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TNT-Equivalency Concepts[2]

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ABSTRACT: TNT equivalency is often used to quantify the approximate destructive potential of a rapidly reacting material when ignited or to assess the amount of damage that resulted from certain ignition or system failure events. The basic concept is introduced along with several of the common equations that apply to chemical or physical energy releases.

KEY WORDS: oxygen, oxygen compatibility, TNT, flammability, flammability limits, fire, explosion.

Trinitrotoluene (TNT) is a well-known high explosive. It is neither the most nor least destructive of explosives. However, its reaction is reproducible and the relative predictability of its performance (including safety of use) have led to a large amount of work with the material.

As a result, it is common practice to compare other explosive events to those that result from the use of TNT. In the extreme case, military weapons are rated in equivalent kilotons or megatons of TNT. However, the concept is equally useful in assessing the damage potential of resultant rapid reactions and explosions of much smaller scale in industrial chemical processes and pressure systems, including those involving oxidants.

There are references that discuss this concept [*1*,*2*], and one popular course taught by Grelecki [*3*] is provided by the AIChE. This paper introduces the concept, derives some of the pertinent equations, and discusses a few of the applications for these data.

TNT equivalencies are not exact predictions or measurements. The destructive potential of a high speed reaction or vessel failure can vary enormously even among

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replicated experiments. Therefore, when TNT equivalencies are estimated, one must always apply appropriate and substantial safety factors.

Among the specific uses to which TNT equivalencies have been put are:

-Estimating the maximum damage potential of an explosion incident.
-Designing barriers to contain explosions.
-Ascertaining whether explosions within systems are likely to produce or to have produced a rupture or failure of a containment vessel.

Explosions

Explosions typically exhibit the production of a pressure wave ("blast wave") the most destructive feature of which is a "shock front' (a relatively abrupt pressure wave moving at the speed of ambient sound or faster) that forms at its leading edge. Shock waves can be produced whenever a differential pressure is abruptly created or released, including when pressure-building combustion occurs at a rate faster than average molecules move (which is the speed of sound). Typically, to generate the most destructive shock wave during combustion, the velocity of the combustion propagation flame front must exceed the local speed of sound. Pressure waves can also be generated with less rapid combustion, however, these waves are less destructive than those that form from rapid combustion. A shock wave may even develop as the result of an extremely rapid combustion of a free exposed material, and it may be developed as the result of a slower combustion that occurs within a vessel that resists dispersion of the pressure increase until the vessel fails.

TNT Equivalency

A TNT equivalency may be cited as either a relative, specific or absolute variable. As a relative number, the TNT equivalency is the damage potential of a subject material divided by the damage potential of a similar mass of TNT (e.g. a material might be reported as having a TNT Equivalency of "3" or of “300%”). As an absolute variable the damage potential would be compared to the amount of TNT that would yield the same damage (that is, a specific mass, for example a damage potential might be equal to 10 grams of TNT).

In estimating TNT equivalencies, it is common to relate the damage potential of a material to the energy release that that material might produce. Therefore one would divide the energy that might be released by a subject material by a standard energy release that has been adopted for TNT. The standard energy release of TNT is taken as approximately 1.1 kcal/g.

Therefore, the TNT equivalency of a material in grams is its energy release (which may include its heat of combustion as well as other other energy derived from mechanical effects) divided by the 1.1 kcal/gram energy release of TNT. In practice, the energy that might be released by a subject material may be very difficult to determine and so coarse, conservative approximations are often used.

Chemical Reactions

Heat may be liberated, when a chemical reaction occurs. Any portion of that heat may become available as mechanical energy in an explosion. A conservative approach assigns all of the heat of the reaction as explosive energy in assigning a TNT equivalency. The heat liberation may result from a chemical combination of two materials (a fuel with an oxidant). It may also result from an internal oxidation (nitrated compounds), decomposition of an endothermic molecule (nitrous oxide, acetylene), polymerization, or other reaction of a single material. These effects may occur in combination as well as individually.

TriNitroToluene (TNT)

TNT is the compound: $C_7H_5(NO_2)_3$, a solid at room temperature and liquid above 82°C. The three nitro- (NO_2) groups contain oxygen that is available for reaction of the carbon and hydrogen. A very high speed combustion reaction is possible, because the oxygen is uniformly (perfectly) distributed throughout the TNT mass.

