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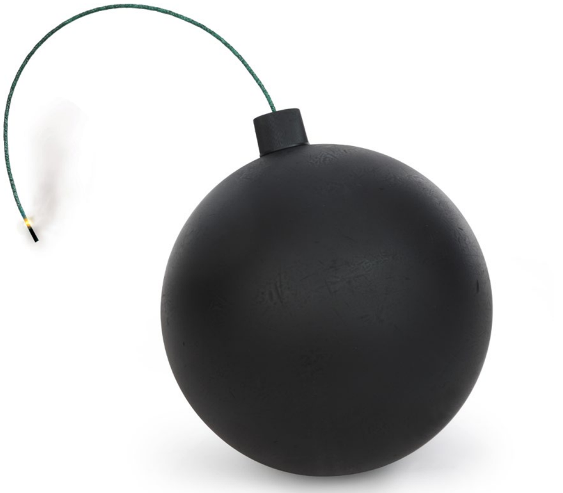
A Calculated Bang:

Explosive Predictions and the Ideal Gas Law



by

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Introduction

From the early use of flames by the caveman to Romans using incendiary compounds in catapults, to fireworks and the development of black powder, various chemical mixtures have historically been designed for specific effects.[5] An explosive is "a pure single substance or mixture of substances, which is capable of producing an explosion by its own energy."[2] Explosives have a wide range of applications such as routine use in construction, mining, demolition, and military training. Media outlets have raised improvised explosive devices to common vernacular following operations in Iraq and Afghanistan. These explosives are associated with solid, liquid, or gaseous components that when exposed to an ignition force, such as heat or friction, generate a reaction. Following detonation, this reaction rapidly generates high temperatures and pressures by the gases produced.

Explosives require direct ignition or initiation to trigger the thermal decomposition of the reactants, which initiates the combustion process. Combustion produces a large volume of gases that rapidly expand in the surroundings. It is the high velocity of movement of gases and rise in pressure that generate a shock wave the can displace material, such as moving rock when mining or blasting through a mountain to establish a road. Explosives are selected for a specific purpose based on their characteristic production of energy. This energy is capable of initiating other reactions, amplifying explosions, or penetrating target material. Some of the more common explosives and their uses are ammonium nitrate (NH_4NO_3) in earthmoving operations; PETN ($C_5H_8N_4O_{12}$ or pentaerythritol tetranitrate) in detonating cords; RDX ($C_3H_6N_6O_6$ or cyclotrimethylenetrinitramine) in blasting caps; TNT ($C_7H_5N_3O_6$) in demolition charges; and composition 4 (C4) in military breaching charges.[3]

Combustion requires three primary components: fuel, energy, and an oxidizer. The fuel is the organic starting material and once the activation energy is achieved, large amounts of energy are rapidly released fragmenting reactants into individual atoms. The components quickly rearrange into smaller and more stable molecules.[5] Oxygen serves as an oxidizer, due to its electronegativity, accepting electrons and forming products including water, carbon dioxide, carbon monoxide, nitrogen, hydrogen, and carbon, among others. Once oxygen levels are depleted, the incomplete combustion products result in the production of elemental carbon and carbon monoxide.

Predicting Reaction Products for Explosives

To facilitate the identification of explosion products, a set of guidelines known as the Kistiakowsky-Wilson' rules (K-W rules) were developed during World War II.[1,5] These six rules are modified to provide additional completeness and are followed in the order in which they appear.

1. All hydrogen atoms in the molecule are oxidized to water.
2. If any oxygen atoms remain, they are used to convert carbon to carbon monoxide.

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3. If any oxygen atoms still remain, they are used by oxidizing their stoichiometric amount of carbon monoxide to CO_2.
4. Any leftover oxygen atoms form oxygen gas (O_2).
5. Nitrogen atoms produce nitrogen gas (N_2).
6. Any remaining carbons form solid carbon (C).

The stoichiometric products for each atom are combined to generate the reaction. Once the reaction is predicted, one can calculate the specific volume of gases produced or displaced to engineer and deliver a particular effect, such as that used in ore mining operations.

For example, suppose that you were using nitroglycerin ($C_3H_5N_3O_9$) to blast through rock to extend a road to a rural area. Applying the modified K-W rules, in a step-wise manner, you could initially predict the reactions products following detonation. These rules are only applicable to molecules containing C, H, N, O elements and are most accurate in moderately oxygen deficient explosives. A simplified "bookkeeping" approach to use the K-W rules is shown below.

