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Comparison of pool scrubbing simulations with SCRUPOS experiment

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ABSTRACT

Numerical simulations of dispersed solid particle behavior inside a scrubbing pool are presented. The goal is to evaluate the decontamination factor of the particles during the pool scrubbing process. The basic phenomena of pool scrubbing are described. The setup used for the simulation validation is presented. Then, the boundary and initial conditions used for simulations are presented. The subgrid model for particle decontamination is presented and, in the end, the results are evaluated and compared with experimental data from the literature.

1 INTRODUCTION

During a hypothetical severe accident in a light water nuclear power plant, the reactor fuel could melt and there is a possibility that some of the radioactive material could be released as particles to the surrounding area. The releases of the radioactive material can be reduced with the application of pool scrubbing, where the release of contaminated gases is filtered through a pool of liquid water. To understand what is happening during pool scrubbing, phenomena at the local scale have to be understood. Specifically, since the gases enter the scrubbing pool as a jet that disperses into bubbles, the behavior of the particle removal from the bubbles is crucial for understanding pool scrubbing phenomena.
In the present paper, the behavior of transition of solid particles from gas phase to liquid phase during the bubble rise in a scrubbing pool was simulated using subgrid modeling. The multi-phase simulations were performed for particles, bubbles and liquid using the open-source Computational Fluid Dynamics (CFD) code OpenFoam, with the solver reactingMultiphase-EulerFoam. In the simulation, the gas, liquid and two particle phases (phase 1 within bubbles and phase 2 within liquid) were simulated. All phases were described in Eulerian frame. The particle densities and bubble diameters were prescribed, based on data from the literature. The

subgrid model takes into account that, due to bubbles rising, the inner air motion moves particles inside bubbles (particle phase 1) due to interfacial drag. The particles first migrate towards the bubble surface and then out of the bubbles. The particles transport from bubbles to liquid is simulated as a transfer via a subgrid model from particle phase 1 to particle phase 2. The subgrid model is programed trough OpenFoam's flexible framework option called fvOptions, which allows users to add source or sink terms to differential equations of the OpenFoam solvers.

Due to the difference in the carrier phase, the behavior of particles inside and outside of bubbles differs. Particles in gas (particle phase 1) raise up with the gaseous phase and, if not transported to the liquid, leave the pool scrubbing tank. The particles in liquid (particle phase 2) stay inside the tank. The difference between modelling of motion of the particle 1 and particle 2 phases is only in the drag correlations due to their connection with the carrier phases. In the end, the simulation results were analyzed and the decontamination factor, which is the resulting measure of the scrubbing efficiency, was calculated.

2 BASIC PHENOMENOLOGY OF POOL SCRUBBING

The goal of pool scrubbing is to remove as much radioactive substances as possible (which can be gases or particles) from a mixture of condensable and non-condensable gases that pass through the liquid pool (in most cases filled with water). An additional purpose is to condense steam and, with this, reduce a possible pressure surge in the nuclear power plant containment.

The main factor in pool scrubbing is the scrubbing or filtration efficiency (β) which can be expressed in terms of the Decontamination Factor (*DF*), which is defined as the ratio of the radioactive material mass entering and leaving the pool with the gaseous phase:

$$DF = \frac{m_{in}}{m_{out}} = \frac{1}{1-\beta}\,, \tag{1}$$

where m_{in} represents the mass entering the pool and m_{out} the mass leaving the pool.

Because of the different behavior of mixture and scales of interactions, three regions can be defined [1, 2]: injector region around the inlet, rise region and surface region. The DF is also highly affected by the pool temperature, which is especially true for installations with higher steam fraction in the mixture entering the pool [3]. The overall DF can be calculated as a product of DF for each region.

3 SCRUPOS EXPERIMENT

The SCRUPOS (SCRUbbing by Pool and Spray) is an experimental facility at Ricerca sul Sistema Energetico - RSE SpA (RSE), Milano, Italy [4]. The goal of the experimental facility is to test the scrubbing of both pool scrubbing and high pressure spray scrubbing. The layout can be seen on Figure 1. The facility is cuboid shaped with height of 1.5 m, length of 1 m and width of 0.5 m. The structure is built from stainless steel frame and tempered glass. It has six measurement access points on the lateral side. Other components are: aerosol injection line, where air flow mass-rate and pressure are monitored with a thermal mass flow and a piezo-resistive transducer, respectively; water injection line, where demineralized water is fed by high-pressure volumetric pump; pick up line, where samples of the air with particle suspension are diluted and analyzed.

