Physics and modelling of under-expanded jets and hydrogen dispersion in atmosphere

Article · January 2009

3 authors:

Vladimir Molkov
Ulster University

Dmitriy Makarov
Ulster University

Maxim Bragin
Loughborough University

PHYSICS AND MODELLING OF UNDER-EXPANDED JETS AND HYDROGEN DISPERSION IN ATMOSPHERE

Molkov V., Makarov D.*, Bragin M.

HYSAFER centre, University of Ulster, Northern Ireland, UK

dv.makarov@ulster.ac.uk

Introduction. The broad use of hydrogen as an energy carrier to tackle the issue of climate change is unavoidable. The emerging hydrogen economy poses new problems to be solved to ensure a level of safety in hydrogen technologies and infrastructure comparable to that for today's fossil fuels. The pressure of onboard hydrogen storage in early-market vehicles already reaches extremely high value 700 bar. Such high storage pressures make accidental hydrogen release and dispersion a potentially hazardous scenario. An unscheduled release from high pressure hydrogen storage, e.g. through a pressure relief device (PRD), can create underexpanded sonic jets with dispersion of hydrogen and a flammable envelope spreading over tens of meters. Safety or set-back distances for hydrogen refuelling stations and stationary applications require accident consequences analysis, performed by contemporary mathematical models and tools.

Novel notional nozzle model. The mean axial concentration decay of a turbulent free vertical round jet issuing into a calm neutral environment for subcritical pressures (pressures ratio below about 1.9 for hydrogen) is given by Chen and Rodi in the form [1]

$$\overline{\eta}(x) = \frac{5.4 \cdot d}{x + x_0}\sqrt{\frac{\rho_\infty}{\rho_g}}\,, \qquad (1)$$

where the entrainment constant K=5.4, d is the nozzle diameter, x and x_0 – distance along the jet axis and virtual origin of the jet, ρ_∞ and ρ_g are the densities of the ambient and issuing gas, evaluated at ambient pressure and temperature. Different approaches exist to apply Eq.1 for supercritical pressures. They are based on a notional nozzle or pseudo-diameter concept. The results of study by Birch et al. 2 show that the concentration decay behaviour of supercritical jets can be described by Eq.1 for subcritical releases, with the actual nozzle diameter d replaced by a notional (or effective) nozzle diameter d_{eff}. With the notional nozzle diameter calculated by the method described in [2] the entrainment constant for application of the Chen and Rodi equation to supercritical pressures below 10 MPa becomes K=4.9. Three years later Birch and co-authors modified the approach for calculation of the effective diameter d_{eff} and calibrated it using the former experimental data. They found that with the new approach the concentration decay constant is K=5.4 3, i.e. equal to that one in the original Chen and Rodi correlation 1. They also found that the virtual origin for concentration decay x_0 is independent of pressure ratio and can be neglected as being too small (0.6 of the notional nozzle diameter d_{eff}).

In order to apply Eq.1 for hydrogen safety engineering the value of the notional nozzle diameter should be first calculated. The methods of calculation of the notional nozzle diameter similar to 2 are not applicable to hydrogen storage pressures above 10-20 MPa when effects of gas non-ideality must be accounted for. Indeed, the Abel-Nobel equation of state written in the form $P = Z\rho R_{H2}T$ with $Z = 1/(1-b\rho)$ has a compressibility factor equal to Z=1.01 at 1.57 MPa, 1.1 at 15.7 MPa, and 1.5 at 78.6 MPa (temperature 293.15 K). A method of calculation for the notional nozzle diameter, based on the concept of Birch et al. [3], but with application of the Abel-Nobel equation for non-ideal behaviour of highly compressed hydrogen, has been recently published by Schefer et al. [4]. However, this approach predicts supersonic velocity at the pseudo-diameter which superimposes additional complications when carrying out numerical simulations of large scale problems with incompressible codes.

A novel notional nozzle model that takes into account the non-ideal behaviour of hydrogen at extremely high pressures through Abel-Nobel equation of state is reported in this paper. Similar to the approach by Birch et al. [2] the developed model is based on the assumption of uniform sonic flow through notional nozzle. However, the model includes the energy conservation equation. This approach avoids formally supersonic velocities in the notional nozzle as in the model of Schefer et al. [4].

