

Impact of Hydrogen Storage Tanks and Environmental Conditions on the Safety of Nuclear Hydrogen Production Systems

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Abstract

Nuclear hydrogen production is of great significance for China to achieve its national strategic goals of carbon peak and carbon neutrality. Hydrogen production via thermochemical water splitting coupled with ultra-high temperature gas-cooled reactors represents a highly promising method for large-scale green hydrogen production. In research on nuclear hydrogen production systems, hydrogen leakage and diffusion behavior represents a critical safety concern, while the separation distance between nuclear hydrogen production plants and nuclear power stations serves as a key metric for system safety assessment. This study centers on the separation distance between nuclear power plants and hydrogen production facilities, investigating the influence of storage tank intrinsic conditions and environmental parameters on hydrogen leakage and diffusion, primarily including tank pressure, tank volume, and ambient temperature. Additionally, the peak overpressure impact from hydrogen explosions is evaluated using the TNO multi-energy method, and the minimum separation distance required to prevent safety accidents is predicted. The results demonstrate a linear relationship between diffusion distance and tank pressure, ambient temperature shows negligible influence on diffusion distance and hydrogen concentration at various positions, while larger tank volume extends the total duration of leakage and diffusion. Under the most severe operating condition examined in this study, the conservatively estimated separation distance is 253 m. This research can provide valuable references for safety risk assessment and plant site layout design of nuclear hydrogen production systems.

Full Text

The Influence of Hydrogen Storage Tank and Environmental Conditions on the Safety of Nuclear Hydrogen Production Systems

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Abstract

Nuclear hydrogen production plays a crucial role in achieving China's strategic goals of carbon peaking and carbon neutrality. Coupling a high-temperature gas-cooled reactor (HTGR) with thermochemical water splitting represents a highly promising approach for large-scale green hydrogen production. In the development of nuclear hydrogen production systems, hydrogen leakage and diffusion behavior are critical safety concerns, and the separation distance between nuclear hydrogen production plants and nuclear power stations serves as a key indicator of system safety. This study investigates the effects of hydrogen storage tank parameters and environmental conditions on hydrogen leakage and diffusion, focusing primarily on tank internal pressure, tank volume, and ambient temperature. The TNO multi-energy method was employed to evaluate peak overpressure impacts from hydrogen explosions and predict the minimum separation distance required to prevent safety accidents. Results demonstrate a linear relationship between diffusion distance and tank internal pressure, while ambient temperature shows negligible influence on diffusion distance and hydrogen concentration at various locations. Larger tank volumes significantly extend the total leakage and diffusion time. Under the most severe conditions studied, the conservatively estimated separation distance is 253 m. These findings provide valuable references for safety risk assessment and plant layout design of nuclear hydrogen production systems.

Keywords: nuclear hydrogen production; leakage and diffusion; numerical simulation; separation distance

1. Methodology

1.1 Geometric Model

The geometric model of the nuclear hydrogen production system and storage tank within a large spatial domain is illustrated in [Figure 1: see original paper].

A computational flow field domain of $1000 \text{ m} \times 1000 \text{ m} \times 200 \text{ m}$ was established to enable wind field calculations, with the storage tank positioned such that its distances to two domain boundaries are both 200 m . The tank interior maintains high pressure to preserve hydrogen in its stored state. Based on our previous research [17], diffusion distance is maximized when wind direction aligns with the leakage direction. Therefore, this study maintains downwind conditions to investigate safety risks to the nuclear power station located downwind.

1.2 Mathematical Model

When hydrogen storage tanks leak, the high internal pressure causes hydrogen to discharge into the atmosphere at high velocity initially, followed by gradual diffusion and dilution under ambient wind. This process involves flow, heat transfer, and mass exchange between hydrogen and air, which can be described by continuity, momentum, energy, and species transport equations:

Continuity Equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0$$

Momentum Equation:

$$\frac{\partial(\rho \mathbf{U})}{\partial t} + \nabla \cdot (\rho \mathbf{U} \mathbf{U}) = -\nabla P + \nabla \cdot \tau + \rho \mathbf{g}$$

Energy Equation:

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho \mathbf{U} h) = \nabla \cdot (\lambda \nabla T) + S_h$$

where ρ (kg/m^3) represents density, t (s) time, P (Pa) pressure, \mathbf{U} (m/s) velocity, μ ($\text{kg}/(\text{m} \cdot \text{s})$) dynamic viscosity, \mathbf{g} (m/s^2) gravitational acceleration, h (m^2/s^2) fluid enthalpy, T (K) fluid temperature, and λ ($\text{W}/(\text{m} \cdot \text{K})$) thermal conductivity.

