Validation of the heat and mass transfer models within a pressurized water reactor containment using the International Standard Problem No. 47 data

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Abstract A lumped parameter type code, called HEPCAL, has been worked out in the Institute of Thermal Technology of the Silesian University of Technology for simulations of a pressurized water reactor containment transient response to a loss-of-coolant accident. The HEPCAL code has been already verified and validated against available experimental data, which in fact have been taken from separate effect tests mainly. This work is devoted to validation of the latest version of the HEPCAL code against experimental data from more complex tests. These experiments have been performed on three different test rigs (called TOSQAN, MISTRA and ThAI) and a part of them became the basis of the International Standard Problem No. 47 (ISP-47) dedicated to containment thermal-hydraulics. Selected experiments realized within the framework of the ISP-47 project have been simulated using the HEPCAL-AD code. The obtained results allowed for drawing of some important conclusions concerning heat and mass transfer models (especially steam condensation), two-phase flow model and buoyancy effects.

Keywords: PWR; Containment; Thermal-hydraulic analysis; Lumped parameter code; ISP-47

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Nomenclature

c_v	–	specific heat at constant volume
E	–	total energy
$\dot{E}$	–	energy flow rate
h	–	specific enthalpy
g	–	acceleration of gravity
g_a	–	mass fraction of air
$\dot{g}$	–	mass flux
L	–	characteristic dimension
m	–	mass
$\dot{m}$	–	mass flow rate
Nu	–	Nusselt number
p	–	pressure
$\dot{q}$	–	heat flux
$\dot{Q}$	–	rate of heat
r	–	latent heat of evaporation
R	–	individual gas constant
Re	–	Reynolds number
t	–	temperature in Celsius scale
T	–	absolute temperature
u	–	specific internal energy
U	–	total internal energy
v	–	specific volume
V	–	total volume

Greek symbols

α	–	heat transfer coefficient
β	–	mass transfer coefficient
$\Delta\pi$	–	driving force for mass transfer
ΔT	–	temperature difference
$\Delta\tau$	–	time step
λ	–	conductivity
ν	–	kinematic viscosity
ρ	–	density
τ	–	time

Subscripts

1	–	beginning of time step
2	–	end of time step
a	–	air
c	–	condensate
D	–	diffusive mass transport
g	–	gaseous medium
h	–	hydrogen

i	–	i-th medium
in	–	inflow
out	–	outflow
s	–	steam
sat	–	saturation conditions
sc	–	steam condensed in the time step
tot	–	total
w	–	water
$wall$	–	walls and structures
we	–	water evaporated in the time step

Superscripts

$'$	–	saturated water
$''$	–	saturated steam

1   Introduction

There are 436 nuclear reactors operating in the world at the moment, and 272 of them are the pressurized water reactors (PWR) [1]. An experience gained through many years of operation of this type of reactors have shown that. PWR is a reliable and safe source of energy. It is highly probable that a third generation PWR will be installed in the first Polish nuclear power plant. Despite of these facts a special effort is put on analyses and improvement of the safety of nuclear reactors.

A nuclear reactor safety has to be analyzed in two aspects: probabilistic and deterministic. Probabilistic safety analysis is aimed to determine the probability of certain accident occurrence [2,3], while the deterministic safety analysis has to predict the course and potential consequences of the accident under consideration [4].

An accident initiated by a rupture of the primary cooling circuit may threat the integrity of the system of barriers isolating radioactive isotopes from the environment and for that reason it has a crucial role in safety of pressurized water reactors. This is the loss-of-coolant accident (LOCA). The rupture of primary circuit is followed by a leak of the primary coolant into the reactor building — the containment. This causes a rapid temperature and pressure increase and the risk of the containment failure occurs. The engineered safety systems have to be installed in order to mitigate consequences of such accident, but knowledge about the course of LOCA is necessary for a proper design of these systems.

It is obvious that analyses of LOCAs cannot be carried out by means of a full-scale physical experiments. Thus, the mathematical modeling and numerical simulations are widely used. The nuclear industry utilizes two

groups of computer codes for thermal-hydraulic analyses of LOCA: lumped parameter (or system) codes and field codes. The system codes are based on one dimensional models of physical phenomena and use of the so-called control zone method for modeling of physical systems. These codes have, at the moment, reached a high level of maturity, and are approved by many nuclear authorities as the official tools for safety analyses.

There is a large experimental database for system codes validation, as described in [5] for example, and it is growing continuously. Despite of this certain processes still remain beyond the system codes modeling capabilities [6–8]. A number of phenomena taking place within containment during the LOCA, as shown in Fig. 1, is clearly three dimensional and the use of computational fluid dynamics (CFD) tools may solve this problem. Unfortunately, the size of the systems under consideration and lack of experimental database for CFD codes validation limit the applications of such tools so far [9].
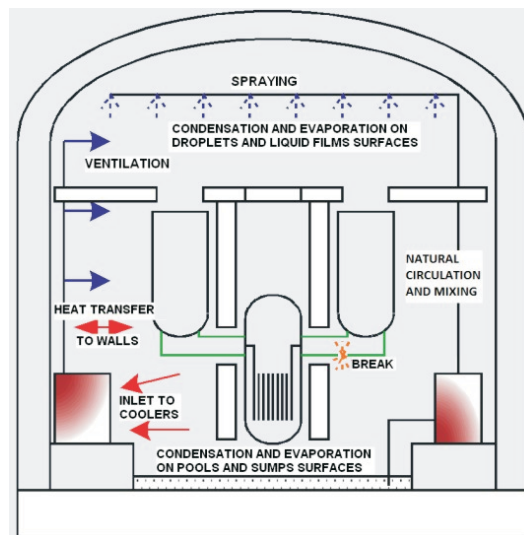

Figure 1. Most important phenomena within a PWR containment during LOCA.

