DISPERSION OF HYDROGEN FROM HIGH-PRESSURE SOURCES

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This paper describes work by Shell Global Solutions and the Health and Safety Laboratory (HSL) to characterise the hazards from jet releases of hydrogen. The objectives were to determine how hydrogen hazards differ from those associated with more traditional hydrocarbon fuels and whether existing models can adequately describe this behaviour.

Controlled release experiments have been carried out with release pressures ranging between 1 and 15 MPa. Concentration measurements were made in unignited free jets to determine the extent of the flammable cloud generated.

The results are compared with predictions from HGSYSTEM, a model developed and validated for jet releases of hydrocarbons. Agreement with model predictions was excellent for 8 out of the 23 releases. The disagreement with the other releases was consistent with the plume being blown off-axis downstream. The strength of this crosswind effect was significant and illustrates the need to include crosswind capability into dispersion models.

KEYWORDS: hydrogen, jet releases, modelling, dispersion, concentration measurements

INTRODUCTION

There is widespread interest in hydrogen and the role it may play as a future energy source. For example, it is the fuel of choice for fuel-cell applications ranging from vehicles to stationary power sources.

To ensure the safe use of hydrogen, through the development of appropriate codes and standards, it is essential to understand all the hazards that could arise following an accidental release. If hydrogen is to be stored, transported and used as a highpressure gas, then the hazards associated with jet releases from accidental leaks must be considered. A jet release in the open will result in a flammable cloud, and if this finds a source of ignition the result will be a cloud fire that burns back leaving a jet fire burning from the leak until the supply is controlled or exhausted. Knowledge of the extent of the flammable cloud is an essential part of managing the potential hazard and quantifying the risk posed.

Shell Global Solutions have contracted the Health and Safety Laboratory (HSL) to assist in an experimental programme aimed at providing realistic demonstrations of the potential hazards.

This paper describes the work performed by HSL to characterise the hazards from medium pressure releases of hydrogen into areas with no obstructions and by Shell Global Solutions to compare the data obtained with the predictions from models. The programme of work involved determination of the downstream concentrations of hydrogen from releases of hydrogen up to 15 MPa (150 bar). Shirvill et al. (2005) describe characterisation of the hazards from un-ignited and ignited releases. In this paper, only the work on un-ignited medium pressure releases is described.

TEST FACILITY

The test facility comprised a purpose-built concrete pad, measuring some 10 m x 50 m and instrumentation was connected to computers located in a control centre located about 300 m from the test area. The releases of hydrogen were initiated manually, but controlled by a PC running software linked to a programmable logic system.

The hydrogen discharge system was designed to have a maximum working pressure of 15 MPa. Discharge orifices of varying diameters (1.0, 3.0, 4.0, 6.0 and 12.0 mm) and various nominal, discharge pressures (between 1 and 15 MPa) were chosen to study a range of momentum jet releases. The orifices consisted of threaded stainless plugs that were 27 mm thick and had holes of the required diameter drilled through them. With the supply system used (eight multi-cylinder packs, each of 17 cylinders), the maximum discharge pressure could only be maintained for a few seconds with the largest orifice before the pressure began to drop. All the releases were aimed horizontally, 1.5 m above the test pad. In each experiment, the hydrogen was released from the orifice and allowed to come to a pseudo steady state during which the concentration measurements were made. A valve located close to the end of the discharge system controlled the release of gas.

EXPERIMENTAL MEASUREMENTS

RELEASE CONDITIONS

The pressure and temperature of hydrogen in the release pipe, close to the release orifice, were recorded during each trial. The pressure was measured either side of the release valve, whereas the gas temperature was only recorded downstream of the release valve, but upstream of the release orifice. The air temperature and relative humidity were measured using a Wessels Type DA 40 H, Digital Hygro/Thermo Anemometer just prior to each trial. The wind speed and direction were measured during the trials at 1.5 m above the ground using a Vector Instruments weather station fixed to the release pipe, 12.5 m from the release orifice.

CONCENTRATION MEASUREMENTS

The concentration of hydrogen in the un-ignited plume was derived from measurements of the oxygen concentration within the cloud. It was assumed that any decrease in the concentration of oxygen was caused by displacement of oxygen by hydrogen gas. The concentration of oxygen in the vapour cloud was measured using "AO2 Oxygen CiTicel" sensors. These are self-powered, electrochemical oxygen sensors capable of measuring oxygen concentrations in the range 0-100 volume percentage (vol. %). The sensors are of a self-powered, metal-air battery type, comprising an anode, electrolyte and an air cathode. The CiTicel oxygen depletion sensors were calibrated against a calibrated oxygen gas analyser. The results showed that the following relationship holds:

Concentration of oxygen =
$$(V_m/V_0) \times 20.9\%$$
 (1)

where V_0 is the sensor output in air, V_m is the sensor voltage in a reduced-oxygen atmosphere. The manufacturer specifies a resolution of $\pm 0.01\%$ oxygen for the sensors. If oxygen is displaced by hydrogen, the concentration is given by:

Concentration of hydrogen =
$$100\% \times (V_0 - V_m)/V_0$$
 (2)

The accuracy of the sensors, including experimental variability, was of the order of $\pm 0.3\%$ hydrogen.

