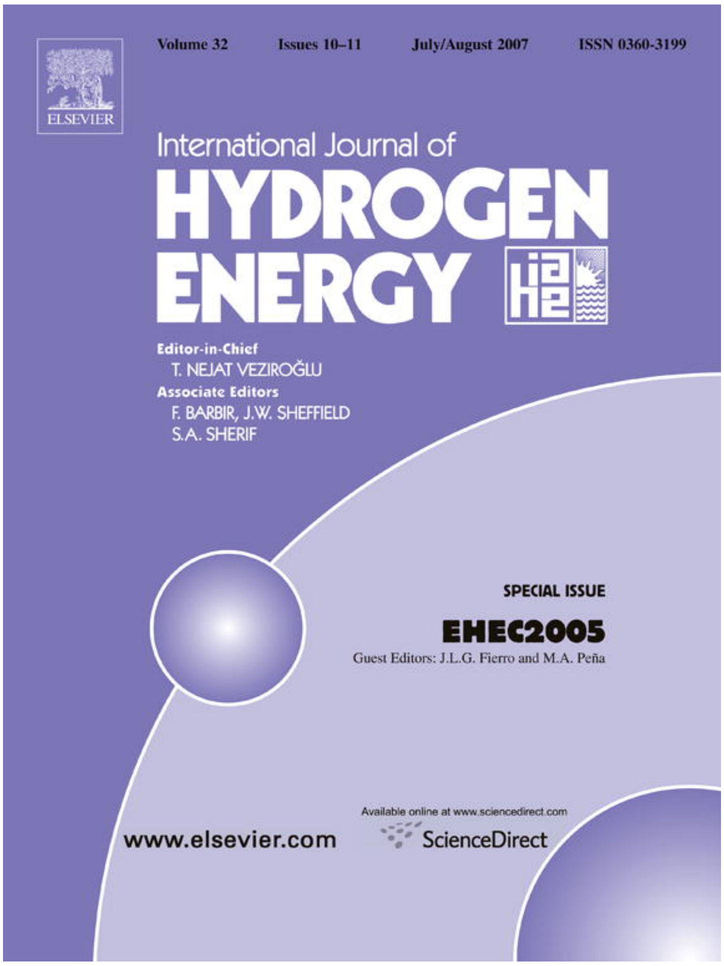
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Effectiveness of small barriers as means to reduce clearance distances

Andrei V. Tchouvelev[a,*], Zhong Cheng[a], Vladimir M. Agranat[b], Serguei V. Zhubrin[c]

[a]*A.V.Tchouvelev & Associates, 6591 Spinnaker Circle, Mississauga, Ont., Canada L5W 1R2*
[b]*Hydrogenics Corp., 5985 McLaughlin Road, Mississauga, Ont., Canada L5R 1B8*
[c]*Flowsolve Limited, 130 Arthur Road, London SW19 8AA, England*

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Abstract

Hydrogen clearance or safety distance can be defined as the minimum distance between a hydrogen leak source and surrounding equipment, property or personnel beyond which the risk to the said recipients associated with existing hydrogen hazards is deemed acceptable. The same principal is applied to determine clearances to ignition sources and air intakes only the criteria in this case are the risk of ignition or the risk of intaking a flammable mixture. The study of effects of small barriers as means to reduce clearance distances for compressed hydrogen releases is important for the development of installation codes and risk mitigation requirements. In this paper, computational fluid dynamics (CFD) modeling techniques were applied to the numerical simulation of the effects of a protective wall of 1 m by 1 m on reducing the size of hydrogen cloud. The protective wall was 1 m away from a 70 MPa (700 bar) 60 L tank, from which an incidental hydrogen release impinged horizontally onto the wall, causing a complicated 3D dispersion of hydrogen cloud. In-house CFD codes first accurately estimated the non-linear hydrogen mass release rate decreasing with time. Then the effects of the wall on the propagation speed of the hydrogen cloud moving behind the wall were investigated using the PHOENICS software package, provided with both the ideal gas law and the real gas law expressed by the Abel-Nobel equation of state (AN-EOS). The distributions of lower flammability limit (LFL) and 50% of LFL hydrogen clouds were described in detail based on the numerical results. It was found that the 50% of LFL hydrogen clouds (2% vol) could propagate behind the wall in less than 0.2 s after the onset of the release. The horizontal extents corresponding to 50% of LFL hydrogen cloud on the central vertical plane are 9.6 m at 5 s when they are predicted using the ideal gas law. When using the real gas law, the predicted extents decrease to 6.3 m at 5 s. The ideal gas law significantly overestimates the hypothetical hydrogen cloud volumes for LFL, or fractions of LFL, for different release times at the current initial stagnation pressure level (700 bar). The current model codes and standards generally specify clearance distances for hydrogen based on the regulators' experience in other flammable gases, like natural gas or propane, rather than on real hydrogen gas properties that particularly deviate from ideal gas law under high pressure. On the other hand, it is relatively more conservative to exploit the ideal gas law to predict the combustible hydrogen cloud extents than using the real gas law for industrial applications. The numerical results from the impingement release also confirm that a small protective wall, or a barrier, can reduce the hydrogen concentration behind the wall. The numerical results can be further applied for defining the zoning requirements for Canadian Electrical Code and clearance distances for Canadian Hydrogen Installation Code.