Oxygen compatibility practitioners are familiar with heats of combustion. The heat of combustion of TNT is cited as 820.7 kcal/mol (mol wt = 227) or 3.6 kcal/g. for a presumed complete reaction in oxygen of:

$$C_7H_5(NO_2)_3 + 5.25O_2 \rightarrow 7CO_2 + 2.5H_2O + 1.5N_2 \qquad (1)$$

It is assumed that the products and reactants are at room temperature with the TNT initially a solid and the final water a liquid.

In comparison, the standard energy release used when calculating TNT equivalencies is only 5.0×10^5 calories per pound (about 1.1 kcal/g). Further, only about 0.6 kcal/g of this would be measured in a calorimeter if the TNT were exploded in an inert atmosphere. Note that this 1.1 kcal/g release (0.6 kcal/g calorimetric component) is less than one third of the heat of combustion of TNT. The principal reason for this is that TNT does not necessarily burn to completion in an explosion. When TNT reacts as a solid, it has a limited supply of oxygen within the molecule upon which to release heat (6 atoms versus the 16.5 atoms needed for complete reaction of the molecule). Also, after TNT has completed its fast reaction and consumed its internal oxygen, the gases produced are hot and an equilibrium between products and reactants may act to limit the extent to which even the available oxygen is reacted, and finally, a significant portion of the heat release that would be reported in a calorimetric test is contained in the latent and sensible heat of the hot gas cloud. Although the TNT might continue to burn in ambient oxidant, the rate of combustion might be far too slow to alter the intensity of the shock wave that was produced.

Indeed, if TNT were to be dispersed in air or to be granulated and mixed into liquid oxygen, so that there would be additional dispersed oxygen available for rapid reaction, then its own TNT equivalency might be as high as several times the standard TNT equivalency of TNT, itself. That is, TNT mixed with liquid oxygen (LOX) might have a TNT equivalency (per unit mass of TNT) approaching and exceeding a value of three.

A typical practice is to use the heat of combustion of a material in estimating its damage potential. The previous observation indicates that this is indeed a very conservative practice, since this method would assign a TNT equivalency of at least 3.3 to TNT, itself. However, if one were to desire a conservative estimate for TNT, one would have to consider that it might in theory be mixed with LOX in a way that might enable the rapid release of all its chemical energy. One also needs to consider whether the reaction of the TNT (or other) material alters other available mechanical energy of a system.

Chemical TNT Equivalencies

Fuel-Based Equivalencies

Table 1 exhibits the heats of combustion, decomposition or reaction of an assortment of materials. Among them are approximate TNT component equivalencies of fuel in abundant oxygen which assume all of the heats of these materials were to be rapidly converted into shock-wave energy. It assumes there are no losses due to equilibria established at high temperature (and therefore incomplete reaction), and no losses due to latent and sensible heats that linger in the combustion products or mechanical energy (to be dealt with later) in the residual gases of a constant volume test. It is presumed that for each of these materials there is an abundance of oxidant intimately available to produce the reaction.

Oxidant-Based Equivalencies

When there is an abundance of fuel and a dearth of oxidant, then the extent of damage is controlled by the amount of rapid reaction of the oxygen. In this case one can consider estimating the damage potential due to the oxidant, and its “TNT Equivalency” in abundant fuel as indicated in Table 1. An example of this might be a spill of LOX onto a porous asphalt. In this case the ambient environment is rich in both hydrogen and carbon. Neglecting the energy in the hydrocarbon bond that must be severed, the extremes of reaction that can occur might be:

$$O_2 + 0.5H_2 \rightarrow H_2O \tag{2}$$

or,

$$O_2 + C \rightarrow CO_2 \tag{3}$$

Equation (2) would yield 3.61 kcal/g of oxygen, while Equation (3) would yield 2.95 kcal/g of liquid oxygen (LOX). Therefore, in this fuel-rich situation, LOX that would be introduced would have a chemical TNT equivalency in the range of 2.7 to 3.3 (this estimate again neglecting latent and sensible heats of the products and incomplete reaction due to expected equilibria at temperature or residual mechanical energy in a constant volume condition). In some (albeit rare) cases, noncompatible materials may be safely used in oxygen if the local inventory of oxygen is both stagnant and small, implying both low TNT equivalency and low damage.

