CABARET scheme for modelling the stratification erosion in gas mixtures in hydrogen mitigation experiments for reactor safety

V Yu Glotov, V M Goloviznin, A A Kanaev, V G Kondakov and A E Kiselev
Nuclear Safety Institute of Russian Academy of Science, 52 Bolshaya Tulskaya Street, Moscow, 115191, Russian Federation
E-mail: glotov-v@yandex.ru, gol@ibrae.ac.ru, kanaev@ibrae.ac.ru, kondakov@ibrae.ac.ru, ksv@ibrae.ac.ru

Abstract. Experiments on atmosphere mixing and stratification in the large scale experimental facility (PANDA), where the initial helium stratification in a vessel is eroded by a vertical jet of steam, were simulated with the CABARET scheme. Good agreement between calculated and measured gas temperature and concentrations has been achieved by refining the mesh and adding the model of radiative heat transfer. The simulation results are presented and discussed.

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 explosive mixture areas that may threaten the integrity of the containment. To ensure hydrogen safety in nuclear power plants, systematic experimental studies are carried out on hydrogen stratification issues (international projects: ERCOSAM-SAMARA [1], HYMERES [2], HYMERES-2). Both simple (basic mechanisms of formation and destruction of light gas stratification) and complex (conditions in more realistic formulation taking into account the operation of safety systems, the effect of obstacles in the flow path, the effects of steam condensation and radiation heat transfer) research is conducted. The enhanced understanding has been achieved by improved modeling capabilities of the computer codes that are used for the safety assessment of current and new nuclear power plants.

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 being developed. It is based on the CABARET scheme [3], which is intended to solve systems of hyperbolic equations. Unlike the semi-empirical approaches used in modern engineering CFD-codes, there are no tuning parameters in the CABARET scheme; as a result, it has an increased predictive capability of modeling the turbulent flows in multicomponent media using grids with incomplete turbulent spectrum resolution.

This article presents the simulation results obtained with CABARET scheme for two experiments conducted on the PANDA facility (HP1_8 HYMERES and H2P1_0 HYMERES-2) to study the process of light gas (helium) stratification destruction under the influence of free and diffuse (scattered on an obstacle) jets of hot steam. The use of a parameter-free approach can allows estimating the effect of thermal radiation on helium stratification process.
2. Experimental facility and initial data

The computational model of the PANDA facility was constructed on the basis of the data of [4, 5]. 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 a total internal volume of 184 m³, a height of 8 m, and a diameter of the cylindrical part of vessels of 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_8.](image)

The experiment H2P1_0 is focused on the helium-rich layer erosion and overall fluid transport and mixing by a free vertical steam jet in Vessel 1 of the PANDA facility for two-gases, for fluid conditions without condensation and under constant pressure (Table 1). The interconnecting pipe (IP) was closed with a lid on the side of the Vessel 1 to stop the flow through IP. The pressure difference between the two vessels has to be minimized by connecting the two vessels with a thin hose. The pressure in the vessels was kept constant throughout the main phase of the test by venting the gas to the atmosphere from the vent located at the top of Vessel 2.

The experiment HP1_8 is aimed at assessing the helium-rich layer erosion and overall fluid transport and mixing by a vertical jet characterized by low momentum in Vessel 1 and Vessel 2 for three-gases, for fluid conditions with condensation and with pressurization, in the presence of a horizontal flow obstruction (circular plate with a diameter of 0.2 m) (Table 1).

| Parameters                      | H2P1_0       | HP1_8       |
|---------------------------------|--------------|-------------|
| Initial vessel pressure, bar    | 1.3          | 1.3         |
| Vessel 1 helium molar fraction  | 25% (above 6 m) | 25% (above 6 m) |
| Vessel 1 steam + air molar fraction | 100% steam (below 6 m), no air | 75% steam + 25% air (below 6 m) |
| Vessel 2 steam + air molar fraction | 100% steam, no air | 75% steam + 25% air |
| Vessel wall temperature, °C     | 108          | 100         |
| Vessel fluid temperature, °C    | 108          | 100         |
| Steam inj. flow rate, g/sec     | 30           | 30          |
| Steam inj. temperature, °C      | 150          | 118         |
| Reynolds number                  | ~14000       | ~14000      |
| Richardson number                | ~0.45        | ~0.25       |

