The simulate of the stratification of an explosive mixture of hydrogen and air in the RBMK-1000 spent-fuel storage pool

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Abstract. Currently, in Russia, codes with concentrated parameters are used as software tools to justify the hydrogen explosion safety of nuclear power units, which use the concept of "average concentration of hydrogen" in the calculated volume and do not take into account the stratification of hydrogen, due to which local concentrations of hydrogen can significantly exceed the "average". This paper presents the hydrogen explosion safety analysis results during a beyond-design accident in the RBMK-1000 spent-fuel storage pool taking into account local concentrations of gas components using the gas dynamic code ANSYS FLUENT. The vapor-gas mixture propagation problem in the spent-fuel storage pool was solved in a two-dimensional approximation. The following sources of hydrogen were considered radiolysis hydrogen generation, hydrogen generation by reducing its solubility in water and the vapor-zirconium reaction. As a result of modeling, the possible accumulation areas of an explosive mixture and their sizes were determined. It is shown that under certain combinations of boundary conditions, due to the presence of convective flows, an explosive concentration is not achieved even if the mixture components stratification is taken into account.

1. Introduction
Interest in hydrogen explosion safety arose after the accident at the Fukushima Daiichi NPP on March 11, 2011. For almost ten years, the main tasks have been formulated, the solution of which is aimed at increasing hydrogen safety.

The modern understanding of the justification of hydrogen explosion safety of NPP power units includes the exclusion of the possibility of detonation of a hydrogen-containing mixture under any operating conditions of the power unit, including design, beyond design basis and even severe stages of accidents [1, 2].

The main way to solve this problem is to demonstrate that a possible mixture of gases (hydrogen, air and steam) is outside the concentration limits of flammability and detonation: $C_{H2}^{\text{LCL}} < \text{LCL}$ or $C_{H2}^{\text{UCL}} > \text{UCL}$ (LCL - lower concentration limit, UCL - upper concentration limit of explosiveness of hydrogen, $C_{H2}$ - volume fraction of hydrogen).

The Shapiro-Maffetti diagram (figure 1) is widely used to determine the explosive limits for uniformly mixed gases.
Figure 1. Shapiro-Moffette flammability diagram for hydrogen-air-steam mixtures at 1 bar and 25° (Shapiro et al., 1957) Models of Combustion.

The main conclusion that can be drawn from the diagram (Figure 1) is as follows: for uniformly mixed gases (steam-hydrogen-air mixture) at atmospheric pressure and a temperature of 25 °C, a mixture containing less than 8% hydrogen by volume and more than 70% steam can be considered safe. At the same time, the Shapiro-Moffetti diagram does not reflect the possible change in concentration limits from temperature and pressure, typical for a LOCA-type accident at a reactor facility [3-9]. However, during the development of an emergency process at an open pool type spent fuel storage facility, the environmental parameters change slightly, which makes it possible to use the Shapiro-Moffetti diagram in the form in which it is shown in Figure 1.

Another feature of the substantiation of hydrogen explosion safety is the high buoyancy of hydrogen, which with a large free space of the internal premises of the nuclear power plant with a high probability can lead to a significant local or global stratification of the steam-hydrogen-air gas mixture [10].

The existing approach to modeling the propagation of a steam-hydrogen-air gas mixture is based on codes with lumped parameters, which cannot fully answer the questions posed. Therefore, the only possible way to determine the possible stratification of gas mixture components is to use gas dynamic codes (CFD - Computational Fluid Dynamics). However, even when obtaining information about the three-dimensional distribution of gas components in space, it is difficult to quantitatively assess the hazard of stratified mixtures, in which the characteristic hydrogen concentration of one part of the mixture is outside the concentration limits, and the other is within these limits.

This article presents the results of numerical modeling of the distribution of the components of the steam-hydrogen-air gas mixture in the space under the slatted slab of the RBMK-1000 reactor spent fuel pool in the course of a beyond design basis accident with a complete power unit blackout. The calculation was carried out using a CFD code for modeling ANSYS FLUENT flows of liquids and gases.

2. Setting up the calculation tool
To demonstrate the possibility of the ANSYS FLUENT computational code, the experimental data from [11] were calculated. Was taken one of the experiments presented in the work (experiment No. 5).
The experimental tank was a sealed vessel of the "barrel" type with a volume of 4 m³ and a diameter of 1.28 m, into which hydrogen was released in a wide range of gas flows (from $0.005 \times 10^{-3}$ to $0.53 \times 10^{-3}$ m³/s) controlled by automatic gas dispensers. The gas mixture preparation device allows you to set and control a constant gas flow rate from $5 \times 10^{-6}$ to $7 \times 10^{-4}$ m³/s.

![Diagram of the spatial distribution of hydrogen concentration and temperature sensors in an experimental barrel-type tank.](image)

**Figure 2.** Diagram of the spatial distribution of hydrogen concentration and temperature sensors in an experimental barrel-type tank.

