with the heat of detonation ($\Delta E_{det}^{TNT} = 4495 \text{ kJ/kg}_{TNT}$), and γ is obtained from Edri’s heat capacity chart (Edri et al., 2013) (blue curve).

The comparison between Edri’s curve and AUTODYN results without AB (linear trend) shows that numerical simulations based on independent EOS for each gas (JWL and ideal gas EOS) are inaccurate to predict the gas pressure as compared to the chemical equilibrium analysis, that is, the heat of detonation and a unique equivalent final gas mixture modeled by an ideal gas EOS with a variable heat capacity ratio (Edri et al., 2012). Furthermore, Figure 5 shows that the chemical

energy released by HE gas products ($\Delta E^{TNT} = E^{TNT} - E_0^{TNT}$) (Price and Ghee, 2009) is less than the initial TNT internal energy because TNT gas products are not expanded to standard atmosphere for the fully confined case. Observe that the detonation energy tends to the initial TNT internal energy when the loading density is zero. As a consequence, the chemical released energy is also not linked to the heat of detonation value that the chemical equilibrium analysis suggests ($\Delta E_{det}^{TNT} = 4495 \text{ kJ/kg}_{TNT}$) (Edri et al., 2012). In other words, direct application of AUTODYN cannot accurately simulate the case without AB when confined explosions occur.

Note that a better agreement between the AUTODYN's curve and the simplified Edri's curve can be obtained by assuming a heat capacity ratio (γ) equal to 1.30. However, the heat capacity ratio for air is 1.40, and it is 1.35 for TNT according to EOSs employed in AUTODYN; thus, this value cannot be justified.

Edri et al. (2013) have also proposed that the absolute QS gas pressure for analysis in AUTODYN with AB (P_{QS}^{AF}) can be estimated from the absolute QS gas pressure obtained from AUTODYN simulations without AB (P_{QS}) through a simplified AB coefficient ($K_{ab} = P_{QS}^{AF} / P_{QS}$), which is calculated as the ratio between the heat of combustion ($\Delta E_{total}^{TNT} = \Delta E_{ad} + \Delta E_{det}^{TNT}$, where ΔE_{ad} is the additional AB energy derived from chemical equilibrium), and the heat of detonation ($\Delta E_{det}^{TNT} = 4495 \text{ kJ/kg}_{TNT}$), that is, $K_{ab} = \Delta E_{total}^{TNT} / \Delta E_{det}^{TNT}$. Therefore, the proposed AB coefficient relies on the following two assumptions: (1) the release of TNT energy per unit of mass (ΔE^{TNT}) obtained from AUTODYN analysis without AB is in agreement with the heat of detonation that the chemical equilibrium analysis provides, and (2) the additional AB energy value (ΔE_{ad}) is consistent with the value that the chemical equilibrium analysis provides. The first assumption is inaccurate as it was discussed above; the second assumption is also incorrect due to the fact that the additional AB energy required to reliably predicting QS gas pressure with AB energy (e.g. UFC gas pressure) is generally smaller than the value provided by the chemical equilibrium analysis as will be discussed in section "Simplified AB energy approach" (Figure 7). Therefore, the AB coefficient based on chemical equilibrium analysis will not lead to accurate predictions due to the fact that AUTODYN employs separate EOS for air and TNT gas products which is in disagreement with the chemical equilibrium assumption (where a unique VG ideal gas EOS is employed for the final mixture). In fact, the ratio between the AUTODYN's curve (black line in Figure 4) and the UFC QS gas pressure (red line in Figure 4) should be a more appropriate AB coefficient; however, this ratio is not a well-defined function because of the high variability of the UFC curve (note that this ratio is less than one for $m_{TNT} / V_{vessel} \geq 6.5 \text{ kg/m}^3$ as we can observe in Figure 4 and discussed above).

Figure 5 shows that the released TNT chemical energy is perceptibly higher for cubical chambers; however, they follow the same trend and values are not significantly different. This difference is because the spherical chambers were modeled with deformable chambers and cubical with rigid chambers. Therefore, a small fraction of the internal energy was absorbed owing to the spherical chamber deformation. Despite that these differences are observed in the TNT chemical energy, the QS gas pressures show the same trend, implying that the error does not affect significantly the QS gas pressure.

Additional energy approach

The AB energy modifies the secondary shock waves due to the fact that the HE gas internal energy is gradually increased during the time (Figure 6). Therefore, the secondary reflected peak pressures are slightly enhanced, and their corresponding arrival times are in the same way reduced. The rate that the AB energy is released defines the degree that the secondary pulses are modified, that is, the train of secondary shock waves is increased as the AB is released faster. However, the

Figure 6. AUTODYN simulations with and without afterburning energy, spherical chamber $m_{TNT}=7$ kg, $R=1500$ mm.

AB energy release rate is usually described by subsonic combustions (deflagrations). Thus, the AB can be commonly considered as a pseudo-static process in comparison to the detonation reaction if normal AB release rates are observed. As a result, the AB energy works mainly as an isentropic process despite the fact that it slightly modifies the secondary shock waves. With this assumption, the final state for the air with additional energy methods can be estimated from the QS air state of simulations without AB. In other words, the QS air volume for simulations with AB energy (V_{air}^{Af}) can be derived by a simple isentropic relationship based on results for the QS air state from models without AB (i.e. the QS air volume and the absolute QS gas pressure, V_{air}^{QS} and P_{QS}) and a reliable absolute QS gas pressure value (with AB), that is, an absolute pressure value in agreement with experimental data (e.g. UFC pressure, P_{UFC}) or another more sophisticated model, such as analyses of the residual gas mixture according to a VG ideal gas EOS (e.g. Edri et al., 2013); therefore

$$V_{air}^{Af} = V_{air}^{QS} \cdot \left(\frac{P_{QS}}{P_{UFC}} \right)^{1/\gamma_{air}} \quad (8)$$

After the AB energy is fully released, we can assume that the work done by the TNT gas products is equal to

$$\Delta W_{TNT} = (E_{TNT} - E_0^{TNT} - \Delta E_{ad}) \cdot m_{TNT} \quad (9)$$

where ΔE_{ad} is the additional specific energy by unit mass released by the HE during the AB reaction (kJ/kg).

Based on the isentropic assumption (equation (8)), it is possible to describe the following procedure to determine the additional energy value in order to use AUTODYN to reliably predict QS gas pressure in confined explosions:

1. Select a reliable experimental or theoretical absolute QS gas pressure (e.g. from UFC's chart for TNT charges, P_{UFC}) (with AB).
2. Calculate the air volume V_{air}^{Af} based on results obtained from simulations without AB (equation (8)).
3. Determine the AB TNT volume from the volume conservation assumption, that is, $V_{TNT}^{Af} = V_{vessel} - V_{air}^{Af}$.
4. Gas densities are calculated by $\rho_{TNT}^{Af} = m_{TNT} / V_{TNT}^{Af}$ and $\rho_{air}^{Af} = m_{air} / V_{air}^{Af}$ (air and TNT masses are constant and equal to the values employed by simulations without AB).
5. The EOSs (equations (4) and (5)) are employed to determine the specific mass energies (E_{TNT}^{Af} and E_{air}^{Af}) from the computed densities and the selected QS gas pressure.
6. From the internal energy conservation criterion, the proper AB energy value is calculated as

$$\Delta E_{ad} = (E_{TNT}^{Af} - E_0^{TNT}) + (E_{air}^{Af} - E_0^{air}) \cdot m_{air} / m_{TNT} \quad (10)$$

It should be noted that the AB energy derived above can be used in AUTODYN to accurately predict more complex confined explosion cases with different chamber stiffness and chamber geometries that are not covered in the UFC or experimental data and empirical relations. For instance, the procedure detailed in this section can be also used when UFC curve is not valid, such as the following: (1) the selected QS gas pressure is different from the UFC value, for example, the experimental one, or another value based on another more accurate model or experimental curve. The user can also choose a design QS gas pressure value different from UFC (e.g. twice of the UFC value); (2) another software package which uses the same physical principles; (3) another kind of HE or a combination of different HEs; (4) another medium of propagation different to air at "stm" condition; (5) when other EOSs are used for the HE or air, for example, the second JWL EOS for TNT that AUTODYN suggests or when different initial internal energies are used; and (6) obtain more accurate values of the additional AB energy when significant numerical errors occur during solution.