	Number of Atoms	
Starting Material: $C_3H_5N_3O_9$	*Used*	*Remaining*
1. All H atoms are oxidized to water.	5 H	0 H
5 H yield **2.5 H_2O**	2.5 O	(9–2.5) 6.5 O
2. Unused oxygen atoms become CO.	3 O	(6.5–3) 3.5 O
3 O yield **3 CO**	3 C	0 C
3. Unused oxygen oxidizes CO to CO_2.		
3 O yield **3 CO_2**	3 O	(3.5–3) 0.5 O
4. Any leftover oxygen atoms form oxygen gas (O_2).		
0.5 O yield **0.25 O_2**	0.5 O	0 O
5. Nitrogen atoms produce N_2.		
3N yield **1.5 N_2**	3 N	0 N
6. N/A *All carbon atoms have been used.		

The products (shown above in bold) are written in the chemical equation, as shown below for the detonation of nitroglycerin ($C_3H_5N_3O_9$). Note that residual carbon would be listed as solid carbon and all other components are gases.

$$C_3H_5N_3O_9(s) \longrightarrow 2.5\ H_2O(g) + 3\ CO_2(g) + 0.25\ O_2(g) + 1.5\ N_2(g)$$

As a final verification, ensure that the equation is balanced to validate that all atoms are accounted for following detonation.

The Ideal Gas Law: PV = nRT

The actual effects of a combustion reaction are governed by the ideal gas law (IGL). Whether working in a mine, discussing the ecological impact of strip mining, or watching a fireworks display, engineers have considered the initial reactants and resulting products. These relationships influence the pressure available to do work on or within a system to generate a specific effect, such as displacing rock when building a tunnel or determining the optimal operating temperature for pyrotechniques during a fireworks display.

Beginning with practice of applying the K-W rules, you will predict the combustion products of select reactants and perform stoichiometric calculations using the ideal gas law at varying conditions. The ideal gas law (IGL) compares the pressure (P) and volume (V) relative to the number of moles (n), Universal Gas Constant (R), and temperature (T). Rearranging this equation, one can see how volume is impacted by variations in temperature and pressure ($V = nRT/P$). Thus, if temperature increases so does the volume (Charles's Law)[6] while increases in pressure are inversely related to volume (Boyle's Law)[8].

Once the reaction products of an explosive are identified, the IGL can be applied to determine either the initial explosive mass required to generate an effect or the volume of by-products produced at a given temperature and pressure. The IGL requires the conversion of units in similar terms, that are comparable with the units used in the ideal gas constant. Common units of conversion are as follows:

Mass	*Temperature*
1 ounce (oz) = 28.35 grams (g) = 0.0283 kg	T(K) = (1K / 1 °C) × (T(°C) + 273.15 °C)
1 pound (lb) = 16 oz = 453.592 g = 0.453592 kg	T(°C) = (5 °C / 9 °F) × (T(°F) – 32 °F)
1 ton (metric) = 2204.62 lb = 1000. kg	T(°F) = [(9 °F / 5 °C) × T(°C)] + 32 °F
Volume	*Pressure*
1 liter (L) = 1000 milliliters (mL)	1 pascal (Pa) = 1 kg/(m × s^2)
1 gallon (gal) = 3.7854 L	1 atmosphere (atm) = 760 torr = 101325 Pa
Avogadro's number	*Universal Gas Constant (R)*
n = 6.022×10^{23} atoms/mole	R = 0.08206 (L)(atm)/(K)(mol)

Problems

1. The common military explosive PETN ($C_5H_8N_4O_{12}$) belongs to the same chemical family as nitroglycerin, a compound with medicinal uses as a vasodilator.[11] Aside from sanctioned use, the "shoe bomber" attempted to detonate a PETN device on a commercial airline flight to Miami in 2001.[9]
   a. Predict the reaction products for the combustion of 1 mole of PETN.
   b. Calculate the total volume of gas (in liters) produced if 15.0 pounds of PETN explodes at 1.3 atmospheres and 70.0 °F.
2. Trinitrotoluene (TNT) is commonly used for commercial mining purposes. The process used to extract oil and gas from shale relies on components of TNT.[10] Given the equation for the detonation of TNT:

   $$C_7H_5N_3O_6(s) \longrightarrow 3.5\ CO(g) + 2.5\ H_2O(g) + 1.5\ N_2(g) + 3.5\ C(s)$$

   Calculate the volume (in liters) of carbon monoxide formed when 10.0 pounds of TNT combusts at 1.2 atmospheres of pressure and 28.4 °C.
3. Nitroguanidine ($CH_4N_4O_2$) is used in select fertilizers and more commonly as a component to propel munitions.[4] Suppose a field artillery soldier was calculating how much nitroguanidine was needed to propel a round. The soldier would need to consider the desired volume of gas to displace along the gun tube and the ambient operating conditions.
   a. Predict the reaction products for the detonation of 1 mole of nitroguanidine ($CH_4N_4O_2$).
   b. Calculate the amount of explosive needed (in pounds) to produce 1500.0 liters of gas at standard temperature and pressure (STP), 1.0 atmosphere of pressure and 32 °F.

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