Consequence analysis of fire and explosion hazards with potential applications to the power generation sector

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Outline

- Introduction about Warwick FIRE

- Snapshots of our activities in fire and explosion modelling
  - Spontaneous ignition in pressurized hydrogen releases
  - Fire modelling using modified FireFOAM
  - Explosion modelling using modified OpenFOAM
    - Vented explosions
    - Deflagration to detonation transition (DDT)
Warwick FIRE

Cross cutting safety issues related to energy, buildings and the environment.
Research projects in the last 5 years

2017-2020: In situ stress analysis of lithium-ion battery cell, €195.5K, EU Horizon 2020.
2015-2018: Pre-normative research on vented deflagrations, €450.4K, EU Horizon 2020
2014-2016: Fire and explosion hazards on offshore installations £180K, UK Technology Strategy Board and DNV-GL.

2013-2018: High performance computing (£20K plus HPC time), EPSRC.

2011-2014: Dense Phase CO2 PipeLine TRANSPORTation, £320K National Grid.
Spontaneous ignition in pressurised hydrogen release
The motivation
Numerical Methods

- **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 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
Following sprouting from the tube

Shileren density

Temperature
Fire modelling using modified FireFOAM
Current fire modelling activities

- Façade fires
- Fully coupled fluid-solid simulation of upward flame spread and fire growth
- Modelling flame spread with FireFOAM
- Hydrogen jet fires
- Enclosure fires
Flame spread over Polymethyl methacrylate (PMMA)

Flame tip ($x_f$)

Pyrolysis gas from wall
C$_5$H$_8$O$_2$

Gas reaction
C$_5$H$_8$O$_2$+6O$_2$ → 5CO$_2$+4H$_2$O

Soot formation and oxidization

Grid size change due to surface regression

Radiative and convective heat transfer

In depth radiative heat transfer

Rear surface Front interface

PMMA

Solid region Gas region

Leading edge

Rear face Wall

Interface

Outlet

Ambient or wall

Solid region

Gas region

$X_{wall}$ $X_f$

$Y_{max}$ $Z_{max}$

$X_{max}$

$x$, $y$, $z$
Sample results of flame spread

The predicted and measured flame height $x_f$ vs pyrolysis height $x_p$.
ISO surfaces of the flame volume defined as the criteria $R_o = 0.99$. The continuous flame (CF), intermittent flame (IF), and plume (PL) regions are specified at 380 s.
Figure 1. Sketch of the computational domain: boundaries and dimension (top), grid layout in the base plane (bottom, left), and zoomed-in grid layout in the nozzle plane (colored in red) (bottom, right).
SYNGAS jet fires

Instantaneous flame temperature fields at $t = 0.35$ s.
Vented explosion modelling using modified OpenFOAM
The configurations considered

ISO containers in hydrogen energy applications
**Base test case**

<table>
<thead>
<tr>
<th>Test #</th>
<th>Vent</th>
<th>Obstructions</th>
<th>Hydrogen concentration</th>
<th>Ignition position</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>Door open</td>
<td>Empty frame</td>
<td>15% (+/- 0.2%)</td>
<td>Mid back wall</td>
</tr>
<tr>
<td>1b</td>
<td>Door open</td>
<td>Empty frame</td>
<td>15% (+/- 0.2%)</td>
<td></td>
</tr>
<tr>
<td>1c</td>
<td>Door open</td>
<td>Cylinder bundle</td>
<td>15% (+/- 0.2%)</td>
<td>Mid back wall</td>
</tr>
<tr>
<td>2a</td>
<td>Door open</td>
<td>Cylinder bundle</td>
<td>15% (+/- 0.2%)</td>
<td></td>
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<tr>
<td>2b</td>
<td>Door open</td>
<td>Cylinder bundle</td>
<td>15% (+/- 0.2%)</td>
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</tr>
</tbody>
</table>
Congestion

(a) Container corrugation

(b) Obstacle holding frame

(c) Bottle stack
Empty container with frame 15% hydrogen concentrations

(a) Instantaneous pressure profile

(b) Time averaged profile for 5 ms

Pressure trace curve for P1 pressure probe location along with experiment measurements
Container with bottles and frame
Container with bottles and frame 15% hydrogen concentration

Numerical predicted of pressure trace curve for pressure probes inside container (a) instantaneous curves, (b) time averaged 5 ms and (c) time averaged curves for probes inside the container.
Flame acceleration and deflagration to detonation transition (DDT) in hydrogen-air mixtures with concentration gradients
Motivation

Accidental releases of combustible mixtures are usually inhomogeneous and subject to both vertical and horizontal concentration gradients.
Experiments considered

Deflagration to detonation transition (DDT) in a rectangular channel filled with hydrogen-air mixture with concentration gradients (Boeck et al., 2015)


Ignition:
- Weak spark ignition in the experiment
- For simulation, patch cells within a radius of 10 mm around the point of ignition (x=0, y=0.03m) to the burnt state (isobaric, adiabatic burnt mixture).
Initial conditions

Initial conditions in the experiment

The ignition patch is assumed as a burned area with high temperature and combustion product.
Animation with temperature Contour

BR30S300
30% H2
Pressure contours
Comparison between the predicted and measured flame position

BR30

BR60
Comparison between the predicted and measured flame speed

Increasing Blockage ratio faster deflagration
Summary

- The KIVA-3V CFD code has been modified to simulate spontaneous ignition in pressurized hydrogen releases.

- OpenFOAM ®, an open source CFD code, has been modified by Warwick FIRE for the following applications:
  - Jet fire, flame spread and coupled fire and mass burning rate
  - Explosion modelling using modified OpenFOAM
    - Vented explosions
    - Deflagration to detonation transition (DDT)
    - Hydrodynamic instabilities during flame acceleration and DDT
Acknowledgement

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