Following the example studied in the preceding section and the above steps, the selected absolute gas pressure is obtained from the UFC's chart (for $m_{TNT} / V_{vessel} = 0.51$, Figure 4) and equal to $P_{UFC} = 1570 \text{ kPa}$; then, $V_{air}^{Af} = 6.111 \text{ m}^3$, $V_{TNT}^{Af} = 7.648 \text{ m}^3$, $E_{TNT}^{Af} = 4861 \text{ kJ/kg}$, $E_{air}^{Af} = 1423 \text{ kJ/kg}$, and the AB energy is equal to $\Delta E_{ad} = 4085 \text{ KJ/Kg}$ (Table 2).

Figure 6 shows a comparison between the pressure time-histories obtained with and without additional AB energy. First, we can observe that the QS gas pressure obtained through AUTODYN with the correct additional energy value (i.e. according to the procedure described in this section) gives accurate prediction of (relative error less than 1%) the QS gas pressure estimated according to UFC charts. Second, the pressure time-history has been also computed according to the AB energy value suggested by the chemical equilibrium analysis. That is, the additional energy was estimated by the Edri's approach and equal to the product between the maximum AB energy $10,005 \text{ kJ/kg}_{TNT}$ (for chamber rich in oxygen) and an air/TNT mass fraction factor equivalent to $\mu = 0.775$ (Edri et al., 2013) with the additional energy according to Edri's chemical analysis of 7821 kJ/kg , which is 191% higher than the value predicted in this section. The obtained QS gas pressure according to this AB energy value is equal to 2240 kPa and 43.5% higher than the UFC's value.

Figure 7. Additional afterburning energy for calculation of UFC QS pressures.

Observe that the QS gas pressure value corresponding to the simulation with AB (the appropriate AB value and the value obtained from Edri's approach) was predicted from the "advanced time-steps" (similar to the previous section but including the additional energy value for the calculation of the TNT gas product work). Alternatively, the QS gas pressure associated with any AB energy value can also be predicted from simulations without AB, that is, by employing the same procedure described in this section, but using the AB energy as the known variable and the QS gas pressure as the unknown parameter.

This procedure has been repeated for the set of cases detailed before (spherical and cubical chambers in Table 2), showing that the approach is always effective to establish the appropriate AB energy in order to accurately predict the QS gas pressure. The additional AB energies for all cases are plotted in Figure 7.

The AB process is a complex phenomenon which involves the turbulent interaction between TNT detonation products and air. In fact, few researchers (e.g. Donahue et al., 2013 or Kuhl et al., 2011) have used more sophisticated CFD model in combination with chemical equilibrium and sophisticated EOSs in order to accurately simulate the turbulent combustion of flammable HE gas products. In this study, it is assumed that the AB energy is released linearly, starting just after the arrival of the first shock wave and concluding when the third shock wave has finished to impinge the chamber walls, in agreement with the simplified gas pressure component approach described by Baker et al. (1983) (based on experimental observation) for spherical chambers subjected to centered TNT detonations. In general, the AB energy release rate does not modify the simulation results since it does not cause a significant non-isentropic work (i.e. a very fast release). In other words, the QS gas pressure acting on fully confined vessels is not prominently affected by the AB rate because the final QS state is associated with the residual quiescent equilibrium. However, the AB rate affects the shock wave propagation, that is, the pressure time-history profiles (peak and arrival times of secondary pulses). It should be noted that the utilization of simplified methods requires less computational times, and using reliable AB rates can also lead to accurate prediction of pressure time-history, besides the QS pressure. Using the

simplified methods is more effective than using sophisticated turbulent combustion models which also involve a high level of uncertainties.

Simplified AB energy approach

The previous two sections have described the procedure to estimate the appropriate AB energy value in order that the QS gas pressure can be reliably predicted through AUTODYN simulations of fully confined HE detonation inside rigid vessels (for any type of chamber's geometry). In this section, the additional AB energy value is derived and can be used to accurately predict QS gas pressure.

The final state associated with the QS gas pressure for rigid chambers without AB energy can be described by the following six equations (two equations from mass conservation, one equation from volume conservation, one equation from Internal energy conservation, and two equations from uniform pressure):

$$\text{Mass: } m_{air} = \rho_{air} \cdot V_{air}; \quad (11a)$$

$$m_{TNT} = \rho_{TNT} \cdot V_{TNT};$$

$$\text{Volume: } V_{air} + V_{TNT} = V_{vessel}; \quad (11b)$$

$$\text{Energy: } E_f^{TNT} \cdot m_{TNT} + E_f^{air} \cdot m_{air} = E_0^{TNT} \cdot m_{TNT} + E_0^{air} \cdot m_{air}; \quad (11c)$$

$$\text{Pressure: } P_{QS} = P_{air}^{ideal}(V_{air}, E_{air}); \quad (11d)$$

$$P_{QS} = P_{TNT}^{JWL}(V_{TNT}, E_{TNT})$$

The masses associated with each gas and their respective initial internal energies are known from initial conditions. Therefore, there are seven unknown parameters ($\rho_{air}, \rho_{TNT}, V_{air}, V_{TNT}, E_f^{air}, E_f^{TNT}$ and P_g) and six equations. To solve for these parameters, one more equation or condition is needed. It can be noted in Figure 4 that a linear trend between the QS gas pressure and m_{TNT} / V_{vessel} (without AB) can be assumed for spherical and cubical chambers, which provides another extra equation; then, the system of equations can be solved to determine the unknown variables. A simplified iterative procedure is established to determine the additional AB energy described by the following steps:

1. The QS gas pressure for simulations without AB is estimated from the linear trend, that is, $P_{QS} = 1326.5 \cdot (m_{TNT} / V_{vessel}) + 148.7(\text{kPa})$.
2. V_{air} is assumed (e.g. $V_{air} \in [0.01 - 0.9999999] \cdot V_{vessel}$).
3. $V_{TNT} = V_{vessel} - V_{air}$.
4. ρ_{air} and ρ_{TNT} are obtained from the mass conservation equations.
5. E_{air} and E_{TNT} are obtained from pressure equations.
6. The energy equation is checked (equation (6)); if it is not satisfied, assume another V_{air} value and return to step 2.
7. Based on converged results of the previous iterative steps (i.e. 1–6), associated with the QS equilibrium for the case without AB, the procedure described in the previous section (i.e. steps 1–6) is employed to estimate the additional AB energy.