An international cooperation on the codes development is organized, in some cases, within the framework of international standard problems (ISP) [10]. The goal of these projects is creating experimental databases for validation of computer codes and working out standards for doing simulations. International consensus is that a detailed knowledge of containment thermal-hydraulics is necessary to predict the local distribution of hydrogen, steam

and air inside the containment. Considerable international efforts have been undertaken to better understand the associated phenomena by conducting a large number of experiments and then subjecting the test results to extensive analytical assessment: ISP-23 [11], ISP-29 [12], ISP-35 [13], ISP-37 [14].

This work is devoted to validation of an in-door computer code HEPCAL developed for simulations of a pressurized water reactor thermal-hydraulics [17]. The code have been already partially validated against the separate effect test results mainly [17]. In this paper the code's response to more complex integral effect test have been analyzed. As scaling issues may have some influence on results of simulations three different testing facilities (containment models) have been chosen for analysis. Sizes of these testing rigs range from relatively small with very simple internal structure to large ones featuring more complex internal geometry.

2 The computer code HEPCAL

2.1 General description

The computer code HEPCAL, worked out at the Institute of Thermal Technology of the Silesian University of Technology [15,16], has been originally designed for simulations of LOCAs within the water-water energetic reactor VVER 440/213 (from Russian: vodo-vodyanoi energetichesky reactor) containment with the bubble condenser tower. This is a lumped parameter system code using the so-called control volume method to reproduce physical phenomena. This approach is in fact a specific kind of the finite volumes method. The whole containment is simulated by a couple of zones (volumes), connected to each other in the specific way. Usually the geometry and dimensions of a control volume correspond to the real dimensions of the specified compartment of the containment. The control volumes are connected through open channels, orifices, valves, membranes or siphon closures. For each zone homogeneous conditions (perfect mixing) are assumed.

The energy balance equation for a given control zone may be written in the following general form:

$$\dot{E}_{in} = U_2 - U_1 + \dot{E}_{out} \, , \tag{1}$$

where $\dot{E}_{in}$, $\dot{E}_{out}$ are the energy inflow and outflow rates, respectively and U_1, U_2 are the total internal energy at the beginning and the end of the time step.

The energy flow rates flowing into the zone and out of the zone are connected with heat transfer between walls and structures and media within the zone, as well as with the intercompartments substance flow rates. Effects of safety systems operations (pumps, fans, spraying system) should be also taken into account. These energy flow rates and initial internal energy in the control zone are determined based on thermal parameters within the zone at the beginning of time step:

$$\dot{E}_{in} = \sum_{i=1}^{n} \dot{m}_{i,in} h_{i,in} + \dot{Q}_{in,walls} \, , \tag{2}$$

$$\dot{E}_{out} = \sum_{i=1}^{n} \dot{m}_{i,out} h_{i,out} + \dot{Q}_{out,walls} \, , \tag{3}$$

where n is the number of media fluxes.

$$U_1 = \sum_{i=1}^{n} \dot{m}_{i,1} u_{i,1} \, . \tag{4}$$

Next, the internal energy at the end of time step, $\Delta\tau$, can be calculated:

$$U_2 = \left(\dot{E}_{in} - \dot{E}_{out} \right) \Delta\tau + U_1 \, . \tag{5}$$

Unknown thermal parameters at the end of time step are dependent on the value of internal energy.

The model applied in the HEPCAL code allows to determine the thermal parameters (temperature, pressure, density) in the specified volumes and the mass and energy flow rates between the control zones. Safety systems work is taken into account as well as the heat transfer between phases and heat accumulation in the structures of the containment. The code is continuously supplemented and developed. Its latest version, marked as HEPCAL-AD [17] allows for simulations of LOCAs within containment of advanced PWRs (EPR, AP-1000).

2.2   Mathematical basis

The mathematical basics of the model describing changes of thermodynamic parameters of state equations of mass and energy balance for specified phases and equations of state [17]. The equations of mass and energy balance apply to the time step $\Delta\tau$, however the equations of state pertain

to the end of each time step. All the equations are non-linear and their form depend on the state of specified agents in the control volume. The basic set of equations constituting the mathematical model consists of:

- equations of the energy and mass balance for each control volume,
- equations describing intercompartment flows,
- equations of state for the specified gaseous agents (air, steam, hydrogen),
- equations describing additional phenomena, e.g. heat transfer to walls and structures.

The governing equations of the model can be written as follows:

- energy balance for gaseous phase in the time step

$$
F_1 = (m_s + m_{we} - m_{sc})\, h_s - p_s V_g + (m_a c_{va} + m_h c_{vh})\, t_g +
$$
$$
+ m_{sc} h'_s\,(t_g) - m_{we} h''_s\,(t_w) - U_{g1} - \Delta E_g = 0 \,, \qquad (6)
$$

- energy balance equation for liquid phase in the time step

$$
F_2 = \delta_1 \big[\, (m_w - m_{we} + m_{sc})\, c_w t_w - m_{sc} h'_s\,(t_g) +
$$
$$
+ m_{we} h''_s\,(t_w) - U_{w1} - \Delta E_w \big] = 0 \,, \qquad (7)
$$

- equation expressing the sum of the agents volumes

$$
F_3 = (m_s + m_{we} - m_{sc})\, v_s + (m_w - m_{we} + m_{sc})\, v_w - V_{tot} = 0 \,, \qquad (8)
$$

- equation expressing the sum of partial pressures

$$
F_4 = \delta_2 \left[p_a + p_h + p_s\,(t_g) - p_s\,(t_w) \right] = 0 \,. \qquad (9)
$$

Constants δ_1 and δ_2 amount to 0 or 1 depending on the state of steam and water in the specified control volume. These basic equations are supplemented by additional relationships describing heat and mass transfer conditions and intercompartment flows of two phase mixture.

