Hazards Induced by Breach of Liquid Rocket Fuel Tanks: Physics-Based Modeling of Cavitation-Induced Self-Ignition and Radiation-Induced Aerosol Explosion of Cryogenic H2-Ox Fluids

Ekaterina Ponizovskaya-Devine
Viatcheslav Osipov
Cyrill Muratov
Halyna Hafiychuk
Vadim Smelyanskiy

Physics Based Methods, Ames - NASA
Fire starts between Orbiter and External tank at 73.213sec.

Flame emerging from the right SRB aft field joint

Dark smoke from SRB leak appears on the ground beginning 0.678 sec after ignition of the boosters

Source of ignition near the broken interface, localized far from hot nozzle gas was puzzling

1. Review of the hydrogen-oxygen vertical impact (HOVI) tests.
2. Detailed analysis of detonation and deflagration flames in GH2/GOx/air mixtures.
3. Key differences between the HOVI test data and the conventional deflagration and detonation.
4. The proposed mechanism of the explosion of GH2/GOX mixture.
7. Dynamics of escape of H2 and Ox liquids from ruptured tanks.
8. Evaporation of escaped cryogenic LH2/LOx on hot ground.
9. Fragmentation of escaped liquid streams and formation of droplets (aerosols) as a result of vertical impact of the ruptured tanks. Structure of sprays.
11. Flame acceleration by aerosol combustion.
12. Interpretation of HOVI 9 and other tests.
13. Cavitation-induced scenarios of ignition of GH2/GOx/LOx cryogenic mixtures and formation of their detonation or deflagration.
Hydrogen/Oxygen Vertical Impact (HOVI) tests

LOx and LH₂ tanks in HOVI 9, 13, and 14 were fixed on a 76 m (250 ft)-high drop tower. Then both tanks were dropped to the ground. In HOVI 2 and 5 only LOx tank was dropped to the LH₂ tank situated on the ground.

The impact velocity was within 30÷35m/sec.

The main purpose of these tests was to obtain explosion data that would be more typical or more representative of a launch vehicle failure than the distributive mixture tests.
Yield from 0.5 to 3.2 percent. Cloud briefly visible before ignition. Prompt ignition.

- Rupture devices between the tanks.
- Polyurethane shell
- Bottom is not ruptured

before

after
**Group 2**: Yield is below about 2 percent. Prompt ignition.

Test 13.

Bottom and top are ruptured.
• Analysis of detonation and deflagration as stable modes of combustion is based on published work and our simulations

• Study of detonation characteristics as functions of H2/O2/N2 mixture composition and conditions necessary for detonation initiation

• Analysis of the main parameters of turbulent deflagration flames in premixed H2/O2/N2 mixtures

• Comparison of detonation and deflagration combustion characteristics with HOVI data
### Hydrogen-oxygen mechanism (CANTERA)

<table>
<thead>
<tr>
<th>Reaction</th>
<th>(A)</th>
<th>(b)</th>
<th>(E) (cal/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(H_2 + O_2 = OH + OH)</td>
<td>1.70 (\times) (10^{13})</td>
<td>0</td>
<td>47 780</td>
</tr>
<tr>
<td>(H_2 + O_2 = H_2O + H)</td>
<td>2.57 (\times) (10^{12})</td>
<td>0</td>
<td>19 626</td>
</tr>
<tr>
<td>(H + O_2 = OH + O)</td>
<td>2.65 (\times) (10^{16})</td>
<td>-0.67</td>
<td>17 041</td>
</tr>
<tr>
<td>(O + H_2 = OH + H)</td>
<td>5.06 (\times) (10^4)</td>
<td>2.67</td>
<td>6290</td>
</tr>
<tr>
<td>(OH + H_2 = H_2O + H)</td>
<td>1.17 (\times) (10^9)</td>
<td>1.3</td>
<td>3626</td>
</tr>
<tr>
<td>(OH + OH = H_2O + O)</td>
<td>6.30 (\times) (10^8)</td>
<td>1.3</td>
<td>0</td>
</tr>
<tr>
<td>(H + OH + M = H_2O + M)</td>
<td>1.60 (\times) (10^{22})</td>
<td>-2.00</td>
<td>0</td>
</tr>
<tr>
<td>(H + H + M = H_2 + M)</td>
<td>1.00 (\times) (10^{18})</td>
<td>-1.00</td>
<td>0</td>
</tr>
<tr>
<td>(H + O + M = OH + M)</td>
<td>6.00 (\times) (10^{16})</td>
<td>-0.6</td>
<td>0</td>
</tr>
<tr>
<td>(H + O_2 + M = H_2O + M)</td>
<td>3.61 (\times) (10^{17})</td>
<td>-0.72</td>
<td>0</td>
</tr>
<tr>
<td>(H_2O + H = H_2 + O_2)</td>
<td>1.25 (\times) (10^{13})</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(H_2 + H = OH + OH)</td>
<td>1.40 (\times) (10^{14})</td>
<td>0</td>
<td>1073</td>
</tr>
<tr>
<td>(H_2O + H_2O = H_2O_2 + O)</td>
<td>2.00 (\times) (10^{12})</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(H_2O + O = O_2 + OH)</td>
<td>1.40 (\times) (10^{13})</td>
<td>0</td>
<td>1073</td>
</tr>
<tr>
<td>(H_2O_2 + OH = H_2O + H_2O)</td>
<td>1.00 (\times) (10^{13})</td>
<td>0</td>
<td>1800</td>
</tr>
<tr>
<td>(O + OH = H + O_2)</td>
<td>3.61 (\times) (10^{14})</td>
<td>-0.5</td>
<td>0</td>
</tr>
<tr>
<td>(H + H_2O = H_2 + H_2O)</td>
<td>1.6 (\times) (10^{12})</td>
<td>0</td>
<td>3800</td>
</tr>
<tr>
<td>(H + H + H_2 = H_2 + H_2O)</td>
<td>6.00 (\times) (10^{19})</td>
<td>-1.25</td>
<td>0</td>
</tr>
<tr>
<td>(H + H + H_2 = H_2 + H_2O)</td>
<td>9.2 (\times) (10^{16})</td>
<td>-0.6</td>
<td>0</td>
</tr>
<tr>
<td>(H_2O_2 + M = OH + OH + M)</td>
<td>1.3 (\times) (10^{17})</td>
<td>0</td>
<td>45 500</td>
</tr>
<tr>
<td>(O + O + M = O_2 + M)</td>
<td>1.2 (\times) (10^{13})</td>
<td>-1.788</td>
<td>0</td>
</tr>
<tr>
<td>(H_2O + OH = H_2O + O_2)</td>
<td>7.50 (\times) (10^{12})</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

#### Output data:

- **Density:** 2.71653 kg/m^3
- **Mean mol. weight:** 14.8652 amu
- **Chem. Pot. / RT:**
  - H2: 0.154075, 0.0208942, -19.5842
  - H: 0.0639392, 0.00433541, -9.79212
  - O2: 0.0428297, 0.0921948, -30.3961
  - O: 0.0305995, 0.0329341, -15.1981
  - OH: 0.138622, 0.158598, -24.9901
  - HO2: 0.000287541, 0.000638456, -40.1881
  - H2O2: 4.34225e-005, 9.93595e-005, -49.9802
  - H2O: 0.569603, 0.690306, -34.7822

