Letter

A computer model for formulation of ANFO explosives

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Abstract

A novel computer model has been designed to aid in the formulation of powdered Ammonium Nitrate/Fuel Oil (ANFO) explosives. This mathematical model calculates heats of explosion, oxygen balances and raw material costs as a function of explosive ingredients. The best theoretical formulation consists of 91.5 % ~ 92.0 % ammonium nitrate (AN), 4.5 % ~ 5.0 % wood powder (WP), 3.0 % ~ 3.5 % composite fuel oil (CFO). This formulation results in an oxygen balance of zero or close to zero.

Keywords: ANFO explosive, Ammonium nitrate, Computer aid, Formulation design.

1. Introduction

One of the primary industrial explosives employed in China consists of ANFO. In order to decrease raw material costs, Fuel Oil (FO) is occasionally replaced with WP by explosive manufacturers. The net result, however, is that non-optimum explosive formulations are manufactured which results in: decreased fuel oxidation; poor blast performance; and an increase in noxious fumes, all of which are detrimental to the overall blasting objectives.

This paper reports on the following: 1) a novel computer aided method for the formulation of powdered ANFO explosives; 2) the establishment of a mathematical model for the formulation of ANFO explosives; 3) the computer aided formulation design and optimization of ANFO explosive and, 4) numerous reasonable formulations with different raw material costs.

2. A mathematical model for the formulation design of ANFO explosives containing C, H, O, and N

Explosive properties as a function of cost are usually the primary consideration during the formulation of industrial explosives. However, the ratios of Heats of Explosion as a function of cost should be the determining factor, not just cost alone. Explosive properties are a function of the heat of explosion (Qv) of an explosive, so the heat of explosion is selected as the primary figure of merit for our mathematical model. However, since cost is also an important factor in the manufacturing of explosives, the ratio of the amount of energy per unit cost (how much bang for the buck) should be the decisive factor as long as raw materials are the only cost consideration. However, while manpower should also be included in the equation, our model does not take this into manpower factors into consideration as these values vary with geographic location. Powdered ANFO explosives consist of Carbon (C), Hydrogen (H), Oxygen (O) and Nitrogen (N). The general empirical formula for ANFO is "$C_aH_bO_cN_d$". Assuming the specific empirical formula is, "$C_{ai}H_{bi}O_{ci}N_{di}$", then the molar mass of component "i" is given as "m_i" and the molar number of component "i" in 1 kg explosive is 10 $x_i\ m_i^{-1}$, where "x_i" is the percent mass content of component "i".

The equation for the reaction of an explosive containing C, H, O, N is given in equation (1).

$$C_aH_bO_cN_d = \sum \frac{10\ x_i}{m_i} C_{ai}H_{bi}O_{ci}N_{di} \rightarrow$$
$$\frac{b}{2}\ H_2O + (c - \frac{b}{2} - a)\ CO_2 + (2a - c + \frac{b}{2})\ CO + \frac{d}{2}\ N_2 \quad (1)$$

Where $a = \Sigma 10\ a_i x_i\ m_i^{-1}$, $b = \Sigma 10\ b_i x_i\ m_i^{-1}$, $c = \Sigma 10\ c_i x_i\ m_i^{-1}$, and $d = \Sigma 10\ d_i x_i\ m_i^{-1}$.

The mathematical formula (where the primary figure of merit is Heat of Explosion) is shown in equation (2).

$$\mathrm{Max}Q_v = \Delta H_{f(H_2O)} \cdot g_1 + \Delta H_{f(N_2)} \cdot g_2 + \Delta H_{f(CO_2)} \cdot g_3 + \Delta H_{f(CO)} \cdot g_4 - \sum \frac{10\ x_i \cdot \Delta H_{f(i)}}{m_i} \quad (2)$$

Where $g_1 = b\ 2^{-1}$, $g_2 = d\ 2^{-1}$, $g_3 = (c - b\ 2^{-1} - a)$,
$g_4 = 2\ a - c + b\ 2^{-1}$.

The mathematical expressions for the other figures of merit are:

Oxygen Balance (OB) = $\Sigma a_i x_i = 100\ \eta$
Variable Sum (VS) = $\Sigma x_i = 100$
Cost Sum (CS) = $\Sigma p_i x_i = p 10^{-1}$
Lower limits and upper limits = $s_i < x_i < t_i$, where i = 1, 2,..., n.

In this mathematical model the following definitions are employed:

ΔH_f Heat of formation for the ingredients, the entire explosive or explosive products (kJ mol^{-1})
g the molar number of the explosion products;
x_i the content of component "i" of the explosive;
m_i the molar mass of component "i";
a_i the oxygen balance of component "i" (%);
η the oxygen balance of the explosive (%);
p_i raw material cost of component "i", RMBy t^{-1};
p raw material cost of explosive, RMBy t^{-1};
s_i lower limit of component "i"; (%);
t_i upper limit of component "i"; (%).

3. Mathematical expression for ANFO explosive formulations

3.1 Commercial ANFO explosives ingredients and their chemical parameters

The oxidizer for ANFO explosives usually consists of: common Ammonium Nitrate; improved Ammonium Nitrate; or porous Ammonium Nitrate. The fuel is typically WP or CFO (which generally consists of a mixture of fuel oil and wax). The formulas, molar mass, heats of formation, oxygen balances and raw material costs of these components are listed in Table 1 [1)-5)].