The concept is based, similar to others, on assumptions of uniform velocity and undiluted gas concentration at the notional nozzle. The pressure at the notional nozzle is atmospheric and the velocity is equal to the speed of sound in hydrogen at a temperature derived from equations of conservation of mass, total energy and the Abel-Nobel equation for isentropically expanding gas being issued from a high pressure reservoir (level 1), through a nozzle orifice (level 2) and, finally, through a notional nozzle at atmospheric pressure (level 3). The procedure for calculation of the notional nozzle diameter d_3=d_{eff} is as follows. Calculate density in the reservoir from the Abel-Nobel equation of state $\rho_1 = P_1 / ZR_{H2}T_1$. Solve a transcendental equation of isentropic expansion to find density at the orifice:

$$\left(\frac{\rho_1}{(1-b\rho_1)}\right)^{\gamma} = \left(\frac{\rho_2}{(1-b\rho_2)}\right)^{\gamma}\left[1+\frac{(\gamma-1)}{2(1-b\rho_2)^2}\right]^{\frac{\gamma}{\gamma-1}} . \quad (2)$$

Find temperature T_2 at the orifice from the relationship:

$$T_1 / T_2 = 1 + (\gamma - 1)/2(1-b\rho_2)^2 , \quad (3)$$

and then pressure P_2 from the Abel-Nobel equation of state. At the orifice, flow is chocked and hydrogen velocity can be calculated using the formula for the speed of sound:

$$V_2^2 = \gamma R_{H2} T_2 /(1-b\rho_2)^2 . \quad (4)$$

From the energy conservation equation written per unit mass,

$$c_p T_2 + V_2^2/2 = c_p T_3 + V_3^2/2 , \quad (5)$$

with the assumption that the hydrogen velocity at the notional nozzle is equal to the local speed of sound

$$V_3^2 = \gamma R_{H2} T_3 , \quad (6)$$

it is easy to derive that the temperature at the notional nozzle is

$$T_3 = \frac{2T_2}{(\gamma+1)} + \frac{(\gamma-1)}{(\gamma+1)}\frac{P_2}{\rho_2(1-b\rho_2)R_{H2}} . \quad (7)$$

Then, hydrogen density at the notional nozzle can be calculated with P_3 equal to the ambient pressure as well as the velocity of gas V_3. Finally, from the continuity equation it follows that

$$d_3 = d_2(\rho_2 V_2 / \rho_3 V_3)^{1/2} . \quad (8)$$

Blowdown dynamics model. The described above notional nozzle model was used to simulate pressure dynamics in the hydrogen storage tank during an underexpanded jet release (blowdown) in experiments by UK Health and Safety Laboratory (HSL). The HSL high-pressure hydrogen experimental facility was equipped with 2 vessels of 98 litres capacity each, initial pressure was P_1=208 bar, initial temperature was estimated as T_1=288 K. These conditions correspond to 3.025 kg of hydrogen mass stored in the facility. Valve with throat wide open provided a minimum orifice Ø9.5 mm in the pipeline. The discharge pipeline was installed at 1.2 m height and directed horizontally.

Schefer et al. [4] demonstrated that the heat transfer in a storage system and elements of release manifold may play important role in the blowdown dynamics. It was not possible to account for the heat transfer processes in the described experiment in detail and the blowdown dynamics was modelled for two limiting cases – adiabatic discharge from the high-pressure vessel (no heat transfer), and discharge under the constant temperature conditions (ideal heat transfer). Simulated pressure dynamics in the hydrogen storage vessel in comparison with the experimental pressure record is shown in Fig.1. One can see that the heat transfer didn't play significant role in the considered experiment (about 20% longer discharge time to reach the same pressure as in the adiabatic case). The experimental pressure dynamics is closer to the simulation results corresponding to the adiabatic case. This may be attributed to the relatively small storage pressure and volume, resulting in a short discharge period, when the heat transfer processes don't have time to take the effect.