TABLE 1—*Typical Max. Chemical Components of TNT Equivalencies*[a]

Material[b]	ΔH_c- Kcal/g	Max. Chem. TNT Equiv.
Hydrogen in abundant Oxygen	34. (/g H_2)	30.9
Oxygen in abundant Hydrogen	4.27 (/g O_2)	3.88
Hydrogen/Oxygen mixture (stoichiometric)	3.79 (/g mix)	3.45
Carbon in abundant Oxygen	7.84 (/g O_2)	7.13
Oxygen in abundant Carbon	2.94 (/g C)	2.67
Carbon/Oxygen mixture (Stoichiometric)	2.14 (/g mix)	1.95
Methane in abundant Oxygen	13.2 (/g O_2)	12.
Oxygen in abundant Methane	3.29 (/g CH_4)	2.99
Methane/Oxygen mixture (stoichiometric)	2.64 (/g mix)	2.4
Aluminum in abundant Oxygen	7.43 (/g O_2)	6.75
Oxygen in abundant Aluminum	4.17 (/g Al)	3.79
Aluminum/Oxygen mixture (stoichiometric)	2.67 (/g mix)	2.42
Buna-N in abundant Oxygen	8.3 (/g O_2)	7.5
Neoprene in abundant Oxygen	3.0 (/g O_2)	2.7
Silicone in abundant Oxygen	3.7 (/g O_2)	3.4
Viton (FKM) in abundant Oxygen	3.6 (/g O_2)	3.3
PTFE in abundant Oxygen	1.0-1.4 (/g O_2)	0.91-1.3
TNT in abundant Oxygen	3.6 (/g O_2)	3.3
C_2H_2[b]	2.1[b] (/g C_2H_2)	1.9[b]
N_2O[b]	0.44[b] (/g N_2O)	0.4[b]

[a] Material burned rapidly in gaseous oxygen.
[b] Based on heat of decomposition without supplemental oxygen present.

Mechanical TNT Equivalencies

Shock waves can also propagate from an abrupt pressure release. This can be the result of a high-speed vessel rupture under pressure. The maximum energy that can be released in this instance relates to the mechanical energy stored in the gas. Table 2 cites numerous common pressure systems and the maximum mechanical TNT equivalencies that might be assigned to each. The mechanical energy in a pressurized ideal gas may be estimated two extremal ways: isothermally and adiabatically. In both cases, the gas of initial volume, V_i, and absolute pressure, P_i, is allowed to expand to a lower absolute pressure P_f (typically atmospheric pressure), and final volume V_f.

TABLE 2—*Typical Mechanical Energy Components of TNT Equivalents.*[a]

Pressure System	Pressure psig (MPa)	Adiabatic[b] lb (kg)-TNT	Isothermal[b] lb (kg)-TNT
“BX” DOT 3AA6000 gas cyl., 10x55in (25x130-cm)	6000 (40.9)	1.65 (0.75)	4.40 (2.00)
“BY” DOT 3AA6000 gas cyl., 9x51in (23x130-cm)	3500 (23.9)	0.93 (0.42)	2.36 (1.07)
“A” DOT 3AA2400 gas cyl., 9x55in (23x140-cm)	2640 (18.1)	0.78 (0.36)	1.92 (0.87)
“B” DOT 3AA2400 gas cyl., 9x51-in.(23x130-cm)	2265 (15.5)	0.58 (0.26)	1.40 (0.64)
“C” DOT 3AA2015 gas cyl., 7x33-in.(18x84-cm)	2015 (13.8)	0.18 (0.083)	0.44 (0.20)
“D-1” DOT 3AA2015 gas cyl., 4x19-in.(10x48-cm)	2015 (13.8)	0.085 (0.039)	0.20 (0.92)
“D” DOT 3AA2015 gas cyl., 4x17-in.(10x43-cm)	2015 (13.8)	0.033 (0.015)	0.078 (0.036)
DOT 3EE1800 Lecture Bottle., 2x12-in.(5x30-cm)	1800 (12.3)	0.004 (0.002)	0.010 (0.005)
10,000-gal (40,000-L) vessel	250 (1.8)	35.5 (16.1)	67.4 (30.6)
50,000-gal (200,000-L) vessel	5 (0.13)	0.35 (0.16)	0.50 (0.23)
10 x 20 Truck Tire	105 (0.81)	0.009 (0.004)	0.016 (0.007)
185-70-R14 Car Tire	32 (0.32)	0.0014 (0.0006)	0.0022 (0.001)

[a] Assuming expansion to a one-atmosphere final pressure in a one-atmosphere ambient pressure of an ideal gas having $\gamma = 1.4$ (approximately that of oxygen or nitrogen).

