CFD based modelling approaches for hydrogen safety issues

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Outline

• Spontaneous ignition

• Hydrogen jet fires

• Hydrogen deflagration, DDT and detonation
Safety relevant properties of hydrogen/methane/propane/gasoline vapour

- Density
- Buoyancy
- Diffusion coefficient
- Minimum Ignition energy
- Flammability range
- Laminar burning velocity
- Heat of combustion
- Detonation sensitivity

http://www.warwick.ac.uk/warwickfire
Spontaneous ignition
Spontaneous ignition: two types of release scenarios

Direct release into air

Release through a section of tube
Spontaneous ignition

- Own modified version of KIVA-3V
- 2-D Unsteady Compressible Navier-Stokes equations solved with an Implicit Large eddy simulation (ILES) method
- Arbitrary Lagrangian Eulerian (ALE) numerical scheme: convective term solved separately from diffusion terms;
- In Lagrangian stage, 2\textsuperscript{nd}-order Crank-Nicolson scheme + 2\textsuperscript{nd}-order central differencing for diffusion and pressure related terms;
- In Eulerian phase, 3\textsuperscript{rd}-order Runge-Kutta method + 5\textsuperscript{th}-order upwind weighted essentially non-oscillatory (WENO) scheme for convection terms;
- Detailed chemical-kinetic scheme - 8 reactive species and 21 elementary steps –third body and “fall off” behavior considered (Williams 2006);
- Multi-component diffusion approach for mixing - thermal diffusion;
- Iris model mimics the rupture process
Validation - Comparison of 1-D release case with theoretical results based on 1-D shock wave theory

10-micron grid size and a 5th-order WENO scheme
Release through a tube D=3mm, L=6cm)
Release tubes with varied cross-sections – all with 50 bar pressure

(a) Local contraction
(b) Local enlargement
(c) Abrupt contraction
(d) Abrupt enlargement

Figure 5. Maximum temperature versus release time for five different internal geometries under the release pressure of 50 bar.
Hydrogen Jet Fires
Hydrogen Jet Fires - Two Modelling Approaches

- Pseudo-source approach (Ewan and Modie 1985)
  - Leak modelled from downstream as a sonic jet with the same mass flow rate

\[ D_{eq} = D_j (0.536 C_D \frac{P_o}{P_a})^{0.5} \]

\[ P_e = P_o \left( \frac{2}{\gamma + 1} \right)^{\gamma / (\gamma - 1)} \]

\[ \rho_e = \rho_o \left( \frac{2}{\gamma + 1} \right)^{\gamma / (\gamma - 1)} \]

\[ Y_o = \frac{4.99 D_s}{z} \left( \frac{\rho_g}{\rho_a} \right)^{1/2} C_D^{1/2} \]

- Two-domain approach
  Numerically solving the under-expanded shock structure

- Results used as inflow for the subsequent large eddy simulation of the jet
Comparison of the predicted mean temperatures by the two approaches

Hydrogen jet flame test
Sandia Laboratory

The two-domain approaches

the Pseudo source approach

Temperature

Jet Exit
Flame Envelope
Hydrogen Flow
Hydrogen jet fires

- **FireFOAM** code with own modified EDC

- Finite volume discrete ordinates model (fvDOM)
- Weighted sum of grey gas model for radiation

\[
e = \sum_{i=0}^{I} a_{e,i}(T)(1 - e^{-\kappa_i P S})
\]

\[
a_{e,i} = \sum_{j=1}^{J} b_{e,i,j} T^{j-1}
\]