Keywords: Hydrogen release; Ideal gas law; Real gas law; Abel-Nobel equation of state; Impingement jet; Clearance distance; Protective wall

1. Introduction

As well as many other gases, merchant hydrogen is stored and transported in large quantities in gaseous form under high pressure. An incidental release of hydrogen generally arises from a failure in the process or storage equipment in which the gas is kept in a safe condition and can result in a large combustible cloud, which, when ignited, could be harmful to personnel, equipment and property. To mitigate these potential harmful effects, model codes prescribe clearance distances. A straightforward method to reduce clearance distances is to install a mechanical barrier in the most probable direction of the release and, thus, reduce the size of dispersed cloud beyond the barrier and potential consequences of the release. The study of effects of small barriers as means to reduce clearance distances for compressed hydrogen releases is important for the development of installation codes and risk mitigation requirements.

Up to now, direct experiments are still the most accurate approach to address the effectiveness of barriers on reducing cloud

* Corresponding author. Tel.: +1 416 464 5888; fax: +1 905 696 7007.
E-mail address: atchouvelev@tchouvelev.org (A.V. Tchouvelev).

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extents caused by hazardous gas releases and dispersion. Meanwhile, CFD simulations provide an inexpensive alternative to the quantitative prediction of mitigation effects. The mitigated hazardous zones and separation distances among components within hydrogen fuelling stations as well as distances from stations to off-site buildings, personnel and equipment can be fully investigated with the CFD techniques.

Hydrogen at a high pressure displays thermodynamic properties different from those predicted by the ideal gas model. The volume required for storing a specific mass of high-pressure hydrogen is larger than the volume the ideal gas law predicts. As a result, the real gas model should be used for more accurate prediction of compressed hydrogen releases and dispersion. Using the real gas model, Venetsanos et al. [1] simulated the hydrogen release rate, the resulting concentration volume and combustion of hydrogen in an actual hydrogen explosion, which took place in a built up area of central Stockholm, Sweden. The simulation results were consistent with the reported real situations. Mohamed and Paraschivoiu [2] used Beattie–Bridgeman equation of state (BB-EOS) to derive the thermodynamic relations describing the specific heats, internal energy, and speed of sound of hydrogen at high pressure. The numerical and analytical results based on BB-EOS accurately predicted the hydrogen mass release rate from a high-pressure chamber. Cheng et al. [3] executed the numerical simulations of compressed hydrogen releases and dispersion using the Abel-Nobel equation of state (AN-EOS) [4]. The numerical results showed that the hydrogen mass release rate was significantly overestimated by the ideal gas law during the choked portion of the release. The authors recommended that the hydrogen cloud caused by the incidental release could be more accurately predicted by the real gas law.

However, the previous CFD works [1,3] assumed that there were no barriers in the hazard cloud zone and that the cloud dispersion was controlled by convection, diffusion and buoyancy resulting from the compressed hydrogen release. To investigate the effectiveness of a small barrier on the hydrogen dispersion, a CFD modeling technique is applied in this paper to the numerical simulation of the effects of a protective wall of 1 m by 1 m on reducing the size of hydrogen cloud. The focus is on the quantitative predictions of the extents of lower flammability limit (LFL) and 50% of LFL hydrogen clouds during high-pressure release impingement against a protective wall, and of the hydrogen dispersion propagation speed behind the wall.