[b] Using Equations (8) for isothermal and (17) for adiabatic cases.

Isothermal Case

In the case of an isothermal expansion, energy is added to the expanding gas to ensure that its temperature remains the same. Typically, this type of expansion is done slowly, so that heat transfer to the gas can be effected. However, if there is a rapid method to transfer the heat, an isothermal expansion could be accomplished at any speed.

The differential mechanical work, dE, that a gas does in isothermally expanding is given by

$$dE = \mathbf{F} \bullet d\mathbf{x} = P\mathbf{A} \bullet d\mathbf{x} = PdV \qquad (4)$$

Where **F** is the vector force the gas pressure, P, exerts on a vector surface of area, **A**, that moves a vector differential distance, d**x**. In this case the force is the product of the gas pressure, P, and the area (**A**); the differential volume, dV, is the dot product of the area and d**x**; and the area differential, **A**•d**x**, is equal to the change in the gas volume, dV. The ideal gas law teaches that PV= nRT, where n is the number of moles, R is the Universal Gas Constant, and T is the absolute temperature in consistent units.

Substitution allows that:

$$E = \int PdV = \int (nRT/V)dV = nRT\ln [V_f /V_i] \tag{5}$$

However, $V_f /V_i = [(nRT/P_f)/(nRT/P_i)] = P_i /P_f$. Further, $nRT = P_tV_t$, where P_t and V_t are the pressure and temperature, respectively, at any point in the process. Therefore, at the initial time,

$$E = P_iV_i \ln [P_i /P_f] \tag{6}$$

In the above equation, V_i is the volume of the vessel. This derivation applies to a gas expanding in a vacuum. However, if there is an environmental pressure (such as atmospheric pressure) present, then the gas expansion will be opposed by the ambient pressure and the gas will cease to deliver energy when its pressure matches the environment.

If the ambient pressure is given by P_a, then P_f ³ P_a and this term alters equation (6) as follows:

$$E = P_iV_i \ln [P_i /P_f] - P_a[V_f - V_i] \tag{7}$$

Since isothermally, $V_f = P_i V_i / P_f$:

$$E = P_iV_i \ln [P_i /P_f] - P_aV_i[(P_i/P_f) - 1] . \tag{8}$$

Adiabatic Case

In the case of an adiabatic expansion, the gas is allowed to perform work on its surroundings without the transfer of heat. Typically an adiabatic expansion is accomplished quickly, because heat transfer is a slow process. However, if the expanding gas can be effectively insulated, then an adiabatic expansion could be effected at any speed.

The mechanical work, E, that an ideal gas does in isothermally expanding is, as in Equation (4), given by

$$E = \mathbf{F}\bullet d\mathbf{x} = P\mathbf{A}\bullet d\mathbf{x} = PdV \tag{9}$$

However, in an adiabatic condition, the relationship between pressure and volume is given by:

$$PV^\gamma = C = P_iV_i^\gamma = P_f V_f^{\gamma} \tag{10}$$

Where, C is a constant value based on the pressure and volume at any point in time, and $\gamma = C_p/C_v$ where C_p is the specific heat at constant pressure and C_v is the specific heat at constant volume. Therefore: $P = (P_i V_i^{\gamma})/V^{\gamma}$, and

$$E = \int P dV = \int [C/V^{\gamma}] dV = \int C\, [1/V^{\gamma}] dV \qquad (11)$$

or

$$E = [C/(\gamma\text{-}1)]\, [(1/V_i^{\gamma-1}) - (1/V_f^{\gamma-1})] \qquad (12)$$

but since $C = P_i V_i^{\gamma} = P_f V_f^{\gamma}$, then

$$E = [1/(\gamma\text{-}1)]\, [(P_i V_i^{\gamma}/V_i^{\gamma-1}) - (P_f V_f^{\gamma}/V_f^{\gamma-1})] \qquad (13)$$