The aerosols are particles of monodisperse amorphous silica, SiO_2, which has a density of 2650 kg/m^3. The major feature of this experiment is that the hydro-dynamic part and the pool scrubbing part were done at the same conditions and is therefore highly suitable for verification of numerical simulation in CFD approach.

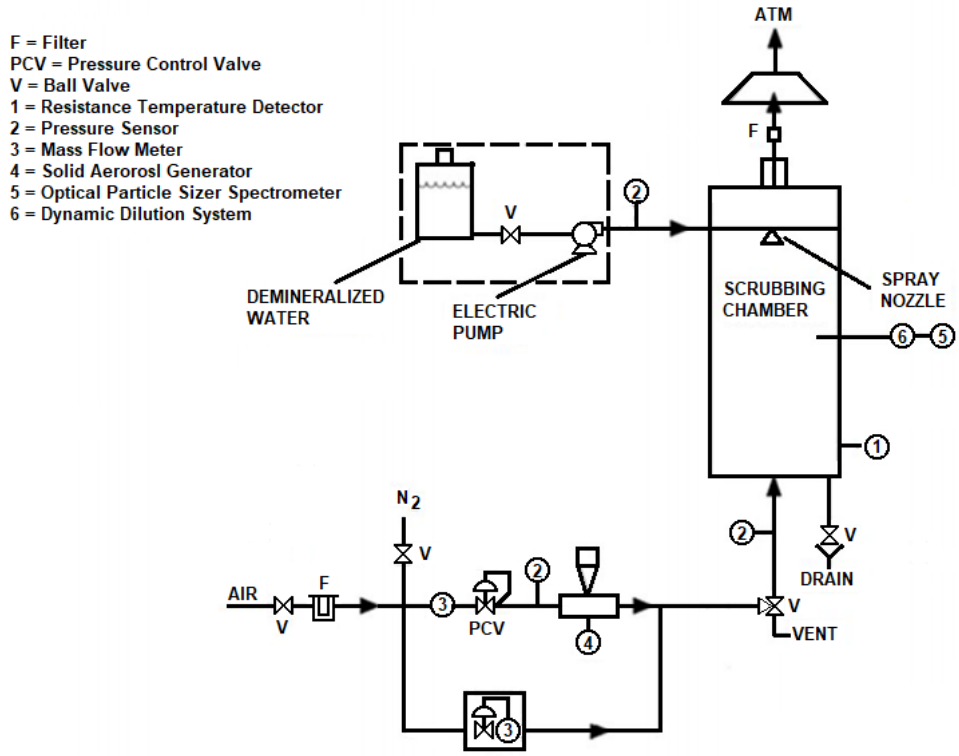

Figure 1: Layout of SCRUPOS facility. [4]

4 NUMERICAL SIMULATION

The importance of the theoretical modelling, using numerical simulations, for the investigation of pool scrubbing is increasing and contributes to experimental investigations, which are costly and time consuming. However, computers are still not powerful enough to directly solve the Navier-Stokes equations for multi-phase flows in large domains [5, 6].

One of better-suited approaches for relatively large systems, to be modelled using a much lower amount of numerical cells than if the phases were considered separately, is two-fluid (or multi-fluid) modelling[1, 7]. All phases are treated as inter-penetrating continua, represented by averaged conservation equations. The averaging process adds the phase fraction for each phase into the equation set, which is defined as the probability that this phase is present at the observed location.

The inter-phase momentum transfer is phase-fraction dependent and is determined from the instantaneous forces acting on the dispersed phase, comprising drag, lift and virtual mass. Problems arise from complex interactions between the fluids, which have different interactions depending on the volumetric fraction of each fluid at the observed location. In order to obtain a numerical solution, the calculation domain has to be divided into calculation cells. Because a higher number of cells directly corresponds to a longer computation time, models for subgrid scales are used in most multi-fluid simulations. Because these models do not need large numbers of cells to run, they are well-suited for use in industrial and nuclear installations. The current state of modelling techniques is described in [8]. In short, the particle transport is modelled with the use of transport equations, which take into account size distribution, coagulation, deposition and mechanical resuspension of particles.