The additional AB energy (ΔE_{ad}) obtained with the above approach (black line) is shown in Figure 7. This figure also shows the additional AB energy obtained according to the procedure described in the previous sections but without considering the linear approximation and utilizing

direct results from AUTODYN simulations (Table 2). We can conclude that the above approach is reliable in estimating the additional energy based on AUTODYN results without AB; owing to that, the linear trend approximation shows a relatively small error. As we can conclude from Figure 7, results are also insensitive to chamber dimension and geometry (sphere or cube) as well as the charge mass; therefore, this chart can be used directly to determine the additional AB energy for spherical or cubical chambers instead of using the procedure detailed in the previous sections, which involves the computation of a prior AUTODYN simulation without AB. It should be noted that the small variation is due to the UFC curve variability and zero additional energy assumption for $m_{TNT}/V_{vessel} \geq 6.5 \text{ kg/m}^3$. Further studies are required to check the validation of this chart for other chamber geometries.

Figure 7 also compares the current results with those obtained using the AB additional energy according to Edri's chemical equilibrium approach (blue curve) (Edri et al., 2013). As shown, the current results (black line) and Edri's curve (blue curve) show a similar global trend; however, the chemical equilibrium approach always displays AB energy values higher than the results obtained by the procedure described in this article. The proposed curve does not show a plateau for chambers rich in oxygen ($m_{TNT}/V_{vessel} \leq 0.387 \text{ kg/m}^3$). The proposed curve tends to the chemical approach (Edri's curve) when the charge mass density is very low; it occurs because TNT concentration is insignificant and the residual mixture is mainly described by the ideal EOS associated with the air. It is interesting to note that if a factor of 0.5 is applied to the additional AB energy suggested by Edri's chemical equilibrium approach, the two approaches give quite similar predictions when $m_{TNT}/V_{vessel} \geq 0.387 \text{ kg/m}^3$. Therefore, the following simplified equation for AB additional energy based on 50% of that suggested by Edri et al. (2013) is proposed to be used for AUTODYN simulations. It is defined by equation (12) and expressed as the green curve in Figure 7; it should be noted that the proposed additional AB energy equation leads to slightly higher additional AB energy, and therefore a slightly higher QS gas pressure prediction than that given by the UFC's chart

$$\Delta E_{ad} = \frac{10005}{2} \cdot \frac{\text{kJ}}{\text{kg}} \begin{cases} 2 - \frac{m_{TNT}}{V_{vessel}} \cdot \frac{1}{0.387 \text{ kg/m}^3} & , \frac{m_{TNT}}{V_{vessel}} \leq 0.387 \frac{\text{kg}}{\text{m}^3} \\ \frac{0.387 \text{ kg/m}^3}{\left(\frac{m_{TNT}}{V_{vessel}}\right)} & , 0.387 \frac{\text{kg}}{\text{m}^3} < \frac{m_{TNT}}{V_{vessel}} < 6 \frac{\text{kg}}{\text{m}^3} \\ 0 & , 6 \frac{\text{kg}}{\text{m}^3} \leq \frac{m_{TNT}}{V_{vessel}} \end{cases} \quad (12)$$

As it was explained in section "Additional energy approach," the QS gas pressure associated with any additional AB energy can be obtained from the QS equilibrium without AB. That is, the procedure described in section "Additional energy approach" can be inverted to estimate the QS gas pressure associated with any additional AB energy value. Similarly, the QS equilibrium without AB can be estimated with the simplified approach described in section "Simplified AB energy approach," that is, using the linear trend detailed in Figure 4. Therefore, the QS gas pressure associated with (1) the simplified method, (2) analyses without AB energy, (3) Edri's AB energy, or (4) the simplified equation (equation (12)) can be obtained and plotted in Figure 8.

Figure 8. Absolute QS gas pressure obtained with different additional afterburning values.

Figure 9 shows the relative error of the absolute QS gas pressure obtained with the additional AB energy in AUTODYN according to the values proposed by (1) the simplified method (black curve in Figure 7), (2) without additional AB energy, (3) Edri's AB energy, and (4) the Edri's modified equation (equation (12)).

From Figures 8 and 9, one can conclude the following: (1) the simplified method predicts a QS gas pressure in agreement with UFC values at relatively small loading density, but it overpredicts the QS gas pressure when $m_{TNT}/V_{vessel} \geq 6.5 \text{ kg/m}^3$; (2) analysis without AB tends to underestimate significantly the QS gas pressure, showing a maximum error of -52% for oxygen deficient chambers; however, the error is reduced as the detonation energy is substantially higher than the combustion energy for chambers rich in oxygen; (3) Edri's AB energy overestimates significantly the QS gas pressure, for example, it predicts a QS gas pressure 53% higher than the UFC value when $m_{TNT}/V_{vessel} = 0.387 \text{ kg/m}^3$. One can observe that the relative error is smaller than 10% when $m_{TNT}/V_{vessel} \leq 0.07 \text{ kg/m}^3$ because the final gas mixture is mainly governed by the ideal gas EOS associated with air. Similarly, the higher differences are observed when $0.12 \text{ kg/m}^3 \leq m_{TNT}/V_{vessel} \leq 2.19 \text{ kg/m}^3$ where error ranges from 20% to 53% . For high loading densities $m_{TNT}/V_{vessel} \geq 2.19 \text{ kg/m}^3$, the relative error is about 15% – 20% ; (4) the simplified equation (12) shows a maximum relative error of 8.6% , it tends to overestimate slightly the UFC QS gas pressure, and can be used accurately for design.

Examples for using the procedure for two experimental cases are shown in Appendix 1. The first case (Kuhl et al., 1998) refers to Lawrence Livermore National Laboratory (LLNL) test of a fully confined explosion of 875 g of TNT inside a 16.6-m^3 cylindrical tank (radius 1.17 m , height: 3.87 m) that was previously studied by Edri et al. (2013). The second case (Donahue et al., 2013) conducted at Defense R&D Canada Suffield refers to a fully confined explosion of 4 kg of TNT inside a 26-m^3 chamber of 3 m interior diameter and 4.2 m long. These examples are

Figure 9. Percentage relative error of the QS gas pressure according to different additional afterburning methods in AUTODYN.

used to validate the procedure and show advantages of the procedure in comparison to the Chemical approach.

Highly deformable chambers

The effect of highly deformable chambers is associated with two main effects: (1) part of the internal energy is transferred to the chamber strain energy associated with chamber deformation and (2) the chamber's volume grows; thus, the final chamber's volume is not equal to the initial one. For these reasons, the derivation of energy conservation presented in section "QS gas pressure" that neglects the chamber deformation may not give accurate predictions.

The deformation of the chamber depends on several structural factors such as the chamber geometry, the material properties, the elements connections, the damage, and the dynamic response, among others. It also depends on the blast load such as the shock wave distribution, the shock wave pattern, shock wave arrival times, the peak and impulse values associated with each shock wave, and the gas pressure component. In some cases, the internal energy (i.e. elastic, plastic and damage) and the volume variation of the chamber can be theoretically related.

Theoretical derivations of the chamber internal energy are not straightforward in many cases. In this study, the final chamber volume and its internal energy are obtained directly from AUTODYN simulation. It should be noted that the deformation energy of the chamber is associated with only the internal energy at the QS state as the kinetic energy has been already attenuated.