An in-house software, based on the analytical simulation codes developed by Mohamed and Paraschivoiu [2], was used to address the changes of pressure, density and flow rate variations at the leak orifice during the release, while the PHOENICS software package developed by CHAM Limited [5], was used to predict the extents of various hydrogen concentration envelopes as well as the velocities of gas mixture for the dispersion in the domain. Using the same approach as that used by Cheng et al. [3], the AN-EOS was incorporated into the CFD model and implemented through the PHOENICS software to simulate the real gas hydrogen release and dispersion. The numerical results are compared with those obtained from using the ideal gas law. The numerical results can be further applied

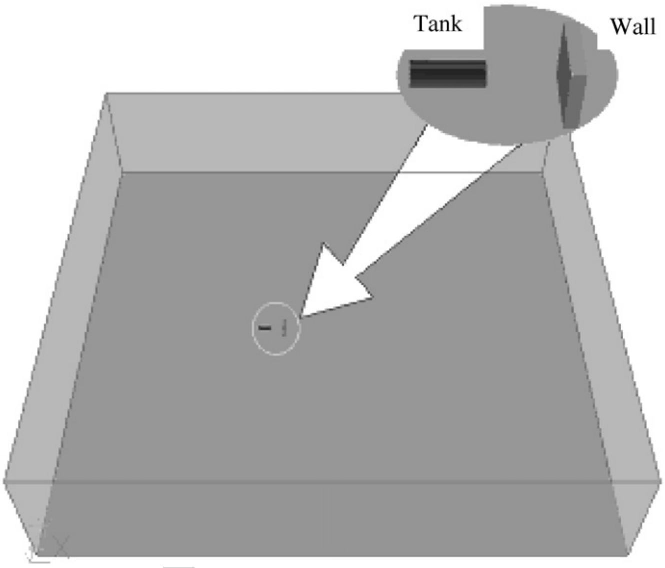

Fig. 1. High-pressure tank and preventive wall inside the domain.

for defining the zoning requirements for Canadian Electrical Code and clearance distances for Canadian Hydrogen Installation Code.

The current modeling approach has been validated, improved and calibrated with experimental data and published research results through various projects, including CFD validation, calibration and enhancement project, a research project sponsored by Natural Resources Canada [6].

2. Modeling scenario description

The CFD problem is to simulate the effects of a 70 MPa (700 bar) horizontal release out of a 60 L tank, through a 6 mm (1/4″) opening onto the plain front face of a 1×1 m wall. The tank is on the centerline of the wall. The wall is located on the floor 1 m away from the tank inside a large warehouse with a 9 m (30 ft) ceiling and without ventilation. A large rectangular domain with the ground area of 40 m by 40 m has been used. Of particular interest is the progression of concentrations at the wall, around the wall, and on the ceiling. Fig. 1 shows the geometry for the current problem.

The tank length is 0.94 m and its outside diameter is 0.356 m. The hydrogen leak location is as follows: 15 m from the west side of domain, 0.5 m from the ground and in the middle of the domain.

The objective of the research is to investigate the effect of high-pressure release impingement against a protective wall, or a wall of process equipment, or an electrical box:

- How fast will the release propagate behind the wall?
- What are the distributions of LFL and 50% of LFL clouds?

3. Mathematical formulations and numerical simulations

Results quoted below were obtained using a general CFD approach, where all the important physical processes were accounted for. Hydrogen convection, diffusion, buoyancy and transcience were modeled based on the 3D compressible Navier–Stokes equations and hydrogen mass conservation equation with the proper initial and boundary conditions. The compressible model assumed that the temperature gradients were small in the domain and thus the gases (hydrogen and air) had compressible properties: the mixture gas density was a function of local hydrogen mass concentration and pressure at the specified temperature.

The complicated 3D hydrogen dispersion, which followed a high-pressure choked release, was controlled by the turbulent flow. PHOENICS software was chosen for the purpose of modeling of the dispersion because it contains a number of validated turbulence models that allow for modeling of complex flow conditions. The LVEL model was selected as a proper turbulence model for computational tasks herein. The LVEL model allows for both laminar and turbulent flow conditions to be considered within one model. The LVEL subroutine computes local Reynolds numbers in every cell of the computational mesh and applies the local effective viscosity based on this number. The effective viscosity includes both laminar and turbulent components, allowing for accurate modeling of fluid flow conditions within the whole domain.

