Fire and Explosion Modelling

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Preliminaries
The Fire Triangle

- **Oxidizers**
  - **Liquids**
  - **Gases**
    - Oxygen, fluorine, chlorine
    - Hydrogen peroxide, nitric acid, perchloric acid
  - **Solids**
    - Metal peroxides, ammonium nitrate

- **Fuels:**
  - **Liquids**
    - Gasoline, acetone, ether, pentane
  - **Solids**
    - Plastics, wood dust, fibers, metal particles
  - **Gases**
    - Acetylene, propane, carbon monoxide, hydrogen

- **Ignition sources**
  - Sparks, flames, static electricity, heat
Fires and explosions can be prevented by removing any single leg from the fire triangle.

Problem: Ignition sources are so plentiful that it is not a reliable control method.

Robust Control: Prevent existence of flammable mixtures.
Vapor Mixtures – Definitions

• **Flash Point**
  – Lowest temperature at which a flammable liquid gives off enough vapor to form an ignitable mixture with air

• **Flammable / Explosive Limits**
  – Range of composition of material in air which will burn
    • UFL – Upper Flammable Limit
    • LFL – Lower Flammable Limit
    • HEL – Higher Explosive Limit
    • LEL – Lower Explosive Limit
Flammability Relationships

Concentration of Fuel

Mist

Vapour Pressure

Upper Limit

Lower Limit

FLAMMABLE REGION

FLASH POINT

Temperature
Flash Point From Vapor Pressure

- Most materials start to burn at 50% stoichiometric
- For heptane:
  - $C_7H_{16} + 11 O_2 = 7 CO_2 + 8 H_2O$
  - Air = $11 / 0.21 = 52.38$ moles air /mole of $C_7H_{16}$ at stoichiometric conditions
  - At 50% stoichiometric, $C_7H_{16}$ vol. % $\approx 0.9$
  - Experimental is 1.1%
  - For 1 vol. %, vapor pressure is 1 kPa temperature $= 23^\circ F$
  - Experimental flash point temperature $= 25^\circ F$
Flammability Diagram

Limiting O\textsubscript{2} Concentration:
Vol. % O\textsubscript{2} below which combustion can’t occur
Flammability Diagram

Limiting $O_2$ Concentration: Vol. % $O_2$ below which combustion can’t occur
Effect of Temperature on Lower Limits of Flammability
## Typical Values - 1

<table>
<thead>
<tr>
<th></th>
<th>LFL</th>
<th>UFL</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane:</td>
<td>5%</td>
<td>15%</td>
</tr>
<tr>
<td>Propane:</td>
<td>2.1%</td>
<td>9.5%</td>
</tr>
<tr>
<td>Butane:</td>
<td>1.6%</td>
<td>8.4%</td>
</tr>
<tr>
<td>Hydrogen:</td>
<td>4.0%</td>
<td>75%</td>
</tr>
</tbody>
</table>

### Flash Point Temp. (deg F)

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol:</td>
<td>54</td>
</tr>
<tr>
<td>Benzene:</td>
<td>12</td>
</tr>
<tr>
<td>Gasoline:</td>
<td>-40</td>
</tr>
</tbody>
</table>
Typical Values - 2

<table>
<thead>
<tr>
<th></th>
<th>AIT (deg. F)</th>
<th>MOC (Vol. % Oxygen)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane:</td>
<td>1000</td>
<td>Methane: 12%</td>
</tr>
<tr>
<td>Methanol:</td>
<td>867</td>
<td>Ethane: 11%</td>
</tr>
<tr>
<td>Toluene:</td>
<td>997</td>
<td>Hydrogen: 5%</td>
</tr>
</tbody>
</table>
More Definitions

• Auto Ignition Temperature
  – Temperature above which spontaneous combustion can occur without the use of a spark or flame.
  – The value depends on concentration of the vapor, material in contact and size of the containment

• Minimum Ignition Energy
  – Lowest amount of energy required for ignition.