and therefore,

$$E = [1/(\gamma\text{-}1)]\, [(P_i V_i) - (P_f V_f)] \qquad (14)$$

In the above equation, V_i is the initial volume of the vessel, and if an uncontrolled release of the pressure is anticipated, then P_f is zero in a vacuum and may not exceed the ambient pressure (typically atmospheric). But, again, since $C = P_i V_i^{\gamma} = P_f V_f^{\gamma}$, then

$$V_f = V_i\, [(P_i/P_f)^{1/\gamma}] \qquad (15)$$

So that,

$$E = [1/(\gamma\text{-}1)]\, [(P_i V_i) - (P_f^{([\gamma-1]/\gamma)} V_i P_i^{1/\gamma})] \qquad (16)$$

As was the case for isothermal expansions, this derivation applies to a gas expanding in a vacuum. However, if there is an environmental pressure (such as atmospheric pressure) present, then the gas expansion will be opposed by the ambient pressure and the gas will cease to deliver energy when its pressure matches the environment.

If the ambient pressure is again given by P_a, then $P_f \geq P_a$, and the energy the ambient expends on the gas must be subtracted. Since P_a is constant, this energy, $\int PdV$, is simply given by $[P_a(V_f - V_i)]$, which by Equation 14 is $[P_a(V_i\, [(P_i/P_f)^{1/\gamma} - V_i]\,)]$. When subtracted from equation (15), the energy liberated in a background pressure is as follows:

$$E = \{[1/(\gamma\text{-}1)]\, [(P_i V_i) - (P_f^{([\gamma-1]/\gamma)} V_i P_i^{1/\gamma})]\} - \{P_a V_i [(P_i/P_f)^{1/\gamma} - 1]\}. \qquad (17)$$

Advanced TNT Equivalencies

In most instances, these TNT equivalency components are additive. If a cylinder contains a high-pressure ideal gas with a mechanical TNT equivalency of 0.5 pounds, and the gas has a chemical TNT equivalency of 1 pound, then the approximate combined mechanical and chemical TNT equivalency would be the 1.5 pound sum. This estimation may still contain significant errors for real materials.

Chemical and mechanical TNT estimation methods described thus far are typically conservative, sometimes by wide margins. However, in some other cases, they underestimate the TNT equivalencies. Where greater accuracy is required, one must assess the specific extent to which a material will react, the speed of the reaction, the ideality of the reactants and products, the nature of the products, and other variables. In Kinney and Graham [*2*], these analyses are done on the basis of changes in the Helmholtz Free Energy.

For example, consider a carbon dust burning in stoichiometric oxygen. If the mixture burned completely to carbon dioxide, and one were to estimate its TNT equivalency by adding the heat of combustion to the mechanical energy in the original oxygen, the result might be in error. This product gas, carbon dioxide, has a significantly lower γ ratio (which would increase the estimated mechanical energy) and might be less ideal than the original oxygen (which would decrease the estimated mechanical energy). In this case, the carbon might well not react fully to carbon dioxide, therefore might not liberate its full heat of combustion (which would decrease the estimated chemical energy). However, if it were to react to carbon monoxide, and if one were to sum the mechanical energy of the initial oxygen and chemical energy (ΔH_c) of the reaction, one would again fall short, because the post-reaction vessel would contain twice the number of moles of gas as the original oxygen. This will increase the mechanical energy component substantially.

Conversely, one might overestimate the TNT equivalency of the reaction of hydrogen with stoichiometric oxygen by adding the heat of combustion to the mechanical energy of the original system. In this case, one must factor in that the product water is present in one-third fewer moles as the reactants, and that water is very nonideal. Following a heat of combustion test, one would find that the products had condensed to yield virtually no pressure, and no mechanical energy in the products.

In the case of TNT itself, the chemical reaction component is about 0.6 kcal/g and the remaining energy to yield the approximate 1.1 kcal/g is due to the mechanical energy contributed by the gaseous reaction products it generates in going from a condensed phase (liquid or solid) to a gaseous phase.

Methods for more precise estimation of TNT equivalencies are found in Kinney and Graham [*2*] and Grelecki [*3*].

Damage Potential

There is a traditional dichotomy in science and engineering between the use of data to achieve a physical effect and to prevent that same effect. This analysis conservatively estimates TNT equivalencies as the maximum damage potential for the sake of designing adequate containment. Those who seek to exploit the shock wave for demolition or military reasons would estimate these equivalencies quite differently. They are interested in the minimum damage potential.