Another important feature of the modeling approach was the use of transient conditions for computing the releases and dispersion of hydrogen clouds, accounting for the time histories of all calculated variables (pressure, gas density, velocity and hydrogen concentration) and the movement of hydrogen clouds with time.

To account for the effect of hydrogen buoyancy, the density difference model implemented in the PHOENICS was used. The dispersed hydrogen was driven by the buoyancy force contributed by the density difference between the local mixed gas and the standard reference air density.

3.1. Time-dependent release rates (source terms)

The modeling of the impingement release of compressed hydrogen, stored in a high-pressure tank, on a vertical wall was used to predict the decrease of pressure due to gas outflow, convection and diffusion as well as the distributions of LFL and 50% of LFL hydrogen clouds.

Due to the release of hydrogen, the remaining hydrogen in the tank expands, causing cooling, depressurizing at the leak orifice, as well as a nonlinear hydrogen mass flow rate decreasing with time. The same approach as shown in [3] was used to predict the time-dependent release rates through the orifice, $\dot{m}(t)$, and consequently the source terms for the hydrogen dispersion. The ideal gas model and the real gas model using the AN-EOS [4] were incorporated into the underlying CFD models.

3.1.1. Ideal gas law correlations

For any time t, $T_{\mathrm{T}}(t)$, $P_{\mathrm{T}}(t)$ and $\rho_{\mathrm{T}}(t)$ are the hydrogen temperature, pressure and density in the tank, respectively. The mass flow rate for gas outflow through an orifice can be estimated by a generalized equation for the ideal gas law [8]:

$$\dot{m}(t) = C_{\mathrm{d}}(t)\sqrt{\gamma}\left(\frac{2}{\gamma+1}\right)^{\gamma+1/2(\gamma-1)} \frac{P_{\mathrm{T}}(t)A}{\sqrt{RT_{\mathrm{T}}}} = C_{\mathrm{d}}\sqrt{\gamma}\left(\frac{2}{\gamma+1}\right)^{\gamma+1/2(\gamma-1)} A\sqrt{P_{\mathrm{T}}(t)\rho_{\mathrm{T}}(t)}, \quad (1)$$

where $C_{\mathrm{d}}(t)$ is the discharge coefficient at time t; γ is the ratio of specific heats ($\gamma = 1.41$ for hydrogen); R is the gas constant: $R = 4124\,\mathrm{J/(kg\,K)}$ for hydrogen; A is the orifice cross-sectional area.

At $t = 0$, the initial hydrogen release rate is

$$\dot{m}_0 = \dot{m}(0) = C_{\mathrm{d}}\sqrt{\gamma}\left(\frac{2}{\gamma+1}\right)^{\gamma+1/2(\gamma-1)} \frac{P_{\mathrm{T}}(0)A}{\sqrt{RT_{\mathrm{T}}}} = C_{\mathrm{d}}\sqrt{\gamma}\left(\frac{2}{\gamma+1}\right)^{\gamma+1/2(\gamma-1)} A\sqrt{P_{\mathrm{T}}(0)\rho_{\mathrm{T}}(0)}, \quad (2)$$

where $P_{\mathrm{T}}(0)$ and $\rho_{\mathrm{T}}(0)$ are, respectively, the initial hydrogen stagnation pressure and density in the tank: $P_{\mathrm{T}}(0) = 700\,\mathrm{bar}$, $\rho_{\mathrm{T}}(0) = 57.9\,\mathrm{kg/m^3}$ using the ideal gas law. Note that this initial stagnation density is overestimated by 45% compared with the real hydrogen properties at 700 bar, as shown in Fig. 2.