### Hydrogen-air mechanism

<table>
<thead>
<tr>
<th>Reaction</th>
<th>(A)</th>
<th>(b)</th>
<th>(E) (cal/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(N_2 + O = NO + N)</td>
<td>1.4 (\times) (10^{14})</td>
<td>0</td>
<td>75 800</td>
</tr>
<tr>
<td>(N + O_2 = NO + O)</td>
<td>6.4 (\times) (10^9)</td>
<td>1</td>
<td>6280</td>
</tr>
<tr>
<td>(OH + N = NO + H)</td>
<td>2.65 (\times) (10^{16})</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(N_2 + M = 2N + M)</td>
<td>3.7 (\times) (10^{21})</td>
<td>-1.6</td>
<td>22 4928</td>
</tr>
</tbody>
</table>
Detonation wave of the $\text{H}_2/\text{O}_2$ stoichiometric mixture (2:1) explosion

Chapman–Jouguet theory, extended by Zeldovich, Von Neumann and Doering (ZND)

Huguenot Curves and Rayleigh Line

- Pressure, atm
- Temperature, K
- Initial point: $p_0=1\text{ atm}, T_0=100\text{ K}$
- $\rho_{\text{H}_2}=0.16, \rho_{\text{O}_2}=1.28\text{ kg/m}^3$

Chapman–Jouguet point

- $\rho_0 v_0 = \rho v$
- $p_0 + \rho_0 v_0^2 = p v^2$
- $c_p T_0 + \frac{v_0^2}{2} = c_p T + \frac{v^2}{2} + Q$

With constant specific heat assumption

Rayleigh Line:

$P = a \left( \frac{1}{\rho} \right) + b$

Huguenot Curve

$h(T) = Q + c_p (T - T_0)$

$Q = \sum Y_i h_{f_i}^0$
- reaction enthalpy

Major species profiles

$\rho_{\text{H}_2}$
$\rho_{\text{H}}$
$\rho_{\text{O}}$
$\rho_{\text{O}_2}$
$\rho_{\text{H}_2\text{O}}$
$\rho_{\text{H}_2\text{O}_2}$

$v_0 \approx 3000 \text{ m/s}$

Initial point,

- Pressure $p_0$
- Temperature $T_0$
- $\rho_{\text{H}_2}$
- $\rho_{\text{O}_2}$

Detonation wave curve

- Chapman–Jouguet theory, extended by Zeldovich, Von Neumann and Doering (ZND)

Detonation - supersonic combustion induced by strong shock wave

Detonation wave structure

Physics Based Methods, Ames - NASA

November 5-8, 2012
## Detonation parameters of H2/O2/N2 mixtures for initial mixture temperature $T_{mix} = 100K$

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$T$, K</td>
<td>2865</td>
<td>1450</td>
<td>3295</td>
<td>3261</td>
<td>3388</td>
<td>2806</td>
<td>2598</td>
</tr>
<tr>
<td>$P_{cj}$, atm</td>
<td>44</td>
<td>24</td>
<td>49</td>
<td>49</td>
<td>50</td>
<td>43</td>
<td>42</td>
</tr>
<tr>
<td>$P_{max}$, atm</td>
<td>82</td>
<td>44</td>
<td>92</td>
<td>91</td>
<td>94</td>
<td>81</td>
<td>76</td>
</tr>
<tr>
<td>Velocity, m/s</td>
<td>1972</td>
<td>1310</td>
<td>2234</td>
<td>2408</td>
<td>2278</td>
<td>2279</td>
<td>2614</td>
</tr>
</tbody>
</table>

### Species composition behind the detonation wave for various composition of mixture

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>After burning</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H2</td>
<td>0.02</td>
<td>$10^{-3}$</td>
<td>10^{-5}</td>
<td>10^{-6}</td>
<td>0.08</td>
<td>10^{-3}</td>
<td>0.20</td>
</tr>
<tr>
<td>O2</td>
<td>0.01</td>
<td>0.01</td>
<td>0.18</td>
<td>0.2</td>
<td>0.02</td>
<td>0.03</td>
<td>10^{-3}</td>
</tr>
<tr>
<td>N2</td>
<td>0.65</td>
<td>0.76</td>
<td>0.71</td>
<td>0.72</td>
<td>0.45</td>
<td>0.6</td>
<td>0.38</td>
</tr>
</tbody>
</table>

**11/16/2012 Physics Based Methods, Ames - NASA**
Detonation wave characteristics vs. hydrogen-oxygen mixture parameters

Detonation pressure strongly depends on temperature $T_{mix}$ of the mixture and relatively weakly on composition. Detonation temperature $T_{max}$ and velocity $v_{dw}$ strongly depend on composition and weakly on the mixture temperature $T_{mix}$.

**Hugoniot curves for $T_{mix}$**

- Dash lines – $p_{max}$
- Solid lines – $p_{cj}$

**Initial species mole fractions:** $H_2:O_2=2:1$

**Detonation pressure** strongly depends on temperature $T_{mix}$ of the mixture and relatively weakly on composition.
Detonation blast in H₂/air mixtures accompanied by high luminescence:
high speed video frames from a detonation experiment*

10 g of C-4 high explosive was used to initiate detonation in the stoichiometric hydrogen/air mixture. The detonation velocity was 1980 m/s, which is in good agreement with the C–J detonation velocity for a stoichiometric mixture of hydrogen and air: (*M. Groethe, E. Merilo, J. Colton, S. Chiba, Y. Sato, H. Iwabuchi, “Large-scale hydrogen deflagrations and detonations”, International Journal of Hydrogen Energy 32 (2007) 2125 – 2133.)
Conditions necessary for a detonation blast of $H_2:O_2:N_2$ mixture

- Strong local explosion that generates a shock wave with high pressure $p > p_{\text{max}}$.
- Critical pressure of initiating shock wave increases when radius of the localization of initiating shock wave decreases.
- The critical pressure in the initiating shock wave depends on the mixture composition, periphery temperature of the mixture, and exceeds $40 \text{atm} ÷ 100 \text{atm}$.
- The formation of detonation weakly depends on temperature in the initiating shock wave.

Data of pressure sensors show that the condition $p_{\text{max}} > 40 \text{atm}$ are not fulfilled in most of the HOVI tests.
Deflagration flame of H2/Ox mixtures at atmospheric pressure

Three processes determining deflagration flame dynamics:

1. Conductive heat flow from the flame front to the cold mixture. \( P=1\text{atm} \)

   \[ v_D = \frac{L_D}{\tau_B} = \sqrt{\frac{\kappa_{\text{air}} R_b}{C_{\text{air}} \rho_{\text{air}}}} \approx (2 \div 2.5)\text{m / sec} \]

   \[ R_b = \tau_B^{-1} \approx 3 \times 10^5 \text{sec}^{-1} \quad \text{combustion rate (see below)} \]

2. Turbulent acceleration of the burning rate according to experimental and numerical studies is:

   \[ v_{\text{Turb}} \approx 3.6 v_D \approx (7.2 \div 9)\text{m / sec} \]

   Velocity increases due to growth of effective combustion area.

3. Thermal expansion of hot combustion products and formation of fast deflagration flame at pressure close to atmospheric: \( p \approx 1 \text{ atm} \).

   \[ v_{\text{front}} \approx v_{\text{Turb}} \frac{T_{\text{flam}}}{T_{\text{mix}}} \approx (30 \div 70)\text{m / sec} \]

   Flame speed increases due to expansion of hot gas (water and nitrogen) forming as a result of the combustion:

   \[ T_{\text{flame}} = \frac{\rho_{H_2} Q_h}{\rho_{\text{products}} C_{p,\text{products}}} + T_{\text{atm}} \approx (2800 \div 3500)K \]

   \( Q_h \) - heat of combustion, \( C_{p,\text{products}} \) - specific heat of combustion products

   \( T_{\text{mix}} = 300K \)
Visible and IR pictures of an explosion of stoichiometric H2/O2 mixture in atmosphere*

Flame front velocity $v_f = 20\text{m/sec-33m/sec}$ for $x_{H2} = 0.867-0.999$ and pressure about 1atm.