The simulation of single bubble scrubbing was performed using the transient multi-phase solver reactingMultiphaseEulerFoam, which is part of the open-source Computational Fluid Dynamics (CFD) software OpenFOAM 3.0.0 and is based on the finite volume method of

equation discretization. In the simulation, a multi-dimensional case for four incompressible phases (liquid water, air, particles 1 and particles 2) was calculated. The only mass transfer is via the subgrid model for phase pair particle 1 and particle 2 which is explained in chapter 6. There was no mass transfer for other phase pairs. The multi-phase solver uses standard multi-phase balance equations for mass, momentum and energy for each phase, which are solved by the PIMPLE coupling algorithm [9].

Mass equation:

$$\frac{\partial \alpha_i \rho_i}{\partial t} + \nabla(\alpha_i \rho_i \vec{v}_i) = \Gamma_i \,, \tag{2}$$

where $\alpha_i$is the volumetric fraction of phase i, ρ_i the phase i density, $\vec{v}_i$ the phase i velocity and Γ_i the inter-phase mass transfer rate of phase *i*.

Momentum equation:

$$\frac{\partial \alpha_i \rho_i \overrightarrow{v_i}}{\partial t} = -\vec{\nabla}(\alpha_i \rho_i \vec{v}_i \vec{v}_i) - \alpha_i \vec{\nabla} p_i + \vec{\nabla}\alpha_i(\bar{\bar{\tau}}_i + \tau_i^t) + \alpha_i \rho_i \vec{g} + \vec{v}_i \Gamma_i + \overrightarrow{M_\iota} \,, \tag{3}$$

where $\vec{\nabla} p_i$ is the pressure gradient of phase *i*, $\bar{\bar{\tau}}_i$ the average viscous stress of phase *i*, τ_i^t the Reynolds stress of phase *i*, $\vec{g}$ the gravity and $\overrightarrow{M_\iota}$ the average inter-phase momentum transfer of phase *i*.

Energy equation:

$$\frac{\partial \alpha_i \rho_i H_i}{\partial t} = -\vec{\nabla}(\alpha_i \rho_i H_i \vec{v}_i) - \vec{\nabla}\alpha_i(\bar{\bar{q}}_i + q_i^t) \; + \alpha_i \frac{Dp_i}{Dt} + H_i \Gamma_i + q''_{ki} a_i + \Phi_i \,, \tag{4}$$

where H_i is the enthalpy of phase *i*, $\bar{\bar{q}}_i$ the conductive heat flux, q_i^t the turbulence enhanced heat flux, Dp_i/Dt the reversible rate of enthalpy change due to compression, q''_{ki} the conductive heat flux between phases, a_i the interfacial area concentration and Φ_i the heat source for phase *i*.

In the simulation, the lift and virtual mass coefficients were set to 0.5 for air and particle phase 1 in water. Turbulent dispersion was turned off. The used drag model was the Schiller-Naumann model [10]:

$$\overrightarrow{M_\iota} = \sum_j \frac{3}{4} \rho_j \alpha_i \alpha_j C_D \frac{\left|\overrightarrow{v_\iota} - \overrightarrow{v_j}\right|\left(\overrightarrow{v_\iota} - \overrightarrow{v_j}\right)}{d_i}, \tag{5}$$

$$C_D = \begin{cases} \dfrac{24(1 + 0.15Re^{0.683})}{Re}, & Re \le 1000 \\ 0.44, & Re > 1000 \end{cases} \tag{6}$$

where M_i is the interface momentum transfer for phase i with phase j, C_D the drag coefficient, d_i the dispersed phase diameter and Re Reynolds number.

The drag between the undesired phase pairs, (air-particle 2, water-particle 1 and particle 1-particle 2) was multiplied by 10^{-3} to simulate that the particle phase 1 is mostly connected with gas phase and particle phase 2 with liquid phase. Namely, in a multi-phase model, each phase acts on each other via drag. With multiplication by a small number, the drag between an undesired phase pair becomes negligible and the equations become “semi-separated”. The four momentum equations in the solver can therefore become separated to air-particle 1 part and water-particle 2 part. This corresponds to the idea of the subgrid model, where particle phase 1

does not interact with water and particle phase 2 does not interact with air. The multiplication factor (10^{-3}) was chosen arbitrarily.