The QS gas pressure that is suggested by experimental curves (such as the UFC's chart) has been commonly determined by tests sustained in highly stiff structures, that is, rigid vessels such as thick monobloc spherical chambers and/or bomb calorimeters (UFC-3-340-02, 2008). In the

same way, most of the chemical equilibrium analyses assume an isochoric combustion (e.g. Edri et al., 2013, or Cheetah software package). The QS gas pressure determined by an isovolumetric process assumption is generally an upper limit for the deformable case. That is, the volume variation causes the enclosed gases to display pressure–volume work which consequently reduces the gas internal energy (pressure and temperature). As a simplified approach to derive the QS gas pressure in highly deformable vessels subjected to internal HE detonations, we modify the QS gas pressure for rigid chambers (P_{UFC}) considering first the effect of gas energy loss and then the effect related to the volume variation. For the derivation, we assume that the final mixture is described by the ideal gas EOS and its respective heat capacity ratio.

Based on the energy conservation law, we can derive the effect of the gas energy loss by assuming that the chamber is isolated from the surroundings. That is, the final gas energy should be equal to the initial internal gas energy (plus the additional AB energy) less the internal energy transformed to the chamber due to deformation. Then, the QS gas pressure variation ($\Delta P^{\Delta U_{chamber}}$) due to only the variation of the internal energy of the chamber ($\Delta U_{chamber}$) is obtained as (i.e. an isochoric process)

$$\Delta P^{\Delta U_{chamber}} = \frac{-\Delta U_{chamber} \cdot (\gamma_{mix} - 1)}{V_{vessel}^0} \quad (13)$$

where γ_{mix} is the heat capacity ratio for the QS mixture and V_{vessel}^0 is the initial vessel volume.

The heat capacity ratio (γ_{mix}) depends mainly on the concentration of reaction products in the final mixture (detonation and AB):

In general, γ_{mix} decreases with increasing temperature and increase with increasing pressure. For the range of temperatures and pressures used in most of these types of calculations ($25^\circ\text{C} < T < 4000^\circ\text{C}$, and $1\text{ bar} < P < 1\text{ kbar}$), the value of γ_{mix} at 15°C and 1 atm can be considered to be constant throughout the range without introducing a significant error. (Edri et al., 2013)

For the case of TNT charges, Edri et al. (2013) have determined the heat capacity ratio for fully confined chambers as a function of the charge mass density (m_{TNT} / V_{vessel}^0). The mentioned Edri's heat capacity ratio is used in this study.

The chamber deformation is generally described by a relatively slow process; therefore, we can assume again that the effect of the chamber volume change is described as an isentropic process. As a result, the theoretical QS gas pressure for deformable chambers (P_{teo}^{DCH}) can be described by

$$P_{teo}^{DCH} = \left(P_{UFC} - \frac{\Delta U_{chamber} \cdot (\gamma_{mix} - 1)}{V_{vessel}^0} \right) \cdot \left(\frac{V_{vessel}^0}{V_{vessel}^f} \right)^{\gamma_{mix}} \quad (14)$$

where V_{vessel}^f is the final chamber volume.

P_{teo}^{DCH} is determined from the experimental/theoretical QS gas pressure (P_{UFC}), and it is modified assuming a simplified approach to account for the energy and volume variation in agreement to the QS mixture modeled as an ideal gas and the chemical equilibrium analysis derived for rigid chambers (Edri et al., 2013). Alternatively, more sophisticated chemical equilibrium models or experimental results (considering the gas energy loss and the volume variation) could be employed to determine the QS gas pressure for deformable chambers. Based on this approach, the obtained P_{teo}^{DCH} is now the objective pressure that matches with the additional AB energy value in AUTODYN (equivalent to P_{UFC} for rigid chambers).

Based on the fact that the chamber deformation occurs slowly in comparison with the shock wave reflection process, we can assume that the QS air volume in highly deformable vessels with AB energy (V_{air}^{Af+DCH}) can be linked to the air volume obtained from simulations with rigid chambers and AB energy (V_{air}^{Af}) according to an isentropic relationship

$$V_{air}^{Af+DCH} = V_{air}^{Af} \cdot \left(\frac{P_{UFC}}{P_{teo}^{DCH}} \right)^{1/\gamma_{air}} \quad (15)$$

Therefore, V_{air}^{Af+DCH} can also be related to the air volume obtained from simulations with rigid chambers and without AB (V_{QS}^{air}). That is, we can substitute equation (8) into equation (15) to obtain

$$V_{air}^{Af+DCH} = V_{air}^{QS} \cdot \left(\frac{P_{QS}}{P_{teo}^{DCH}} \right)^{1/\gamma_{air}} \quad (16)$$

The sum of the QS air and HE gas product volume (V_{air}^{Af+DCH} , V_{TNT}^{Af+DCH}) should be equal to the final chamber volume (V_{vessel}^f)

$$V_{air}^{Af+DCH} + V_{TNT}^{Af+DCH} = V_{vessel}^f \quad (17)$$

According to the conservation of energy, we need to consider also the energy of chamber deformation; therefore

$$\Delta W_{TNT} = \Delta W_{air} + \Delta U_{chamber} \quad (18)$$

where ΔW_{TNT} is described by equation (9), ΔW_{air} is defined by equation (6) and $\Delta U_{chamber}$ is the chamber deformation energy at the QS state.

Based on the above equations and assumptions, a simplified procedure to determine the appropriate AB energy value (ΔE_{ad}^{DCH}) is proposed, in order that AUTODYN gives accurate predictions of the QS gas pressure as compared with the theoretical QS gas pressure for deformable chambers (P_{teo}^{DCH}):

1. Obtain the equilibrium based on simulations without AB and assuming a rigid chamber. Note that steps 1–6 in section “Simplified AB energy approach” can be used to estimate the solution for spherical and cubical chambers. It can be done using a rigid material in AUTODYN.
2. Assume a value for the chamber deformation energy ($\Delta U_{chamber}^*$) and the final volume (V_{vessel}^{f*}). As a first attempt, these values can be estimated from simulations for the deformable chamber and without AB energy. Alternatively, these results can also be obtained by simulations of deformable chambers with the additional AB energy derived for rigid chambers (sections “Additional energy approach” and “Simplified AB energy approach”). The asterisk symbol has been employed to indicate that these values change iteratively (point IX).
3. The QS gas pressure for deformable chambers (P_{teo}^{DCH}) can be obtained from the simplified theoretical equation (equation (14)) or by another accurate chemical equilibrium or experimental data.
4. The QS air volume (V_{air}^{Af+DCH}) is determined from the results of rigid chamber analyses without AB (point I and equation (16)). Alternatively, it can be estimated from analysis or simulations with a specific AB value (e.g. the additional AB energy derived for rigid chambers) (equation (15)).

5. Calculate the TNT volume from equation (17). That is, $V_{TNT}^{Af+DCH} = V_{vessel}^{f*} - V_{air}^{Af+DCH}$.
6. Gas densities are calculated by $\rho_{TNT}^{Af+DCH} = m_{TNT} / V_{TNT}^{Af+DCH}$ and $\rho_{air}^{Af+DCH} = m_{air} / V_{air}^{Af+DCH}$ (air and TNT masses are constant and equal to values employed by simulations without AB).
7. The EOSs (equations (4) and (5)) are employed to determine the specific mass energies (E_{TNT}^{Af+DCH} and E_{air}^{Af+DCH}) from the computed densities and the selected QS gas pressure (P_{teo}^{DCH}).
8. From the internal energy conservation criterion, the proper AB energy value is calculated as

$$\Delta E_{ad}^{DCH} = (E_{TNT}^{Af+DFC} - E_0^{TNT}) + (E_{air}^{Af+DFC} - E_0^{air}) \cdot m_{air} / m_{TNT} + \Delta U_{chamber}^* / m_{TNT} \quad (19)$$

9. The simulation should be carried out with the additional AB energy estimated by equation (19). If the chamber deformation energy ($\Delta U_{chamber}$) and/or the final volume (V_{vessel}^f) is/are significantly different from the values assumed in step II, it is required to return to step II and repeat the analysis with the new values in order to improve the prediction accuracy.