• Minimum Oxygen Concentration (MOC)
  – Oxygen concentration below which combustion is not possible.
  – Expressed as volume % oxygen
  – Also called Limiting Oxygen Concentration (LOC)

• Max. Safe Oxygen Conc. (MSOC)
Minimum Ignition Energy

MIE is dependent on temperature, % of combustible in combustant, type of compound
Flammability Relationships

- Flash Point
- Auto Ignition Temperature (AIT)
- Flammable Region
<table>
<thead>
<tr>
<th>Material</th>
<th>Variation</th>
<th>Autoignition Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pentane in air</td>
<td>1.50%</td>
<td>1018 °F</td>
</tr>
<tr>
<td></td>
<td>3.75%</td>
<td>936 °F</td>
</tr>
<tr>
<td></td>
<td>7.65%</td>
<td>889 °F</td>
</tr>
<tr>
<td>Benzene</td>
<td>Iron flask</td>
<td>1252 °F</td>
</tr>
<tr>
<td></td>
<td>Quartz flask</td>
<td>1060 °F</td>
</tr>
<tr>
<td>Carbon disulfide</td>
<td>200 ml flask</td>
<td>248 °F</td>
</tr>
<tr>
<td></td>
<td>1000 ml flask</td>
<td>230 °F</td>
</tr>
<tr>
<td></td>
<td>10000 ml flask</td>
<td>205 °F</td>
</tr>
</tbody>
</table>
Autoignition Temperature (Some Data)
Auto-Oxidation

- The process of slow oxidation with accompanying evolution of heat, sometimes leading to autoignition if the energy is not removed from the system.

- Liquids with relatively low volatility are particularly susceptible to this problem.

- Liquids with high volatility are less susceptible to autoignition because they self-cool as a result of evaporation.

- Known as **spontaneous combustion** when a fire results; e.g., oily rags in warm rooms; land fill fires.
## Ignition Sources of Major Fires

<table>
<thead>
<tr>
<th>Source</th>
<th>Percent of Accidents</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrical</td>
<td>23</td>
</tr>
<tr>
<td>Smoking</td>
<td>18</td>
</tr>
<tr>
<td>Friction</td>
<td>10</td>
</tr>
<tr>
<td>Overheated Materials</td>
<td>8</td>
</tr>
<tr>
<td>Hot Surfaces</td>
<td>7</td>
</tr>
<tr>
<td>Burner Flames</td>
<td>7</td>
</tr>
<tr>
<td>...</td>
<td></td>
</tr>
<tr>
<td>Cutting, Welding, Mech. Sparks</td>
<td>6</td>
</tr>
<tr>
<td>...</td>
<td></td>
</tr>
<tr>
<td>Static Sparks</td>
<td>1</td>
</tr>
<tr>
<td>All Other</td>
<td>20</td>
</tr>
</tbody>
</table>
Fire Models
Flash Fire

- Flash fire is the non explosive combustion of a vapour cloud resulting from a release of flammable material into the open air, which, after mixing with air, ignites.

- Combustion in a vapour cloud develops an explosive intensity and attendant blast effects only in areas where intensity turbulent combustion develops and only if certain conditions are met.

- Where these condition are not present, no blast should occur.

- The cloud then burns as a flash fire, and its major hazard is from the effect of heat from thermal radiation.
Raj and Emmons Model (Flash Fire)

• The model is based on the observation;

  – The cloud is consumed by a turbulent flame front which propagates at a velocity which is roughly proportional to ambient win speed.

  – When a vapour cloud burns, there is always a leading flame from propagating with uniform velocity in the unburned cloud. The leading flame front is followed by a burning zone.

  – When gas concentrations are high, burning is characterized by the presence of a tall, turbulent diffusion, flame plume.