Both particle phases were simulated as a dispersed liquid phase with a droplet diameter of 0.35 µm which corresponds to the AMMD (aerodynamic mean mass diameter) of particles in the POSEIDON experiment [11]. Namely, the difference in dispersed solid or dispersed liquid phase in OpenFoam is only in the phase density change according to local parameters [9], which is, for this case, negligible.

5 COMPUTIONAL DOMAIN, MESH, BOUNDARY AND INITIAL CONDITIONS

A numerical mesh representing a cuboid with sides of 1 and 2 m and a height of 2 m was developed. The gas inlet is located in the middle of the bottom plane with a diameter of 10 cm. Around the inlet region the mesh was refined to better describe its shape. The actual inlet in the experiment was much smaller with a diameter of only 10 mm. The mesh was made using OpenFoam utility snappyHexMesh and is composed of around 140,000 computational cells. The mesh at the immediate proximity of the inlet was refined with a 2 times denser mesh.

The boundary conditions of the cases on the inlet were velocity of 0.64 m/s for case 1 and 0.85 m/s for case 2 and particle phase volume fractions of $2 * 10^{-8}$ for case 1 and $6 * 10^{-8}$ for case 2; the remaining volume fraction in both cases was air as were the conditions in SCRUPOS experiment. The outlet was specified as an opening with constant pressure 10^5 Pa and free outlet condition for volumetric fraction with air fraction of 1 for returning flow. The walls were treated with no-slip condition for velocity fields and as zero gradient for phase fractions.

The initial conditions was whole tank filled with water with velocity field 0 m/s with initial seeding for every other phase (particle phases and air phase with volumetric fraction 10^{-12}) to prevent discontinuities.

6 SUBGRID MODEL

The subgrid model of particle transport from particle phase 1 (particles in bubbles) to particle phase 2 (particles in water) was based on the parametric modeling of the two-phase Euler-Euler simulation of single bubble decontamination during rise [12]. The mesh represented a 5 ° wedge geometry which simulated rotational symmetry of a spherical bubble (Figure 2). Boundary conditions were set to symmetry and the rotation bubble wall with fixed rotational velocity. The tested bubble diameters were from 0.8 cm to 2 cm and the rotational velocities ranged from 20 to 400 rad/s.

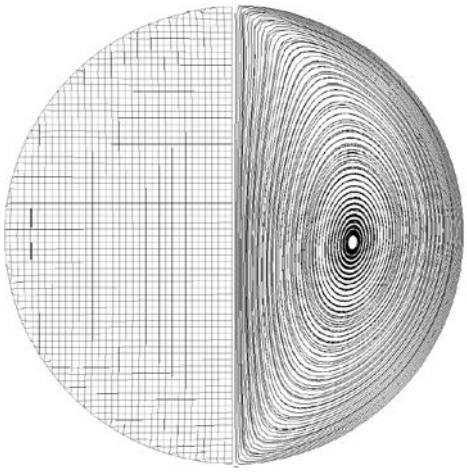

Figure 2: Computational wedge domain (left: schematic of numerical mesh with 196,000 cells; right: fully developed air streamlines).

The single bubble decontamination plots were drawn for each tested condition and then fitted (Figure 3) with an analytical function. From all results the model constants were produced. In the present paper the subgrid model is based only on bubbles with 1 cm diameter.