Deflagration dynamics of GH2/GOx/GN2 mixture (2:1:4) (simulation results)

Initial conditions: $T_0=2000K$, $p_0=1$atm, and radius $R_0=1$cm

Deflagration propagates with temperature $T_{max}=3400K$, pressure $p_{max}=1.02$atm, and flame front velocity $V_f \approx 25$m/s

Pressure is very close to 1atm. The pressure length scale is much greater than that of temperature, i.e. the “temperature wave” is more localized than the “pressure wave”. Deflagration velocity is equal to

$$v_f \approx v_D \left( \frac{T_{\text{flame}}}{T_{\text{gas}}} \right) \approx 25 m / \text{sec}, \quad v_D = \sqrt{\frac{k_{\text{gas}} R_b}{C_{\text{gas}} \rho_{\text{gas}}}}$$

The simulation results of the simplified model agree with the results obtained from an analytical estimation.
Deflagration dynamics depending on the initial local pressure (simulation results)

Ignition condition: local temperature $T_0=3000\text{K}$ and pressure $p_0=25\text{atm} - 65\text{atm}$ inside area of the radius $R_0=1\text{cm}$.

Periphery temperature of mixture $T_{\text{mix}}=100\text{K}$ and pressure $p_{\text{mix}}=1\text{atm}$

Stationary pressure, temperature and velocity of the deflagration wave are $p=1\text{atm}$, $T=2400\text{K}$, $v=30\text{m/s}$ and do not depend on the ignition conditions.
### Hydrogen/Oxygen Vertical Impact (HOVI) tests: location of pressure sensors

<table>
<thead>
<tr>
<th># sensor / range</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>ft</td>
<td>4</td>
<td>5.75</td>
<td>8.4</td>
<td>12.3</td>
<td>17.8</td>
<td>25.8</td>
<td>37.67</td>
<td>54.7</td>
<td>79.2</td>
<td>115</td>
</tr>
<tr>
<td>m</td>
<td>1.2</td>
<td>1.7</td>
<td>2.5</td>
<td>3.6</td>
<td>5.4</td>
<td>7.7</td>
<td>11.5</td>
<td>16.4</td>
<td>23.8</td>
<td>35.5</td>
</tr>
</tbody>
</table>
Shape of shock wave impulse inside the mixtures (sensor data for distances 4ft and 5.8ft from explosion center)

The pressure in the blast waves of all HOVI tests (except for HOVI 9) is smaller than 5.5atm, i.e. the detonation conditions are not fulfilled and the explosion is a fast deflagration.

HOVI 13, $p_{\text{max}} = 4.2$atm
HOVI 2, $p_{\text{max}} = 5.4$atm
HOVI 5, $p_{\text{max}} = 3$atm

HOVI 9, $p_{\text{max}} \approx 80$atm-110atm, $V=2966-2625$ m/sec

The maximum pressure in the blast waves of HOVI 9 exceeds the critical pressure $p_{\text{max}}$. Such high pressure can be created by a strong shock wave of collapsing vapor bubble near LO2 surface or the formation of deflagration to detonation transition due to aerosol combustion.
Hazards induced by breach of liquid fuel tanks: Hydrogen-oxygen vertical impact (HOVI) tests

Outstanding problems:

(i) HOVI tests showed that cryogenic H2/Ox mixtures always self-ignite without any external sources when gaseous hydrogen and oxygen mix with a liquid Ox stream; Source of self-ignition was enigmatic!

(ii) HOVI tests data (pressure $p_f \sim 5$ atm and velocity $v_f \sim 600$ m/s of explosion front) cannot be explained by existent theory of detonation ($p_f > 50$ atm, $v_f > 2000$ m/s) and deflagration ($p_f = 1$ atm, $v_f < 30$ m/s).

<table>
<thead>
<tr>
<th>HOVI test</th>
<th>Pressure data, atm</th>
<th>Experimental shock velocity, m/sec (different directions)</th>
<th>Duration of shock wave msec</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>4.46 ÷ 5.4</td>
<td>740 ÷ 825</td>
<td>~ 3.5</td>
</tr>
<tr>
<td>5</td>
<td>2.5 ÷ 3</td>
<td>620 ÷ 660</td>
<td>~ 4.0</td>
</tr>
<tr>
<td>2</td>
<td>3.2 ÷ 4.7</td>
<td>730 ÷ 780</td>
<td>~ 3.4</td>
</tr>
<tr>
<td>9</td>
<td>80 ÷ 110</td>
<td>2625 ÷ 2966</td>
<td>~ 0.7</td>
</tr>
</tbody>
</table>

Delay time of ignition $t_{ign} = 10$ ms - 100 ms
Key differences between the HOVI test data and the conventional deflagrations

• High speed in excess of 700 m/sec

• Relatively high pressure of the blast waves from 3 atm to 5 atm (>100 atm for HOVI 9)

• High luminescence accompanying the blast
Conclusions about ignition conditions from HOVI tests

• Ignition always occurred in the LH2/LO2 pan tests. Tests demonstrated that this ignition is not due to external sources.

• The HOVI tank test data later verified the tendency for self-ignition of liquid hydrogen and liquid oxygen, because each HOVI test ignited without external assistance.

• The HOVI test data also showed that a liquid hydrogen spill alone is not likely to self-ignite, because in every HOVI test with a ground cloud of hydrogen, caused by a breach in the bottom of the hydrogen tank, the ground cloud did not ignite until liquid oxygen was released.

• HOVI test data showed that the ignition occurs when gaseous hydrogen (GH2) and oxygen (GOx), and liquid oxygen (LOx) mixture is available.
The cavitation-induced mechanism of ignition can arise just when gaseous hydrogen (GH2) and oxygen (GOx), and liquid oxygen (LOx) mixture is available.

Cavitation is collapse of oscillating bubbles of vapor GOx in LOx.

Cavitation-induced ignition of H2/Ox mixtures is determined by injection of super-heated and super-compressed gas formed in a bubble collapsing near the LOx surface into the space above LOx surface and ignition of the GH2/GOx mixture in this space.

The ignition effect intensifies when GH2 is inside the collapsing vapor bubble in LOx.

The cavitation ignition is a random process that is characterized by different maximum temperature and pressure of gases injected form the collapsing bubble in gaseous H2/O2 mixtures.
Inertial collapse of bubbles with rarefied gas

A simple analogy of this effect is inertial adiabatic compression of a gas in a cylinder under the action of the piston. In this case

\[ \frac{p}{p_0} = \left( \frac{V_0}{V} \right)^\gamma = \left( \frac{H}{x} \right)^\gamma; \quad \frac{T}{T_0} = \left( \frac{V_0}{V} \right)^{\gamma-1} = \left( \frac{H}{x} \right)^{\gamma-1} \]

and the equation of motion of piston of mass \( M \) is

\[ M\ddot{h} = Mg + p_{atm}S - pS; \quad h = H - x \]

\[ \frac{M}{S} \ddot{x} = p_0 \left( \frac{H}{x} \right)^\gamma - p_L; \quad p_L = p_{atm} + \frac{Mg}{S} \]

Initial condition: \( t = 0 \), \( \dot{x} = v = 0 \), \( x = H \)

Final condition: \( t = t_f \), \( \dot{x} = v = 0 \), \( x = x_{\text{min}} \)

\( p_0 \) is initial vapor pressure.