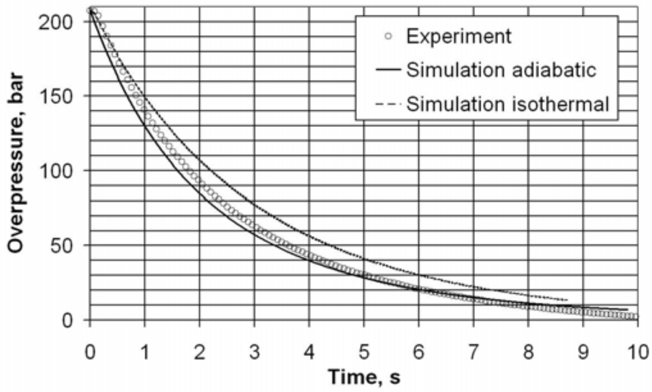

Fig.1. Simulated blowdown pressure dynamics.

CFD simulation of blowdown jet. Accurate simulation of hydrogen dispersion and flammable mixture envelope is important for risk assessment of hydrogen technologies. Computational Fluid Dynamics (CFD) is used routinely nowadays for simulation of gas distribution dynamics in space and time. However, transient character of hydrogen discharge from a storage with changing in time pressure and temperature within the vessel results in the variation of the notional nozzle diameter, and hydrogen velocity and temperature at the notional nozzle, which makes implementation of the boundary conditions in CFD application non- trivial.

To avoid simulation of changing with time effective diameter, hydrogen mass inflow was modelled using volumetric sources of hydrogen mass, momentum, and energy. With such approach the release volume is constant, but the volumetric sources are changing to reflect changing parameters at the notional nozzle. The standard k-ε turbulence model was used in simulations, thus the CFD model included volumetric sources for the turbulent kinetic energy and the turbulent kinetic energy dissipation rate equations as well.

First, the applicability limits of the model were studied using the example of another HSL experiment on underexpanded hydrogen jet: Run 7 described in [5], where at particular quasi-steady state conditions the hydrogen storage pressure was equal to p_1=10.0 MPa and temperature T_1=14^{0}C, discharge rate was estimated as m=0.045 kg/s, nozzle diameter was d_2=3 mm. Comparison of the measured hydrogen concentrations with simulation results corresponding to different ratios of the release volume size to the notional nozzle diameter are shown in Fig.2. As can be seen, the simulated and experimentally observed hydrogen concentrations are in a good agreement, provided that ratio of the release volume size to the effective diameter d_{eff} is up to 4.

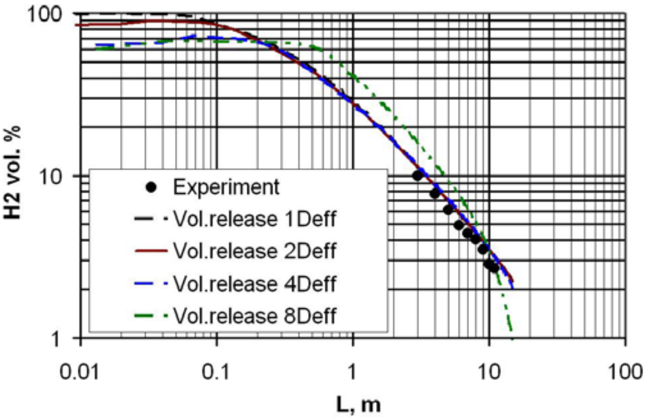

Fig.2. Comparison of measured and simulated H_2 concentration for various sizes of the release volume.

After this validation procedure, the volumetric release strategy was employed to simulate the HSL blowdown experiment described in the previous section (see Fig.1 for the blowdown pressure dynamics). The dependence of volumetric hydrogen mass, velocity, and energy sources on time were obtained using the described above adiabatic notional nozzle concept.

Calculation domain dimensions were LxWxH= 101.4x39.8x21.2 m. Numerical grid consisted of 784204 control volumes (CV). Initial value of the notional nozzle diameter was equal d_{eff}=0.1 m and hydrogen was released using a cylindrical volume LxD = 0.1x0.1 m. CV size varied from 0.025 m in the hydrogen release volume to ~5.0 m in the far field.

