Synthesis of Modelling and Simulation for Hydrogen Gas Release and Explosion

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Abstract. The article presents the results of two methods for modelling and simulation of the leakage, dispersion and explosion of hydrogen in the event of major accidents in urban areas. Modelling of flammable substances by standard methods fully based on input data. Therefore, the predictions from common software packages should be extended to experimental results. The aim of this paper is to present the synthesis of modelling and simulation for one component gas-air dispersion and explosion to demonstrate the rational approach to loss prevention based on understanding of the nature of incidents and of the type of loss that actually occur.

1 Introduction

1.1 Interest

In the present article we obtained a set of experimental data needed to evaluate the explosion severity of hydrogen using a combination of experimental methods and suitable standard software simulation procedures. Consequence evaluation is an important part in risk assessment even if the results often contain many uncertainties. A method to identify and quantitatively evaluate such uncertainties would be to carry out a comparative study of experimental models and CFD models [1]. Selected application cases include the solution of current research tasks related to fundamental aspects of the effective syngas cleaning with the aim of increasing the hydrogen gas component [2].

1.2 Previous studies

Modelling the consequences of accidents in the Czech Republic has a long tradition among safety-oriented fields [3]. This research is located in the analytical field of industrial safety. The article offers a unique opportunity to present results of modelling with world-renowned computing models for predicting emergency situations. In fact, the data obtained can be used by professionals in the fields of fire prevention, explosions and toxic releases, but also in risk analysis and prevention. The results will help to orientate and avoid quickly mistakes in accepting absurd, overly conservative or overly optimistic results [4].

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2 Experimental model

2.1 High-speed camera

The high-speed camera Photon FASTCAM SA-Z (speed >1M fps; resolution >12k fps) has been used to capture high-resolution digital images at ultra-high speeds. The high-speed camera has been installed in a chamber opening and focused on ignition source. FASTCAM Viewer tools allow image calibration and measurement of angles and distances from explosion image data [5].

2.2 Experimental Setup

The experimental setup used for determination of hydrogen-air explosion limits is schematically described in described in [5].

2.3 Experimental procedure

Lower explosion limits of the hydrogen-air mixture were determined experimentally according to the [6]. Procedure for gas explosion starts with evacuation to leave a space for the hydrogen gas. For example, the use of hydrogen concentrations of 30 vol. % and 35 vol. % require the partial pressures of hydrogen to be added are 0.30 bar and 0.35 bar respectively. Then the evacuation pressures should be 0.70 bar and 0.75 bar respectively. PLC starts the experiment where 600 ms is counted as ignition delay time, and then the gas is mixed by blowing dispersion air into the hydrogen-air mixture inside the chamber. After that the mixture is ignited by the electric discharge. The explosion characteristics are measured and calculated [7].

2.4 Calculation procedure

The explosion pressure in a constant volume chamber have been simulated based on the adiabatic assumption through thermal equilibrium. The element potential approach in the thermochemical equilibrium calculations applied in the Chemkin subroutine has been used for explosion pressure calculations. This approach represents "ideal" deflagrations in closed systems well and gives the highest possible attainable explosion pressures. Explosion pressures are calculated using the species and their thermodynamic values from the GRI 3.0. The mechanism used for the simulation was developed by Burcat. For the calculation we used Chemical Equilibrium Calculator [8].

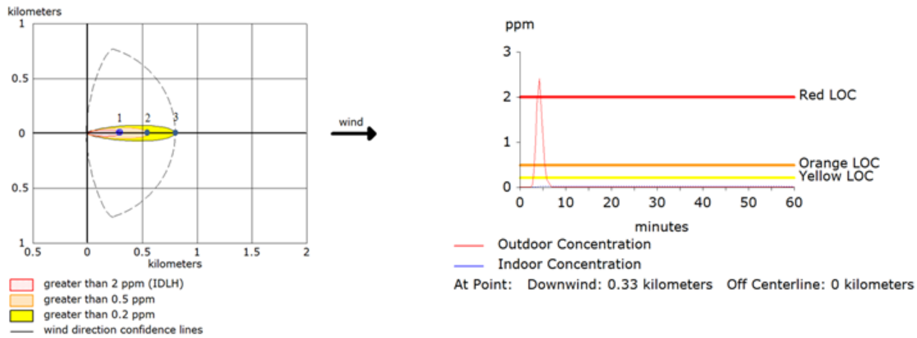
3 SW simulation

3.1 Simulation setup

Areal Locations of Hazardous Atmospheres is the hazard modelling program for the CAMEO® software suite, which is used widely to plan for and respond to chemical emergencies. Threat zones can also be shown in Google Earth using KML export feature [8]. The SW package represents well-known pre-accident modelling tools commonly employed in assessment of dangerous substances releases, dispersion, and other effects and consequences [1].