Effect of strong compression of vapour bubble and initiation of extremely high temperature and pressure in it is determined by inertia of the heavy piston motion.

The role of the piston in cavitation of a vapor bubble is played by the liquid. The effect intensifies due to the condensation and burning of GOx/GH2 mixture inside the bubble

If the initial gas temperature \( T_0=300 \text{K} \) and pressure \( p_0 < 0.1p_a \) then the maximum pressure and temperature in both the piston and the collapsing bubble are

\[ p_{\text{max}} \geq 125 \text{atm} \]

\[ T_{\text{max}} \geq 1200 \text{K} \]
Inertial cavitation of bubbles with vapor and rarefied neutral gas: simplified analytical calculation

**Initial LOx temperature** $T_0 = 90K$ and pressure $p_0 = 1\text{ atm}$. The overpressure shock jump is $0.5\text{ atm}$ ($p_L - p_0 = 0.5\text{ atm}$), then the maximum vapor pressure and temperature in the collapse bubble are

(a) **Without considering condensation**

Rayleigh-Plesset equation of bubble motion

$$ R \frac{d^2 R}{dt^2} + \frac{3}{2} \left( \frac{dR}{dt} \right)^2 + 4\nu \frac{dR}{dt} + \frac{2\sigma}{\rho_L R} = \frac{p_b(R) - p_L}{\rho_L} \quad \text{for } R < R_0 $$

$p_b(R) = p_0 \left( \frac{R_0}{R} \right)^{3\gamma}$, $p_L = p_L + 2\sigma / R_0$

$$ R_{\min} = R_0 \left( \frac{p_0}{(\gamma - 1)p_L^*} \right)^{\frac{1}{3(\gamma - 1)}} $$

$$ p_{\max} = \Gamma p_L \left( \frac{p_L^*}{p_0} \right)^{\frac{1}{(\gamma - 1)}} \quad \text{for } \Gamma = \frac{(\gamma - 1)p_L^*}{p_0} $$

$T_{\max} = T_0 \left( \frac{(\gamma - 1)p_L^*}{p_0} \right)$

$p_0$ is initial pressure of the neutral gas.

(b) **With considering of condensation**

The Ox vapor bubble contains saturated oxygen vapor and a small portion of gaseous hydrogen (GH2). $p_v$ is pressure of saturated oxygen vapor, $p_{g0}$ is initial GH2 pressure: $p_{g0} << p_v$. The saturated vapor condenses on the bubble wall and its pressure remains low down to a very small radius for $t < t_c$.

$$ p_b(t) = p_v + p_{g0} \left( \frac{R_0}{R} \right)^{3\gamma} \quad \text{at } t < t_c = \left( \frac{R_o}{\Sigma} \right)^{2/3} \propto \left( \frac{\rho_L}{\rho_v} \right)^{4/3} $$

$$ \Sigma(T_L) = \frac{q_L^2}{c_L T_L D_L^{1/2}} \left( \frac{\rho_v}{\rho_L} \right)^2 $$

$$ t_f = 0.915 \left( \frac{\rho_L R_0^2}{(p_L - p_v)} \right)^{1/2} \approx 4 \times 10^{-4} \text{ sec for } R_0 \leq 1 \text{ mm} \quad \text{Time of bubble collapse} $$

This is condition of the effect: condensation is intensive enough.

It is valid for LOx but not for LH2 due to different of $T_L$ and relation $\left( \frac{\rho_L}{\rho_v} \right)$

(a) without considering of condensation:

$$ \Delta p_{\max} \approx 0.017 \text{ atm} \quad \Delta T_{\max} \approx 54K $$

(b) with considering of condensation for $p_L - p_0 = 0.5\text{ atm}$:

$$ p_{\max} \approx p_{g0} \left[ \frac{(\gamma - 1)p_L^*}{p_{g0}} \right]^{\frac{1}{(\gamma - 1)}} \left( \frac{(\gamma - 1)p_L^*}{p_{g0}} \right) $$

$$ T_{\max} \approx T_0 \left( \frac{(\gamma - 1)p_L^*}{p_{g0}} \right) $$

$$ R_{\min} \approx R_0 \left( \frac{p_{g0}}{(\gamma - 1)p_L^*} \right) \left( \frac{(\gamma - 1)p_L^*}{p_{g0}} \right) \quad \text{for } p_{g0} = 0.01(0.005)\text{ atm} $$

$$ p_{\max} \approx 300(800)\text{ atm} \quad T_{\max} \approx 5400(11000)\text{ K}, $$

$$ R_{\min} \approx 0.03(0.02)\text{ mm} \quad \text{for } p_{g0} = 0.01(0.005)\text{ atm} $$

11/16/2012
Equations for radius of the collapsing vapor bubble in liquid

For the incompressible liquid

\[ \frac{\partial \rho_L}{\partial t} = 0 \implies \frac{\partial}{\partial r} (\rho_L u_L) + \frac{2 \rho_L u_L}{r} = 0 \]

Using the boundary condition

\[ \rho_L (u_L - \dot{R}) = -j_{cd} \]

we find:

\[ u_L(r, t) = \left( \frac{R}{r} \right)^2 \dot{R} - \frac{j_{cd}}{\rho_L} \left( \frac{R}{r} \right)^2 \]

Then the conservation moment equation

\[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial r} = -\frac{1}{\rho} \frac{\partial p}{\partial r} + \frac{\mu}{\rho} \Delta u \]

can be written as

\[ -\frac{1}{\rho_L} \frac{\partial p_L}{\partial r} = \ddot{R} \left( \frac{R}{r} \right)^2 + \frac{2R}{r^2} \dot{R}^2 - \frac{1}{\rho_L} \left( \frac{R}{r} \right)^2 \frac{dj_{cd}}{dt} \frac{R\dot{R}}{\rho_L r^2} - \frac{2R^4}{r^5} \dot{R}^2 + \frac{2j_{cd} R^4}{\rho_L r^5} \dot{R} + \frac{2R^4}{r^5} \frac{j_{cd}}{\rho_L} \dot{R} - \frac{j_{cd}^2}{\rho_L^2} \frac{2R^4}{r^5} \]

Integrating this equation from R and taking into account boundary condition for the pressure at \( r=R \)

\[ p_L + \frac{2\sigma}{R} = p_m + \frac{j_{cd}^2 \rho_m (\rho_L - \rho_1)}{\rho_L \rho_1} - \frac{2\mu}{3R} \left( \frac{R}{\rho_L} \right) \left( \frac{\dot{R} - j_{cd}}{\rho_L} \right) \]

we obtain the modified Rayleigh-Plesset equation for the bubble radius:

\[ \ddot{R} + \frac{3}{2} \left( \frac{\dot{R}}{\rho_L} \right)^2 - \frac{\dot{R} j_{cd}}{\rho_L} - \frac{R}{\rho_L} \frac{dj_{cd}}{dt} - \frac{j_{cd}^2}{2 \rho_L^2} = \frac{p_L}{\rho_L} + \frac{p_m}{\rho_L} - \frac{2\sigma}{R \rho_L} + \frac{j_{cd}^2 \rho_m (\rho_L - \rho_1)}{\rho_L \rho_1} - \frac{2\mu}{3R \rho_L} \left( \frac{\dot{R} - j_{cd}}{\rho_L} \right) \]
A high-fidelity model of collapsing of Ox vapor bubbles with admixed GH2 taking into consideration the burning inside the bubble was developed. The equations for the incompressible liquid phase \(r > R(t)\) may be reduced to the equation for the bubble radius \(R\):