2.3   Simplified heat and mass transfer model

The heat and mass transport from the gaseous atmosphere to walls and structures is one of the most important processes within the containment in LOCA conditions.

The mass transport is linked with the energy flow in every case. As each medium has its specific enthalpy the heat flux related to the diffusive mass transport can be described, in general, as follows:

$$\dot{q}_D = \sum_{i=1}^{n} \dot{g}_i h_i \; . \tag{10}$$

The mass flux is given by the following formula [18]:

$$\dot{g}_i = \beta_i \Delta \pi_i \; , \tag{11}$$

where β_i is the mass transfer coefficient and $\Delta \pi_i$ is the driving force for the mass transfer of i-th medium.
Solubility of hydrogen and air in water is low, so these agents were considered as the inert ones and only the mass diffusion related to steam condensation is taken into account.

The heat is transported in one of three ways as the temperature difference exists. It is the convective heat transport in the case under consideration, so it may be written:

$$\dot{q} = \alpha \Delta T + \dot{g}_s h_s \; . \tag{12}$$

It was assumed that the process is stationary in the given time step and the temperatures of gas and walls, as well as the composition of the gaseous atmosphere in the near wall region are known. Values of these parameters are determined on the basis on computations for the end of the previous time step.

The heat transfer coefficient from internal atmosphere to containment walls and structures may be calculated using three methods:

- Marshall-Holland formula,

- Tagami relationships,

- standard correlations for Nusselt number considering the mass and energy transport related to steam condensation or evaporation.

The first two methods have been implemented into the previous version of the HEPCAL code (marked as HEPCAL-AU), and the last one in the latest version – HEPCAL-AD [17]. The Marshall-Holland correlation relies on experimental results [19] and it relates the heat transfer coefficient value to the current mass of air m_a and steam m_s into the considered control volume:

$$\alpha = C \left(\frac{m_a}{m_s}\right)^{-0.8} . \tag{13}$$

The constant C in Eq. (13) is equal to 320 for concrete walls and 450 for steel walls. It is however not explicitly indicated whether the phase change is considered or not. Moreover, the heat transfer coefficient value computed by this formula is limited to 1580 W/(m²K) in the HEPCAL code.

The maximum value of the heat transfer coefficient determined by Tagami relationships is a function of the energy release rate from the primary circuit to the control volume [20]:

$$\alpha_{\mathrm{max}} = f \left(\frac{\text{energy released to the containment}}{\text{containment volume} \times \text{time peak pressure}}\right) . \tag{14}$$

Experiments have shown that usually the maximum pressure value is reached at the end of the blowdown phase of the accident. The maximum value of the heat transfer coefficient is given by the following formula:

$$\alpha_{\mathrm{max}} = 425 \left(\frac{E_{coolant}}{V \tau_{blowdown}}\right)^{0,6} , \tag{15}$$

where $E_{coolant}$ stands for the energy released along with the coolant from the primary circuit, V is the volume of the control zone where the break takes place and $\tau_{blowdown}$ is the blowdown phase time (it amounts to about 20 s for a large LOCA and rises while the rupture becomes smaller).

The researches realized by Tagami [20] have proved that the increase of the heat transfer coefficient during the blowdown phase has a parabolic trend and it can be written as:

$$\alpha = \alpha_{max} \sqrt{\frac{\tau}{\tau_{blowdown}}} . \tag{16}$$

The heat transfer coefficient value falls down after the blowdown phase till the stagnation phase is achieved. This decrease is described by the following relationship:

$$\alpha = \alpha_{stag} + (\alpha_{max} - \alpha_{stag}) e^{-0.05(\tau - \tau_{blowdown})} d , \tag{17}$$

where α_{stag} is the heat transfer coefficient in the stagnation phase.

The value of heat transfer coefficient stabilizes in the stagnation phase and it is calculated as:

$$\alpha_{stag} = 11.3 + 283.4 \frac{m_s}{m_a} \, d \, . \tag{18}$$

The heat transfer coefficient values computed according to Eqs. (15)–(18) are right for the steel walls. The values equal to 40% of them are assumed for the concrete walls.

Following relationships are implemented in the model for the case of pure steam condensation on a vertical wall [21,22], Nusselt number:

$$\mathrm{Nu} = 0.943 \left[\frac{r \left(\rho_c - \rho_s \right) g L^3}{\left(T_{sat} - T_{wall} \right) \nu_c \lambda_c} \right]^{\frac{1}{4}} \tag{19}$$

for the laminar flow of the condensate and:

$$\alpha = \frac{\mathrm{Re} \nu_c \rho_c r}{L \left(T_{sat} - T_{wall} \right)} \tag{20}$$

for the turbulent flow of condensate. The Reynolds number is calculated from formula:

$$\mathrm{Re} = C A^m \, . \tag{21}$$

The constants $C = 3{\cdot}10^{-3}$ and $m = 3/2$ in Eq. (21) are determined according to [22]. The parameter A is described by the following formula:

$$A = \frac{g^{\frac{1}{3}} \lambda_c L \left(T_{sat} - T_{wall} \right)}{\nu_c^{\frac{5}{3}} \rho_c r} \, . \tag{22}$$

The presence of inert gases decreases the heat transfer coefficient significantly. This is taken into account by calculation of the correction factor, f, dependent on the air mass fraction in the mixture [23]. This parameter is the ratio of the real heat transfer coefficient and the heat transfer coefficient for condensation of pure steam:

$$f = \begin{cases} 1.00 - 1.165 g_a^{0.26} & \text{for } g_a < 0.3, \\ 0.21 - 0.16 g_a & \text{for } g_a > 0.3. \end{cases} \tag{23}$$

It is also assumed that no hydrogen is present in the control volume – only steam-air mixture.

