IMPACT CALCULATIONS

Objective

To study the variation in peak overpressures with the mass of a potentially explosive substance using TNT analysis and to quantify the consequences of calculated overpressures using probit correlations.

Probit Correlations*

1. Deaths from Lung Hemorrhage
   $Y = -77.1 + 6.91 \ln p_0$ 0% fatalities, $p_0 = 93.64$ kPa and 10% fatalities, $p_0 = 120.1$ kPa
2. Eardrum Ruptures
   $Y = -15.6 + 1.93 \ln p_0$ 0% fatalities, $p_0 = 9.13$ kPa and 10% fatalities, $p_0 = 22.26$ kPa
3. Structural Damage
   $Y = -23.8 + 2.92 \ln p_0$ 0% structural damage, $p_0 = 6.87$ kPa and 10% structural damage, $p_0 = 12.39$ kPa
4. Glass Breakage
   $Y = -18.1 + 2.79 \ln p_0$ 0% glass breakage, $p_0 = 1.34$ kPa and 10% glass breakage, $p_0 = 2.49$ kPa

**These correlations have been obtained from the textbook referenced at the end of the report.*

TNT Analysis and Overpressure Calculations

$$m_{TNT} = \frac{\eta m_{hc} \Delta H_c}{E_{TNT}} \qquad z_e = \frac{r}{m_{TNT}^{1/3}} \qquad \frac{p_o}{p_a} = \frac{1616\left[1 + \left(\frac{z_e}{4.5}\right)^2\right]}{\sqrt{1 + \left(\frac{z_e}{0.048}\right)^2}\sqrt{1 + \left(\frac{z_e}{0.32}\right)^2}\sqrt{1 + \left(\frac{z_e}{1.35}\right)^2}}$$

Parameters are defined in the nomenclature section at the end of this report. An explosion efficiency of 5% was assumed in all the calculations presented in this report.

Overpressure Vs Heat of Combustion Calculations

The figure below depicts the variation in overpressure with heat of combustion for 1 mg, 10 mg, 100 mg and 1000 mg of explosive substance. The distance 'r' was assumed to be 1 m. The overpressure increases with an increase in heat of combustion and also increases with an increase in the mass of explosive substance.

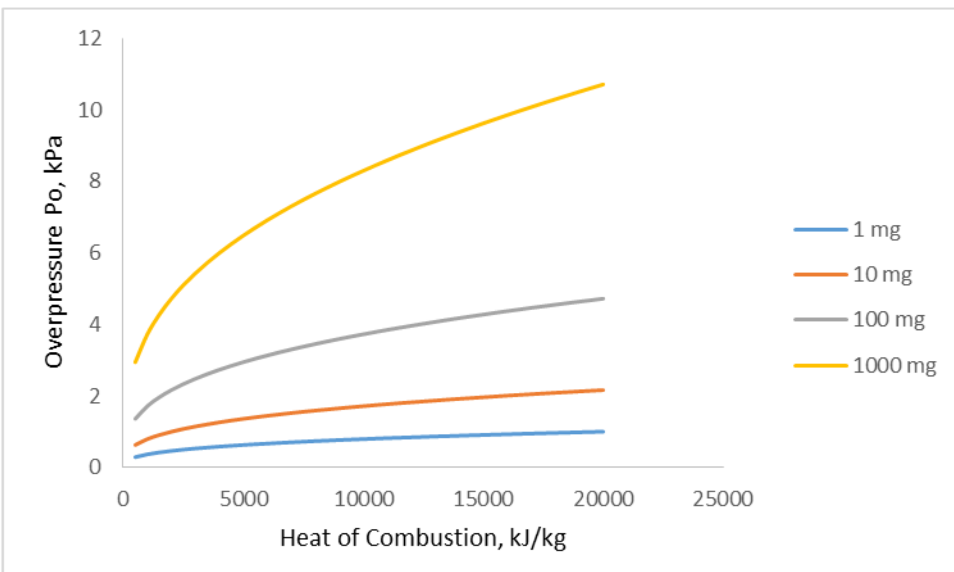

Figure 1: Overpressure Vs Heat of Combustion in kJ/kg for Different Masses of Substance