\[
R \frac{d^2 R}{dt^2} + \frac{3}{2} \left( \frac{dR}{dt} \right)^2 + \frac{j_{cd}}{\rho_L} \frac{dR}{dt} - \frac{R}{\rho_L} \frac{dj_{cd}}{dt} = \frac{p_m - p_L}{\rho_L} - \frac{2\sigma}{R\rho_L} + \frac{j_{cd}^2 (2\rho_L - \rho_m)}{2\rho_L^2\rho_m} - \frac{4\mu}{R\rho_L} \left( \frac{\dot{R}}{\rho_L} - j_{cd} \right)
\]

the advection-diffusion equation for the liquid temperature \(T_l\):

\[
\frac{\partial T_l}{\partial t} + \left( \frac{R}{r} \right) \left( \frac{dR}{dt} \right) \frac{\partial T_l}{\partial r} = \frac{\kappa_L}{C_L \rho_L r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial T_l}{\partial r} \right)
\]

with initial and boundary conditions:

\[
R(t = 0) = R_0, \quad \dot{R}(t = 0) = 0, \quad T_L(0) = T_m(0) = T_{L0}, \quad T_L(r \to \infty) = T_{L0}, \quad (T_L(r = R) = T_m(r = R) = T_s).
\]

Due to high gas temperature in the bubble the equations for gas phase are:

\[
\begin{align*}
\frac{\partial E}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 u_m (p_m + E) \right) &= \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \kappa_m \frac{\partial T_m}{\partial r} \right) + Q_h G_{comb} \\
E &= \frac{5}{2} R_0 T_m c_m + \frac{1}{2} \rho_m u_m^2, \quad \rho_i = c_i M_i, \quad \rho_m = \sum_i c_i M_i, \\
\frac{\partial u_m}{\partial t} + u_m \frac{\partial u_m}{\partial r} &= -\frac{R_0}{\rho_m} \frac{\partial (T_m c_m)}{\partial r}, \quad \kappa_m = \sqrt{\frac{T_m}{T_0} \sum_i c_i \kappa_i(T_0)}
\end{align*}
\]

Here \(r\) is the radial coordinate, \(\rho_L, C_L\) and \(r_L\) are the liquid density, specific heat and thermal conductivity, \(p_m\) and \(\rho_m\) are the pressure and gas mass density, respectively, \(\rho_L\) is pressure in liquid far from the bubble; \(R_0, c_p\) are the gas constant and mole concentration \(i\) – gas; \(\rho_m, T_m, u_m,\) and \(E\) are the total density, temperature, velocity, and energy of gas mixture (H2,O2, H2O).
Basic model for collapsing bubbles in a liquid

Dynamics of the gas mixture inside a bubble, taking into account the combustion and high diffusivity of the light GH2 molecules, can be written as

\[
\begin{aligned}
\frac{\partial c_{Ox}}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 c_{Ox} u_m \right) &= -\frac{1}{2} G_{comb}, \\
\frac{\partial c_{H2O}}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 c_{H2O} u_m \right) &= G_{comb}, \\
\frac{\partial c_{H2}}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 c_{H2} u_m \right) + G_{comb} &= \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 D_{H2} \left( \frac{\partial c_{H2}}{\partial r} - \frac{c_{H2}}{2T_m} \frac{\partial T_m}{\partial r} \right) \right]
\end{aligned}
\]

Here

\[
D_{H2} = \left( \frac{T_m}{T_0} \right)^{3/2} \left( \frac{p_0}{p_m} \right) D_{H2}(T_0, p_0)
\]

is hydrogen diffusion coefficient.

\(q_h\) is the latent heat of vaporization.

The initial and boundary conditions for above equations are:

\[
\frac{\partial T_m}{\partial r} \bigg|_{r=R} = 0, \left( \kappa_m \frac{\partial T_m}{\partial r} - \kappa_i \frac{\partial T_i}{\partial r} \right) \bigg|_{r=R} = j_{cd} q_h, \quad \frac{\partial c_i}{\partial r} \bigg|_{r=R} = 0, \quad c_i \bigg|_{r=0} = c_{i,0}, \quad u_m \bigg|_{r=0} = 0, \quad u_m \bigg|_{r=R} = \frac{\partial R}{\partial t} - \frac{j_{cd} c_{H2}}{c_{Ox} M_{Ox}}, \quad \frac{j_{cd} c_{H2}}{c_{Ox} M_{Ox}} = D_{H2} \left( \frac{\partial c_{H2}}{\partial r} - \frac{c_{H2}}{2T_m} \frac{\partial T_m}{\partial r} \right) \bigg|_{r=R},
\]

The burning of GOx/GH2 mixture is described by 20 chain chemical reactions in CANTERA CODE that include generation of O, H, OH species. For simplicity here we consider a simplified model of the burning that takes into account only main gas components that can arise in a collapsing bubble (at 0 < r < R): oxygen vapor, non-condensable gaseous hydrogen and water generated as a result of the burning. The simplified model based on the assumption that the burning rate is limited by the initiation reactions having the lowest rates:

\[
\text{H2} + \text{O2} \rightarrow \text{OH} + \text{OH} \quad \text{and} \quad \text{H2} + \text{O2} \rightarrow \text{HO2} + \text{H},
\]

Thus, we modeled the GH2/GOx combustion by the brutto reaction H2+O2 → H2O+ 1/2O2 with the rate: (T is in degrees Kelvin).

\[
G_{comb} = c_{H2} c_{Ox} \left[ 1.1 \cdot 10^8 \exp(-19680 / T) + 1.48 \cdot T^{2.433} \exp(-26926 / T) \right] m^3 / mol / s
\]

This simplified combustion model predicts the same parameters of steady detonation and deflagration waves as those obtained with the help of the full model describing all main chain reactions of GOx/GH2 mixture combustion.
Cavitation-induced ignition (scenario 1)

Cooling of surface of O2/H2 bubbles, their collapse and generation of a strong shock wave

(1) Cooling of surface of LOx fragments by cold GH2

(2) Formation of bubbles with thin cooled liquid layers and low pressure

(3) Collapse of the bubble and generation of the strong shock wave by the bubble collapsing near the liquid-gas interface.

Over 30 msec ignition delay time

0.1 mm surface layer of LOX fragment submerged into ~ 30K GH2 atmosphere will be cooled down to 60K - 70K.

\[ p = p_c \left( \frac{T_s}{T_c} \right)^7 \]

\[ T_c = 154.6K \quad p_c = 50.4\text{atm} \]

\[ p = 0.12\text{atm at 65K} \]
Simulation results (scenario 1): Formation of collapsed bubble with gigantic pressure and temperature

Code based on high-fidelity physics-based complex model for collapsing bubble was developed. The model takes into account the dynamic condensation-evaporation processes and combustion of Ox/H2 mixture inside the bubble.

An algorithm and a computer code were developed.

The algorithm MUSCL scheme with variable mesh that is thinner near the gas/liquid boundary. We use variable time-step algorithm that is applicable to stiff problems.

Collapsing of bubble of radius $r_0=2$mm, surface temperature $T_s=65$K (blue) and 70K (red), ambient pressure $p=1$atm, and initial partial GH2 pressure 0.01atm for different Hertz-Knudsen accommodation coefficient $\alpha=1$ (solid) and 0.3 (dashed).
Scenario 2: Formation in a LOx fragment of a “weak” shock producing of vapour bubble collapsing and cavitation-induced ignition of GH2/Ox mixture

Model of formation of a “weak” shock as a result of impact of a LOx piece on a solid wall

After the impact, the weak shock wave induces collapse of bubble near the liquid- mixture interface (result simulation).