The leakage diffusion model involves two species: air and hydrogen. Their distribution in the large space is calculated using a species transport model:

$$\frac{\partial(\rho \phi)}{\partial t} + \nabla \cdot (\rho \mathbf{U} \phi) = \nabla \cdot (\Gamma \nabla \phi)$$

where Γ ($\text{kg}/(\text{m} \cdot \text{s})$) represents diffusivity and ϕ denotes species volume fraction. During hydrogen-air mixing, mixture properties (density, viscosity, specific heat) are calculated using volume-fraction-weighted averaging, which subsequently affects all governing equations.

Turbulence model selection significantly impacts leakage calculations, particularly for the high-speed jet during initial leakage. Among conventional CFD

turbulence models, k - ε and k - ω satisfy most turbulence computation requirements. Yu et al. [18] demonstrated that the SST k - ω model further improves accuracy for high-speed leakage calculations, including high-pressure scenarios. Consequently, this study employs the SST k - ω model [19]:

Turbulent Kinetic Energy (k) Equation:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho k U_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left[(\mu + \sigma_k \mu_t) \frac{\partial k}{\partial x_j} \right] + P_k - \beta^* \rho \omega k$$

Specific Dissipation Rate (ω) Equation:

$$\frac{\partial(\rho \omega)}{\partial t} + \frac{\partial(\rho \omega U_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left[(\mu + \sigma_\omega \mu_t) \frac{\partial \omega}{\partial x_j} \right] + \alpha \rho S^2 - \beta \rho \omega^2$$

where P_k represents the production of turbulent kinetic energy, Ω (s^{-1}) vorticity magnitude, F_1 and F_2 are blending functions, and σ_k and σ_ω are turbulent Prandtl numbers. Model constants are: $\sigma_{k1} = 0.85$, $\sigma_{k2} = 1$, $\sigma_{\omega1} = 0.5$, $\sigma_{\omega2} = 0.856$, $\alpha = 0.09$, $\alpha_1 = 0.31$, $\beta_1 = 0.075$, $\beta_2 = 0.0828$.

1.3 Boundary Conditions and Mesh Generation

The numerical simulations were conducted using the CFD software in:Flux, which employs a finite volume method (FVM) solver with the SIMPLE algorithm for pressure-velocity coupling. The global domain was discretized using structured grids of varying sizes. Due to the large computational domain and limited resources, coarser grids were used in horizontal and vertical regions far from the leakage source, while grid refinement was applied near the leakage opening to ensure accuracy, as shown in [Figure 2: see original paper]. Grid independence studies monitoring hydrogen concentration along the leakage horizontal line demonstrated that approximately 150,000 cells provide sufficient accuracy.

Boundary Conditions: - Ambient wind: velocity inlet boundary - Hydrogen leakage opening: mass flow inlet boundary - Hydrogen discharge from the storage tank constitutes an under-expanded high-pressure jet, forming complex flow structures near the release point. Based on previous analysis [20], the CFD software simplifies near-field calculations using isentropic flow conditions. Parameters at the Mach disk downstream of the release point are calculated based on tank orifice diameter and fluid properties, serving as boundary conditions to improve computational efficiency. - Domain side boundaries (Surfaces 1-4): zero pressure gradient to allow free outflow - Bottom surface (Surface 5): no-slip wall to restrict vertical flow

This study maintains constant wind speed, leakage height, and orifice diameter while investigating pressure, temperature, and volume effects. Calculation conditions are summarized in .

TABLE:1 Calculation Conditions | Parameter | Values | |———|———| | Tank Pressure (MPa) | 5, 7, 9, 11, 13 | | Wind Velocity (m/s) | 5 | | Ambient Temperature (°C) | -25, -15, -5, 5, 15, 25 | | Hydrogen Temperature inside Tank (°C) | -25, -15, -5, 5, 15, 25 | | Leakage Height (m) | 5 | | Tank Volume (m³) | 31.42, 49.09, 70.69, 96.21, 125.66 | | Leakage Diameter (mm) | 50 | | Leakage Direction | Horizontal leakage along the ground |

2. Analysis of Tank and Environmental Factors

For hydrogen leakage and diffusion, both storage tank conditions and environmental parameters influence gas dispersion. This study analyzes specific factors including tank internal pressure, tank volume, and ambient temperature to determine their effects on critical accident assessment parameters such as diffusion distance and duration. Since hydrogen's flammability limits are approximately 4-75% by volume, hydrogen clouds with volume fractions exceeding 4% are considered combustible, with the farthest distance where hydrogen concentration drops to 4% defined as the diffusion distance.