The mass flux is calculated by elimination by the convection driving force, ΔT of the mass transport driving force, $\Delta \pi_s$. According to [18] the

ratio of heat transfer coefficient and mass transfer coefficient is denoted as φ, whereas the ratio of the mass driving force and heat transfer driving force is ψ.

$$\varphi = \frac{\alpha}{\beta_s} \, , \tag{24}$$

$$\psi = \frac{\Delta\pi_s}{\Delta T} \, . \tag{25}$$

Applying the analogy between heat and mass transfer one obtains [18,22]:

$$\varphi = \frac{c_p}{m} \left(\frac{m\eta}{0.74\delta_s} \right)^{0.66} \tag{26}$$

and

$$\psi = \frac{rX}{Rm^*T_{sat}T_g} \, , \tag{27}$$

where: c_p – specific heat capacity at constant pressure for the steam-air mixture, m – ratio of the steam and the steam-air mixture molar masses, m^* – ratio of the steam and air molar masses ($\sim$0.622), T_g – temperature of the steam-air mixture, δ_s – dynamic diffusion coefficient of the steam through the inert gas (air), η – dynamic viscosity of the steam-air mixture, X – the mass fraction of the steam in the air-steam mixture.

2.4   Numerical algorithm

The calculations of unknown quantities are realized in several steps. First, all the mass and energy fluxes are calculated (the leakage of coolant from the primary circuit, the flow rates of agents through the valves, orifices, water flow rate in the spraying system, heat accumulation in walls and structures). Heat transfer between gaseous and liquid phase is also determined. All these calculations refer to the thermal parameters at the beginning of time step and allow to determine the internal energy of gas and liquid at the end of time step. Eventually, one obtains a set of n nonlinear equations which is being solved using the Newton-Rapshon method. At the last step of calculations all the remaining quantities (partial pressures, total volumes of gas and water etc.) are calculated. The computational procedure is repeated in the each time step for each control volume.

The convergence of numerical solution is determined by controlling the residuals of energy balance equations. The default value of a residuum is 0.01. The time step may be defined by the user. It is usual to set short

time steps for the initial phase of simulation (0.001–0.01 s) and next increase
them during calculations.

3   The International Standard Problem No. 47

3.1   General objectives of the ISP-47 project

Despite of all the tests accomplished under the Nuclear Energy Agency
management containment the thermal-hydraulics remains an open ques-
tion, as stated in the report [6]. The main objective of the ISP-47 is to
demonstrate the actual capability of CFD and lumped parameter codes in
the field of containment thermal-hydraulics, e.g. to predict the hydrogen
distribution under LOCA conditions [24]. The proposed activities will lead
to a significant improvement of the reliability of severe accident contain-
ment models/codes. As recommended in the State-oOf-the-Art ReportT
[6] this approach follows a strategy being progressive in modeling difficulty
and it is proposed to realize this ISP in two main steps, the first one is
dedicated to the validation of refined models in the separate effect facility
TOSQAN (7 m^3) and at larger scale in MISTRA (100 m^3), whereas the sec-
ond one addresses the validation of codes in a complex and more realistic
compartmented geometry ThAI (60 m^3).

3.2   TOSQAN testing station

The TOSQAN (TOnus Qualification ANalytique) project has been created
to simulate separate effect tests representative of typical accidental thermal-
hydraulic flow conditions in the reactor containment (wall condensation,
spray, sump, aerosol).

Testing station (see Fig. 2) is a closed cylindrical vessel (total volume
of 7 m^3, inert diameter of 1.5 m, total height of 4.8 m) into which steam
or non-condensable gases can be injected through a vertical pipe located
on the vessel axis. The spray is injected on the vessel axis, 0.7 m from
the top of the facility. Over 150 thermocouples are located in the vessel
(in the main flow and near the walls). For mass spectrometry 54 sampling
points are used for steam volume fraction measurements. Optical accesses
are provided by 14 overpressure resistant viewing windows permitting non-
intrusive optical measurements along the enclosure diameter at 4 different
levels (laser Doppler velocimetry and particle image velocimetry techniques
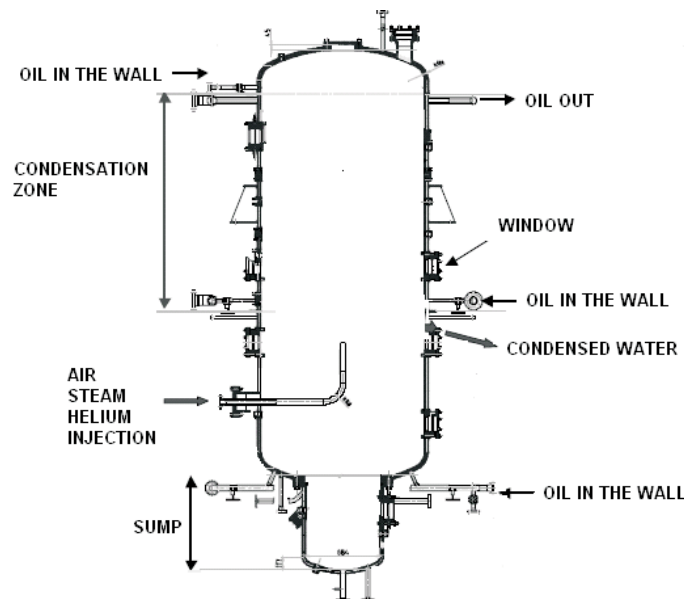for the gas velocities, Raman spectrometry for steam volume fractions).