Secondary cavitation shock wave

GOx vapor bubble with GH2 admixture will collapse with very high P and T if initial pressure jump > 0.3 atm

Collapsing of bubble of radius $r_0 = 2\text{mm}$, temperature $T_L = 90\text{K}$, pressure $p = 1\text{atm}$, and initial partial GH2 pressure $0.003\text{atm}$ (red), $0.01\text{atm}$ (blue) under the initiating shock wave with over pressure $\Delta p_L = 0.5\text{atm}$ (red), $1\text{atm}$ (blue). (see next slide for detail).

Pressures of the shock waves induced by impact of the LOx fragment at solid surface

$$p \approx \rho_L v^2 / 2 \approx 2.5 \text{ atm}, \quad v = 20 \div 30 \frac{m}{\text{sec}}$$

Conclusion: The pressure in the weak shock wave is too small to directly induce ignition of GH2/GOx mixture of any composition but is large enough to induce bubble collapse in the liquid oxygen.
Scenario 2: Dynamic of main variables in the collapsing bubble

- **Time (ms)**
  - Initial time: $t_0 = 0.29\,\text{ms}$
- **Radius (mm)**
  - Minimum radius: $r_{\text{min}} = 0.07\,\text{mm}$
- **Temperature (K)**
  - Maximum temperature: $T_{\text{max}} = 1700\,\text{K}$
- **Total pressure (atm)**
  - Maximum pressure: $p_{\text{max}} = 2200\,\text{atm}$
- **Condensation $J_{\text{cd}}$ (kg/m$^2$/s)**
  - Maximum condensation rate: $J_{\text{cd, max}} = 18000\,\text{kg/m}^2/\text{s}$
- **H$2$ pressure (atm)**
  - Maximum H$2$ partial pressure: $p_{H_2,\text{max}} = 1300\,\text{atm}$
- **Reaction rate, sec$^{-1}$**
  - Maximum reaction rate: $G_{\text{max}} = 3\times10^4/\text{sec}$
Shock formation in LOx pieces as a result of their impact on Challenger surface and cavitation-induced ignition of released GH2/Ox (Scenario 2)

First Fireball Area
In O2/H2 mixture cloud
Dynamics of detonation wave formation in gaseous stoichiometric H2/O2/N2 mixture induced by cavitation ignition

The parameters of steady detonation wave $p_{\text{max}}=100\,\text{atm}$, $p_{\text{cj}}=60\,\text{atm}$, $T_{\text{max}}=3800\,\text{K}$, $v_{\text{dw}}=3000\,\text{m/s}$ in stoichiometric H2/Ox mixture coincide with those that we obtained using the model (CANTERA) taking into account 19 main chain reactions in GOx/GH2 mixture detonation.

Numerical and analytical calculations showed that the pressure in the collapsing bubbles can exceed 2000 atm. Radial shock wave of the radius $r>0.15\,\text{mm}$ and the pressure $p > 250\,\text{atm}$ induced by a collapsing bubble can lead to detonation ignition of the H2/Ox mixture. Dynamics of this process is shown in the figures.

Cavitation-induced ignition of a stoichiometric H2/Ox mixture (2:1) with the mixture temperature $T=100\,\text{K}$ and pressure $p=1\,\text{atm}$ for radius $r>0.15\,\text{mm}$. Initial cavitation condition: temperature $T_0=1500\,\text{K}$ and pressure $p_0=350\,\text{atm}$ for $r<0.15\,\text{mm}$ (in red).
In reality the super-hot and compressed O, H, and OH species are formed in the process of GH2/GOx combustion inside bubbles. They will be ejected into the space above the LOx surface and easily ignite the GH2/GOx mixture nearby.

Ignition induced by injection of hot atom gases from bubbles collapsing in a liquid into GH2/GOx mixture

In the case of injection of the atomic species into the explosive H2/Ox mixture the ignition rates is limited by the following very fast reactions:

\[ O + HO_2 \rightarrow O_2 + OH, \quad O + H_2 \rightarrow OH + H, \quad H + O_2 \rightarrow HO_2, \quad HO_2 + OH \rightarrow H_2O + O_2 \]

The first and last reactions have activation energy \( \Delta = 0 \) and other \( \Delta \) is closed to zero.

Our calculation based on CANTERA Code showed that the explosive mixture containing 0.05 mole fraction of atomic hydrogen self-ignites at the temperatures \( T \geq 85K \).
The detonation wave rapidly dissipates in the area with zero H2 density and heat wave initiates a deflagration in the mixture at the other side of zero H2 area. The parameters of the deflagration wave:

- Maximum temperature $T_{\text{max}} = 2600K$
- Flame front velocity $V_f = 30m/s$
- Pressure $p$ is about 1atm

Transition of local detonation induced by cavitation ignition to aerosol deflagration

Initial conditions:

- $T_{\text{mix}} = 200K$, $p_{\text{mix}} = 1\text{atm}$
- $T = 3000K$, $p = 3000\text{atm}$ inside area $r < r_0 = 0.1\text{mm}$

Results of simulation

- For radius of collapsing bubble $r_{\text{min}} = 0.1\text{mm}$, size of hydrogen exhaustion area $R_{\text{inh}} = 1\text{cm}$

White is area with zero H2 density

The detonation wave rapidly dissipates in the area with zero H2 density and heat wave initiates a deflagration in the mixture at the other side of zero H2 area.
Proposed mechanism of the explosion of GH2/GOX mixture

- HOVI test explosions of GH2/GOX mixture are intensified by the combustion of cryogenic H₂/O₂ aerosols.

- Aerosol vaporization is controlled by infrared radiation of hot combustion products.

- Aerosols form as a result of an impact of the liquid jet escaping from the ruptured tanks against solid surfaces.
Sequence of events leading to explosion

1. Breach of the LH2 tank and escape of the LH2 jet
2. Fragmentation of the LH2 jet and formation of LH2 droplets (aerosol) in the air
3. Partial evaporation of LH2 droplets
4. Breach of the LOx tank and formation of LOx aerosol cloud near the top of the LH2 tank
5. Mixing of LH2 and LOx aerosols
6. Cavitation-induced ignition upon direct contact of large Lox pieces with LH2 droplets
7. Onset of fast deflagration combustion of GH2 with atmosphere oxygen and formation of hot luminous combustion products
8. Enhanced LH2 and LOx droplet evaporation by infrared radiation
9. Initiation of radiation-mediated LH2-LOx aerosol combustion behind the flame front
10. Rapid flame acceleration as a result of pressure, temperature, and product density buildup due to the aerosol combustion
11. Formation of a super-fast deflagration or detonation flame that may trigger deflagration-to-detonation transition
12. Formation of detonation due to cavitation-induced ignition
Dynamics of escape of H2 and Ox liquids from ruptured tanks (the first group of HOVI Tests)

Conservation of mass of escaped liquid in time $dt$ (adiabatic process)

\[
\frac{\rho_L v^2}{2} S_h dh = \frac{\rho_L V_0^2}{2} S_h dh + (p - p_{at}) S_h dh, \quad dh_g = -dh_L = \frac{S_h}{S_0} v dt, \quad dm_L = \rho_L S_0 dh_g,
\]

\[
p = \left( \frac{V_{g0}}{V_g} \right)^\gamma \quad \frac{dV_g}{dt} = a \left( \frac{V_{g0}}{V_g} \right)^\gamma - \frac{p_{at} + \rho_L V_0^2}{2 p_0} \right) \frac{1}{2}, \quad a = \frac{S_h}{S_0} \left( \frac{2 p_0}{\rho_L} \right) \frac{1}{2}
\]

\[
t = \int_{V_{g0}}^{V_g} \frac{dV}{a \left[ \left( \frac{V_{g0}}{V} \right)^\gamma - \frac{p_{at} + \rho_L V_0^2}{2 p_0} \right]^{1/2} \frac{\rho_L v_0^2}{2 p_0} < \frac{p_{at}}{p_0} \quad \text{for impact velocity} \quad v_0 < 45 \text{m/sec}
\]

Hydrogen is a light liquid

Maximum volume of escaped LH2 occurs in tanks with relatively large initial gas volume $V_{g0}$ or when bottom (but not tops) of tanks are ruptured (group 2 HOVI)

\[
V_{max} = V_{g0} \left( \frac{p_{at} - \rho_L V_0^2}{2 p_0} \right)^{-1/2}
\]

$V_{g0} = \alpha V_0$

- $\alpha = 20\%$
- $\alpha = 15\%$
- $\alpha = 7.36\%$

$v_0 = 33\text{msec}$ – velocity of the tank on impact; $V_{g0}$ and $p_0$ are initial volume and pressure of gas in the H2 tank.