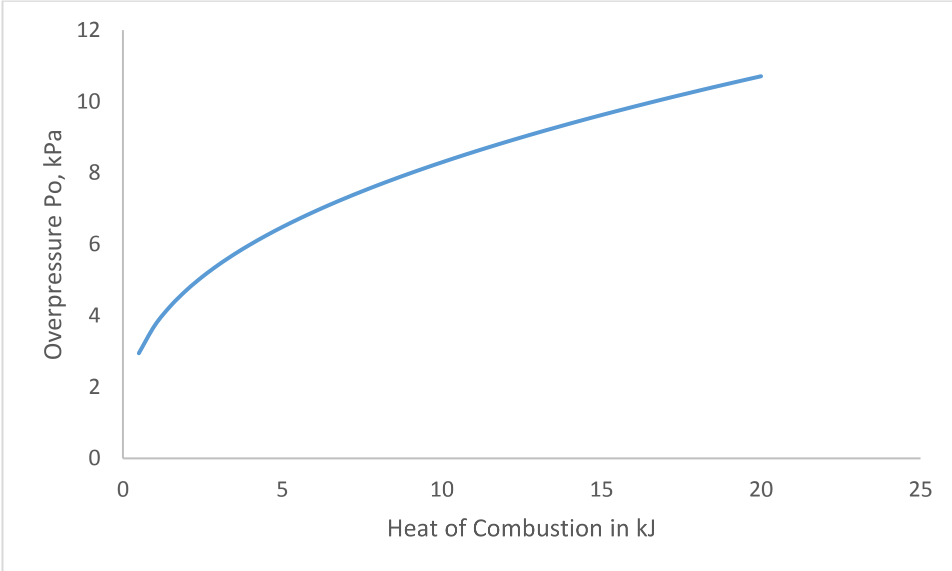

Figure 2: Overpressure Vs Heat of Combustion in KJ

The resulting overpressures in the figures above are in the range between 0.1 kPa and 11 kPa. The table below describes what these overpressures mean in terms of fatalities and damage caused.

Table 1: Estimated Damage due to Overpressure

Overpressure, kPa	% Lung Hemorrhage	% Eardrum Ruptures	% Structural Damage	% Glass Breakage*
0.1	0	0	0	0
1	0	0	0	0
2	0	0	0	2.9
3	0	0	0	22
4	0	0	0	51.5
5	0	0	0	75
6	0	0	0	88
7	0	0	0	94.5
8	0	0	0	97.5
9	0	0	1.5	99
10	0	0	2.8	99.5
11	0	0	5	99.8
12	0	0	8.5	100

Glass breakage refers to the shattering of glass, typically, those of windows and occasional failure of frames.

Summary of Calculations for some Potentially Explosive Lab Chemicals

1. Acetyl Peroxide

Mass of Substance, g	Overpressure, kPa	% Fatalities, Lung Hemorrhage	% Fatalities, Eardrum Ruptures	% Structural Damage	% Glass Breakage (shattering of glass)
0.1	5.81	0	0	0	86
1	13.51	0	1.5	15	100
10	38.75	0	42	98	100
100	171.24	88	99.6	100	100

2. Dinitrophenol

Mass of Substance, g	Overpressure, kPa	% Fatalities, Lung Hemorrhage	% Fatalities, Eardrum Ruptures	% Structural Damage	% Glass Breakage
0.1	4.24	0	0	0	58
1	9.54	0	0	1.9	99.4
10	24.45	0	13.8	76	100
100	89.74	0	92	100	100

3. Trinitrotoluene

Mass of Substance, g	Overpressure, kPa	% Fatalities, Lung Hemorrhage	% Fatalities, Eardrum Ruptures	% Structural Damage	% Glass Breakage
0.1	2.88	0	0	0	19
1	6.33	0	0	0	90.6
10	14.91	0	2	23	100
100	44.41	0	52	99.2	100

Relationship between Distance from Explosion Site and Overpressure

All the above overpressure calculations were made with the assumption, r = 1 m. The table below depicts the relationship between ‘r’ and overpressure. The overpressure was calculated for 10 mg of TNT. It can be observed that for distances of the order of magnitude 0.1 cm from the site of explosion, the calculated overpressures are very high. For this case, the values are significantly lower at distances above 10 cm.

Distance from Explosion Site, r (m)	Calculated Overpressure, Po (kPa)
0.001	533.4
0.01	11.9
0.1	0.147
1	0.013

Fume Hoods

A fume hood is designed primarily to exhaust chemical fumes, vapors, gasses, dust, mist and aerosol. They offer some protection against inhalation exposure, chemical spills, run-away reactions and fires by acting as physical barriers between the reactions and the laboratory. However, they are not designed to contain explosions, even when the sash is fully closed. Explosion Proof Fume Hoods, or Combustible Hood Enclosures are designed to eliminate igniting spark potential of fume hood components by using rated explosion proof components like light fixtures, switches, receptacles, motors and wiring on the fume hood. If an explosion hazard exists, the user should provide anchored barriers, shields or enclosures of sufficient strength to deflect or contain it. 3M offers safety and security window films which help protect people from flying glass shards, one of the most common causes of blast-related injuries and fatalities. It might be possible to incorporate such films in laboratory fume hoods.

Nomenclature

m_{TNT} = equivalent mass of TNT

η = empirical explosion efficiency (assumed as 5%)

m_{hc} = mass of hydrocarbon

ΔH_c = energy of explosion of the flammable gas

E_{TNT} = energy of explosion of TNT

M = molecular mass

z_e = scaled distance

r = distance from ground-zero point of explosion (assumed as 1 m)

p_s = scaled overpressure

p_o = peak side-on overpressure

References

Crowl, D.A. and Louvar, J.F. (2011). *Chemical Process Safety: Fundamentals with Applications*. Prentice Hall, Englewood Cliffs, NY.