

## Prediction of Overpressure Caused by Hydrogen Detonation from the Perspective of Detonation Cells

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### 1. Introduction

With the recent focus on hydrogen energy, there has been growing interest in producing hydrogen using nuclear energy. However, given the flammable nature of hydrogen, safety concerns must be addressed when siting hydrogen production facilities near nuclear power plants. In the event of a hydrogen leak at a production facility, any resulting explosion must not compromise the safety of the nuclear power plant. Following a hydrogen leak, the gas is dispersed by the wind and if its concentration falls within the flammable range and an ignition source is present, a hydrogen explosion may occur. In this paper, the density and velocity profiles of hydrogen are modeled as Gaussian distributions for performing dispersion analysis. Based on the results of the dispersion analysis, the amount of hydrogen exploding is determined, and the explosion overpressure for the corresponding amount is calculated using the Bauwens model.

### 2. Methodology

#### 2.1 Concentration distribution

In accordance with the assumption presented in [1], that the density ( $\rho$ ), velocity ( $v$ ), and mass fraction ( $Y$ ) of hydrogen in the dispersion of jet and plume follow a Gaussian distribution, we can employ Gaussian distribution to analysis the hydrogen dispersion. In Eqs (1-3),  $B$  is a characteristic half-width.  $\lambda$  is the ratio of density spreading relative to velocity. The subscript  $cl$  refers to the centerline, while  $amb$  indicates the ambient conditions.

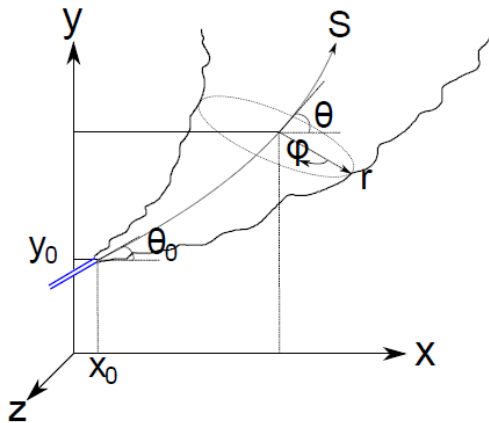


Fig. 1. Plume model coordinate [1]

$$v = v_{cl} \exp\left(-\frac{r^2}{B^2}\right) \quad (1)$$

$$\rho = (\rho_{cl} - \rho_{amb}) \exp\left(-\frac{r^2}{\lambda^2 B^2}\right) + \rho_{amb} \quad (2)$$

$$\rho Y = \rho_{cl} Y_{cl} \exp\left(-\frac{r^2}{\lambda^2 B^2}\right) \quad (3)$$

$$\frac{dx}{dS} = \cos\theta \quad (4)$$

$$\frac{dy}{dS} = \sin\theta \quad (5)$$

Eqs (6-10) represents a set of conservation equations, which include continuity, x-momentum, y-momentum, species continuity, and energy Eqs, respectively. In following Eqs,  $u$  is wind speed and  $E$  is air entrainment rate.

$$\frac{d}{dS} \int_0^\infty \rho v r dr = \frac{\rho_{amb} E}{2\pi} \quad (6)$$

$$\frac{d}{dS} \int_0^\infty \rho v^2 r \cos\theta dr = \frac{\rho_{amb} u E}{2\pi} \quad (7)$$

$$\frac{d}{dS} \int_0^\infty \rho v^2 r \sin\theta dr = \int_0^\infty (\rho_{amb} - \rho) g r dr \quad (8)$$

$$\frac{d}{dS} \int_0^\infty \rho v Y r dr = 0 \quad (9)$$

$$\frac{d}{dS} \int_0^\infty \rho v \left( h + \frac{v^2}{2} - h_{amb} \right) r dr = 0 \quad (10)$$

By substituting Eqs (1-3) into Eqs (4-10) and solving the resulting set of integral Eqs, we can determine the concentration distribution of hydrogen in the atmosphere.

#### 2.2 Hydrogen Detonation

From the perspective of overpressure on nuclear power plant structures located at a distance, a hydrogen detonation is considered the worst-case scenario for a hydrogen explosion. In accordance with the scientific literature, a hydrogen detonation can be defined as an explosion resulting from the ignition of a vapor cloud

formed by the mixing of leaked hydrogen with air. The overpressure generated by the detonation is directly proportional to the mass of hydrogen that is involved in the explosion. However, it is unclear which part of the flammable cloud should be considered due to the strong concentration gradients caused by the release.