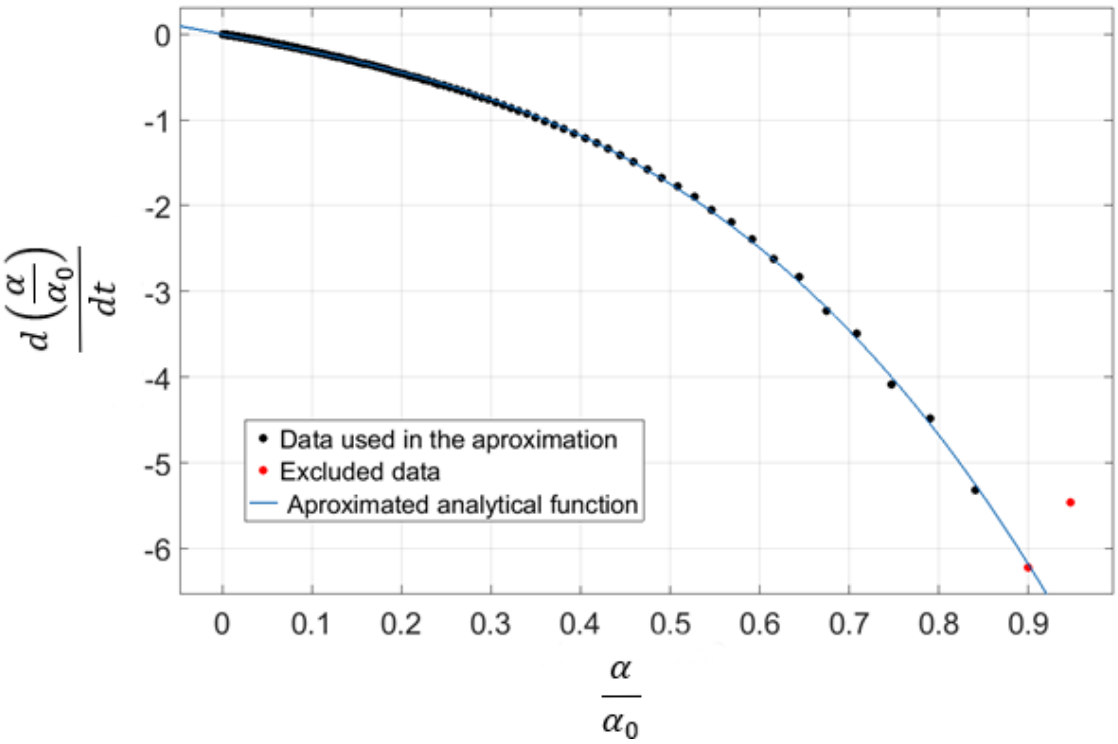

Figure 3: Results of a single bubble decontamination and approximated function for one of the test conditions. The α_0 represents the initial value of particle volumetric density inside bubble.

The produced model can be described as the sum of cubic and linear function and can be written as:

$$\frac{\partial \alpha_{par}}{\partial t} = \mathrm{B} * \omega * \alpha_{par} * \left(1 + \frac{A}{B} * {\alpha_{par}}^2\right), \tag{7}$$

where α_{par} is the particle volumetric fraction, ω the bubble rotational velocity, A and B constants with values of $-4.14 * 10^{-4}$ and $-2.28 * 10^{-9}$ respectively. Thus, eq. (7) should not be considered as empirical, but as a summary of results of simulations, based on basic physical laws and equations, which were performed earlier.

The model described in eq. (7) is valid for decontamination of a single bubble wedge, which means that the model should be changed to suit the dispersed bubble multi-phase case in 3D geometry. This can be achieved with division with the wedge wall surface and the multiplication with the cell volume and air-water interfacial area concentration in multi-phase numerical simulation. With that, the surface decontamination flow is multiplied with the surface of bubbles in each computational cell.

The inverse of the bubble wedge surface C_{bs} can be therefore written as:

$$C_{bs} = \frac{2}{\vartheta * D_{Sm}^2}, \tag{8}$$

where ϑ is the wedge angle and D_{Sm} the Sauter mean diameter of bubble. The interfacial area concentration a_1 for spherical bubbles is taken from [13] and can be written as:

$$a_1 = \frac{6 * \alpha_{air}}{D_{Sm}}. \quad (9)$$

In addition, the rotational velocity ω can be expressed as

$$\omega = \frac{2 * U_r}{D_{Sm}}, \quad (10)$$

where U_r is the magnitude of the relative velocity between gas and liquid phase which corresponds to the bubbles rise velocity in stagnant water.

Combining the eqs. (7)-(10) the final model for 3D dispersed spherical bubbles in bubble regime can be written as:

$$\frac{\partial \alpha_{par}}{\partial t} = \frac{4}{\vartheta * D_{Sm}^3} * V_{cell} * a_1 * \left(U_r * B * \alpha_{par} * \left(1 + \frac{A}{B} * {\alpha_{par}}^2 \right) \right). \quad (11)$$

Equation (11) is then used in the fvOptions subroutine.

