Mathematical modelling of hydrogen safety problems with CABARET scheme

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Abstract. Experiments on overall fluid transfer and mixing in the large scale experimental facility (PANDA), where the initial helium-rich layer is eroded by a flow resulting from the interaction of a jet/plume with horizontal flow obstruction, were simulated with the CABARET scheme. Computational simulation results are provided for two mesh resolutions and are compared with the experimental data. Good agreement between calculated and measured gas temperature and the breakup of the helium layer dynamics was achieved by refining the mesh in the jet area and by adding the model of radiation heat transfer.

1. Introduction
During a severe accident with loss of coolant, a large amount of hot steam and hydrogen can enter the atmosphere of the containment of a pressurized water reactor. The non-uniform distribution and stratification of hydrogen in the containment can lead to the formation of an explosive mixture areas that threatens the integrity of the containment. To ensure hydrogen safety of nuclear power plants, systematic experimental studies are carried out on hydrogen stratification issues (international projects: ERCOSAM-SAMARA [1], OECD/NEA HYMERES [2], OECD/NEA HYMERES-2).

HYMERES project HP1 test series addressed helium (simulating hydrogen) layer erosion by the flow, resulting from the interaction of a steam jet with flow obstructions. One of these tests was selected for a benchmark exercise. The comparison between calculated and experimental results, as well as between simulations, raised a few questions about the actual importance of considering radiative heat transfer, the relation between mesh topology and other modelling aspects (turbulence model, numerical methods, boundary conditions, etc.) [3]

At Nuclear Safety Institute (IBRAE RAS), a software tool for numerical modeling of hydrogen safety problems based on innovative approaches to constructing detailed multidimensional and multiphysical transport models for gas mixtures is developed. It is based on the CABARET scheme [4], which is intended to solve systems of hyperbolic equations. The method is second-order accurate on non-uniform grids in space and time, has a very small dispersion error and computational stencil defined within one space–time cell. For shock-capturing, the scheme uses a conservative non-linear correction procedure which is directly based on the maximum principle. Unlike the semi-empirical approaches used in modern engineering CFD-codes, there
are no tuning parameters in the CABARET scheme. The use of a parameter-free approach can make it possible to estimate the effect of thermal radiation on helium stratification process.

2. Experimental facility and Initial data
The experimental investigation is performed in the PANDA facility. The computational model of the PANDA facility was constructed on the basis of the data in [5, 6]. The main modeling elements are the pressure vessels Vessel 1 and Vessel 2, the interconnecting pipe IP and the tubes for injecting steam and helium (Figure 1) with total internal volume 184 m$^3$, height 8 m, diameter of the cylindrical part of vessels 4 m. The vessels were carefully insulated using rock-wool mats, which was simulated by a heat transfer coefficient based on experimentally determined heat loss rate.

![Figure 1. Experimental configuration and nominal initial condition for HP1_6_2.](image)

The test is aimed at assessing the helium-rich layer erosion and overall fluid transport and mixing in Vessel 1 and Vessel 2 for two-gases, for fluid conditions without condensation and with constant pressure, in the presence of a horizontal flow obstruction by a jet characterized by high momentum (Table 1).

| Parameters                              | Nominal Value                                      |
|-----------------------------------------|----------------------------------------------------|
| Initial vessel pressure, bar            | 1.3                                                |
| Vessel 1 helium molar fraction          | 25% (above 6 m)                                    |
| Vessel 1 steam + air molar fraction     | 100% steam (below 6 m), no air                     |
| Vessel 2 steam + air molar fraction     | 100% steam, no air                                 |
| Vessel wall temperature, °C             | 108                                                |
| Vessel fluid temperature, °C            | 108                                                |
| Steam injection flow rate, g/sec        | 60                                                 |
| Steam injection temperature, °C         | 150                                                |
| Pressurization                          | -                                                  |
| Flow obstruction                        | + (horizontal circular plate)                      |
| Steam condensation                      | -                                                  |
3. Mathematical model

The low-speed turbulent convective flow of a multi-component (helium-air-vapor) mixture that occurs in the field of gravity is simulated. The system of defining equations includes the equations of balance of mass, momentum and energy for the mixture as a whole, as well as the equations of components transfer:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0, \\
\frac{\partial (\rho u_i)}{\partial t} + \nabla \cdot (\rho u_i \mathbf{u}) &= -\nabla P^* + \nabla \cdot (\rho \tau_{ij}) + (\rho - \bar{\rho}) g_i, \quad i, j = 1, \ldots, 3, \\
\frac{\partial \rho C_v T}{\partial t} + \nabla \cdot (\rho C_v T \mathbf{u}) &= -\nabla \cdot (\mathbf{q} + \sum_{k=1}^{N} C_{p,k} j_k T), \\
\frac{\partial \rho_k}{\partial t} + \nabla \cdot (\rho_k \mathbf{u}) &= -\nabla \cdot (j_k), \quad k = 1, \ldots, N.
\end{align*}
\]