For a given TNT equivalency, the damage potential of an explosion is often dependent upon many properties in addition to the heat of combustion. The immediate (local) affect is especially dependent upon the brisance (or “sharpness”) of the explosion. The effect at distance depends on other factors such as the total energy release.

Before a vessel will fail due to overpressure, at least two criteria must be met. The internal pressure must develop a force on the vessel’s walls in excess of the vessel’s

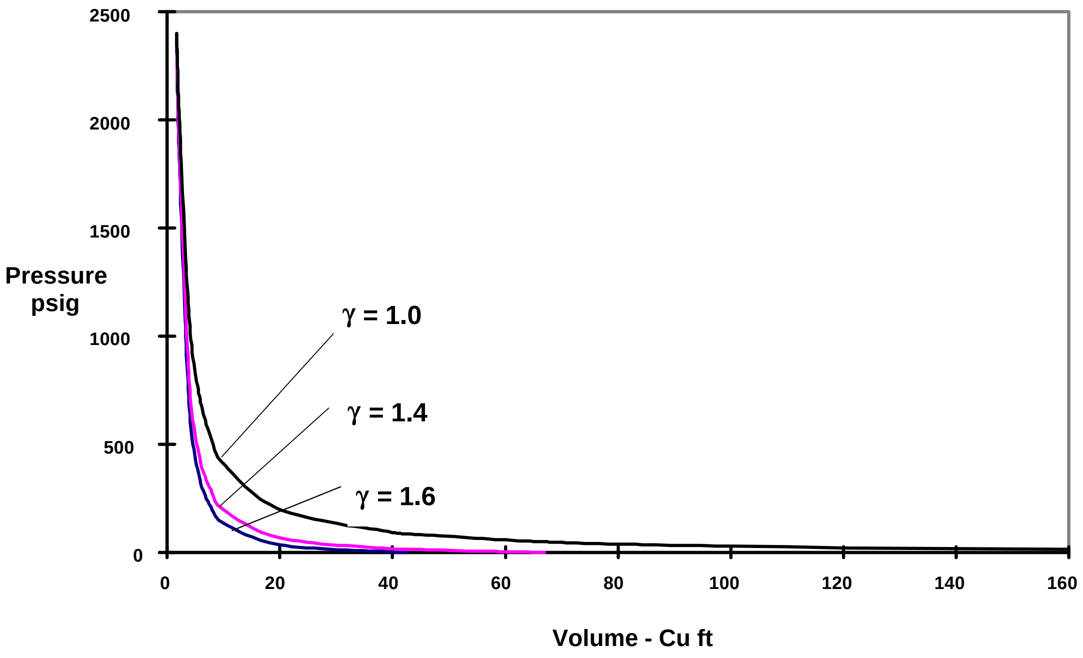

FIG. 1—*Idealized adiabatic expansions*.

strength, and the force must be sustained as the vessel stretches and fails (that is, the energy the gas can deliver must exceed the vessel's toughness). If the pressure decays below the burst pressure as the vessel stretches, then rupture may not result.

Fig. 1 exhibits the mechanical energy (characteristic adiabatic case) in a 3AA2400 gas cylinder containing ideal gases of differing γ. The three curves illustrate the gas initially at 2640 psig (18.1 MPa) expanding to atmospheric pressure at three different points on the abscissa. The energy is the area under each curve. Notice that as γ increases, the energy decreases. Table 3 tabulates the effect. Typically, a large γ is associated with small molecules (such as monatomic gases: argon and helium) and smaller γ is associated with larger molecules (such as CO_2, SF_6, etc.). Indeed, as molecule size increases, γ approaches unity. Therefore, if a cylinder ruptures at a given pressure, the destruction will be appreciably greater if it contains a small-γ gas, such as CF_4, than if it contains a large γ gas, such as argon (the comparative mechanical TNT equivalence of CF_4 is about twice that of argon at comparable initial pressures). Indeed, as γ approaches unity, the adiabatic mechanical energy approaches that for the isothermal (maximum) case.