The "barrel" was placed inside a concrete dome. In the experiments, hydrogen was released into the chamber through a round hole of constant diameter $D_0 = 14$ mm located in the lower part of the cylindrical volume. Figure 1 shows the layout of the sensors: a matrix of 24 sensors with hydrogen and temperature sensors was installed in a “barrel” on seven vertical rods, which made it possible to fix the position of each sensor in the plane of the vertical axial section of the cylinder.

Hydrogen was injected into the chamber for 300 s at a speed of 1.88 m/s.

To simulate the experimental chamber, a three-dimensional mesh was created, consisting of ~ $9 \times 10^5$ nodes.

The coefficient of mass diffusion was used as the selected parameter. Figure 3 shows the picture of the distribution of the molar concentration of hydrogen in the chamber at the value of the coefficient taken "by default" ($2.88 \times 10^{-5}$ m²/s).

![Picture of the distribution of molar concentration of hydrogen.](image)

**Figure 3.** Distribution of the molar concentration of hydrogen in the chamber at the default value of the mass diffusion coefficient ($2.88 \times 10^{-5}$ m²/s).
Additionally, a series of calculations was carried out with different values of the mass diffusion coefficient. Figure 4 shows graphs of the vertical distribution of the molar concentration of hydrogen in the experimental chamber at different values of the mass diffusion coefficient. For comparison, the graph also shows the experimentally measured vertical distribution of the hydrogen concentration.

![Mass Diffusivity Dependence](image)

**Figure 4.** Dependence of the vertical distribution of the molar concentration of hydrogen in the experimental chamber on the mass diffusion coefficient

Figure 4 shows that when the mass diffusion coefficient is $2.88 \times 10^{-4}$ m$^2$/s, the altitude distribution of the molar concentration of hydrogen is closest to the experimental dependence. Thus, it was concluded that it is possible to use the ANSYS FLUENT computational code to analyze the stratification of the components of the steam-hydrogen-air gas mixture.

Analysis in 2-D and 3-D approximation gave identical results.

3. **Description of the research object**

The standard spent fuel storage system at NPPs with RBMK-1000 reactors provides storage of case with spent fuel assemblies and spent fuel assemblies without case in two near-reactor storage pools. Within the central hall of the power unit, there are two spent fuel pool with the following dimensions: length - 10.3 m; width - 4.2 m; depth - 17.2 m. To provide biological protection, the pools are filled with water.

The slotted floor of the spent fuel pool is made of cantilever beams fixed in the wall of the pool and reinforced with braces made of stainless pipes. The cantilever beams form two rows of slots along the spent fuel pool with a step of 250 mm, separated by a central slot. The length of the beams is 2 m. The slotted ceiling is closed by hinged stainless steel covers. Removable and hinged covers partially prevent the escape of water vapors and "dirty" gases into the central compartment, and also protect the stored SNF from flying objects. During normal operation of the power unit, water vapor leaving the pool surface, radioactive gases from under the cladding of leaky fuel elements, radiolytic hydrogen are discharged into the air purification and ventilation system of the central hall. In the event of an accident with a complete de-energization of the power unit, the blowing off of gases from under the
slotted ceiling stops, and they begin to fill the free space. An additional source of hydrogen in this case is its release from the water due to a decrease in gas solubility when the water in the pool is heated.

At the first stage of the accident with water heating in the storage pool, the sources of gases are:

- hydrogen:
  - radiolytic: \(0.47 \cdot 10^{-5}\) kg/s;
  - due to a decrease in solubility: \(0.3 \cdot 10^{-5}\) kg/s;
- steam due to evaporation \(1.85 \cdot 10^{-3}\) kg/s;
- the air of the central hall of the power unit.

These numerical values were obtained by an expert method and are consistent with the substantiating materials of the RBMK-1000 SNF near-reactor spent fuel pools.

4. Description of the design model
The simulation was carried out using the ANSYS FLUENT design code in a 2-dimensional approximation. All calculations were carried out using a "pressure-based" solver, in a stationary mode, taking into account gravity. Models with a three-component mixture of the working fluid were used. Molecular hydrogen, air and water steam were taken as components from the internal libraries of the software product.

The modeled area can be conditionally divided into two sub-areas. The first subarea simulates the space in the storage pool between the water surface and the slit and has dimensions \(4.2 \cdot 0.75\) m. The second sub-area simulates a part of the central hall of the power unit, adjacent directly to the slot floor and serving as a source of reverse gas flow under the slot floor. The second subregion has dimensions of \(5.2 \cdot 0.75\) m.

Both subregions are interconnected by 5 slots. The largest slot is 0.2 m wide, located in the middle of the pool and simulates a technological slot. The remaining four slots simulate the gaps between the slabs, have a width of 0.01 m and are located two at the edges of the pool, and two in the middle between the technological slot and the edges of the pool. The slots are 0.005 m high.

A structured computational grid with an adaptive step, consisting of \(\sim 8 \cdot 10^4\) nodes, was used. The design scheme is shown in Figure 5.
5. Results
The calculation results are shown in figure 6 and table 1.