Figure 2. Cross section of the TOSQAN vessel (prepared according to [24]).

The TOSQAN vessel has thermostatically controlled walls so that the wall temperatures can be kept constant.

3.3   MISTRA testing station

The MISTRA testing station consists of a stainless steel vessel with 99.5 m^3 in volume, 7.3 m in height and 4.25 m in diameter. Three independent condensers are inserted inside the containment close to the external walls. A lower centered injection is concerned in these ISP-47 tests. Figure 3 shows the main characteristics of the facility and the location of the measurements in the so-called highly instrumented half plane (gas temperature, gas concentration, laser Doppler anemometry).

3.4   ThAI testing station

The ThAI facility can be characterized as a coupled-effects test facility. It allows investigation of natural convection and atmospheric stratification, heat exchange between solid structures and vessel atmosphere, heat conduction in solid structures, as well as steam condensation on walls and in the atmosphere, and transport of condensed water. The ThAI containment
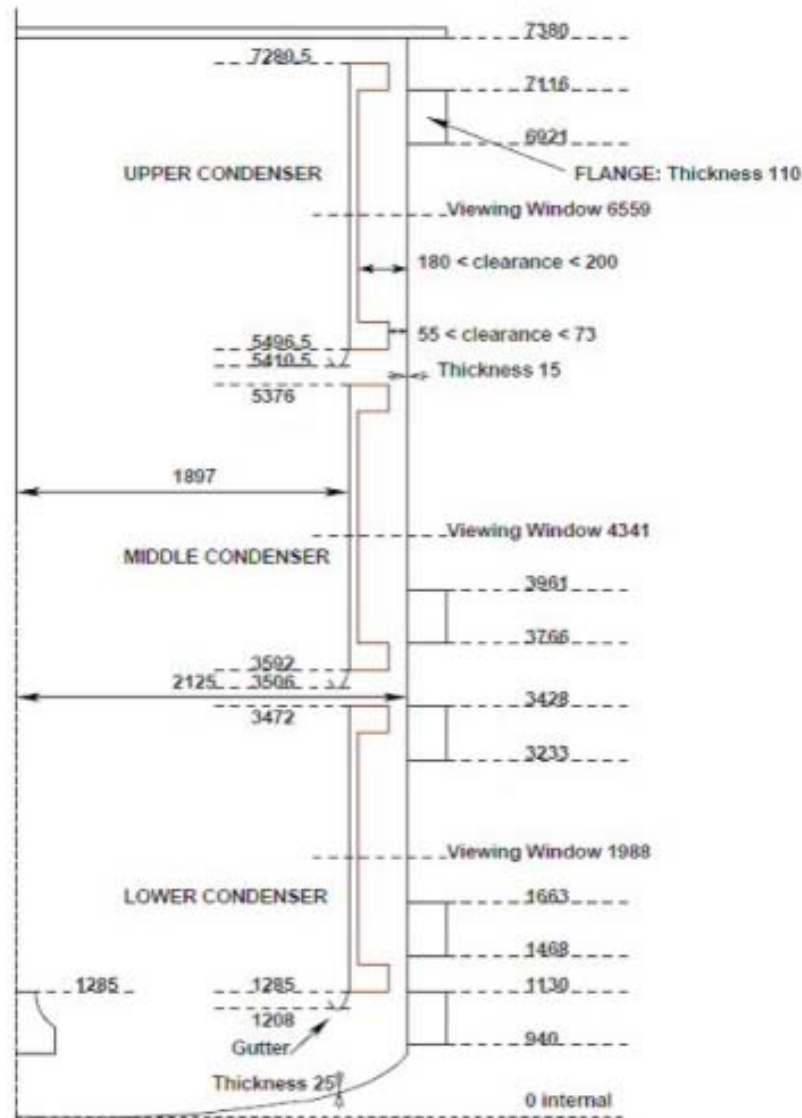
Figure 3. MISTRA vessel – symmetry half plane [24].