It is assumed that the discharge coefficient is a constant: $C_{\mathrm{d}}(t) = 0.95$ throughout the release process, as suggested by Beek [8]. The initial release rate is therefore 1.3166 kg/s using the ideal gas properties in Eq. (2). Solving the first-order ordinary differential equation for the mass release rate depending on time by assuming a critical temperature, $T_* = (2/(\gamma+1))T_{\mathrm{T}}$, at the leak orifice, the time-dependent ideal gas release rate can be approximated as the following correlation:

$$\dot{m}(t) = -V\frac{\mathrm{d}\rho}{\mathrm{d}t} = \rho(t)u(t)A \approx \dot{m}_0 \mathrm{e}^{-(C_{\mathrm{d}}A/V)t\sqrt{\gamma(2/\gamma+1)^{\gamma+1/\gamma-1}RT_{\mathrm{T}}}} \approx 1.3166\mathrm{e}^{-0.378443t}, \quad (3)$$

where V is the tank volume and $u(t)$ is the gas velocity. It takes about 15.45 s to finish the underlying choked release. It should be noted that approximation correlation 3 is also derived using Eq. (1), where $P_{\mathrm{T}} = \rho_{\mathrm{T}}RT_{\mathrm{T}}$ and assuming a constant temperature, T_{T}, in the tank.

3.1.2. Real gas law calculations

As shown in Fig. 2, there is more than 20–50% density deviation for the ideal gas law in comparison to the real gas law for storage pressures in the hundreds of bars. As a result, hydrogen release rate needs to be recalculated using the real gas law as well.

Fig. 3 shows the mass release rates calculated with using the real gas law and the ideal gas law. In-house software modified from the analytical simulation codes developed by Mohamed and Paraschivoiu [2] was used for calculating the corresponding release rates with the assumption of an adiabatic process. The stagnation properties of hydrogen inside the tank, as well as sonic properties of hydrogen at the orifice, were simulated by using the real gas model. It is assumed that the thermodynamic properties are distributed uniformly throughout the

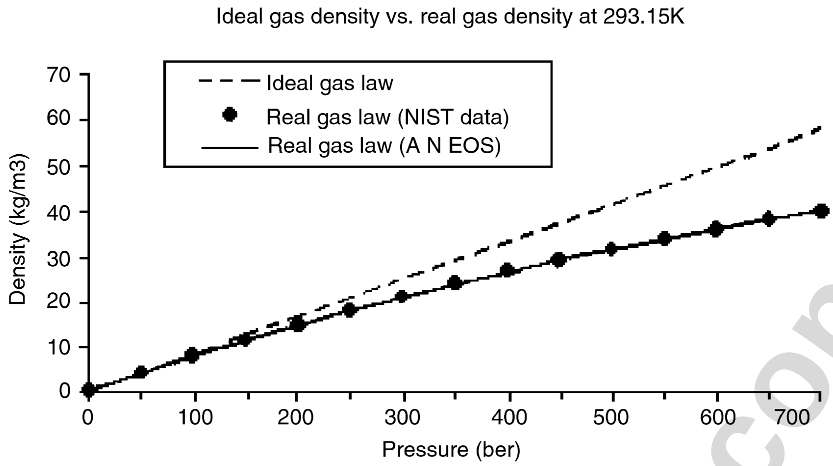

Fig. 2. Density deviation from ideal gas law as a function of pressure at 293.15 K. At 700 bar, the real gas density is about 40 kg/m^3 but is overestimated by 45% when using the ideal gas law. Solid line: ideal gas law. Dots: NIST data [7]. Dash line: real gas law using AN-EOS.

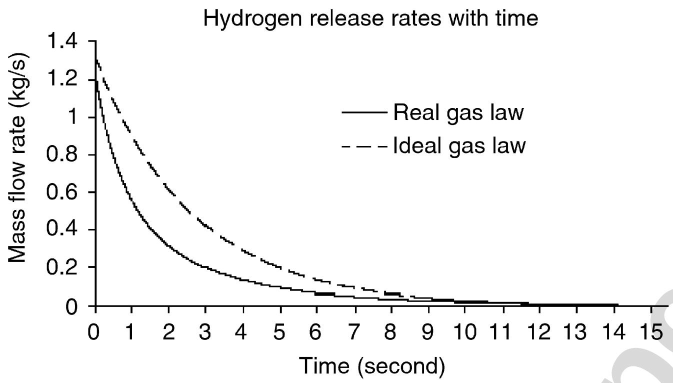

Fig. 3. Choked hydrogen release rate for the impingement release. Initial tank pressure: 700 bar. The leak orifice size: $\frac{1}{4}''$. Solid line: the choked release rate with using real gas properties (The predicted choked release lasts 14.14 s). Dash line: the choked release using ideal gas law (The predicted choked release lasts 15.45 s). The ideal gas law overestimates the hydrogen release rate by up to 53% 3 s after the onset of the release.