Physics Based Methods, Ames - NASA

11/16/2012

Maximum volume of escaped LH2 does not depend on the ignition delay time and hole cross-section $S_h$

\[
\rho_L = 70 \text{kg/m}^3, \quad \gamma = C_p / C_v = 1.4, \quad p_0 = 1.45 \text{atm}, \quad p_{at} = 1 \text{atm}
\]
Maximum volume of escaped Ox liquid in HOVI tests

\[ t = \int_{V_{g0}}^{V_g} \frac{dV}{a \left[ \left( \frac{V_{g0}}{V} \right)^\gamma - \frac{p_{at}}{p_0} + \frac{\rho_L V_0^2}{2 p_0} \right]^{1/2}}, \quad a = S_h \left( \frac{2 p_0}{\rho_L} \right)^{1/2} \]

\[ V_g (t) = V_{g0} + tS_h \left( \frac{2 p_0}{\rho_L} \right)^{1/2} \left( \frac{\rho_L V_0^2}{2 p_0} - \frac{p_{at}}{p_0} + \left( \frac{h_{g0}}{h_0} \right)^\gamma \right)^{1/2} \]

for \( t \leq t_{esc} = h_{at} / v_0 \leq 25 \text{ m sec} \)

LOX  \quad \text{t}_{ex} \text{ is time of escape of the main column of Ox liquid of cross section } S_h

Oxygen is a heavy liquid

Maximum volume of escaped liquid

\[ \eta_m = \frac{S_h}{S_0} + \frac{h_m - h_g (t_{ex})}{h_0 - h_g (t_{ex})} \geq 33\% \]

for the delay time about 180 m sec

\[ V_m = V_{g0} (t_{ex}) \left( \frac{p_{at}}{p_1} \right)^{-1/2} \quad \text{for } t > t_{esc} \]

The time of the fall of the escaped Ox liquid to the ground

\[ t_{ex} = \left( h_{H2} + h_{O2} \right) / v \geq 100 \text{ m sec} \]

\[ h_{H2} = 2.24 \text{ m and } h_{O2} = 0.86 \text{ m are heights of hydrogen and oxygen tanks} \]

Maximum volume of escaped Ox liquid can occur only when bottoms (but not tops) of both tanks are ruptured (group 1) and there is a relatively large delay time.

\[ V_0 = 33 \text{ m/s} \quad \text{velocity of the tank on impact; } V_{g0} \text{ and } p_0 \text{ are initial volume and pressure of gas in the O}_2 \text{ tank} \]

\[ \rho_L = 1141 \text{ kg/m}^3, \quad \gamma = C_p / C_v = 1.4 \]

\[ p_0 = 2.1 \text{ atm, } p_{at} = 1 \text{ atm} \]

\[ \rho_L V_0^2 > \frac{p_{at}}{2 p_0} \]

for impact velocity \( v_0 > 13 \text{ m/sec} \)
Escape of $GH_2$ in the second group of HOVI tests (HOVI 2 and 5)

Breach of $H_2$ tank top results in escape of gaseous $H_2$

Dynamics of escape of gaseous $H_2$

- $V_{g0}$ and $p(0)$ are initial volume and pressure of gas in the $H_2$ tank,
- $S_h$ – cross section of the rupture

\[
V_{g0} \frac{d \rho_v}{dt} = -jS_h, \quad S_h = \pi r_h^2,
\]

\[
p = R_v \rho_v T,
\]

\[
j(t) = \left( \frac{p_0}{p} \right)^{1/\gamma} \sqrt{\frac{2\gamma}{\gamma - 1} p \rho_v \left( 1 - \left( \frac{p_0}{p} \right)^{1-1/\gamma} \right)}
\]

\[
M_{H_2} = S_h \int_0^{t_{esc}} j \, dt, \quad M_{H_2}^{max} \approx \frac{p(0) - p_0}{p_0} \rho_v V_{g0}
\]

For $r_h > 10cm$
- $M_{H_2} = 0.9kg$ for HOVI 5 and $M_{H_2} = 0.5kg$ for HOVI 2.

Time of escape $t_{esc}$ is determined by the area $S_h$

Total escaped mass $M_{H_2}$ does not depend on $S_h$

For $r_h > 10cm$ escape time $t_{esc}$ is less than the explosion delay time $\tau_d$
Evaporation is slowed down by film boiling

A vapor cushion forms between the liquid and hot solid surface (Leidenfrost effect). Due to this effect a drop of water that is vaporized almost immediately at 334 °F (168 °C) persists for 152 seconds at 395 °F (202 °C).

We emphasize that in the case of LH2 spills the temperature of the ground is 15 times higher than the boiling temperature of the liquid.

The equation for the height of vapor cushion:

\[
\frac{q_h \rho_L \rho_v g}{12 \mu \kappa_v (T_0 - T_L)} \frac{d}{dr} \left( r h^3 \frac{d}{dr} \left( h + a^2 \frac{d^2 h}{dr^2} \right) \right) = \frac{r}{h}
\]

Characteristic length scales of:
- vapor cushion thickness and droplet radius

\[
h_0 \left( \frac{\mu \kappa_v (T_0 - T_L)}{q_h \rho_v \rho_L g} a^2 \right)^{1/5} a = \sqrt{\frac{\sigma_L}{\rho_L g}}
\]

Estimating evaporation time \( t_0 \):

\[
\pi R^2 q_h \rho_L H = \pi R^2 t_{L, evap} \kappa_v (T_0 - T_L) / h_0
\]

For \( R = H = 5 \text{mm} \): \( t_0 = 5 \text{sec} \)

Predicted evaporation time is very long in comparison with conductivity time \( t_{evap} = 30 \text{msec} \).

Physics Based Methods, Ames - NASA
Impact of the liquid jet with the ground results in turbulence and breaks the liquid into droplets. Fragmentation of liquid droplets is a complex and poorly understood phenomenon. Droplet sizes may vary significantly. The typical droplet radius depends both on the parameters of the liquid and gas [1]. Very recent experimental studies of liquid jets impinging on a flat smooth surface established the following empirical correlation for the mean droplet radius [2]:

\[ r_d = 2.53 \times 10^5 d_{or} \, Re^{-1.28} \, We^{0.4} \left( \frac{\mu_{LH2}}{\mu_{air}} \right)^{-1.16}, \]

\[ Re = \frac{d_{or} v \rho_L}{\mu_{LH2}} \] - Reynolds number, \[ We = \frac{d_{or} v^2 \rho_L}{\sigma_{LH2}} \] - Weber number,

\( \mu_{air} = 1.63 \times 10^{-5} \, Pa \, sec, \)

\( \mu_{LH2} = 1.32 \times 10^{-5} \, Pa \, sec, \mu_{LO2} = 1.96 \times 10^{-4} \, Pa \, sec \)

Typical droplet radius

\[ r_{d,H2} \approx 8 \text{mm}, \quad r_{d,O2} \approx 0.5 \text{mm} \]

Typical radius of the droplets in the H\(_2\) cloud is about \( r_{d,H2}=8\text{mm} \) and in the O\(_2\) cloud is about \( r_{d,O2}=0.3\text{mm} \). These values are almost independent of the stream diameter \( d_{or} \).