2.1 Effect of Tank Internal Pressure

[Figure 3: see original paper] illustrates the influence of tank internal pressure on diffusion distance. Under conditions of 1.5 m tank radius, 10 m tank height, and 25°C ambient temperature, higher internal pressure results in greater hydrogen exit velocity and longer velocity decay time. The results show a linear increase in combustible hydrogen cloud diffusion distance with pressure, reaching approximately 160 m at 13 MPa. Han et al. [21] conducted experiments on high-pressure hydrogen leakage through small orifices at 10-40 MPa, reporting similar linear trends in diffusion distance.

Increased initial leakage velocity releases more hydrogen mass into the large space within the same timeframe, compromising safety. However, higher velocity also entrains more ambient air to dilute hydrogen concentration, which enhances safety. Concentration variations along a horizontal line parallel to the ground through the leakage origin are shown in [Figure 4: see original paper]. At equivalent distances from the leakage source, higher-pressure leaks consistently exhibit higher hydrogen concentrations, indicating that the negative effect of hydrogen mass accumulation outweighs the positive effect of concentration dilution. High-pressure leaks not only increase diffusion distance but also maintain relatively higher concentrations, representing greater safety risks. Comparing 13 MPa and 5 MPa conditions along the leakage horizontal line, the concentration difference initially increases then decreases, with a maximum difference exceeding 20% occurring near the leakage source. This indicates that initial concentration is most significantly affected, with the gap narrowing as ambient wind dilutes the plume.

2.2 Effect of Ambient Temperature

Ambient temperature affects gas cloud density differences and atmospheric turbulence [22], thereby influencing diffusion concentration and distance. Analysis was conducted at 5 MPa pressure, 1.5 m tank radius, and 10 m tank height. presents diffusion distances for combustible hydrogen clouds at various temperatures after reaching steady state. Results show slight increases in diffusion distance with rising temperature, but the effect is minimal. Wang [23] investigated large-scale liquid hydrogen leakage, while Liu et al. [24] studied short-duration high-pressure hydrogen leakage, both concluding that ambient temperature has limited impact on hydrogen diffusion. In current calculations, the slight distance increase with temperature may result from hydrogen volume expansion at higher temperatures. [Figure 5: see original paper] shows the combustible hydrogen cloud contour at 25°C, with horizontal diffusion distance of approximately 98 m and vertical diffusion distance of about 16 m.

TABLE:2 Diffusion Distance Under Different Ambient Temperatures | Ambient Temperature (°C) | Diffusion Distance (m) | ————— | —————
 ——— | -25 | 95 | | -15 | 96 | | -5 | 96 | | 5 | 97 | | 15 | 97 | | 25 | 98 |

Parameter variations at different ambient temperatures were calculated to analyze specific effects. Figure 6: see original paper shows temperature effects on hydrogen flow velocity, which drops sharply within 0-5 m from the leakage source before stabilizing and eventually matching ambient wind speed. Ambient temperature significantly affects velocity near the leakage source, with diminishing influence farther downstream. Figure 6: see original paper displays hydrogen temperature variation along the leakage horizontal line, showing rapid temperature decrease upon exiting the tank, followed by gradual warming through mixing with ambient air until approaching environmental temperature. Temperature increases rapidly within 30 m of the source, then rises slowly thereafter. Figure 6: see original paper demonstrates minimal temperature effect on horizontal line concentration, confirming that ambient temperature has negligible impact on combustible hydrogen cloud diffusion distance and concentration distribution.

2.3 Effect of Tank Volume

Tank volume was varied by changing radius while maintaining 10 m height. Radii of 1 m, 1.25 m, 1.5 m, 1.75 m, and 2 m correspond to volumes of 31.42 m³, 49.09 m³, 70.69 m³, 96.21 m³, and 125.66 m³, respectively. Transient calculations were performed to investigate volume effects. Since tank pressure decreases over time, a time-stepping algorithm was implemented to describe parameter variations near the leakage source [25]:

$$\frac{d\rho}{dt} = -\frac{q}{V}$$

$$\frac{dP}{dt} = -C_v \frac{d\rho}{dt}$$

where V (m^3) is tank volume, q (kg/s) mass flow rate, and C_v ($\text{J}/(\text{kg} \cdot \text{K})$) specific heat at constant volume.

[Figure 7: see original paper] shows tank parameter variations during leakage. Figures 7(a) and 7(b) indicate that tank volume does not affect initial leakage pressure or mass flow rate. Over time, tank pressure equilibrates with atmospheric pressure, eventually ceasing outflow. However, larger tank volumes require significantly longer leakage durations, increasing safety risks. Figure 7: see original paper demonstrates that tank volume directly determines initial hydrogen mass, necessitating longer leakage times. The time difference between minimum and maximum volumes exceeds 250 s, indicating greater safety risks for large-volume tanks.