\[
(\text{Re} = \frac{\rho v_{inj} D}{\mu}, \text{D } = 0.2 \text{m})
\]

\[
(\text{Ri} = \frac{\Delta \rho g L}{\rho v_{inj}^2}, \text{L } = 1 \text{m})
\]
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 governing 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:

\[
\frac{\partial \rho}{\partial t} + \text{div} (\rho \vec{u}) = 0 \\
\frac{\partial \rho u_i}{\partial t} + \text{div} (\rho u_i \vec{u}) = -\nabla_i P^* + \nabla_j \tau_{ij} + (\rho - \bar{\rho}) g_i, \quad i, j = 1, ..., 3 \\
\frac{\partial \rho C_v T}{\partial t} + \text{div} (\rho C_v T \vec{u}) = -\text{div} \left( \bar{q} + \sum_{k=1,N} C_{p,k} \vec{j}_k \right), \\
\frac{\partial \rho \vec{j}_k}{\partial t} + \text{div} (\rho \vec{j}_k \vec{u}) = -\text{div} (\vec{j}_k), \quad k = 1, ..., N
\] (1)

Here \( \rho, P, u \) and \( T \) are the density, pressure, speed and temperature of the mixture. When \( w/c << 1 \) (\( c \) - speed of sound), the pressure \( P \) may be represented as a sum of thermodynamic pressure, averaged over the volume of the mixture \( P_0 = P_0(t) \), and dynamic pressure \( P^* = P^*(x, t) \), ensuring the propagation of sound waves in the medium [5]. 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

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

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

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

3.1. Wall condensation model
Wall condensation is determined by diffusion processes and calculated using additional boundary conditions. It is assumed that the water vapor condensation on the cooled surface is accompanied by the formation of an infinitely thin film of condensate, which flows down under the action of gravity. At the film boundary, the temperature is taken to be equal to the wall temperature, and the longitudinal velocity component is assumed to be zero. In the case of equilibrium, the partial vapor pressure on the surface of the condensate film is equal to the saturation vapor pressure at the corresponding temperature \( P_v = P_{sat}(T_{wall}) \). The mass flow rate of the condensate film \( j_v \) can be deduced from both Fick’s law and the advective mass transfer at the interface, in addition to the mass balance [7]:

\[
j_v = \frac{M_v}{M} \rho D_v \frac{\partial \ln(x_v)}{\partial n}
\] (3)
Here $M_v$ and $D_v$ are the molecular mass and the diffusion coefficient of water vapor, and $x_g = 1 - x_v$ is the molar fraction of non-condensable gases. The diffusion layer model is a direct numerical model. It has no empirical dependences, but it requires a good near wall grid resolution. Thus, it is necessary to analyze the solution convergence on refined grids.

3.2. Radiative heat transfer model

For the problems of low-temperature gas dynamics, radiation has an effect only on the redistribution of energy in the medium. However, this is often sufficient 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 a water vapor, which comes in a large volume from the break in the primary circuit during severe accidents. 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 1bar and a temperature equal to 500K, the optical thickness of 1m thick layer is $\tau \approx 120 >> 1$ [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 the conductive flux in the Fourier law

$$\dot{q}_{rad} = -k_{rad} \cdot \nabla T, \quad k_{rad} = \frac{16\sigma T^3}{3a_R}$$

(4)

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

$$q_w = \varepsilon_{gw}\sigma(T_g^4 - T_w^4), \quad \varepsilon_{gw} = 1/(1/\varepsilon_g + 1/\varepsilon_w - 1)$$

(5)

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

4. Results

Hexahedral unstructured meshes were used in the calculations. In order to check the influence of mesh resolution, two simulations were performed with the fine mesh (2.33 mil. cells) and the coarse mesh (0.98 mil. cell), respectively. The mesh cells were modified locally to reduce the cell size (from 2.5cm to 1cm) inside the boundary layers and near the jet area. Non-dimensional wall distance, $y^+$, in average is around 8 for fine mesh and 20 for coarse mesh (it depends on time and velocity distribution on the surface).