Similarly, in situations where a given thermal energy is introduced into a gas, the effect can be most destructive for a gas of high γ. Consider an energy input, say a fractional combustion, in either a bulk argon or CF_4 gas. The resulting pressure rise in the argon gas will be greater than in the CF_4. However, upon rupture of both vessels at a common pressure, the pressure decay is faster and of shorter range than for the CF_4.

Another dramatic example of the role of γ is for the combustion of aluminum in oxygen. Aluminum is a very energetic material that is often added to high explosives to enhance the destructive potential. As aluminum burns, its oxide typically condenses into a hot liquid having little vapor pressure. It is the heat transfer from this liquid that enhances

TABLE 3—*Effect of g on Mechanical TNT Equivalencies*[a]

g[b]	TNT Equivalence	
	Pi = 2640 psig (18.1 MPa) Lb (kg) TNT	Pi = 500 psig (3.5MPa) Lb (kg) TNT
1.66	0.549 (0.25)	0.083 (0.038)
1.40	0.784 (0.36)	0.112 (0.051)
1.33	0.881 (0.40)	0.123 (0.056)
1.22	1.09 (0.49)	0.147 (0.067)
1.10	1.44 (0.65)	0.183 (0.083)
1.01	1.86 (0.84)	0.224 (0.102)
1.001	1.916 (0.869)	0.2287 (0.1037)
1.0001	1.9217 (0.8717)	0.2292 (0.104)
1.0	1.9221 (0.8720)	0.2292 (0.104)
Isothermal	1.9221 (0.8720)	0.2292 (0.104)

[a] For a 3AA2400 cylinder (1.76 ft^3, 0.0419 m^3, water volume) containing the indicated pressure for which expansion to one atmosphere occurs in a one atmosphere counteracting pressure.

[b] Argon has a value of about 1.66, oxygen a value of about 1.4, and CF_4 a value of about 1.22.

explosives. An aluminum/oxygen mixture transfers its greatest heat when it is burned in near-stoichiometric conditions. However, aluminum/liquid-oxygen mixtures that are near stoichiometric do not yield the greatest explosive potential, because the final pressure collapses towards zero.

Aluminum is far more destructive when there is an excess of oxygen present (Kirshenbaum [*4*]). This is because it is the heat transfer from the low vapor pressure liquid aluminum oxide product into the nonreacting portion of the oxygen that produces high pressures, and therefore high mechanical energy. When aluminum is mixed with LOX, the combined mixture can be more destructive than TNT, *provided there is an excess of oxygen in the mixture*. By the previous simplistic analysis, one might expect an explosive comprising aluminum, stoichiometric oxygen, and an excess of a monatomic material such as argon to be even more destructive, however, in most cases, a large presence of argon would prevent the reaction from proceeding.

Isothermal versus Adiabatic

If a pressure vessel at ambient temperature ruptures, then the rapidly expanding, nearly adiabatic, gas will decrease in temperature. Any heat transfer will be from the surroundings into the gas and result in an increase in the TNT equivalency to some value

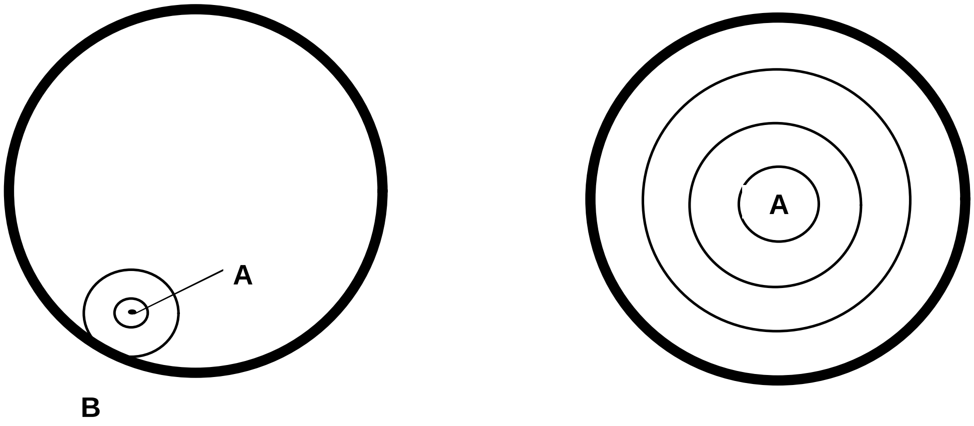

FIG. 2—*Idealized explosions*.

between the adiabatic and isothermal approximations. The adiabatic approximation is a lower-bound estimate.