  – At point that cloud’s vapour had already mixed sufficiently with air, the vertical depth of the visible burning zone is about equal to the initial, visible depth of the cloud.
Raj and Emmons Model (Flash Fire)

\[ H = 20d \left[ \frac{S^2}{gd} \left( \frac{\rho_o}{\rho_a} \right) \frac{wr^2}{(1-w)^3} \right] \]

- **H** is visible flame height in m, **S** is constant velocity (burning speed) in m/s, **d** is cloud depth, **r** is stoichiometric mixture air fuel mass ratio, **g** is gravitational acceleration.

- \( \rho_o \) and \( \rho_a \) is fuel-air mixed and air density. **w** is represent the inverse of the volumetric expansion due to combustion in the plume, is highly dependent on the cloud’s composition.
W can be determine using the following equation;

\[
w = \frac{\phi - \phi_{st}}{\alpha(1 - \phi_{st})} \quad \text{for } \phi > \phi_{st}
\]

\(\alpha\) is a constant pressure expansion ratio for stoichiometric combustion (typically 8 for hydrocarbon),

\(\phi\) is a fuel-air mixture composition

\(\phi_{st}\) is stoichiometric mixture composition.

- If the cloud consist of pure vapour, \(w\) represents the inverse of the volumetric expansion resulting from constant pressure stoichiometric combustion: \(w = 1/9\).
- If the mixture in the cloud is stoichiometric or lean, there no combustion in the plume; the flame height is equal to the cloud depth, \(w = 0\). the behaviour of the expression for \(w\) should smoothly reflect the transmission from one extreme condition to the other.
- The model gives no solution for the dynamics of a flash fire, and requires an input value for the burning speed \(S\). the burning speed can be estimated as follows \(S=2.3U_w\) where \(U_w\) is the ambient wind speed.
Other Flash Fire Model

• Eisenberg, Lynch and Breeding (See Lees, 1996)
Jet Fire Model

- The jet fire model by Cook, Baharami and Whitehouse

\[ L = 0.00326 \left[ \dot{m}(-\Delta H_c) \right]^{0.478} \]

\[ R_s = 0.29s \left[ \log_{10}(L/s) \right]^{0.5} \]

$-\Delta H_c$ is the heat of combustion (J/kg)
$L$ is the length of flame (m)
$m$ is the mass flow (kg/s)
$s$ is the distance from the source of release
$R_s$ is the radius of the flame at distance $s$ (m) along with the centre line.
Pool Fire
Pool Fire Model

• Burgess and Hertzberg

\[ m = \frac{0.001 \Delta H_c}{\Delta H_v + c_p (T_b - T_a)} \]

Here, \( m \) is the mass burning rate in \( \text{kgm}^{-2}\text{s}^{-1} \)
\( \Delta H_c \) is the heat of combustion of fuel at its boiling point (kJ/kg)
\( \Delta H_v \) is the heat of vaporisation of fuel at its boiling point (kJ/kg)
\( C_p \) is the heat capacity of the liquid (kJ.\text{kg}^{-1}.\text{K}^{-1})
\( T_b \) is the liquid boiling temperature (K)
\( T_a \) is the initial temperature of the liquid (K)
Pool Fire Model

- The flame length can be estimated using Thomas Correlation

\[
\frac{L}{D} = 42 \left( \frac{m}{\rho_a (gD)^{0.5}} \right)^{0.61}
\]

where

- \( L \) is flame length (m),
- \( D \) is the pool diameter (m),
- \( g \) is the acceleration due to gravity
- \( \rho_a \) is the ambient density (kg/m\(^3\))
Explosion Models
BLEVE is a consequence of holding a pressurized flammable liquids above its boiling point.
Causes of BLEVE

- The immediate cause of the BLEVE is rupture of the container. If the pressure inside the vessel exceeds the outside strength of the walls the vessel will fail.
- If the vessel is overfilled and expansion (due to boiling of liquid) results in a heavy hydrostatic pressure.
- If the vessel is weakened by mechanical damage or by high temperature resulting from immersion in a fire then failure can occur.
Mechanism of BLEVE

- When BLEVE is initiated, the liquid boils off rapidly producing a reaction which turns parts of the ruptured vessel into rockets which can travel 2500 ft or more.