tank during the release, The ordinary differential equations discretized from the conservation equations governing the mass and energy to the control volume containing the hydrogen inside the tank, were numerically solved using the first-order Euler method. The results show that it takes 14.14 s to finish the choked release when using the real gas law. The ideal gas law also overestimates the hydrogen release rate by 6% at the start of the release and then to about 50% from 2 to 5 s. After 10 s of release, the deviation in the mass release rates for the two gas laws reduces to 5%. By comparing the total areas below the ideal and real gas release rates during the choked release time, we can find that the ideal gas law overestimates the total mass of hydrogen released to the atmosphere by about 45%.

3.2. Hydrogen dispersion clouds

Using the two release rates shown in Fig. 3, the CFD modeling of hydrogen dispersion was done separately for real and ideal gas laws as follows [3]:

- An ideal gas dispersion simulation using the PHOENICS software package through PLANT (a FORTRAN code generator in PHOENICS) exploiting the ideal gas release rate obtained by Eq. (3) as initial and boundary conditions at the orifice;
- A real gas dispersion simulation using AE-EOS implemented through PLANT exploiting the real gas release rate obtained by the in-house software modified from [2] as initial and boundary conditions at the orifice.

The compressed hydrogen releases to a domain of 40 m × 40 m × 9 m, which is assumed to be large enough for neglecting the boundary effects. To save the computational time, a global structured grid of 35 × 18 × 21 for half domain (40 m × 20 m × 9 m) was used for the symmetric hydrogen dispersion problem. The mesh was locally refined near the leak orifice so as to capture the local hydrogen physical properties in the jet flow establish region (jet's non-buoyant and intermediately region). The mesh was also refined near the stagnation zone on the barrier. The grid sensitivity studies using a high grid resolution yielded similar numerical results, indicating that this grid density yields sufficiently accurate solutions for the underlying impingement problem.

The CFD modeling of the choked release was performed for 14.14 s by using the AN-EOS real gas model and for 15.45 s by using the ideal gas law. The sufficient accuracy in the calculations of time histories was guaranteed during the transient iterations by controlling the residuals for the momentum, mass and concentration balance equations at each time step.

Fig. 4 shows the hydrogen concentration distributions (from 2% to 20% vol) on the horizontal plane which is 0.5 m above the ground 0.1, 0.2, and 0.5 s after the onset of the release using the ideal gas law and the real gas law, respectively. These top-view pictures illustrate an animated hydrogen impingement process. Both ideal and real gas laws predict that the released hydrogen cloud propagates behind the wall in less

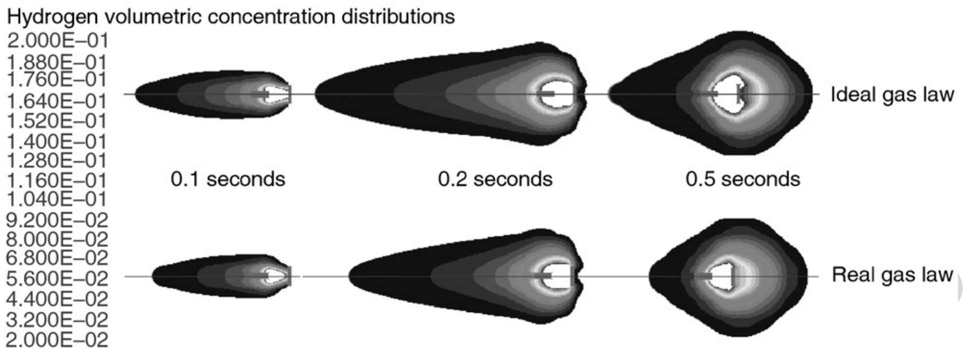

Fig. 4. H_2 concentration distributions on the horizontal plane using ideal gas law and real gas law. The label at the left shows the hydrogen volumetric concentration distributions between 2% and 20%. The six top-view pictures show the concentration distributions (between 2% and 20% vol) on the horizontal plane that crosses the $\frac{1}{4}''$ leak orifice at the beginning of the release. Top three pictures: ideal gas law. Bottom three pictures: real gas law. From left to right: 0.1, 0.2 and 0.5 s after the leak. The 2% vol H_2 cloud touches the ends of the barrier in less than 0.1 s and propagates behind the wall in 0.2 s. It also can be seen that the hydrogen cloud obtained with the real gas law is smaller at the early stage of the leak. (Note: here and below white area inside the boundary contains hydrogen concentration greater than 20%).