However, if a vessel that contains a reacting or heated gas ruptures, the situation is different. In this case, the initial gas temperature is greater than the surroundings. Initially, any heat transfer is from the gas to the surroundings and results in a decrease in the TNT equivalency, until the expanding gas cools to ambient level. When the expanding gas cools below ambient temperature, the direction of heat transfer will reverse. In the initial portion of this expansion, the adiabatic TNT estimation is an upper-bound estimate.

Application to Oxygen Systems

Energy Needed to Fail Vessels

An estimate of the energy required to fail a given vessel when a material inside burns in oxygen is extremely difficult and far beyond the introductory scope of this paper. The reasons for this are many. Because the most hazardous reactions are very rapid, the consequence of a combustion event can be highly localized (as at point A in Fig. 2, left). It is possible for a high explosive to fail the wall of a strong vessel (at point B) and yet not fail a low pressure rupture disk located just a short distance away. This scenario is much more severe than if the combustion event is centralized as at the right of Fig 2. Materials that burn in oxygen will tend to be concentrated in very local positions (a valve seat, or a droplet of oil) and so the result of a combustion is most significant at the site of the reactive material. In addition, if a shock wave is established, it can reflect onto itself and increase its ability to cause local vessel failure.

However, this paper can relate the energy that might be needed in an explosion to fail a specific component, allowing that even in this case the precision is not great.

Consider a hydraulically driven metal tensile-strength tester. In this case, consider the energy that is expended in a 2-in (5-cm) long gage region of a metal tensile test specimen, of area 0.2 in^2 (1.3 cm^2). As the force on the specimen is increased, energy

TABLE 4—*Estimated Energy to Fail Metal Specimens*[a]

Metal	**Energy to Fail Tensile Test Specimens**[b]	
	ft-Lb (cal)	**TNT Equiv - g**
hard copper	250 (81)	0.07
soft copper	370 (120)	0.11
carbon steel	690 (223)	0.20
nickel alloy 400	1390 (449)	0.41
304 stainless steel	2330 (754)	0.68

[a] Obtained by gravimetric integration of stress-strain curves.
[b] 2- in. (5-cm) long x 0.2 in.^{2} (1.3 cm^2) area test section.

would be transferred to the test specimen that would initially produce elastic deformation and later plastic deformation (assuming the rate of loading were not so rapid as to cause a brittle response in the specimen). The energy, E, the specimen would absorb is given by:

$$E = \int \mathbf{F} \cdot d\mathbf{l} = \int P dV \tag{18}$$

Where P is the pressure in the hydraulic cylinder and dV is the hydraulic volume differential, **F** is the force the pressure would produce and d**l** is the stretch in the specimen. The integration limits would be from the ambient-pressure volume to the volume at which the specimen fails. Table 4 exhibits maximum energy containment estimates based on these constraints and is obtained by integrating the stress/strain curves for typical metals during tensile strength tests.

These data coarsely approximate the maximum energy required to fail metal components of different alloys, and they relate to the toughness of the metals (as is also measured by Charpy impact apparatuses). Clearly, there are substantial difference in the abilities of various metals to contain the energy of explosive events. Indeed, Bartknecht [5] indicates that if such a frangible disk is stressed rapidly, it may exhibit an artificially higher ultimate tensile strength (he presents data suggesting at least a 10% increase). However, One must also be wary that if the vessel is stressed at extremely high rates, it may exhibit a brittle failure mode that will contain even less energy. For these reasons, estimates of vessel containment capacities may require very large safety factors (even as high as one or two orders of magnitude).

Summary

The most basic principles and practices of estimating maximum TNT equivalencies were introduced. This very approximate but useful tool allows one to bracket the maximum damage that an oxygen reaction might cause and may allow one to justify the use of a particular material in oxygen on the basis of a system's ability to withstand the worst-case damage. The significance of the ratio of a gas's specific heats has been illustrated. The significance of stress on vessel failures has been illustrated. More advanced and sophisticated use of these estimates can give insight into the amount of damage that would result from an oxygen incident and the scale of the combustion or mechanical event that could cause it. As a result, hypotheses that explain or predict incidents may be tested and validated or excluded.

References

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