model is presented in Fig. 4. The ThAI is a cylindrical steel vessel with 60 m³ in volume, 9.2 m in height and 3.2 m in diameter. Internal structures are an inner cylinder of 1.4 m in diameter and 4 m in height, and a horizontal separation plate with vent flow openings.
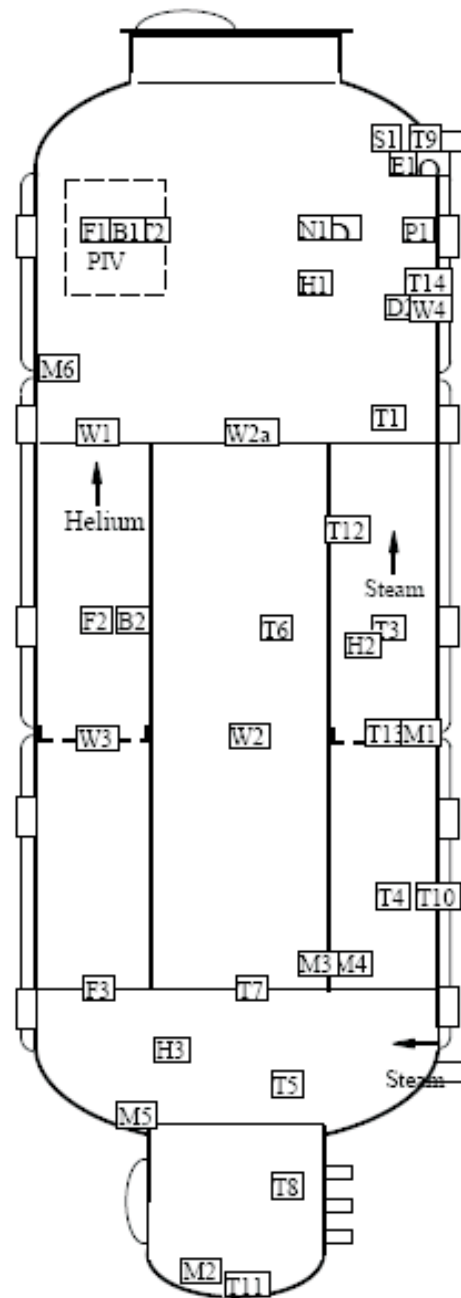
Figure 4. ThAI vessel with localization of injection and measuring points [24].

4 Experimental scenarios and results of simulations

The numerical results presented further in this section have been obtained by using the newest version of the code – HEPCAL-AD. The numerical models (nodalization of the vessels and boundary and initial conditions) have been prepared according to report [24]. The HEPCAL models of the systems under consideration consist of 4 control zones for the TOSQAN facility, 3 control zones (next changed into 7) for the MISTRA facility and 10 control zones for the ThAI vessel. Due to limited availability of detailed experimental data only pressure trends are compared and shown for TOSQAN and MISTRA tests. The presented values of parameters are the average values over the whole vessel volume, if not otherwise specified.

4.1 TOSQAN experiment

The TOSQAN ISP test is composed of a succession of different steady-state conditions obtained by varying the injection conditions in the test vessel. The main stages of interest for the measurements are the four steady-state conditions: three steady-state conditions of air-steam mixture at two different pressure levels (Phase A), and one steady-state condition of air-steam-helium mixture (Phase B). Each steady-state condition is reached naturally by keeping a constant steam injection flow rate [24]. The mass flow rates of the all mediums during the ISP experiment are shown in Fig. 5.

The first stage of simulation consists of three code runs with applying three methods of the heat transfer coefficient determination. Only the initial phase of experiment has been simulated. The results are compared in Fig. 6. This comparison confirmed observations made in [26] and [27]. Considering this the heat transfer coefficient has been calculated using the Nusselt number correlations in all remaining simulations.

The measured and calculated pressure trends inside the TOSQAN vessel there are presented in Fig. 7. These results are very similar, both qualitatively and quantitatively. Some more visible discrepancies appear while helium is injected into the vessel. A plausible explanation of this is neglecting the influence of this gas on the heat transfer coefficient.
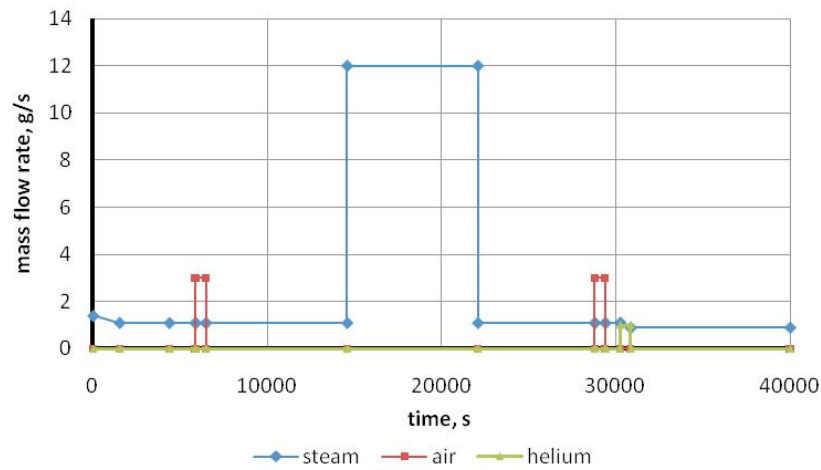
Figure 5. TOSQAN ISP-47 experiment – mass flow rates of steam, air and helium (prepared according to [24] and [25].
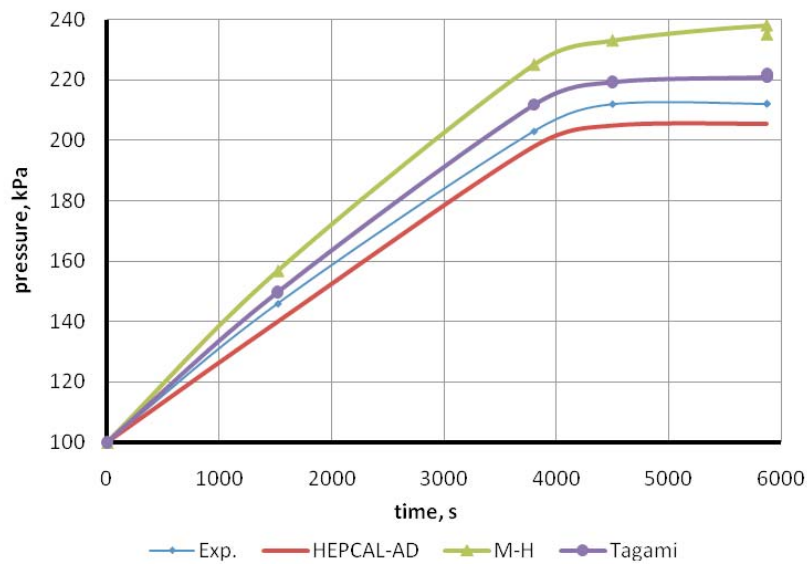