![Figure 6. Volume fraction of hydrogen (hydrogen source \( \sim 1.0 \times 10^{-5} \text{ kg/s} \).](image)

**Table 1. Volume fraction of gas components of the mixture (hydrogen source \( \sim 1.0 \times 10^{-5} \text{ kg/s} \)).**

|        | Average | Min | Max |
|--------|---------|-----|-----|
| Hydrogen | 2.42    | \(~1.5\) | 4.27 |
| Water steam | 54.0    | \(~6.0\) | 95.1 |
| Air    | 43.6    | 0   | \(~60.0\) |

The results show that the explosive concentration in the gas mixture is not achieved in any of the design cells (\(C_{\text{H}_2}>8\%\) and \(C_{\text{H}_2\text{O}}<70\%\)). For a quantitative assessment of the hazard of stratified mixtures, it is convenient to use the diagram shown in figure 7, which shows what fraction of the computational domain is occupied by one or another fraction of the volumetric concentration of gases.

![Figure 7. The distribution of the volume fraction of hydrogen (hydrogen source \( \sim 1.0 \times 10^{-5} \text{ kg/s} \)).](image)
For example, it can be seen from figure 7 that more than \( \frac{3}{4} \) of the entire volume of the computational domain is occupied by a gas mixture with a volume concentration of hydrogen of about 2.5\%, which is significantly lower than the concentration limit of explosiveness of a vapor-hydrogen-air gas mixture.

To assess the uncertainty of the initial data, an additional calculation was carried out with a tenfold increase in the hydrogen consumption (~1.0·10^{-4} kg/s). The results are shown in figures 8, 9 and table 2.

**Figure 8.** Volume fraction of hydrogen (hydrogen source ~1.0·10^{-4} kg/s).

**Figure 9.** Hydrogen volume fraction distribution (hydrogen source ~1.0·10^{-4} kg/s).

**Table 2.** Volume fraction of gas components of the mixture (hydrogen source ~1.0·10^{-4} kg/s).

| Component        | Average | Min  | Max  |
|------------------|---------|------|------|
| Hydrogen         | 4.68    | ~2.0 | ~9.5 |
| Water steam      | 11.1    | ~5.0 | ~20  |
| Air              | 84.2    | 0    | ~95  |
In this case, a significant proportion (~4%) of the calculated space under the slotted ceiling is occupied by a mixture of gases in an explosive ratio.

6. Conclusions
The results presented in this paper show that the use of CFD codes, like ANSYS FLUENT, makes it possible to analyze the propagation of gas mixture components in a closed space, taking into account their possible stratification.

The analysis of the first stage of an accident with a power unit blackout at the near-reactor cooling pool showed that the formation of an explosive concentration with the expected gas flow rate is not expected. With an increase in hydrogen consumption by 10 times, compared with the expected, an explosive gas mixture is formed in ~4% of the volume of the space under the slot floor.

References
[1] NP-001-15. General provisions for ensuring the safety of nuclear power plants 2015 (Moscow: Federal Nuclear and Radiation Safety Supervision Authority of Russia)
[2] NP-040-02. Rules for hydrogen explosion protection assurance at nuclear power plants 2002 (Moscow: Federal Nuclear and Radiation Safety Supervision Authority of Russia)
[3] Basevich VY et al. 2019 Three-Dimensional Direct Numerical Simulation of Turbulent Combustion of Hydrogen-Air Mixtures in a Synthetic Turbulent Field, Phys. Chem. №13 636-645
[4] Agrawal N, Prabhakar A and Das S K 2015 Hydrogen distribution in nuclear reactor containment during accidents and associated heat and mass transfer issues: a review Heat Transf. Engin. №36 10
[5] Hoyes J R and Ivings M. J. 2016 CFD modeling of hydrogen stratification in enclosures: Model validation and application to PAR performance Nucl. Engin. and Design №310 142-153
[6] Reinecke E A et al. 2010 Open issues in the applicability of recombiner experiments and modeling to reactor simulations Progr. in Nucl. Energy №52 136–147
[7] Della Loggia E 1992 Hydrogen behavior and mitigation in water-cooled nuclear power reactors. ISBN 92-8263364-0 114
[8] Gupta S et al. 2015 THAI test facility for experimental research on hydrogen and fission product behavior in light water reactor containments Nucl. Engin. and Design №294 183-201
[9] Buben N Ya 1946 Collection of works on physical chemistry J. of phys. chem. Additional volume 148, 154
[10] Kirillov I A, Kharitonova N L, Sharafutdinov R B and Khrennikov N N 2017 Ensuring hydrogen safety at nuclear power plants with water-cooled reactors current state of the problem J. Nucl. and rad. safety №2 84
[11] Denisenko V P, Kirillov I A, Korotbsey S V and Nikolaev I I 2013 Hydrogen Distribution in Enclosures - On Distiction Criterion Between Quasi-Homogeneous Mixing and Stratification Modes (Electronic Materials, Conference Paper)