Implicit segregated solver, SIMPLE procedure for pressure-velocity coupling, 3rd order accurate MUSCL discretisation scheme for convective terms, 2nd order accurate central-difference scheme for diffusion terms, 2nd order accurate time discretisation were used for simulations, time step was equal Δt=0.005 s. In CFD simulations the release continued until t=10 s, while simulations continued to t=17 s of real time. Dynamics of H_2 vol. concentration along the centre-line with time is shown in Fig. 3 (t=1-10 s and t=11-17 s).

As it is seen in Fig.3, the maximum propagation distance of a fast-burning hydrogen-air mixture (hydrogen concentration above 20% vol.) is 5 times shorter than the propagation of hydrogen clouds at concentrations close to the low flammability limit (4% vol.). Also, while a hydrogen-air mixture at concentrations close to the low flammability limit propagated further with time, the volume of fast burning hydrogen-air mixture was decreasing when time was above 1 s.

Conclusions. The alternative notional nozzle model, based on Abel-Nobel equation of state and applicable to the extremely high hydrogen storage pressures, was developed. The model was combined with the volumetric source terms approach for CFD simulation of blowdown phenomena and validated against experimental results for a quasi-steady state hydrogen underexpanded jet. The application of the developed approach was demonstrated using the blind prediction of hydrogen concentrations in HSL blowdown experiment. The development will be of interest for modelling a large spectrum of problems associated with underexpanded releases from high-pressure storage facilities, e.g. blowdowns, delayed ignitions, jet fires, etc.

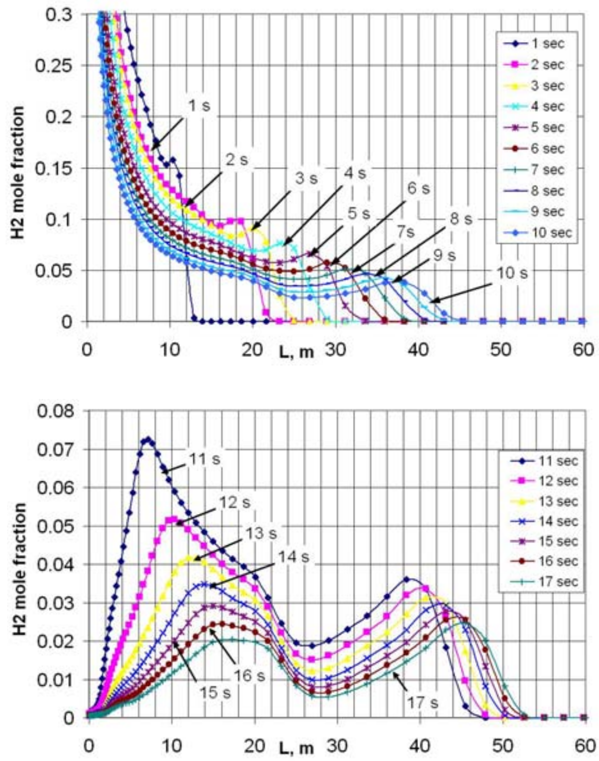

Fig.3. Simulated H_2 concentration dynamics along the jet centre-line: t=1-10 s and t=11-17 s.

1. Chen C., Rodi W. // Vertical turbulent buoyant jets – a review of experimental data. Pergamon Press. Oxford. 1980. P.37.
2. Birch A.D., Brown D.R., Dobson M.G. and Swaffield F. // The structure and concentration decay of high pressure jets of natural gas. Comb. Sci. Tech. 1984. V.36. P. 249-261.
3. Birch A.D., Huges D.J., and Swaffield F. // Velocity decay of high pressure jets. Combustion Science and Technology. 1987. V.52. P.161-171.
4. Schefer R.W., Houf W.G., Williams T.C., Bourne B. and Colton J. // Characterization of high-pressure, underexpanded hydrogen-jet flames. International Journal of Hydrogen Energy. 2007. V.32. P.2081-2093.
5. Roberts P.T., Shirvill L.C., Roberts T.A. // Dispersion of hydrogen from high-pressure sources. Hazards. Proc. of Hazards XIX Conference, 28-30 March 2006, Manchester, UK.