Figure 6. TOSQAN ISP test – initial phase, comparison of different methods of the heat transfer coefficient calculation.
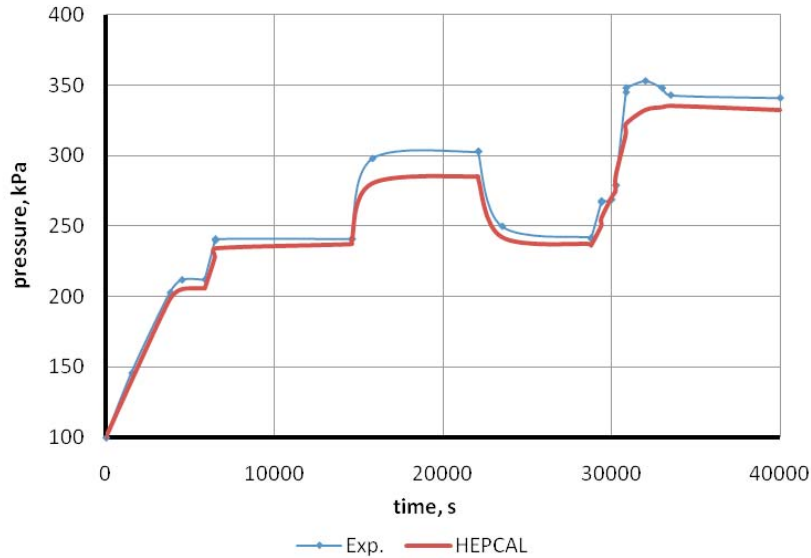
Figure 7. Pressure trends inside the TOSQAN vessel during the ISP-47 test.

4.2   MISTRA experiment

The simplified test sequence related to the ISP-47 exercise done on the MISTRA testing rig is made up of four successive phases:

(1) Preheating phase: superheated steam injection into the facility initially at room temperature and pressure. This is a process phase mainly used to heat up the steel structures.

(2) Air/steam steady state (Phase A) defined from the balance between the injected and condensed mass flows (130 g/s) ensuring the stability of all the parameters: pressure, temperature and gas concentrations.

(3) Air/steam/helium transient mass flow of helium (simulating hydrogen) is added to the main steam mass flow at a rate of 10 g/s for half an hour.

(4) Air/steam/helium steady state (Phase B) with the same definition and boundary conditions as for Phase A.

Two experiments realized on the MISTRA testing station have been simulated using the HEPCAL code. MASP0 test is the reference case and it

encloses only one phase – depressurization due to natural circulation of the internal atmosphere and heat losses to the environment. The MASP1 test consist of two phases: natural depressurization (up to 2100 s) and spraying phase (from 2100 to 3900 s). The comparison of the experimental and numerical pressure trends is presented in Fig. 8. One may see that the numerical pressure trend for the MASP0 test is a little bit overestimated at the beginning of the test and then the pressure falls down below the experimental values. A probable reason for such situation is very coarse nodalization of the vessel. This effect has been previously observed in the real plant simulations also, see [28] for example. Beside of this the similarity of the results is satisfactory.
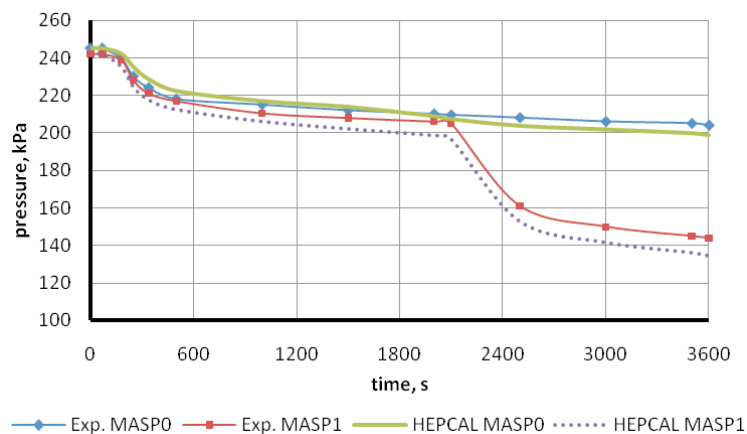

Figure 8. Comparison of pressure trends for the MISTRA test MASP0 and MASP1.

4.3   ThAI experiment

The experiment considered as the ISP-47 project part was divided into 3 phases with gas injections at 3 different locations and the last phase with out gas injection. Initially, air featuring about 70% humidity was present in the vessel. The temperatures of vessel structures, atmosphere and surroundings was 22 ºC, while the atmospheric pressure was 100 kPa. During the 1st phase of the experiment which lasted from 0 to 2700 s, helium at 20 ºC was injected into the vessel with a mass flow rate of 0.59 g/s together with a small amount of steam (0.16 g/s). Later, during the 2nd phase of the experiment, from 2700 to 4700 s, steam at 111 ºC was injected

into the vessel with a mass flow rate of 35 g/s. Steam condenses on the cold structures of the ThAI vessel. Helium and steam were injected upwards during these phases in the upper part of the ThAI vessel. During the 3rd phase, steam at 111 °C was injected into the lower part of the vessel in the horizontal direction with a flow rate of 35 g/s from the time step of 4700 to 5700 s. The last (4th) phase lasted from 5700 to 7700 s without any injection of gases.