3.2 Mathematical expression for formulation of ANFO explosives

If the amount of AN, WP, FO and wax is respectively x_1, x_2, x_3, and x_4, then:
$g_1 = 0.250\ x_1 + 0.304\ x_2 + 0.714\ x_3 + 0.748\ x_4$
$g_2 = 0.125\ x_1$
$g_3 = 0.125\ x_1 - 0.442\ x_2 - 1.492\ x_3 - 1.457\ x_4$
$g_4 = -0.125\ x_1 + 0.856\ x_2 + 2.143\ x_3 + 2.165\ x_4$
and, Formula (3) gives the general formula for Heat of Formation for ANFO explosives.

$$\sum \frac{10\ x_i \cdot \Delta H_{f(i)}}{m_i} = 44.183\ x_1 + 45.562\ x_2 + 29.486\ x_3 + 21.970\ x_4 \quad (3)$$

Table 1 Physical chemistry parameters of ANFO explosive raw materials.

No.	Empirical formula	Ingredient	MW (g $mole^{-1}$)	ΔHf (kJ $mole^{-1}$)	OB (%)	Cost (RMBy t^{-1})
1	$N_2O_3H_4$	AN	80	353.46	+20	1400
2	$C_{15}H_{22}O_{10}$	WP	362	1649.43	–137	400
3	$C_{16}H_{32}$	FO	224	660.44	–342	2000
4	$C_{18}H_{36}$	Wax	254	558.03	–346	4000

Table 2 Calculated properties of ANFO explosives at $\eta = 0$.

Formula No.	%AN	%WP	% FO + Wax	*Qv* (kJ kg^{-1})	OB (%)	Cost (RMBy t^{-1})	*Qv* $Cost^{-1}$ (kJt kg^{-1} $RMBy^{-1}$)
1	92.80	3.00	4.20	3845.2	0	1435.2	2.68
2	92.00	4.00	4.00	3787.8	0	1416	2.68
3	91.74	4.85	3.41	3836.9	0	1400	2.74
4	91.65	5.00	3.35	3832.7	0	1390.1	2.76
5	91.18	5.82	3.00	3821.9	0	1359.8	2.81
6	90.50	7.00	2.50	3820.3	0	1345	2.84

Table 3 Properties of ANFO explosives formulations at $\eta < 0$.

No.	%AN	%WP	% FO + Wax	*Qv* (kJ kg^{-1})	OB (%)	Cost (RMBy t^{-1})	*Qv* $Cost^{-1}$ (kJt kg^{-1} $RMBy^{-1}$)
1	91.03	6.00	2.97	3816.2	–0.2	1372.9	2.78
2	90.98	6.00	3.02	3803.7	–0.4	1373.8	2.77
3	90.92	6.00	3.08	3791.1	–0.6	1374.6	2.76
4	90.87	6.00	3.13	3778.6	–0.8	1375.5	2.75

Then the primary figure of merit (Maximum Heat of Explosion) is given in formula (4).

$$\text{Max } Q_v = 51.084\, x_1 - 50.653\, x_2 - 180.317\, x_3 - 173.169\, x_4 \quad (4)$$

Formula (4) assumes the following conditions:

$20\, x_1 - 137\, x_2 - 342\, x_3 - 346\, x_4 = 100\, \eta$

$x_1 + x_2 + x_3 + x_4 = 100$

$1.4\, x_1 + 0.4\, x_2 + 2.0\, x_3 + 4.0\, x_4 \leqslant p10^{-1}$

$89.0 \leqslant x_1 \leqslant 95.0$

$2.5 \leqslant x_2 \leqslant 7.0$

$1.0 \leqslant x_3 \leqslant 3.0$

$0 \leqslant x_4 \leqslant 1.0$

For formula (4), the values η and p may be assumed, in general $\eta \leqslant 0$.

4. Computer solutions

To arrive at a solution, a computer is employed. The mathematical formulas previously referenced are input into a MS Excel program. The mathematical solution is different with different oxygen balance values (η) and raw material costs. The solutions are detailed in Tables 2 and 3.

From Table 2, we observe that Formulation No. 6 has the higher ratio of heat of explosion to raw material cost than that of other formulations. However, the content of WP in Formulation No. 6 is higher than in the other formulations, resulting in a lower charge density compared to the other formulations, thus the energy per unit volume explosive is lower. Therefore, Formulation No. 4 has the overall best theoretical performance when charge density is considered. As AN content increases, the raw material cost increases, the heat of explosion increases, and overall explosive properties are improved based on formula (4). Since the value $x_1 > 0$, as AN increases, the theoretical heat of explosion increases. If the values of x_2, x_3, and x_4 increase (because of the multiples of x_2, x_3 and x_4 are < 0), then the heat of explosion for ANFO explosives decreases.

From Table 3, we see that, (for conditions when oxygen balance is less than zero ($\eta < 0$)), as oxygen balance becomes more negative, then: the AN weight percent decreases; the weight percent of fuel oil and wax increases; and the ANFO heat of explosion decreases. On the other hand (for oxygen balance values greater than zero (η < 0)), the volume of toxic gases (i.e., CO) produced after the explosion increases. Therefore, it is important that oxygen balances be zero (or close to zero) in order that formulations have high heats of explosion and low toxic gas volumes.

References

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