[Figure 8: see original paper] illustrates combustible hydrogen cloud dilution in the atmosphere. Within 20 s of leakage initiation, combustible hydrogen cloud volume and mass increase rapidly. Under various tank volume conditions, maximum cloud volumes range from 3400-3800 m^3 with masses of 18-21 kg, peaking at 11-15 s. Maximum cloud volumes and masses are similar across conditions, differing primarily in dissipation time. Larger initial hydrogen mass in big tanks provides sustained mass supply to the combustible cloud despite similar transient maxima, resulting in longer dissipation times. Statistical analysis shows maximum diffusion distances of 95-98 m across volume conditions, reached at 17-19 s.

3. Worst-Case Scenario Analysis

Based on the above factor analyses, the worst-case scenario was defined by combining the most severe conditions: 13 MPa tank pressure, 5 m/s wind speed, 25°C ambient temperature, 5 m leakage height, 125.66 m^3 tank volume, 50 mm leakage diameter, and horizontal ground-level release.

[Figure 9: see original paper] shows hydrogen concentration distribution below 4% under worst-case conditions. High initial hydrogen momentum dominates over buoyancy effects, with upward floating trends emerging as velocity decreases. The red region represents concentrations exceeding 4% (combustible), with horizontal diffusion distance of approximately 162 m. While vertical diffusion also affects safety, this study focuses on downwind nuclear power stations, where vertical diffusion distance of about 28 m poses relatively minor risk compared to horizontal dispersion.

Safety assessment of nuclear hydrogen production systems primarily concerns separation distance between chemical plants and nuclear power stations, determined by hydrogen diffusion distance and deflagration distance. The sum of these distances constitutes the required separation. In practice, plant construction distances should exceed this conservative separation distance to ensure

safety during leakage accidents. Structural peak overpressure limits represent critical safety indicators; Japan's standard of 10 kPa as the threshold for no public damage [25] was adopted for this estimation.

Various methods exist for estimating explosion peak overpressure. This study employed the TNO multi-energy method [26] for deflagration distance calculation, which requires actual hydrogen volume, explosion severity, combustion energy, and other parameters to compute dimensionless and actual distances. Under worst-case conditions at stable diffusion, combustible hydrogen cloud volume is approximately 815 m^3 , with combustion energy of 3.5 MJ/m^3 . Without obstacle blockage, explosions resemble strong deflagration (Severity Level 7) [27].

The calculated separation distance is approximately 253 m, with deflagration distance accounting for 36% of the total. This indicates that ignition risk during hydrogen diffusion cannot be neglected, requiring mitigation measures during both diffusion and deflagration phases.

FIGURE:10 Separation distance under worst-case conditions

4. Conclusions

This study investigated the influence of hydrogen storage tank conditions and environmental parameters on leakage accident safety in nuclear hydrogen production systems. Key conclusions are:

1. **Tank internal pressure significantly affects hydrogen diffusion distance**, exhibiting a linear increase with pressure. Higher-pressure leaks also produce higher hydrogen concentrations at equivalent locations, further increasing safety risks. Comparison of high and low-pressure scenarios reveals larger concentration gaps during initial leakage stages that gradually narrow over time.
2. **Ambient temperature variation shows negligible effects** on combustible hydrogen cloud diffusion distance and concentration distribution. While temperature substantially affects velocity near the leakage source, with higher temperatures increasing exit velocity, this effect diminishes within 5 m. Hydrogen temperature rises rapidly within 30 m of the source, then approaches ambient temperature.
3. **Tank volume differences determine initial hydrogen mass**, affecting total diffusion time. Across volume conditions, maximum diffusion distances range 95-98 m, with maximum combustible cloud volumes of $3400\text{-}3800 \text{ m}^3$ and masses of 18-21 kg. Larger tanks contain more hydrogen mass, requiring longer dilution times.
4. **Combined worst-case scenario analysis** yields a hydrogen diffusion distance of approximately 162 m. If ignited at stable diffusion, the deflagration distance is about 91 m under the no-public-damage overpressure

criterion, resulting in a conservative separation distance of 253 m. These findings provide valuable references for safety evaluation of nuclear hydrogen production systems.

Author Contributions

GAO Qunxiang: Conceptualization, numerical simulation, results analysis, original draft writing

ZHANG Zixuan: Data validation, figure preparation, manuscript revision

LIN Xiangdong: Model optimization

PENG Wei: Supervision, manuscript revision and finalization

ZHANG Ping: Computational model guidance, resource provision

ZHAO Gang: Computational model validation

ZHANG Han: Data processing

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