Figure 7 shows that ΔE_{ad}^{DCH} is generally smaller than the value determined with rigid chamber assumptions. Therefore, $\Delta U_{chamber}$ and V_{vessel}^f determined from deformable chamber analyses should show intermediate values between the case without AB and the case with the AB energy value derived for rigid chambers (ΔE_{ad}). Likewise, the AB energy for deformable analysis (ΔE_{ad}^{DCH}) is overestimated when the assumed $\Delta U_{chamber}$ and V_{vessel}^f values (smaller than case with AB) are based on analyses without AB. Therefore, the resultant QS gas pressure will be slightly higher than P_{teo}^{DCH} if the $\Delta U_{chamber}$ and V_{vessel}^f values are effectively higher for the case with AB energy. Hence, $\Delta U_{chamber}$ and V_{vessel}^f computed without AB energy can be considered as conservative, resulting generally in a slightly higher QS gas pressures. On the other hand, the iterative process described in step IX can be done to improve the prediction accuracy.

Example of deformable chamber procedure

The procedure for deformable chambers discussed in this section is applied to almost the same example analyzed in previous sections. That is, the same conditions and parameters are utilized; however, the material yielding strength is significantly reduced to $\sigma_y = 1.5 \cdot 10^5$ kPa in order to increase the chamber's plastic deformation and generates a significant volume variation. Additionally, the one-eighth volume domain has been expanded from 1.6 to 2.5 m because the chamber's radial deformation is larger than 10 cm for this deformable case. Moreover, larger Euler Elements are employed, with edge lengths equal to 20 mm, leading to a total of 1,953,125 Euler elements to cover the Euler's volume in the numerical model.

Because of the remapping process, the computed TNT mass is equal to $m_{TNT} = 7.765$ kg (different from the 7.06 kg obtained for 13.3 mm side length Euler blocks). Note that the Euler elements can be reduced in order to improve accuracy of the charge mass value; however, this step has been avoided because it is possible to work directly with the remapped value, and the difference in charge mass would not affect the observations and discussions on the simulated results. The internal air mass is estimated to be equal to $m_{air} = 16.849$ kg and the initial vessel volume, $V_{vessel}^0 = 13.759$ m³ ($t_a = 27$ mm) (or 14.063 m³ considering the real shell thickness, $t = 5.23$ mm). The analyses and the result are discussed below:

Figure 10. Simulation results for the deformable chamber with the appropriate afterburning energy, (a) kinetic energy of different materials, (b) internal energy of different materials, (c) chamber radial displacement, and (d) pressure time-histories at different points inside the chamber.

1. Based on the procedure described in section “Simplified AB energy approach” which relies on the linear QS gas pressure obtained for rigid fully confined spherical/cubical chambers, the QS equilibrium is obtained for the analysis without AB. That is, the QS gas pressure is calculated through the linear trend (Figure 4) and equal to $P_{QS} = 897.3 \text{ kPa}$ (step I). After that, the QS air volume is iteratively obtained to ensure the energy equilibrium, $V_{air}^{QS} = 10.010 \text{ m}^3$ (step II) and $V_{TNT}^{QS} = 3.749 \text{ m}^3$ (step III). The QS densities are obtained as $\rho_{air}^{QS} = 1.683 \text{ kg/m}^3$ and $\rho_{TNT}^{QS} = 2.071 \text{ kg/m}^3$ (step IV). Then, the QS internal energies are $E_{TNT}^{QS} = 1237.9 \text{ kJ/kg}$ and $E_{air}^{QS} = 1332.7 \text{ kJ/kg}$ (step V). Note that the chemical released energy is equal to $\Delta E^{TNT} = 2443 \text{ kJ/kg}_{TNT}$. It should be noted that all these values are similar to the results reported in section “QS gas pressure.”
2. Based on the iterative results (see point IX), the internal energy transferred to the chamber deformation is $\Delta U_{chamber} = 8016 \text{ kJ}$ and the final chamber volume is $V_{vessel}^f = 23.851 \text{ m}^3$. These values are directly obtained from AUTODYN simulation associated with an advanced time-step (25 ms) (Figure 10); this advanced time-step (25 ms) can be assumed as the equivalent QS state (note that kinetic energies are

- substantially attenuated at this time, Figure 10(a)). The internal energy associated with the chamber material (BHW35) at 25 ms is $\Delta U_{chamber}$ (Figure 10(b)) and multiplied by 8 to account for the whole spherical chamber. The final volume is derived from the residual displacement (Figure 10(c)) $d_{res} = \Delta R = 299.2 \text{ mm}$, assuming that the chamber keeps its spherical shape (in agreement with the observed final deformed geometry). It should be noted that material failure and/or erosion have not been considered.
3. The QS gas pressure for the deformable chamber is obtained from the simplified theoretical equation ($P_{teo}^{DCH} = 632.6 \text{ kPa}$) (equation (14)), assuming that the heat capacity ratio for the final mixture is $\gamma_{mix} = 1.355$ according to Figure 12 reported by Edri et al. (2013) corresponding to a charge mass density $m_{TNT} / V_{vessel}^0 = 0.034 \text{ lb / ft}^3$. Similarly, the QS gas pressure obtained from the UFC chart is equal to $P_{UFC} = 1529 \text{ kPa}$ (UFC-3-340-02, 2008) associated with a charge mass density $m_{TNT} / V_{vessel}^0 = 0.552 \text{ kg / m}^3$. Note that the pressure change due to the gas internal energy loss is $\Delta P^{\Delta U_{chamber}} = -202.3 \text{ kPa}$ (equation (13)).
 - 4–8. The air volume for the QS state inside the deformable chamber is calculated from equation (16), $V_{air}^{Af+DCH} = 12.848 \text{ m}^3$. The TNT gas volume is calculated from equation (17) as $V_{TNT}^{Af+DCH} = 11.004 \text{ m}^3$. The air and TNT densities are $\rho_{air}^{Af+DCH} = 1.311 \text{ kg / m}^3$ and $\rho_{TNT}^{Af+DCH} = 0.620 \text{ kg / m}^3$, respectively. Therefore, the internal energy for air and TNT gas products are $E_{air}^{Af+DCH} = 1206.0 \text{ kJ / kg}$ and $E_{TNT}^{Af+DCH} = 2561.5 \text{ kJ / kg}$. Finally, the additional AB energy required for the deformable case is computed through equation (19) as $\Delta E_{ad}^{DCH} = 2081 \text{ kJ / kg}_{TNT}$. Note that $\Delta U_{chamber} = 8016 \text{ kJ}$ and $V_{vessel}^f = 23.851 \text{ m}^3$ (detailed in point II) have been computed according to the additional AB energy iteratively obtained (see point IX).