- The liquid can take fire if it is flammable and burning material can spread over a large area. If the gas or liquid mixes with air a vapour cloud explosion can occur.
Mathematical Model for BLEVE

- There are many models describing BLEVE. One such model is given below.

\[ t_{10} = 0.60(W_{tot})^{1/6} \]
\[ D = 1.836(W)^{1/3} \]

Here
- \(t_{10}\) is the lift-off time in seconds,
- \(W_{tot}\) is the total weight of combustibles and air,
- \(D\) is the maximum diameter of fireball and
- \(W\) is the weight of combustibles.
Vapour Cloud Explosion

U V C E

N C O F I N D

A P O L X

P O U P L O S I N S

D U D S

O S I N S
Vapor Cloud Explosion

- Cloud will spread from too rich, through flammable range to too lean.
- Edges start to burn through deflagration (steady state combustion).
- Cloud will disperse through natural convection.
- Flame velocity will increase with containment and turbulence.
- If velocity is high enough cloud will detonate.
- If cloud is small enough with little confinement it cannot explode.
- Increasing unsaturation will increase chance of explosion (flame speeds higher).
- Effect of explosion readily modeled by analogy with TNT.
Factors Favoring High Over Pressures

• Size of Clouds
  – probability of finding ignition source
  – likelihood of generating any overpressure
  – magnitude of overpressure

• Cloud composition
  – Highly unsaturated molecules are bad

• Weather
  – Stable atmospheres lead to large clouds.
  – Low wind speed encourages large clouds.

• Source
  – flashing liquids seem to give high overpressure
# Impact of VCEs on People

<table>
<thead>
<tr>
<th>Peak Overpressure psi</th>
<th>Equivalent Wind Velocity mph</th>
<th>Effects</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>70</td>
<td>Knock personnel down</td>
</tr>
<tr>
<td>2</td>
<td>160</td>
<td>Rupture eardrums</td>
</tr>
<tr>
<td>5</td>
<td>290</td>
<td>Damage lungs</td>
</tr>
<tr>
<td>10</td>
<td>470</td>
<td>Threshold fatalities</td>
</tr>
<tr>
<td>15</td>
<td>670</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>940</td>
<td>50% fatalities</td>
</tr>
<tr>
<td>30</td>
<td></td>
<td>99% fatalities</td>
</tr>
<tr>
<td>35</td>
<td></td>
<td></td>
</tr>
<tr>
<td>50</td>
<td></td>
<td></td>
</tr>
<tr>
<td>65</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
## Impact of VCEs on Facilities

<table>
<thead>
<tr>
<th>Peak Overpressure psi</th>
<th>Typical Damage</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5 - 1</td>
<td>Glass windows break</td>
</tr>
<tr>
<td>1-2</td>
<td>Common siding types fail:</td>
</tr>
<tr>
<td></td>
<td>- corrugated asbestos shatters</td>
</tr>
<tr>
<td></td>
<td>- corrugated steel panel joints fail</td>
</tr>
<tr>
<td></td>
<td>- wood siding blows in</td>
</tr>
<tr>
<td>2-3</td>
<td>Unreinforced concrete, cinder block walls fail</td>
</tr>
<tr>
<td>3-4</td>
<td>Self-framed steel panel buildings collapse</td>
</tr>
<tr>
<td></td>
<td>Oil storage tanks rupture</td>
</tr>
<tr>
<td></td>
<td>Utility poles snap</td>
</tr>
<tr>
<td>5</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Loaded rail cars overturn</td>
</tr>
<tr>
<td>7-8</td>
<td>Unreinforced brick walls fail</td>
</tr>
</tbody>
</table>
## Distance Comparison