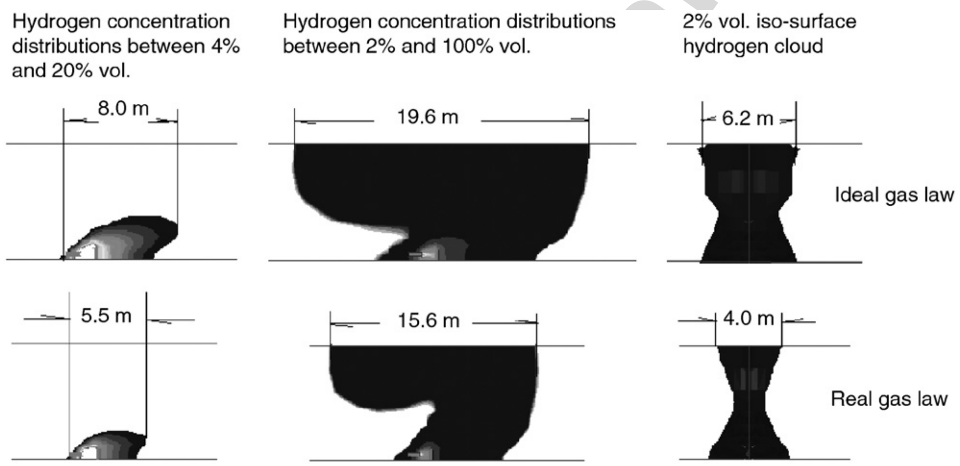

Fig. 5. Hydrogen cloud 1 s after the onset of release using ideal gas law and real gas law. Top three pictures: ideal gas law. Bottom three pictures: real gas law. The two horizontal red lines here and below in each picture mark the ceiling and the ground. Left: hydrogen concentration distributions between 4% and 20% vol on the plane that is in the direction of the release. Middle: hydrogen concentration distributions between 2% and 100% vol on the plane that is in the direction of the release. Right: 50% of LFL (2% vol) hydrogen cloud iso-surface, viewed in the direction of the release. The solid line in the middle marks the symmetric axis of the domain.

than 0.2 s, whereas the real gas law predicts a relatively small cloud size.

Fig. 5 shows side view and cross section of LFL (4% vol) and 50% of LFL (2% vol) hydrogen clouds and their corresponding concentration distributions 1 s after the onset of the leak, obtained by using the ideal and real gas laws. The hydrogen jet impinges on the wall, results in a stagnation zone in which the static pressure exceeds the distant ambient pressure. The jet bounces backwards due to a pressure effect and then floats to the ceiling under the buoyancy effect as well. The hydrogen concentration is relatively high in the stagnation zone. Meanwhile, the cloud bypasses the wall and accumulates behind the wall, causing a 2% vol hydrogen cloud of 19.6 m long and 6.2 m wide, as predicted by the ideal gas law, and a cloud of 15.6 m long and 4 m wide, as predicted by the real gas law. The different hydrogen cloud shapes 1 s after the onset of the leak confirm that the ideal gas law overestimates the hydrogen release rate and the size of hydrogen clouds at this time. To be noted that the cloud cannot disperse very quickly in the vicinity of the leak orifice, and therefore relatively high hydrogen concentrations (more than LFL) appear between the orifice and the wall. The concentrations close to the ceiling are relatively low (less than LFL). The numerical results also show that the hydrogen concentrations near the ceiling obtained by the real gas model are significantly lower than those obtained by the ideal gas law.

It should be noted that the extent of LFL hydrogen cloud for ideal gas law (8.0 m) is by 2.5 m (or more than 30%) larger than for real gas law (5.5 m), as shown on Fig. 5 by images on the left. This suggests that clearance distances could be reduced by 2.5 m for this scenario.