As we can observe in Figure 10(d), the pressure time-history for different points inside the chamber effectively approaches the QS gas pressure value determined by the simplified approach (i.e. $P_{teo}^{DCH} = 632.6 \text{ kPa}$). Therefore, the presented procedure has been effective to reliably predict the QS gas pressure.

As a comparison, the additional AB energy is estimated according to the same procedure, but based on the two extreme cases (without iterations). First, the simulation is run without AB energy. In this case, the chamber's internal energy and the final chamber's volume are obtained as $\Delta U_{chamber}^* = 1571.2 \text{ kJ}$ and $V_{vessel}^{f*} = 15.346 \text{ m}^3$, respectively. Then, the additional AB energy is estimated according to the above steps II–VIII and it has $\Delta E_{ad}^{DCH} = 2876 \text{ kJ / kg}_{TNT}$, which is 38% higher than the iterated value. Re-performing the simulation according to the derived additional AB energy value, the chamber's internal energy and the final volume are significantly increased and new iterations then should be carried out (point IX). Note that for this extreme case, the correct QS gas pressure is equal to $P_{teo}^{DCH} = 1285.9 \text{ kPa}$ (equation (14)), but the QS gas pressure obtained at the end of the simulation is different and equal to 765.5 kPa . In the second case, $\Delta U_{chamber}^* = 17,672 \text{ kJ}$ and $V_{vessel}^{f*} = 45.923 \text{ m}^3$ are computed from simulations if the additional AB energy used in the simulation is determined through the rigid chamber approach ($\Delta E_{ad} = 3130 \text{ kJ / kg}$, Figure 7). In this case, the deformable chamber additional AB energy value is estimated (steps II–VIII) to be equal to $\Delta E_{ad}^{DCH} = 1415 \text{ kJ / kg}_{TNT}$ (32% less than the iterated value). If we perform the simulation with this obtained additional energy value, the chamber's internal energy and final

volume are considerably smaller, implying the iterative procedure should be applied to improve the prediction accuracy (point IX). It should be noted that for the second case considered here, the correct QS gas pressure is equal to $P_{teo}^{DCH} = 209.6 \text{ kPa}$ (equation (14)), but the calculated QS gas pressure is about 313.0 kPa at the end of the simulation.

We can conclude from these two examples that highly deformable chambers are very susceptible to the QS gas pressure, that is, the final deformation and the chamber volume are largely sensitive to the additional AB energy value. Therefore, the iterative procedure needs to be carried out when analyses and designs of highly deformable chambers are performed. This result is in agreement with conclusion discussed by authors in previous studies that show that the QS gas pressure should be properly considered when highly deformable chambers are studied (Hernandez et al., 2014). As it was mentioned above, the case without AB can be considered as a conservative assumption because it implies higher additional AB energy estimation, but it is smaller than the AB energy derived with the rigid chamber assumption.

The rigid chamber analysis (Figure 7 or section “Simplified AB energy approach”) indicates that the additional AB energy should be equal to $\Delta E_{ad} = 3130 \text{ kJ/kg}$ (or 3432 kJ/kg according to equation (12)). Likewise, the chemical equilibrium derivation suggests a value equal to 6865 kJ/kg. All these values are greater than 150% of the value estimated for the deformable case (2081 kJ/kg). Therefore, Figure 7 should not be used for highly deformable chambers. Note that equations (15)–(18) can be employed to determine the QS gas pressure in the deformable chamber using the AB energy derived with the rigid chamber assumption of 313 kPa, which is 49% higher than that derived by the simplified approach. However, Figure 7 or equation (12) can be used conservatively for chamber designs despite that they are not accurate for highly deformable chambers.

The boundary for deriving the additional AB energy with the rigid chamber assumption is not straightforward to define. As it has been discussed, the QS gas pressure for deformable chambers changes due to two phenomena: the energy loss and the volume growth. In the previous sections, it has been discussed that spherical chambers (with the original yielding strength) that show limited ductility (ductility ratio less than 7.0; Hernandez et al., 2014) have behaved as rigid structures, owing to the chamber deformation energy being less than 1% of the energy of the enclosed gases. If we compare equations (19) and (10), it can be concluded that the last term associated with the chamber’s energy is apparently the difference between the deformable case and the rigid chamber; this fact could support that the boundary can be defined in terms of an energy percentage. Nevertheless, the volume variation also plays an important role. Therefore, both parameters, that is, the chamber energy and the chamber volume variation, should be considered in order to establish the limit. For example, there are structures which can show significant volume variation but not absorbing a significant amount of deformation energy. A boundary could be directly defined in terms of the QS gas pressure variation between the deformable and the rigid case. It is suggested that $(P_{UFC} - P_{teo}^{DCH}) / P_{UFC} < 5\%$ is used if the rigid chamber assumption is accurate, that is, the chamber deformation could be ignored. Likewise, rigid chambers should show that the estimation of the AB energy (equation (19)), calculated when the internal energy and final volume are computed from the simulation considering the additional AB energy according to the rigid chamber assumption (Figure 7 or section “Simplified AB energy approach”), is not significantly different from the AB energy defined for the rigid chamber (Figure 7 or section “Simplified AB energy approach”). In other words, iterations are not required for rigid chambers because the AB energy for the deformable case (equation (19)) and the rigid case (equation (10)) should not differ significantly (see point IX) (e.g. $(\Delta E_{ad} - \Delta E_{ad}^{DCH}) / \Delta E_{ad} < 5\%$).

Conclusion

It was found that the AUTODYN's QS gas pressure (without additional energy methods) does not coincide with thermo-chemical equilibrium, that is, the released chemical energy according to JWLEOS is lower than the heat of detonation energy. Therefore, thermo-chemical AB energy values should not be used by software packages which do not accurately model the final gas mixture.

It was found that the AUTODYN's QS gas pressure for chambers subjected to TNT explosions and without AB follows a linear relationship with the charge mass density. Based on the assumption that the AB energy works isentropically, a methodology to determine the appropriate AB energy was described in order that AUTODYN model with additional energy methods reliably predicts QS gas pressure.

A simplified AB energy approach was established for spherical/cubical vessels subjected to TNT explosions based on the QS equilibrium and the linear trend observed for simulations without AB. The AB energy value can be calculated as half of the value proposed by the chemical equilibrium analysis. The AB energy suggested by the chemical approach is in agreement with the appropriate additional energy value when mass densities are very small ($m_{TNT} / V_{vessel} \leq 0.07 \text{ kg/m}^3$). A simplified procedure was also proposed to determine the appropriate AB energy for accurately simulating QS gas pressure in highly deformable chambers. In general, the additional AB energies required for deformable chambers are smaller than the values for rigid chambers.

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References

- Baker WE, Cox PA and Westine PS (1983) *Explosion Hazards and Evaluation*, vol. 5. Amsterdam: Elsevier Scientific Publishing Company.
- Beshara FBA (1994) Modelling of blast loading on aboveground structures—II. Internal blast and ground shock. *Computers & Structures* 51: 597–606.
- Donahue LK (2008) *Afterburning of TNT Detonation Products in Air*. Halifax, NS: Dalhousie University.
- Donahue LK, Zhang F and Ripley R (2013) Numerical models for afterburning of TNT detonation products in air. *Shock Waves* 23: 559–573.
- Edri I, Feldgun VR, Karinski YS, et al. (2012) On blast pressure analysis due to a partially confined explosion: III. Afterburning effect. *International Journal of Protective Structures* 3: 311–332.
- Edri I, Feldgun VR, Karinski YS, et al. (2013) Afterburning aspects in an internal TNT explosion. *International Journal of Protective Structures* 4: 97–116.
- Hernandez F, Hao H and Abdel-jawad M (2014) On the effectiveness of ventilation in high explosive storage chambers to mitigate blasting effects. In: *6th international conference on protection of structures against hazards*, Tianjin, China, 16–17 October.