<table>
<thead>
<tr>
<th>Coefficients for emissivity</th>
<th>(k_i)</th>
<th>(b_{e,i,1} \times 10^4)</th>
<th>(b_{e,i,2} \times 10^4)</th>
<th>(b_{e,i,3} \times 10^4)</th>
<th>(b_{e,i,4} \times 10^4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon dioxide, (P_e \sim 0) atm</td>
<td>0.3946</td>
<td>0.4334</td>
<td>2.620</td>
<td>0.560</td>
<td>2.565</td>
</tr>
<tr>
<td></td>
<td>15.64</td>
<td>-0.4814</td>
<td>2.822</td>
<td>-1.794</td>
<td>3.274</td>
</tr>
<tr>
<td></td>
<td>394.3</td>
<td>0.5492</td>
<td>0.1087</td>
<td>-0.3500</td>
<td>0.9123</td>
</tr>
<tr>
<td>Water vapor, (P_w \sim 0) atm</td>
<td>0.4098</td>
<td>5.977</td>
<td>-5.119</td>
<td>3.042</td>
<td>-5.564</td>
</tr>
<tr>
<td></td>
<td>6.525</td>
<td>0.5677</td>
<td>3.533</td>
<td>-1.967</td>
<td>2.718</td>
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<tr>
<td></td>
<td>120.5</td>
<td>1.800</td>
<td>-2.334</td>
<td>1.008</td>
<td>-1.454</td>
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<tr>
<td>Water vapor, (P_w \sim 1.0) atm</td>
<td>0.4496</td>
<td>6.324</td>
<td>-8.358</td>
<td>6.135</td>
<td>-13.03</td>
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<tr>
<td></td>
<td>7.113</td>
<td>-0.2016</td>
<td>7.145</td>
<td>-5.212</td>
<td>9.888</td>
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<tr>
<td></td>
<td>119.7</td>
<td>3.500</td>
<td>-5.040</td>
<td>5.435</td>
<td>-3.888</td>
</tr>
<tr>
<td>Mixture, (P_{w}/P_e = 1)</td>
<td>0.4303</td>
<td>5.150</td>
<td>-2.303</td>
<td>0.9779</td>
<td>-1.494</td>
</tr>
<tr>
<td></td>
<td>7.055</td>
<td>0.7749</td>
<td>3.399</td>
<td>-2.297</td>
<td>3.770</td>
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<tr>
<td></td>
<td>178.8</td>
<td>1.907</td>
<td>-1.824</td>
<td>0.5808</td>
<td>-0.5122</td>
</tr>
<tr>
<td>Mixture, (P_{w}/P_e = 2)</td>
<td>0.4201</td>
<td>6.508</td>
<td>-5.551</td>
<td>3.029</td>
<td>-5.353</td>
</tr>
<tr>
<td></td>
<td>6.516</td>
<td>-0.2504</td>
<td>6.612</td>
<td>-5.882</td>
<td>6.528</td>
</tr>
<tr>
<td></td>
<td>131.9</td>
<td>2.718</td>
<td>-3.118</td>
<td>1.221</td>
<td>-1.612</td>
</tr>
</tbody>
</table>

\(P_T = 1\) atm, \(0.001 \leq P^5 \leq 10.0 \) atm-m, \(600 \leq T \leq 2400K\)

http://www.warwick.ac.uk/warwickfire
The under-expanded hydrogen jet fire of Schefer et al.


Nozzle Diameter: 5.08mm
Pressure: 104.8atm
Tank temperature: 231.4K

<table>
<thead>
<tr>
<th>Simulated</th>
<th>Experimental</th>
<th>Theoretical</th>
<th>Error between Simulated and Experimental values</th>
<th>Error between Theoretical values</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m)</td>
<td>(m)</td>
<td>(m)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.06</td>
<td>6.7</td>
<td>7.58</td>
<td>+5.4%</td>
<td>-6.9%</td>
</tr>
</tbody>
</table>

http://www.warwick.ac.uk/warwickfire
The under-expanded hydrogen jet fire of Ekoto et al.


<table>
<thead>
<tr>
<th>Jet</th>
<th>$d_j$ [mm]</th>
<th>$m$ [kg/s]</th>
<th>$p_0$ [barg]</th>
<th>$T_0$ [K]</th>
<th>RH [%]</th>
<th>$T_{amb}$ [K]</th>
<th>$p_{amb}$ [mbar]</th>
<th>$U_{wind}$ [m/s]</th>
<th>$\varphi_{wind}$ [$^\circ$]</th>
<th>$L_{vis}$ [m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>20.9</td>
<td>1.0</td>
<td>59.8</td>
<td>308.7</td>
<td>94.3</td>
<td>280</td>
<td>1022</td>
<td>2.84</td>
<td>68.5</td>
<td>17.4</td>
</tr>
</tbody>
</table>

![Fire image](image1)

![Graph image](image2)
Hydrogen explosions

- **Deflagration**: the combustion or reaction wave propagates at a velocity less than the speed of sound.