13 CiTicel AO2 Oxygen sensors were used in the trials. These were positioned between 3 and 11 m from the discharge point as indicated in Figure 1. The sensors were located at heights of 1.5 or 2.0 m above ground level at the release point, depending on their position downstream, relative to the release nozzle. The ground was level for the first 5 m downstream of the release point. Beyond that, the ground fell away slowly, falling approximately 0.2 m in the next 6 m. The sensors were positioned to be at the release



Figure 1. Distance of sensors from release point



Figure 2. (a) Array from release. (b) Array to release

height, or 0.5 m above the release height (the heights quoted for the sensors relate to ground level at the release point and not height above ground at the sensor location). The sensors were orientated so that the opening on the sensor was perpendicular to the direction of gas flow, i.e. across the flow of gas. Figures 2(a) and 2(b) show the array of CiTicel sensors used to measure the concentration of hydrogen at different positions in the gas cloud. The CiTicel AO2 sensors produce an output voltage of 0-62 mV (9-13 mV in air) depending on the concentration of oxygen. This is relatively small, so amplifiers were used to increase the signal before it was logged to the PC.

DATA LOGGING

The concentration data recorded were logged on a Dell Pentium, OptiPlex GX1P PC. The computer was fitted with three Data Translation, DT3000 series, data logging cards, each capable of recording 32 channels of data. During the trials, the computer was programmed to record data at a frequency of 10 Hz. The release conditions were logged on the PC running the hydrogen release rig. Due to the manner in which the PC handled the data, the time-base was not exact and corresponded to ca. 55.6 Hz.

RAW DATA

23 release experiments were performed with orifice sizes ranging from 3 to 12 mm and release pressures from 1.1 to 13.7 MPa. Typical release condition data for a target release pressure of 15 MPa are given for a 4 mm orifice in Figure 3(a) and for a target pressure of 12 MPa and a 3 mm orifice in Figure 3(b). Figure 3(a) illustrates the rapid pressure drop with a higher pressure and larger orifice compared to the pseudo steady state with a slightly lower pressure and smaller orifice Figure 3(b).

The concentration signals comprised either a rapid rise to a plateau, a constant period and then a fall or were very variable due the jet being blown off line. The results for run 7 (10 MPa release through a 3 mm orifice), where the concentration measurements



Figure 3. (a) 15 MPa Target pressure 4 mm orifice. (b) 12 MPa Target pressure 3 mm orifice



Figure 4. (a) Run 7 concentrations. (b) Run 7 wind data



Figure 5. (a) Run 13 concentrations. (b) Run 13 wind data

were steady and the wind speed and direction satisfactory, are illustrated in Figure 4. In Figure 5, the results from run 13 (7.4 MPa release pressure through a 3 mm orifice) are illustrated, indicating the effect of a more variable wind speed and direction on the concentration measurements.

DATA ANALYSIS

Release data were processed as a moving average through the data set. This procedure was adopted to try to compensate for an initial pressure pulse in the signal as the control valve was released and the tendency in runs with the larger orifices for the pressure to fall. The release temperature was taken as the best estimate over the release duration. The temperature signals showed some strong perturbations (see Figure 3) when the release started, probably due to compression of gas expanded through the opened valve and checked at the pipe end holding the (smaller diameter) orifice plate.

Hence, for the experiments, average pressure and temperature data for the release measured just upstream of the nozzle were calculated for the release, but there was no measure of actual release rate. AEROPLUME (see below) has a simple discharge model that, for ideal gases at moderate pressures, yields the same answers as more complicated models, but contains no corrections for non-ideal behaviour and does not account for compressible flow effects, shock formation etc. Consequently, there is some doubt over how well the flow rate and near-field dispersion is calculated. The intention of this data comparison is to see how well the model performs without fine-tuning when given a set of hydrogen-release conditions. The processed release data are summarised in Table 1 along with the flow rate calculated by the AEROPLUME model.

To derive concentrations for model comparison, a moving window of 5 seconds duration was passed through the data and the 5-second mean-concentration calculated. The highest value in the series was used. For all except the sensors at 10 m and 11 m from the source, and where the plume was considerably off-axis (concentration <1 vol.%), the mean defined above was very close to the overall single maximum concentration measured.

MODEL DESCRIPTION

The HGSYSTEM dispersion model, AEROPLUME, was used as the basic model - a full technical description can be found on the HGSYSTEM web site (2005). AEROPLUME is an integral model that is able to predict the dispersion of gases and two-phase hydrocarbon mixtures. It has a complex entrainment mechanism that accounts for jet mixing, mixing due to buoyancy (positive and negative), crosswind entrainment and ambient turbulence for a wide range of atmospheric stability conditions. Unfortunately, the model only allows for differing orientation of the release in the vertical plane so the comparison is limited to horizontal jet predictions in the wind direction only.