- Kuhl AL (2010) Thermodynamic states in explosion fields (LLNL-CONF-425882). In: *14th international detonation symposium*, pp. 1–4. Available at: <https://e-reports-ext.llnl.gov/pdf/388882.pdf>
- Kuhl AL, Bell JB, Beckner VE, et al. (2011) Gasdynamic model of turbulent combustion in TNT explosions. *Proceedings of the Combustion Institute* 33: 2177–2185.
- Kuhl AL, Forbes J, Chandler J, et al. (1998) *Confined Combustion of TNT Explosion Products in Air*. Schaumburg, IL: Lawrence Livermore National Laboratory.
- Miller PJ (1996) A reactive model with coupled reaction kinetic for detonation and combustion in non-ideal Explosives. *MRS Online Proceedings* 418. Available at: <http://journals.cambridge.org/action/displayAbstract?fromPage=online&aid=8050637>
- Price MA and Ghee AH (2009) Modeling for detonation and energy release from peroxides and non-ideal improvised explosives. *Central European Journal of Energetic Materials* 6: 239–254.
- UFC-3-340-02 (2008) *Structure to resist the effects of accidental explosions*. U.S. Departments of the Army, Navy and Air Force. Available at: https://www.wbdg.org/ccb/DOD/UFC/ufc_3_340_02.pdf
- Weibull HRW (1968) Pressures Recorded in Partially Closed Chambers at Explosion of TNT Charges (U). *Annals of the New York Academy of Sciences* 52(1):357–361

Appendix

Validation with experimental data

Two experimental tests are simulated here to demonstrate the validity of the proposed method. The first is the Lawrence Livermore National Laboratory (LLNL) test (Kuhl et al., 1998) of a fully confined explosion with 875 g of trinitrotoluene (TNT) exploding inside a 16.6-m³ cylindrical tank (radius: 1.17 m, height: 3.87 m). This example was also studied by Edri et al. (2013). The second is a test conducted at Defense R&D Canada Suffield (Donahue et al., 2013). It is a fully confined explosion of 4 kg TNT inside a 26-m³ cylindrical vessel with ellipsoidal heads (3 m internal diameter, 4.2 m long) closed explosion chamber.

LLNL test. This example corresponds to a very low TNT mass density, that is, $m_{TNT} / V_{vessel} = 0.053 \text{ Kg} / \text{m}^3$. Therefore, differences between the chemical approach and the proposed procedure are not significant (see Figure 7).

Section “QS gas pressure” gives the procedure to determine the QS gas pressure from analysis without afterburning (AB) based on results obtained from “advanced time-steps.” Alternatively, one can use the linear trend provided in Figure 4, which gives $P_{QS} = 1326.5 \cdot 0.053 + 148.7 = 218.6 \text{ kPa}$. This quick calculation may induce a small error when compared with the AUTODYN simulation without AB. Note that AUTODYN simulation gives $P_{QS} = 189.4 \text{ kPa}$.

Using $P_{QS} = 218.6 \text{ kPa}$, the QS equilibrium is obtained using the procedure described in section “Simplified AB energy approach” (steps 1–6), where $V_{air}^{QS} = 16.59886 \text{ m}^3$, $V_{TNT}^{QS} = 1.141 \cdot 10^{-3} \text{ m}^3$, $\rho_{air}^{QS} = 1.22504 \text{ kg} / \text{m}^3$ ($m_{air} = 20.334 \text{ kg}$), $\rho_{TNT}^{QS} = 767.0 \text{ kg} / \text{m}^3$, $E_{air}^{QS} = 446.1 \text{ kJ} / \text{kg}$ and $E_{TNT}^{QS} = -1881 \text{ kJ} / \text{kg}$, then the energy equation is satisfied (equation (6)). This result shows that the QS pressure (without AB) is so small that the QS air volume is practically equal to the vessel volume, then we can assume that $V_{air}^{QS} = V_{vessel} = 16.6 \text{ m}^3$ and $P_{QS} = 218.6 \text{ kPa}$ to estimate the additional AB energy.

After obtaining the QS equilibrium, the procedure described in section “Additional energy approach” (steps 1–6) is employed to determine the additional AB energy. The absolute Unified Facilities Criteria (UFC) pressure could be selected from the UFC chart (Figure 2-152) of $P_{UFC} = 355.3 \text{ kPa}$ as a reference, or from other references; for example, we can also use the experimental QS gas pressure which is approximately equal to $P_{exp} = 387 \text{ kPa}$ (according

Figure 11. Pressure and impulse time-history comparison between experimental results, analysis without afterburning and with chemical afterburning ($\Delta E_{ad} = 10,005 \text{ kJ/kg}$).

to re-digitalized data, Figure 11). It is observed that the experimental and UFC values are very similar. Following the procedure, if we use P_{UFC} , we obtain that $\Delta E_{ad} = 9072 \text{ kJ/kg}$; if we use P_{exp} , it has $\Delta E_{ad} = 10,696 \text{ kJ/kg}$. If we use the simplified equation (equation (12)), $\Delta E_{ad} = 9324 \text{ kJ/kg}$.

This example is related to a rich-in-oxygen case ($m_{TNT} / V_{vessel} \leq 0.384 \text{ kg/m}^3$); therefore, the AB energy according to the chemical equilibrium can be calculated as $\Delta E_{ad} = 10,005 \text{ kJ/kg}$ (Edri et al., 2013). Using the QS equilibrium, this additional energy implies a QS gas pressure (with AB), $P_{QS}^{Edri} = 373 \text{ kPa}$.

There is no perceptible difference between the chemical equilibrium approach and the proposed methodology in this example because the selected experiment is related to a small TNT mass density. Therefore, the additional AB energy derived from the chemical equilibrium can be used.

A two-dimensional (2D) axisymmetric model was developed in AUTODYN v14.0 (Figure 12) replicating the model which was described by Kuhl et al. (1998) (note that photographs show that tank heads were not flat as the 2D model assumed). The simulation was computed for two cases: without AB and with the AB derived by the Chemical approach ($\Delta E_{ad} = 10,005 \text{ kJ/kg}$). Analyses with the proposed additional energy were not performed because there is no perceptible difference with the chemical approach for this case. Square $5 \text{ mm} \times 5 \text{ mm}$ computational fluid dynamics (CFD) elements were employed and solved with the Euler (2D Multi-material) solver. Chamber was assumed rigid and boundary conditions were chosen as perfect reflective. The AB energy was released linearly from 0.65 to 5 ms.

Figure 11 compares the pressure and impulse time-history obtained from simulations (without and with AB) and the experimental results (Kuhl et al., 1998). Overall, it is observed that analyses with the Chemical AB energy (or the proposed method) are in agreement with experimental data. According to numerical results, QS gas pressures were 189.4 kPa for case without AB and 345.2 kPa for case with AB, similar to the experimental one (387 kPa).