- **Deflagration to detonation transition (DDT)** refers to a phenomenon in ignitable mixtures of a flammable gas and air (or oxygen) when a sudden transition takes place from a deflagration type of combustion to a detonation type of combustion.

- **Detonation**: the combustion or reaction wave propagates at a velocity faster than the speed of sound.
CFD modelling of hydrogen deflagration


Osaka Gas’ Hydrogen station

Chamber structure for explosion experiments

![Diagram of chamber structure](image)

**Fig. 12** Variation in Overpressure (kPa) with distance from open end of chamber

**Fig. 13** Effect of hydrogen concentration on Overpressures generated

[Osaka Gas' Hydrogen station](http://www.warwick.ac.uk/warwickfire)
CFD modelling of hydrogen deflagration induced by ignited jet release

Hydrogen deflagration, DDT and detonation

- Own modified version of OpenFOAM
- Single step reaction was taken from Gamezo et al.
- A single step chemistry derived by ourselves

\[ \dot{\omega} = A[H_2][O_2]\exp\left(\frac{-E_a}{RT}\right) \]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values or Expressions</th>
<th>Annotation</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>$1.13 \times 1015 \text{cm}^3/(\text{mol.s})$</td>
<td>Pre-exponential factor</td>
</tr>
<tr>
<td>$E_a$</td>
<td>46.37RT0</td>
<td>Activation energy</td>
</tr>
<tr>
<td>Q</td>
<td>43.28RT0/M</td>
<td>Chemical heat release</td>
</tr>
<tr>
<td>$\Gamma$</td>
<td>1.17</td>
<td>Specific heat ratio</td>
</tr>
<tr>
<td>$K_0=\mu_0=D_0$</td>
<td>$7.0 \times 10^{-5} \text{g/(cm.s.K0.7)}$</td>
<td>Transport coefficient</td>
</tr>
</tbody>
</table>
Hydrogen deflagration, DDT and detonation – Validation of the single step chemistry

1D steady ZND wave

Free-propagating laminar flame

<table>
<thead>
<tr>
<th>Distance to left end</th>
<th>475mm</th>
<th>595mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak Pressure</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Meas.</td>
<td>3.6MPa</td>
<td>6MPa</td>
</tr>
<tr>
<td>Pred.</td>
<td>3.75MPa</td>
<td>5.81MPa</td>
</tr>
<tr>
<td>Discrepancy</td>
<td>4.2%</td>
<td>3.2%</td>
</tr>
</tbody>
</table>
DDT
DDT - Validation

- 80 mm×2000 mm tube, $L=160$ mm, $BR = 0.5$
- Smallest grid size: 20 micron, structured (AMR)
- Boundary conditions: no-slip reflecting boundaries.
- Fuel: stoichiometric Hydrogen-air mixture
- Ignition: a region of high temperature (2000 K)
Detonation propagation in a bifurcated tube

Summary of modelling approaches presented

• A dedicated code for spontaneous ignition modified from Kiva-3V

• A modified FireFOAM code for hydrogen jet fires

• A modified OpenFOAM with newly developed single step hydrogen reaction cover the full range from laminar to flames, turbulent deflagration, DDT and detonation
Acknowledgement

• **Sponsors**
  European Commission
  The Engineering and Physical Science
  Research Council, UK (EPSRC)
  FM Global
  The National Natural Science Foundation of
  China

• **Collaborators**
  The Heath and Safety Laboratory
  BP
  University of Ulster
  Warsaw University of Technology
  University of Science and technology, China

• **Researchers**
  Baopeng Xu
  Sergio Ferraris
  Changjian Wang
  Zhibin Chen
  Vendra Madhav Rao
  EL Hima
  Jianping Zhang
  Ali Heidari

• **Former colleagues**
  Vincent Tam
  Siaka Dembele
  Siva Muppala