Only first and second phases of experiment have been simulated due to lack of sufficient data for comparison. The results are shown in Figs. 9–11. One may note that numerical results remain in a quite good conformity with the experiment.
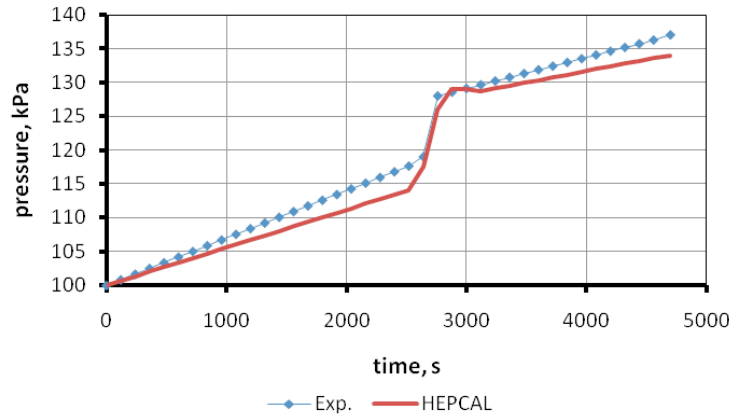

Figure 9. Comparison of pressure trends for ThAI IPP test.

5   Conclusions

The main aim of this work has been to validate the HEPCAL-AD code against experimental results. The heat and mass transfer phenomena are dominant during the loss-of-coolant accident within containment of a pressurized water reactor. For that reason the set of the ISP-47 project experiments has been considered as the most suitable for validation of the mathematical models implemented into the HEPCAL-AD code.

The analyses performed for the TOSQAN and MISTRA experimental stations were aimed at evaluation of different methods of the heat transfer coefficient determination and checking the heat and mass transport models.
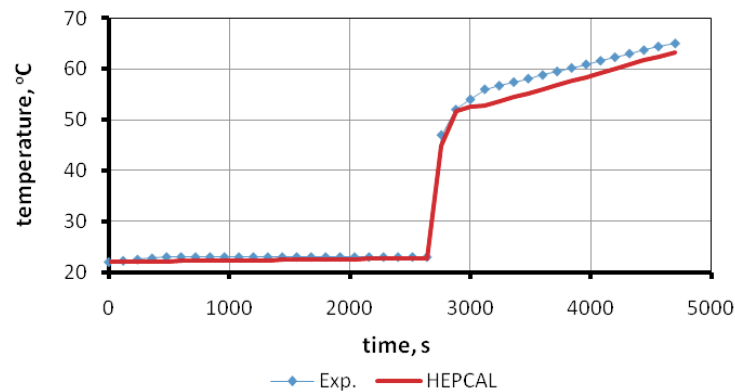
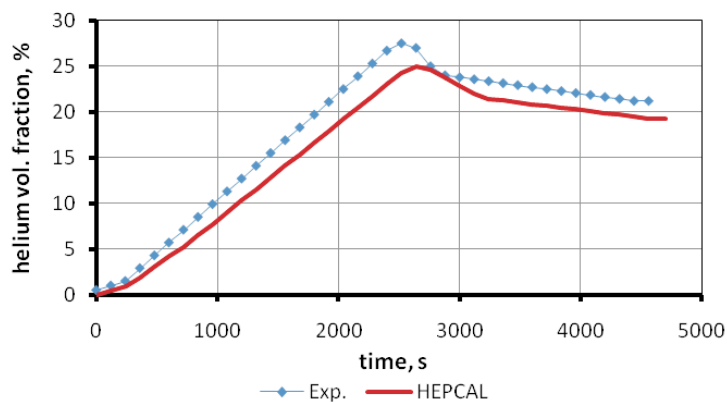Figure 10. Comparison of temperature trends for ThAI ISP test.

Figure 11. Helium concentration in the upper plenum of the ThAI vessel during the ISP
          test.

The heat transfer coefficient may be calculated by using three methods.
The usage of the standard correlations for Nusselt number and consider-
ing the mass transfer related to the steam condensation gave only a fair
consistency of calculations. Application of the methods based on empirical
correlations for the heat transfer coefficient calculation resulted in their val-
ues much smaller than experimental. A probable reason for such situation
is neglecting or not correct implementation of phase change phenomena.
Although the empirical equations are very convenient to implement into
the code and their application makes the simulation shorter, they may lead
however to wrong results. The third applied method for the heat transfer

coefficient determination has given best results in the analysed case, but the use of this method requires a lot of data which may not be always available for a real plant simulation.

The HEPCAL code validation accomplished according to the ThAI experiment results shows that the model may be used for assessing the behaviour of hydrogen (please note that helium was used instead of this gas during measurements) within a containment of a PWR during the loss-of-coolant accident.

It may be noted that numerical results are a little bit underestimated in most of the presented cases. A plausible explanation may be overestimation of the heat transfer coefficient from the gaseous atmosphere to wall and structures caused by neglecting the influence of hydrogen (helium) as the inert gas. Another reason for this situation could be too high efficiency of spraying (actually set equal to 1.0 in all simulations).

Received 4 January 2012

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