Bauwens and Dorofeev aimed to identify and concentration gradients the critical dimensions required to sustain a propagating detonation wave [2]. The sensitivity of a combustible mixture to detonation is characterized by its detonation cell size ( $\lambda_{cell}$ ), which measures the scale of detonation instabilities. The cell size is a material property that is determined experimentally, and it determines the ability of a detonation to propagate. There are two limiting conditions for supporting detonation wave propagation with respect to detonation cells [2]. One relates to the concentration gradient, where  $d\lambda_{cell}/dx$  is less than 0.1, while the other is related to the critical dimensions, where the number of detonation cells within flammable layer ( $n_{\lambda_{cell}}$ ) is greater than 5. The hydrogen mass corresponding to these two limiting conditions is considered as the detonable mass for performing the overpressure analysis.

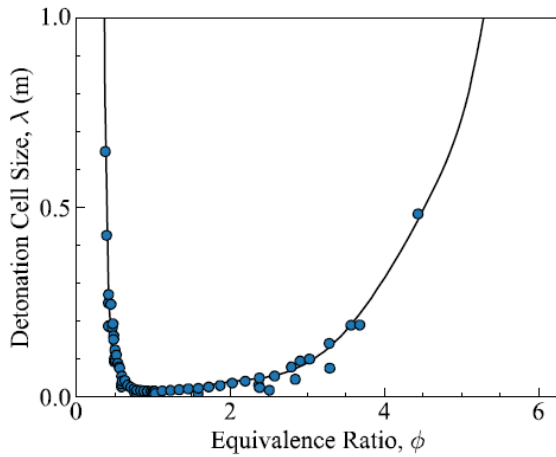


Fig. 2. Detonation cell size fits for hydrogen-air mixtures, based on data from the CALTECH Detonation Database. [3]

### 2.3 Overpressure

When evaluating overpressure as a function of distance, overpressure curves such as TNT, TNO, and BST are commonly used. Dorofeev proposed an equation for the pressure curve generated by an open-air explosion of detonable mass [4].  $P^*$  is overpressure normalized by the ambient pressure and  $R^*$  is dimensionless distance.  $R$  is dimensional distance from the center of the detonable region and  $E$  is the total energy released by the mass of hydrogen contained within the detonable region.

$$P^* = \frac{0.34}{(R^*)^{4/3}} + \frac{0.062}{(R^*)^2} + \frac{0.0033}{(R^*)^3} \quad (11)$$

$$R^* = R \left( \frac{P_{amb}}{E} \right)^{1/3} \quad (12)$$

## 3. Analysis

### 3.1 Analysis assumptions

In this paper, the methodology described above was applied to estimate the concentration distribution and explosion overpressure pressure of leaked hydrogen. We assumed a continuous release of hydrogen stored at 7 MPa and 20°C and analyzed three different cases with leak hole sizes of 50mm, 100mm, and 150mm. The wind speed is assumed to be 1.5m/s.

### 3.2 Concentration distribution

The detonable mass was calculated to be 0.29kg, 3kg, and 11.2kg for leak sizes of 50mm, 100mm, and 150mm, respectively.

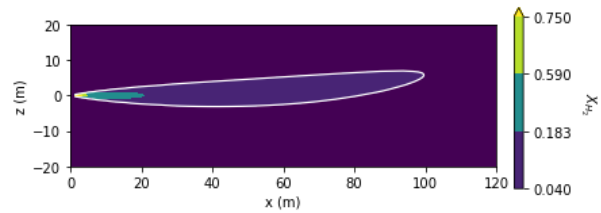


Fig. 3. The molar fraction distribution of hydrogen as a function of distance with leak size of 50mm

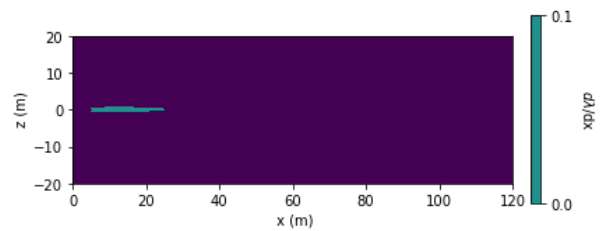


Fig. 4. The gradient of detonation cell size as a function of distance with leak size of 50mm