7 RESULTS

To compare the simulation results with the SCRUPOS experiment, the average decontamination factor is calculated as the ratio of the sums of particle 1 mass fluxes entering ($\dot{m}_{p\_in}(t)$) and exiting ($\dot{m}_{p\_out}(t)$) the computational domain in 10^{-2} s time intervals. Given the time scale of the bubble motion, this arbitrarily chosen value should be small enough.

$$DF = \frac{\sum \dot{m}_{p_{in}}(t)}{\sum \dot{m}_{p_{out}}(t)} \quad (12)$$

The calculated decontamination factor for the first case is 6.33 and 4.70 for the second one. The experimental results of SCRUPOS at similar conditions give decontamination factors of 4.15 and 2.77, respectively.

It should be noted that the calculated average air volume fraction and the relative vertical velocity between gas and liquid phase exceed those measured in the experiment. This results in higher decontamination rates in the subgrid model. The described model also takes into account only the decontamination of dispersed spherical bubbles with no interactions between them.

The first few seconds of the simulation were scrapped because the particles need some time to reach the upper domain boundary. The approximate cut-off time was set by the arrival of air to the water surface (5 s).

One of the important causes for the observed differences could be that the average calculated particle volume fraction is around 10^{-8}, which could lead to numerical errors.

8 CONCLUSIONS

A simulation of decontamination of an air-particle mixture in a pool scrubbing tank with a proposed subgrid model using a CFD solver with multi-phase modelling approach was performed. The simulation is the first attempt to add a subgrid model to the OpenFoam solver and use it as a CFD tool for the studies of the decontamination factor of scrubbing pools at different conditions. The Euler-Euler description was used with the goal of studying large quantities of particles in large pools. However, the use of such description means operating with extremely low volume fractions of the particle phase which could lead to numerical errors. Nevertheless, the subgrid model gives good results in comparison with the experiments and the major error in the simulation appears to come from the hydrodynamic part of the numerical simulation.

In future work, different flow regimes, cap bubble decontamination and also bubble breakage, coalescence and collisions should be added to the subgrid modelling. Other pool scrubbing regions (jet inlet and surface region) should also be added to the studies to be able to quantitatively compare simulations with experiments.

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REFERENCES

[1] Allelein, H.J., et al., "OECD/CSNI Specialist Meeting on Nuclear Aerosols in Reactor Safety-Summary and Conclusions", in: NEA/CSNI, O. (Ed.), Cologne, Germany, 1998.
[2] Herranz, L.E., Fontanet, J., "Analysis of the Effect of Water Ponds on HTR Confinement Behavior Under Accident Conditions", Prog. Nucl. Energ. 67, 2013. 7-14.
[3] Uchida, S., et al., "Temperature Dependent Fission Product Removal Efficiency Due To Pool Scrubbing", Nucl. Eng. Des. 298, 2016. 201-207.
[4]+ Turni, M., "Experimental study and modeling of a pool scrubbing system for aerosol removal". ETH Zurich, 2016.
[5] Rusche, H., "Computational Fluid Dynamics Of Dispersed Two-Phase Flows At High Phase Fractions". Imperial College London (University of London), UK, 2003.
[6] Niceno, B., et al., "Euler-Euler Large Eddy Simulation of a Square Cross-Sectional Bubble Column Using the Neptune_CFD Code", Sci. Technol. Nucl. Ins., 2009. 1-8.
[7] Frank, T., et al., "Validation of Eulerian Multiphase Flow Models for Nuclear Safety Application", ISTP-2004, Pisa, Italy, 2004.
[8] Bonart, H., "Implementation And Validation Of A Solver For Direct Numerical Simulations Of Turbulent Reacting Flows In OPENFOAM". Karlsruhe Institute of Technology, Germany, 2012.
[9] Greenshields, C.J., "Openfoam User Guide", OpenFOAM Foundation Ltd, version 3, 2015.
[10] Wardle, K.E., Weller, H.G., "Hybrid Multiphase CFD Solver for Coupled Dispersed/Segregated Flows in Liquid-Liquid Extraction", Int. J. Chem. Eng. 2013, 1-13.
[11] Dehbi, A., et al., "Aerosol retention in low-subcooling pools under realistic accident conditions", Nucl. Eng. Des. 203, 2001. 229-241.
[12] Kunšek, M., et al., "Parametric study of a single rising bubble scrubbing ", 27th International Conference Nuclear Energy for New Europe - NENE 2018, Porotoroz, Slovenia, 2018.
[13] Ozaki, T., et al., "Code performance with improved two-group interfacial area concentration correlation for one-dimensional forced convective two-phase flow simulation", Journal of Nuclear Science and Technology, 2018. 1-20.