3.2 Simulation procedure

The distances of hazardous zones were taken under the worst condition from the point of view of cloud dispersion weather conditions (stability class F and 2 $m.s^{-1}$). Volume of the vessel was 1000-L. Material characteristics were taken from updated chemical library, including new DIPPR chemical data. Figure 1 illustrates the threat zone estimates on a grid in used SW. A threat zone is an area where a hazard such as ignition concentration, thermal radiation or overpressure have exceeded a user-specified Level of Concern (LOC).



a) b)

Fig. 1ab. Threat Zones for 99 % (red), 50 %(orange) and 1% (yellow) criterion.

4 Results of modelling and simulation

4.1 High-speed images

Figure 2 illustrates the turbulent spherical flame that have been produced in the concentrations close to lower explosion limit.

Fig. 2. High-speed images of hydrogen-air mixture close to lower explosion limit.

4.2 Explosion parameters

Figure 3 illustrates the explosion pressure (P_{ex}) versus hydrogen concentration (C) at initial atmospheric pressure 1 bar and temperature 25 °C. The maximum explosion pressure (P_{max}) and maximum adiabatic explosion pressure ($P_{ad,max}$) give its peak values between C = 30- 35 vol.%. The difference between P_{max} and $P_{ad,max}$ is remarkably increased at highly rich mixtures. This is due to the absence of oxygen and the heat loss through the continuum radiation to the vessel wall.

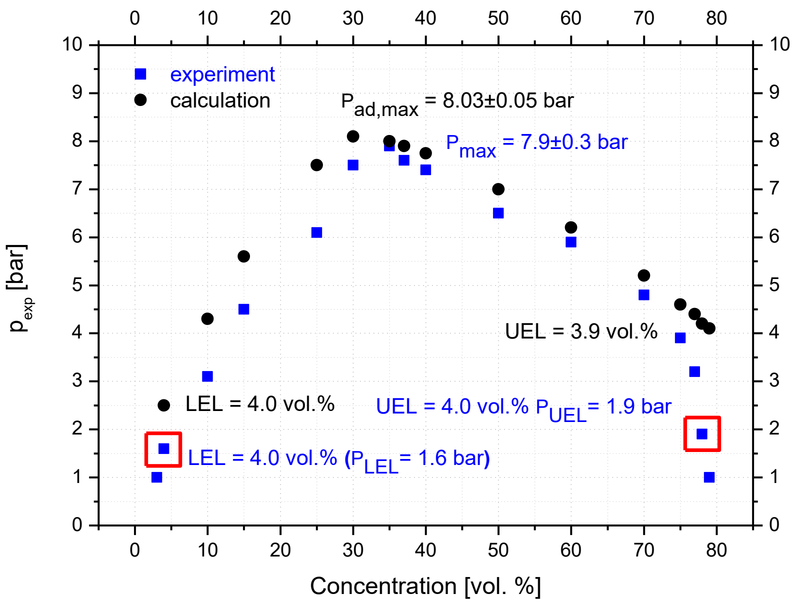


Fig. 3. Explosion pressure versus fuel fraction.

The experimentally obtained LEL = 4.0 vol.% (P_{LEL} = 1.6 bar) have been implemented as the LOC input for SW simulation. The results of SW simulation are therefore supported by real experimental measurement with the knowledge of uncertainties and setup use. This introduces general methodological advantage.

4.3 Numerical simulation

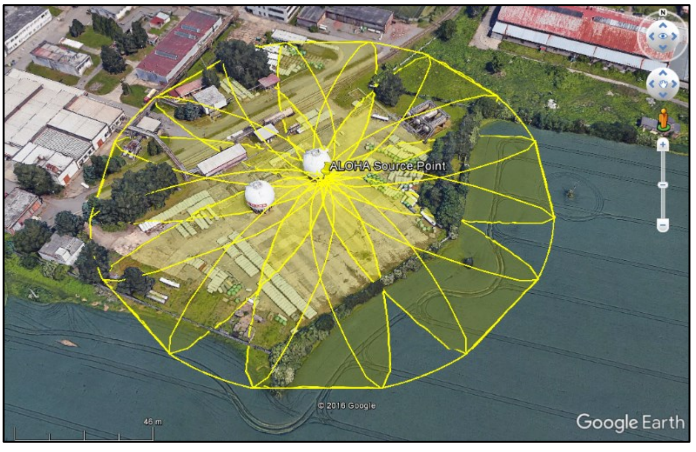


Fig. 4. Results of accident release of hydrogen implemented in Google Earth.

The results of hydrogen leak and dispersion have been implemented in Google Earth and presented in Figure 4. The yellow threat zone represents the ignitable concentration level.

5 Conclusion

In the presented article we presented the methodological synthesis of experimental physical modelling and numeric simulation for hydrogen gas release. First, the explosion limits are investigated by both the 1000-L explosion chamber and chemical equilibrium calculations. Second, the measured and calculated results are implemented as the LOC input for SW simulation of hydrogen leak from real hydrogen storage technology. Combining the SW simulation and experimental modelling for investigation of gas dispersion offers great possibilities for further CFD support and simulations development. This work started a systematic investigation of hydrogen gas behavior that combine heated 1000-L explosion apparatus available at Energy Research Centre, VŠB - Technical University of Ostrava with well-known pre-accident modelling tools.

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