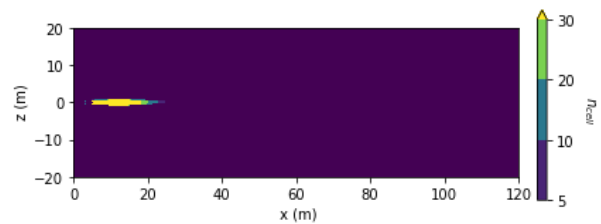


Fig. 5. The number of detonation cell as a function of distance with leak size of 50mm

The detonable mass was calculated to be 0.29kg, 3kg, and 11.2 kg for leak sizes of 50mm, 100mm, and 150mm, respectively (Fig. 6). The explosion of the calculated detonable mass of hydrogen results in overpressure as a function of distance, as shown in Fig. 7.

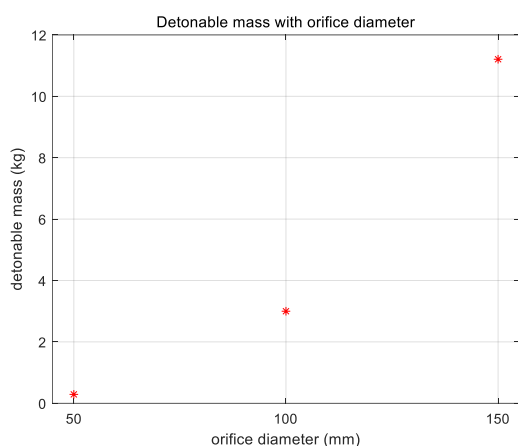


Fig. 6. The detonable mass with leak size of 50mm, 100mm and 150mm

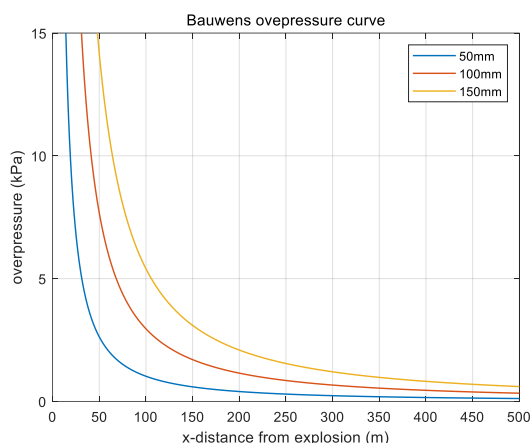


Fig. 7. The overpressure with leak size of 50mm, 100mm and 150mm as a function of distance

### 3. Conclusions

An assessment of the impact of hydrogen explosion on a nuclear power plant should be performed to produce hydrogen for nuclear applications. To predict the overpressure caused by hydrogen explosions, it is important to determine the mass of hydrogen participating in the detonation. For hydrogen jets discharged from high-pressure vessels, not all of the leaked hydrogen explodes due to the strong concentration gradient. Therefore, the concentration distribution in the atmosphere according to the hydrogen leak conditions is predicted, and the detonable mass is determined. In this paper, density and velocity of hydrogen were assumed to follow a Gaussian profile, and

the detonable mass was predicted from the perspective of detonation cells. The detonation cell is a factor that determines the ability of the shock wave to propagate, and there are limitations on the size gradient and the number of the detonation cells. In this paper, hydrogen concentration distribution and overpressure analysis were performed for different leak sizes. We expect that by determining the detonable mass based on the concentration distribution of hydrogen, we can prevent overpressure from being overestimated.

### REFERENCES

List and number all bibliographical references in 9-point Times, single-spaced, at the end of your paper. When referenced in the text, enclose the citation number in square brackets, for example [1]. It is recommended that the number of references does not exceed five.

- [1] B. D. Ehrhart and E. S. Hecht, "Hydrogen Plus Other Alternative Fuels Risk Assessment Models (HyRAM+) Version 4.1 Technical Reference Manual," Tech. Rep. SAND2022-5649, Sandia National Laboratories, April 2022.
- [2] C. R. L. Bauwens and S. B. Dorofeev, "Quantifying the potential consequences of a detonation in a hydrogen jet release," in Proceedings of the International Conference on Hydrogen Safety (ICHS 2019), (Adelaide (Australia)), pp. 612–623, September 24 – 26 2019.
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