![Figure 2. Pressure evolution. Experiment HP1_8.](image1)

![Figure 3. Condensation rate evolution on different grids. Experiment HP1_8.](image2)

![Figure 4. Helium molar fraction along the axis of symmetry of Vessel 1 at heights of 8m and 7m.](image3)
Figures 2-4 show the grid-based convergence of the solution to the experimental data (HP1_8) for the pressure and helium molar fraction. It is seen that the difference lies in the erosion time of the helium cloud. At the beginning of the experiment, the vapor condensation occurred below the helium level while the upper part of the vessel walls remained cold. During the destruction of the helium layer, hot steam gets to the cold walls, which leads to a spike in the rate of condensation (figure 3). On these spikes we can find that the time difference for two meshes is about 170 seconds.

Despite the fact that the vapor temperature is relatively small (below 150 °C), the radiative heat transfer plays a noticeable role. The effect of radiation can be found in the gas temperature distribution: without radiation model, the gas temperature is overestimated by 2-3 °C (figure 5). This leads to a decrease in buoyancy in the jet. As a result, the dynamics of helium erosion is reduced (figure 6).

Similar results take place in a simpler separate effect test (experiment H2P1_0) on the erosion of a helium cloud by a free jet of steam in a two-component medium without pressurization. By the end of the experiment, the gas temperature without radiation is overestimated by more than 5 °C (figure 7), and the erosion process at the top of Vessel 1 is slower (figure 8).

These results are illustrated with figures 9-10. At the time of 1100 seconds, in calculation with the radiation model considered, the mixture is completely mixed, while in calculation without radiation model, a stagnant region with a high concentration of helium remains in the upper part of Vessel 1.
Conclusions
An important advantage of the CABARET technique for the modeling of turbulence is the absence 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 important processes, the use of CABARET can significantly simplify the interpretation of the experimental results in a complex multiphysical formulation. According to the results of the calculations, a high accuracy simulation of erosion of helium stratification has been shown. Both in the separate effect test (H2P1_0), and in more realistic multiphysical test (HP1_8), a significant influence of radiative heat transfer on erosion process was observed. At the moment, the question of the effect of radiation at low temperatures of steam and the choice of numerical models of radiation is open and requires further research.

![Figure 9. Helium distribution in Vessel 1 at the time of 1100 sec with radiation model. Experiment H2P1_0.](image1)

![Figure 10. Helium distribution in Vessel 1 at the time of 1100 sec without radiation model. Experiment H2P1_0.](image2)

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References
[1] Paladino D 2012 The Euroatom-Rosatom ERCOSAM-SAMARA projects on containment thermal-hydraulics of current and future LWRs for severe accident management 2012 Proceedings of ICAPP (USA: Chicago)
[2] Paladino D 2014 OECD/NEA HYMERES Project: For the Analysis and Mitigation of a Severe Accident Leading to Hydrogen Release Into a Nuclear Plant Containment Proceedings of ICAPP (USA: Charlotte)
[3] Goloviznin V M 2013 Novel Algorithms of Computational Hydrodynamics for Multicore Computing (Moscow University Press) p 481
[4] Paranjape S 2015 OECD/NEA HYMERES project: PANDA Test HPI_8 Quick-Look Report TM-42-15-02 Rev-0 HYMERES-P-15-16
[5] Paranjape S 2018 OECD/NEA HYMERES-2 project: PANDA Test H2P1_0 Quick-Look Report TM-41-18-06 Rev-0 HYMERES-2-18-13
[6] Rieper F 2008 On the Behaviour of Numerical Schemes in the Low Mach Number Regime PhD thesis (Bradenburg: University of Technology)
[7] Peterson P F, Schroock V E, Kageyama T 1993 Journal of Heat Transfer 115 (4)
[8] Ozicik M N 1985 Heat Transfer A Basic Approach (McGraw-Hill Book Company) p 800
[9] Sadovnichy V, Tikhonravov A, Voevodin VI and Opanasenko V 2013 “Lomonosov”: Supercomputing at Moscow State University. In Contemporary High Performance Computing: From Petascale toward Exascale (Chapman & Hall/CRC Computational Science, Boca Raton, USA, CRC Press) pp 283–307