The model version used here is not the same as that on the web site. AEROPLUME predicts cross-section jet properties. It generates parameters denoting the horizontal distance travelled, the centroid height position, jet velocity, jet angle, jet temperature

Run number	Pressure (MPa absolute)	Temperature (Celsius)	Hole diameter (mm)	Calculated flow rate (kg s ^{-1})
1	12.0	20	4	0.094
2	13.0	18	4	0.102
3	12.6	17	4	0.099
4	13.7	17	3	0.061
5	12.3	15	3	0.055
6	11.9	15	3	0.053
7	10.0	14	3	0.045
8	9.9	14	3	0.044
9	9.3	13.5	4	0.074
10	9.4	13	4	0.075
11	7.7	13	4	0.061
12	7.4	14	3	0.033
13	7.4	13.5	3	0.033
14	5.0	12.5	3	0.022
15	5.6	13	3	0.025
16	5.1	14.5	4	0.040
17	5.4	14.5	4	0.043
18	4.3	14	6	0.077
19	4.1	14	6	0.073
20	2.3	13.5	6	0.041
21	2.6	14	4	0.021
22	2.5	14.5	3	0.011
23	1.1	14.5	12	0.078

Table 1. Processed release data and calculated flow rate

and jet concentration plus other diagnostics. AEROPLUME has been augmented with a profiling processor to calculate off-axis concentrations and, in this form, appears in the Shell FRED (Shell, 2004) modelling system.

The profile assumption is that the concentration distribution is a simple Gaussian distribution in both horizontal and vertical planes, with a virtual source height defining the "centre" of the vertical. The plume "average" properties calculated directly by the model are identified as being concentration-weighted averages. With this assumption, the highest concentration in the profiled jet is always twice the average concentration calculated by AEROPLUME.

Given a distribution, off-axis concentrations can be calculated. In Shell FRED 4.0 (Shell, 2004), a contour capability is implemented. For this work, the concentration along a straight-line (the experimental axis) was needed and this functionality is not available in FRED. This was the only reason for using HGSYSTEM (v5) for this work.

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PRESENTATION OF RESULTS

The results are presented as log-log plots of the data versus the model predictions. The model predictions were considered:

- Very good if there is an agreement "within a factor of 2" with the data, and the model prediction is conservative. Factor of 2 agreements are often used as a benchmark when comparing dispersion models with data; or
- Not to be in agreement if there was a significant discrepancy, i.e. more than a factor of 2 between the data and the model, particularly if the there was a widening discrepancy with distance.

COMPARISONS

The model predictions were not in agreement with the data for 15 of the 23 runs. The data for the first four runs that were not in agreement (1 to 4 - see Table 1) are illustrated in Figure 6. In all cases, where the data were not in agreement, the jet was clearly affected by a crosswind; as shown by the detailed concentration/time data. At 3 m from the source, the model does quite well in predicting concentrations. As distance increases and the jet velocity decreases, then the difference between the model prediction and data increases.



Figure 6. Runs where the model does not fit the data because of cross-wind influences



Figure 7. (a) Runs where model agrees very well with data – wind direction is always very close to the jet axis. (b) Runs where model agrees very well with data – wind direction is always very close to the jet axis

By about 5.5 m downwind (runs 1 and 2) and 6.5 m downwind (runs 3 and 4) the concentration is lower than could be accounted for by experimental variation in the plume centreline and all data appear to display a change in slope. This is seen in all of the comparisons considered poor. Although ambient wind speed is very low, the wind direction is significantly different to the jet direction. This suggests that crosswind effects are very important at dilutions of \sim 20 fold.

Figure 7 shows the 8 runs for which agreement is very good. The main characteristics of these releases are that the ambient wind is aligned with the axis of jet discharge and the measured time series resemble those of the model.

CONCLUSIONS

A series of hydrogen releases from high pressure has provided useful, but not complete, data on hydrogen dispersion. For a majority of releases the wind-direction was not aligned with the initial jet direction and, even though wind speeds were low, the dispersion appeared to be affected.

Comparison with the predictions of an integral jet model, used with no special modification for hydrogen, was very good when the wind direction was aligned with the jet axis, but degraded as the wind-direction varied. Although there was no direct verification that the model predictions of release rate were correct for the pressure, temperature and hole size combinations, as hazard assessments are set up on the basis of such inputs, the agreement obtained was very encouraging.

In future work, it would be desirable to add the ability to model a release with a horizontal angle between the release and wind direction. This is generally not needed for hazard assessments when worst case assumptions are used, but for assessing discharges from fixed outlets, such as vents, this would be useful. The data model comparison could then be extended.

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