The simulation confirms numerical results obtained by Edri et al. (2013) and shows that the chemical approach leads to accurate prediction when small TNT mass densities are used. That is, the LLNL test and the Naval Civil Engineering Laboratory (NCEL) tests, associated with $m_{TNT} / V_{vessel} = 0.053 \text{ kg/m}^3$ and $m_{TNT} / V_{vessel} = 0.065 \text{ kg/m}^3$, respectively, match experimental data with $\Delta E_{ad} = 10,005 \text{ kJ/kg}$ as Edri et al. (2013) suggested.

Figure 12. 2D axisymmetric model and pressure profile at 100 ms for case without afterburning and with chemical additional afterburning ($\Delta E_{ad} = 10,005 \text{ kJ/kg}$).

Defense R&D Canada Suffield test. This second example is related to a relatively higher TNT charge mass density, $m_{TNT} / V_{vessel} = 0.154 \text{ kg/m}^3$; therefore, differences between the proposed additional AB energy and the chemical approach can be observed (Donahue et al., 2013).

Section “QS gas pressure” indicates the procedure to determine the QS gas pressure from analysis without AB based on results obtained from “advanced time-steps.” Alternatively, we can use the linear trend given in Figure 4, which gives $P_{QS} = 1326.5 \cdot 0.154 + 148.7 = 352.8 \text{ kPa}$. AUTODYN results without AB give $P_{QS} = 381 \text{ kPa}$, which is not significantly different from the linear trend proposed in this study.

Using $P_{QS} = 352.8 \text{ kPa}$, the QS equilibrium is obtained with the procedure described in section “Simplified AB energy approach” (steps 1–6), where $V_{air}^{QS} = 25.988 \text{ m}^3$, $V_{TNT}^{QS} = 1.159 \cdot 10^{-2} \text{ m}^3$, $\rho_{air}^{QS} = 1.22543 \text{ kg/m}^3$ ($m_{air} = 31.847 \text{ kg}$), $\rho_{TNT}^{QS} = 345.1 \text{ kg/m}^3$, $E_{air}^{QS} = 719.7 \text{ kJ/kg}$, and $E_{TNT}^{QS} = -402.8 \text{ kJ/kg}$, then the energy equation is satisfied (equation (6)). This result shows that the QS pressure (without AB) is so small that the QS air volume is practically equal to the vessel volume, then we can assume that $V_{air}^{QS} = V_{vessel} = 26.0 \text{ m}^3$ with $P_{QS} = 352.8 \text{ kPa}$ to estimate the additional AB energy.

After evaluating the QS equilibrium, the additional AB energy is determined following the procedure described in section “Additional energy approach” (steps 1–6). From the UFC chart (Figure 2-152), it is found that $P_{UFC} = 714.6 \text{ kPa}$. Following the procedure described in section “Additional energy approach,” we can obtain $\Delta E_{ad} = 6942.6 \text{ kJ/kg}$. Based on the simplified equation (equation (12)), $\Delta E_{ad} = 8018 \text{ kJ/kg}$. It should be noted that if the QS pressure obtained from the AUTODYN simulation without AB $P_{QS} = 381 \text{ kPa}$ and the experimental pressure ($P_{exp} = 691 \text{ kPa}$) are used, the estimated additional energy is equal to $\Delta E_{ad} = 6544.1 \text{ kJ/kg}$.

This example refers to a chamber rich in oxygen ($m_{TNT}/V_{vessel} \leq 0.384 \text{ kg/m}^3$); therefore, the AB energy can be calculated according to the chemical equilibrium as $\Delta E_{ad} = 10,005 \text{ kJ/kg}$ (Edri et al., 2013). Using the estimated QS equilibrium, the QS gas pressure (with AB) is $P_{QS}^{Edri} = 882.9 \text{ kPa}$ when the chemical approach energy is used. Therefore, differences between the chemical approach and the procedure described in this article are prominent.

The simulation was run in AUTODYN-2D v14.0; the original problem was simplified and some geometrical details have been assumed. These simplifications and assumptions are summarized as follows: (1) the charge was simplified as a spherical charge, ignited on its center, and located in the center of the chamber. The experimental charge was cylindrical (diameter-to-height ratio approximately 1.0) and initiated at the top end by a RP83 detonator (Donahue et al., 2013), and the cylindrical charge was oriented perpendicular to the longitudinal axes of the chamber. Therefore, an axisymmetric model for efficient simulation is not exact as compared to the experimental test. (2) Details of the head geometry or the nozzle were not provided in Donahue et al. (2013) and Donahue (2008); therefore, the nozzle was ignored in the numerical model. (3) Ellipsoidal heads were assumed in order that actual chamber volume, internal radius, and chamber longitudinal dimension are maintained (according to information provided by the authors). These simplifications and assumptions affect mainly the train of reflected waves; however, the QS gas pressure should not be modified by them because it is related to the QS equilibrium (when shock waves are mitigated); therefore, the simulated reflected shock wave peaks will not match the experimental measurements.

Based on these assumptions, an axisymmetric 2D model was created. Square $5 \text{ mm} \times 5 \text{ mm}$ CFD elements were employed and solved with the Euler (2D Multi-material) solver. The chamber was modeled with a rigid material. One-dimensional (1D) wedge model was used to model the first shock wave just before it impinges on the chamber walls in order to improve the simulation accuracy and reduce computational time. 1D results were remapped to the 2D axisymmetric model at 0.684 ms. AB energy was released linearly from 0.784 to 7.684 ms; these times were selected from inspection of the experimental data.

Three simulations have been performed with different additional AB energy values: (1) without AB, (2) according to chemical approach $\Delta E_{ad} = 10,005 \text{ kJ/kg}$, and (3) the additional energy estimated according to the procedure proposed in this study $\Delta E_{ad} = 6942.6 \text{ kJ/kg}$. Figure 13 shows the comparison of the modeled and experimental pressure time-history (at point P3; Donahue et al., 2013). From the results, it is evident that simulations with the proposed additional energy value better match the experimental results.

The QS gas pressure was obtained for each simulation and equal to (1) 381.0 kPa, (2) 925.2 kPa, and (3) 757.3 kPa, respectively. Figure 14 shows the pressure distribution at 100 ms for the three simulations which represent the QS state.

These simulations showed that the total energy was increased during the time due to numerical error during the solution, which has caused the QS gas pressure for the case with the proposed AB (757.3 kPa) not exactly equal to the UFC value (714.6 kPa) or the experimental value (692.7 kPa). Similarly, an increase of energy due to numerical error in the solution was observed for case without AB which may explain that the QS gas pressure without AB (381 kPa) has not perfectly matched

Figure 13. Pressure time-history comparison of (a) experimental and simulation without afterburning $\Delta E_{ad} = 0$, (b) experimental and analysis with chemical afterburning energy $\Delta E_{ad} = 10,005 \text{ kJ/kg}$, (c) experimental and simulation with proposed afterburning energy $\Delta E_{ad} = 6942.6 \text{ kJ/kg}$, and (d) impulse comparison of all analyses.

the linear trend (352.8 kPa). Nonetheless, the proposed procedure leads to better predictions of QS pressure in fully confined explosions.

Figure 14. Comparison of pressures at 100ms (near the QS state) for three cases: (1) without afterburning, (2) $\Delta E_{ad} = 6942.6 \text{ kJ/kg}$ (proposed value), and (3) $\Delta E_{ad} = 10,005 \text{ kJ/kg}$ (Chemical approach).