Two mechanisms of the heat transfer from the hot gas (combustion products to cold H2 droplet:

(i) thermo-conduction and (ii) infrared radiation of hot gas.

(i) The thermo-conduction evaporation is surface heating of a droplet to a temperature $T_s$ due to diffusion heat flow of hot gas.

(ii) Radiation heat is volume process ($a_{abs}r_{bubble} < 1$) that results in heating of whole droplet to $T_L$ and fast evaporation and burning.

Equations describing evaporation and burning LH2 droplet are the same that used for bubble cavitation with the exception of the equation for radius

$$
\rho_L \dot{R} = \rho_g (u_g - \dot{R}) = j_{cd},
$$

$$
j_{cd} = \frac{\beta (p_{Ox} - p_s(T_s))}{\sqrt{2\pi R_{Ox} T_s}},
$$

$$
p_s(T_s) = p_c \left( \frac{T_s}{T_c} \right)^\lambda.
$$

The conduction flow is depressed due to cold GH2 vapor area near the droplet. Therefore the evaporation time a bubble with $R_0>1$mm can be estimated ($T_c=33.2K$ is critical temperature)

$$
(T_c - T_{L0})C_L \rho_L V_R = (\alpha R) \epsilon \sigma T_g^4 S_R t, \quad t_{evap} = \frac{C_L \rho_L (T_c - T_{L0})}{3\alpha \epsilon \sigma T_g^4}.
$$

**Radiation-induced combustion**

$$
d(\rho H2)/dt = - (\rho H2/\tau_{evap})(T(t)/T_0)^4.
$$

$T_0=3500K$, $\tau_{evap} = t_{evap}/e = 10^{-3}/sec.$
The super-hot and compressed O, H, OH species are formed in the collapsed bubble in process of a local explosion the GOx/GH2 mixture inside the collapsing bubble. These species can ejected from the bubble into the space above the LOx interface and easily ignite the GH2/GOx mixture localized under this interface. This effect can induce the fast deflagration of the aerosol mixtures.

The time of radiation-induced combustion

\[ \tau_{\text{evap}} \approx \frac{1}{e} t_{\text{evap}} \approx \frac{C_L \rho_L \left( T_c - T_{L0} \right)}{10 \alpha \varepsilon \sigma T_g^4} \]

does not depend on the droplet radius and averaged density of droplets can be presented as

\[ \frac{d(\rho_{H2\text{drop}})}{dt} = - \rho_{H2\text{drop}} / \tau_{\text{evap}} \left( \frac{T(t)}{T_0} \right)^4 \]

\( T_0 = 3500K, \tau_{\text{evap}} = 10^{-3}/\text{sec.} \)

The value of \( \rho_{H2\text{drop}} / \tau_{\text{evap}} \) was added in the mass balance equations for the gas components. The results are depended on relation of the averaged droplet density to the evaporation time: \( \rho_{H2\text{drop}} / \tau_{\text{evap}} \).

Initial averaged droplet density

\( \rho_{H2\text{drop}}(0) = 0.05 \text{kg/m}^3 \quad r=6\div8 \text{ mm} \)

\( \rho_{O2}(0) = 0.4 \text{ kg/m}^3 \quad r=0.5\text{mm} \)

**Parameters of flame front**

Velocity \( V_f = 620 \text{m/sec} \), Temperature \( T_{max} = 3900K \), Pressure \( p_{max} = 5.5\text{atm} \)
<table>
<thead>
<tr>
<th>HOVI test</th>
<th>Pressure sensor data, atm</th>
<th>Experimental shock velocity</th>
<th>Calculated shock velocity</th>
<th>Mass and density of H$<em>2$ aerosol, $M</em>{H2}$ kg, ($\rho_{H2} = \text{kg/m}^3$, $M_{O2}$)</th>
<th>Duration of shock (calculated and measured)</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>3.3±4.2</td>
<td>≈ 740±825</td>
<td>≈ 760</td>
<td>≈ 0.7kg (0.031kg/m$^3$) 5.6 (0.248)</td>
<td>≈ 3.5msec</td>
</tr>
<tr>
<td>5</td>
<td>2.5±3</td>
<td>≈ 660</td>
<td>≈ 660</td>
<td>≈ 0.45kg (0.02) 3.6 (0.16)</td>
<td>≈ 4.0msec</td>
</tr>
<tr>
<td>2</td>
<td>3.2±5.4</td>
<td>≈ 780</td>
<td>≈ 785</td>
<td>≈ 0.65 kg (0.029) 5.2 kg (0.23)</td>
<td>≈ 3.4msec</td>
</tr>
<tr>
<td>9</td>
<td>80±110</td>
<td>2625±2966</td>
<td>2500±2928</td>
<td>8.3±15.2kg (0.68) 66-121kg (5.44)</td>
<td>≈ 0.7msec</td>
</tr>
</tbody>
</table>
The HOVI test data showed that a liquid hydrogen spill alone is not likely to self-ignite, because in every HOVI test with a ground cloud of hydrogen, caused by a breach in the bottom of the hydrogen tank, the ground cloud did not ignite until liquid oxygen was released. The ignition occurs when gaseous hydrogen (GH2) and oxygen (GOx), and liquid oxygen (LOx) mixture is available.

LOx stream released from the tank serves to ignite the GH2/GOx mixture via the collapse (cavitation) of vapor bubbles in LOx. The ignition effect intensifies when GH2 is contained in the bubbles. Such bubbles can form from the turbulent mixing of H2 and Ox flows escaping from the breached fuel tanks. Very high pressures and temperatures arise in the collapsing bubbles due to ignition of the GH2/GOx mixture inside the bubbles.

Super-compressed and hot gases injected from a bubble near LOx surface into GH2/GOx mixture produces a strong shock wave, followed by hot gas. This cavitation-induced ignition can lead to deflagration or detonation of GH2/GOx mixtures. The combustion characteristics depend on volume, structure and composition of the H2 and Ox clouds.

Impact of the liquid jet with the ground results in turbulence and breaks the liquid into droplets that are partially evaporated and form aerosol clouds with gaseous H2 and Ox present. The aerosol combustion determines the main parameters of the explosion including high pressure, temperature and flame front velocity. Its rate is controlled by the infrared radiation of hot combustion products.

The aerosol combustion can result in detonation of GH2/GOx mixture when H2 and Ox gases and aerosols are well-mixed. Our calculation show that such a situation is realized in the HOVI 9 test and determines the high explosion yield in this case.

In the case of poorly mixed H2 and Ox clouds the aerosol combustion cannot result in detonation but intensifies deflagration, i.e., it increases the pressure, temperature and flame front velocity (HOVI 13 and 14 tests of the first group).

In the second group of the HOVI tests (HOVI 2 and 5) only GH2 has time to escape from the top of the tank before the explosion, i.e. the LH2 aerosols do not arise. Therefore, deflagration occurs with relatively low pressure, temperature and flame front velocity.