Fig. 6 shows 50% of LFL hydrogen clouds and their corresponding concentration distributions 5 s after the onset of the leak, obtained with using the real and ideal gas laws,

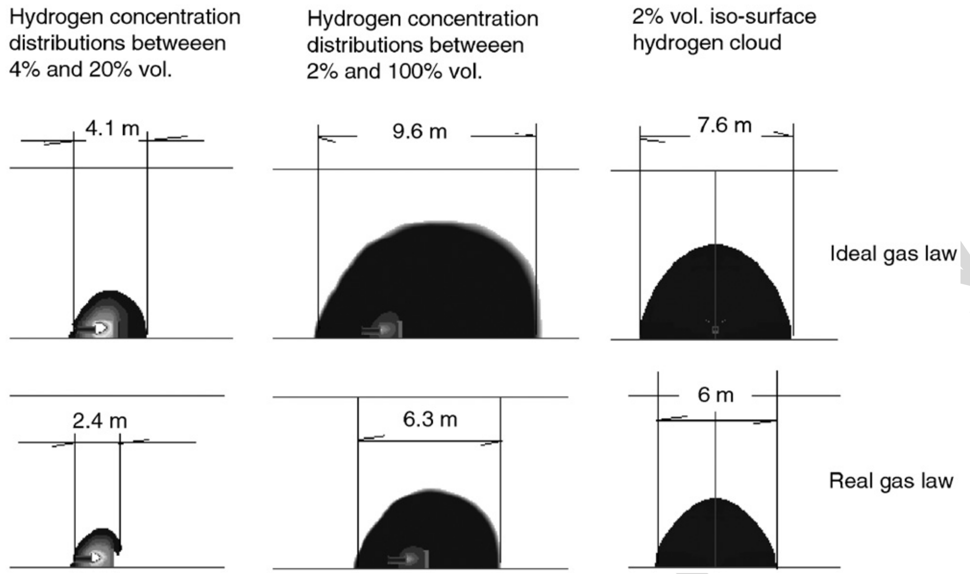

Fig. 6. Hydrogen cloud 5 s after the onset of release using ideal gas law and real gas law. Top three pictures: ideal gas law. Bottom three pictures: real gas law. Left: hydrogen concentration distributions between 4% and 20% vol on the plane that is in the direction of the release. Middle: hydrogen concentration distributions between 2% and 100% vol on the plane that is in the direction of the release. Right: 2% vol of hydrogen cloud iso-surface viewed in the direction of the release.

respectively. At this time, the LFL clouds are smaller than those at 1 s due to the reduced mass release rate so only 50% of LFL (2% vol) clouds are shown in the figure. The ideal gas law yields a larger hydrogen cloud of 9.6 m by 7.6 m while the real gas law yields a smaller one of 6.3 m by 6 m.

Towards the end of the release (at 14 s) the difference between hydrogen cloud extents for the real and ideal gas laws drops to less than 0.5 m for LFL cloud and to about a meter for 50% LFL cloud. The 2% vol hydrogen cloud becomes 7.9 m long and 6.4 m wide by using ideal gas law, and 6.8 m long and 7.0 m wide by using real gas law. It is likely that residual clouds at the end of the release for the real and ideal gas laws will be of similar size.

4. Conclusions

In this paper, an impingement release out of a 60 L tank at 700 bar on a wall 1 m away was simulated by using real and ideal gas laws separately. The AN-EOS was incorporated into the transient CFD model to accurately predict the real gas properties of hydrogen. The sufficient accuracy in the calculations of time histories of hydrogen density, concentration, velocity and pressure was achieved during the transient iterations by controlling the residuals for the momentum, mass and concentration balance equations at each time step. It was predicted that it takes about 15.45 s to finish the choked release using the ideal gas law and 14.14 s using the real gas law. The ideal gas law overestimates the hydrogen mass release rates by up to 50% in the first 5 s of the leak. CFD modeling of hydrogen dispersion shows that the 50% of LFL hydrogen clouds (2% vol) can propagate behind the wall in less than 0.2 s after the onset of the release. The ideal gas law significantly overestimates the hypothetical hydrogen cloud volumes for LFL, or fractions of LFL, for different transient release times at the current initial stagnation pressure level (700 bar). The codes and standards can be relaxed if the real gas law is used. On the other hand, it is more conservative to exploit the ideal gas law to predict the combustible hydrogen separation distances than using the real gas law in the industrial applications.

The obtained numerical results from the impingement release confirm that a protective wall, or a wall of process equipment, can reduce the hydrogen concentration behind the wall. The separation distances can be decreased by the introduction of the wall with a proper size in the leak direction.

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