Here \( \rho, P, u \) and \( T \) are the density, pressure, speed and temperature of the mixture. When \( u/c \ll (c \text{ - speed of sound}) \), the pressure \( P \) might be represented as a sum of the thermodynamic pressure, averaged over the volume of the mixture \( P_0 = P_0(t) \), and the dynamic pressure \( P^* = P^*(x, t) \), ensuring the propagation of sound waves in the medium [7]. In this case, the propagation of small perturbations in the medium is a “fast” process as compared to diffusion phenomena and convective mixing of gases. The change in the internal energy during the passage of the sound wave through the medium occurs due to compressibility. Thus, the dynamic pressure can be found from the equation

\[
P^* = c^2 (\rho - \rho_0), \quad \rho_0 = \rho \left( \frac{P_0}{P} \right)^{1/\gamma}.
\]

To increase the time step (\( \tau \sim 1/c \)), artificial sound speed \( c_a < c \) can be used (artificial compressibility method). Choosing \( c_a \) from the condition \( u/c_a 10^{-1} \), we obtain a weakly compressible approximation of the medium \( \partial \rho/\rho \sim (u/c_a)^2 < 10^{-2} \).

The total diffusion transfer is represented in the system (1) by a stress tensor \( \tau_{ij} \), and vectors of heat \( \mathbf{q} \) and mass \( j_k \) flux density for which gradient approximations are used in the form of Newton, Fourier and Fick laws.

3.1. Radiation heat transfer model

For the problems of low-temperature gas dynamics, a radiation has an effect only on the redistribution of energy in the medium. However, this is often quite enough to drastically change the whole picture of the phenomenon. Only polyatomic gases (CO\(_2\), H\(_2\)O, NH\(_3\), etc.) have a significant ability to emit and absorb radiant energy. For the problems of containment thermal hydraulics, the most interesting is water vapor, which comes in a large volume from the break in the primary circuit during serve accident. With increasing temperature and vapor concentration in the containment rooms, the medium becomes optically dense. For example, with a partial pressure of steam equal to 1 bar and a temperature equal to 500K, the optical thickness of 1 m thick layer is \( \tau \approx 120 \geq 1 \) [8]. In this case, the radiation field becomes isotropic; therefore, the diffusion approximations become valid.

In the Rosseland diffusion model of radiative thermal conductivity, the radiative heat flux is expressed through the temperature gradient, as well as the conductive flux in the Fourier law

\[
\mathbf{q}_{rad} = -k_{rad} \cdot \nabla T, \quad k_{rad} = \frac{16 \sigma T^3}{3a_R}.
\]

Here \( a_R = a_R(x, v, T, P) \) is an average steam absorption coefficient according to Rosseland, \( \sigma \) is a Stefan-Boltzmann constant. On the walls, the isotropic condition of radiation is violated. In
practice, an approximate formula is used

\[ q_w = \varepsilon_{gw} \sigma \left( T_g^4 - T_w^4 \right), \varepsilon_{gw} = \frac{1}{1/\varepsilon_g + 1/\varepsilon_w - 1}. \] (4)

Here \( \varepsilon_g \) and \( \varepsilon_w \) are gas and wall emissivity coefficients, \( \varepsilon_{gw} \) is reduced emissivity.

4. Results
In the experiment, the time histories of gas temperatures and helium concentrations above the injection describe the progression of the erosion process, which is characterized, at each elevation, by helium concentration drop and temperature increase as a result of the rise of the leading edge of the steam jet and its associated mixing zone.

To study the effect of mesh resolution on stratification erosion dynamics, two hexagonal unstructured meshes of 1 million (coarse) and 3.6 million (finer) cells were used. The mesh cells were modified locally to reduce the cell size from 1.5 cm to 0.75 cm in the jet area (Figure 2).

![Figure 2. Mesh refinement in near jet area from 1.5 cm (left) to 0.75 cm (right).](image)

The calculations without the included thermal radiation model showed that for a coarse mesh the time of helium stratification breakup is substantially underpredicted. This is related to the difficulties in modelling the resulting recirculation flow above the plate due to the underpredicted broadening of the free jet on the coarse mesh (Figure 3, right). On the finer mesh, erosion dynamics at the 6926 m level is close to the experimental (Figure 3, left), but at the levels above, the mixing is smoother. Also on both meshes an overprediction of temperature of 5-7 °C is observed.
Despite the fact that the vapor temperature is relatively small (below 150 °C), thermal radiation may have a noticeable role. The calculation with the enabled Rosseland thermal heat transfer model showed significantly better agreement with the measured temperature (Figure 4). The dynamics of the helium layer breakup in the upper region of the facility also demonstrates a better convergence (Figure 5, left), which may be due to increased buoyancy of the plume resulting from the interaction of a jet with the disk.

**Figure 3.** Time history of helium concentration at the level 6926 m for two meshes (left) and comparison of averaged vertical speed fields for two meshes (right).

**Figure 4.** Time history of temperature on the axis line at the level 6926 m (left) and gas temperature horizontal profile at level 5626 m at 300 sec (right).
5. Conclusions
An important advantage of the CABARET technique for the modeling of a turbulence is the lack of semi-empirical models and tuning parameters. The only source of uncertainty is the grid itself, the selection criterion of which is based on the analysis of grid convergence. Since convergence to experimental data is possible only with modeling of all the important processes, the use of CABARET can significantly simplify the interpretation of the results of experiments in a complex multiphysical formulation. According to the results of the calculations, significant influence of considering of radiation heat transfer to erosion process was observed. At the moment, the question of the effect of thermal radiation at low temperatures of steam and the choice of numerical models of thermal radiation is open and requires further research.

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