<table>
<thead>
<tr>
<th>INVENTORY (tons)</th>
<th>UVCE</th>
<th>BLEVE</th>
<th>FIRE</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>120</td>
<td>18</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>150</td>
<td>36</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>200</td>
<td>60</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>250</td>
<td>90</td>
<td>20</td>
</tr>
<tr>
<td>20</td>
<td>310</td>
<td>130</td>
<td>30</td>
</tr>
<tr>
<td>50</td>
<td>420</td>
<td>200</td>
<td>36</td>
</tr>
<tr>
<td>100</td>
<td>530</td>
<td>280</td>
<td>50</td>
</tr>
<tr>
<td>200</td>
<td>670</td>
<td>400</td>
<td>60</td>
</tr>
<tr>
<td>500</td>
<td>900</td>
<td>600</td>
<td>100</td>
</tr>
<tr>
<td>1000</td>
<td>1150</td>
<td>820</td>
<td>130</td>
</tr>
</tbody>
</table>
Mechanical Explosion – Gas Filled Vessel

- Lees (1996) prefers to use Brode equation for the estimation of the explosion energy of gas-filled vessels. The following version of the Brode equation in terms of TNT equivalence has been given in the Second Canvey Report (HSE, 1981)

\[ E = 1.43 \times 10^{-6} \left( \frac{P_1 - P_0}{\gamma - 1} \right) V \]

E is the explosion energy (ton of TNT),
P_1 is the initial pressure in the vessel (kPa)
P_0 is the pressure of the surrounding (kPa)
V is the volume of the vessel (m³).
The volume can be calculated using Ideal gas law.
Chemical Explosion

- Explosion due to exothermic reaction occurring internally.
- Such reaction may involve decomposition of unstable substances, polymerization of monomers, or combustion of fuel – oxidant mixtures.
- Heating and increase of mole-number result in a rise in pressure to the bursting point of the vessel, etc.
- Explosives decomposes quickly that confinement of the development of pressure are self-imposed.
- Fire may or may not ensue.
Energy of Explosion

• It is important that the energy of explosion be estimated correctly

• Use appropriate model to estimate energy
  – Combustion
  – Heat of reaction
  – Physical explosion energy
  – etc
TNT Equivalent

- TNT equivalency is a simple method for equating a known energy of a combustible fuel to an equivalent mass of TNT.

- The approach is based on the assumption that an exploding fuel mass behaves like exploding TNT on an equivalent energy basis.
The equivalent mass of TNT

\[ m_{\text{TNT}} = \frac{\eta m \Delta H_C}{E_{\text{TNT}}} \]

- \( m_{\text{TNT}} \) is the equivalent mass of TNT (mass)
- \( \eta \) is the empirical explosion efficiency (unitless)
- \( m \) is the mass of hydrocarbon
- \( \Delta E_{\text{TNT}} \) is the energy of explosion of TNT

- A typical value for energy of explosion of TNT is 1120 calories/gram. The heat of combustion for the flammable gas can be used in place of the energy of explosion for the combustible gas.
The procedure to estimate the damage associated with an explosion using the TNT equivalent method is as follows:

- Determine the total amount of flammable material involved in the explosion.
- Estimate the explosion efficiency and calculate the equivalent mass of TNT.
- Use the scaling law to estimate the peak side on overpressure.
- Estimate the damage for common structures and process equipment using table guide.
Multi-Energy Models for Blast Effects

- Recent developments in science suggest too many unknowns for simple TNT model.
- Key variables to over pressure effect are:
  - Quantity of combustant in explosion
  - Congestion/confinement for escape of combustion products
  - Number of serial explosions
- Multi-energy is consistent with models and pilot explosions.
ALOHA

- A software offered free of charge by the US EPA.
  - Can model dispersion, fire and explosion

- Part of Cameo Suite
meters

meters

>= 8.0 psi = destruction of buildings
>= 3.5 psi = serious injury likely
>= 1.0 psi = shatters glass
Confidence Lines