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Coupling of CFD and lumped parameter codes for thermal-hydraulic simulations of reactor containment

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The work deals with thermal-hydraulic analyses of a pressurized water reactor containment response to accidents caused by a rupture of primary circuit. The in-house system computer code HEPCAL-AD and CFD ANSYS Fluent have been coupled for these simulations. The aim of this work is verification of possible ways of the codes coupling. The assessment of each method has been done by comparing the computational results with experimental data obtained from testing rigs of the AP-600 reactor containment cooling system. Additional simulations of a loss-of-coolant accident (LOCA) have been carried out as well, and compared with outcomes of the AP-600 reactor simulator.

Keywords: reactor containment, thermal-hydraulic analysis, lumped parameter code, CFD code, coupling.

Nomenclature

Symbols
c – specific heat capacity,
$\dot{E}$ – energy transfer rate,
h – specific enthalpy,
m – mass,
p – pressure,
t – temperature,
U – internal energy,
v – specific volume,
V – total volume,
ΔE – energy change in time step,
$\Delta\tau$ – time step.
Superscripts
$'$ – saturated water conditions,
$''$ – saturated steam conditions,
Subscripts
1 – beginning of time step,
2 – end of time step,
a – air,
g – gas,
h – hydrogen,
in – flowing into a control zone,

out – flowing out of a control zone,
s – steam,
sc – steam condensed in time step,
tot – total,
we – water evaporated in time step.

1. Introduction

Deterministic safety analyses for nuclear reactors are conducted by means of mathematical modeling and computer simulations. Thermal-hydraulic analyses of potential accidents play very important role in overall safety assessment. The nuclear industry has developed two types of computer codes for such analyses: the system codes, also called the lumped parameter codes, based on one-dimensional models of physical phenomena, and the field codes, based on three dimensional models and CFD technique [1]. The latter are mostly specialized CFD codes for nuclear purposes [2].

The system codes have reached a high level of maturity and are well recognized and approved by many nuclear authorities as official tools for safety analyses. There is however a certain number of phenomena which cannot be modeled by system codes properly or at all (mixing, natural circulation, stratification, hydrogen behavior). A meaning of these phenomena for an accident progress may be high, so the detailed knowledge is necessary for proper prediction of the system behavior. The obvious solution to this problem is application of the CFD tools. Unfortunately, there are some limitations at the moment:

- the size of the systems under consideration makes creation of the numerical models and computations very time-consuming;
- there is no sufficient experimental database for validation of the results.

Lumped parameter codes will always require less CPU time than CFD. Therefore, it is evident that these codes will always act as the main "workhorse" for analyzing containment thermal-hydraulics. Lumped parameter codes also have some inherent limitations (some of them mentioned before) mainly due to the applied simplified models of flow processes. This results in a significant user influence on code results. This issue is evidenced in the International Standard Problem No. 47 (see [3]). Therefore, combined use of both lumped parameter codes and CFD codes is recommended. Such a combination would use a lumped parameter code as the main tool for the containment analyses, and a CFD tool will be used to analyze selected accident scenarios. The main objective of the combined approach is to improve and guarantee the quality of the containment thermal-hydraulic analyses. Even CFD codes validation results show some opportunities to improve the reliability of thermal-hydraulic analysis by the use of a combined approach [4].The described approach assumes practically independent use of lumped parameter and CFD codes.

Coupling between system (lumped parameter) and CFD codes for their parallel use and with an exchange of computational data has been postulated as a new method for thermal-hydraulic analyses of nuclear reactor systems a few years ago. Such a coupling may be easily done for steady-state analyses. For example: a coolant flow through the reactor core may be simulated in three dimensions by a CFD tool in order to obtain the velocity and temperature field, while the remaining parts of the primary circuit are simulated by a system code. Application of this method for transient computations is a little bit more complicated.

This work deals with thermal-hydraulic analyses of containment behavior during transients and accidents. The author used an in-house lumped parameter code HEPCAL and a commercial CFD software ANSYS Fluent to try out possibilities of coupling these numerical tools in order to create a more realistic model of an advanced reactor containment. The presented solution is the first of its type or represents the first major attempt to couple these two numerical tools.

2. Characteristics of analyzed object

The AP-600 reactor is a medium-size Westinghouse pressurized water reactor of 600 MW electric rated power. The reactor is similar to the previous generation, but contains a number of new solutions for safety systems. The project utilizes almost exclusively passive safety systems, whose operation is based on the laws of nature – gravity, pressure difference and natural circulation.

The containment construction for the AP-600 reactor is shown in Fig. 1. The steel containment vessel encloses the primary circuit with the passive safety systems. This vessel is an integral part of the containment passive cooling system. The containment is surrounded by the concrete shield building. There is a gap between the steel vessel and the shield building which allows for natural circulation of the air. [5] One unique feature of the AP-600 is its passive containment cooling system (see Fig. 1). This system is required to keep the internal pressure below the design limits for at least 72 hours without any operators action. During the design-basis accident, either a loss-of-coolant or a main-steam line-break, large amounts of steam appear in the containment vessel and come in contact with much cooler walls. Heat is transported to these structures by convection and condensation, and through the steel walls by conduction. Heat is then transported to the air flowing within annular gap formed between the containment steel vessel and the concrete shield building. The external passive spraying system is activated as the internal pressure crosses 115 kPa. The water drains by gravity from the tank located at the top of the shield building. Evaporation of water on the external steel vessel surface intensifies heat transfer to the flowing air.

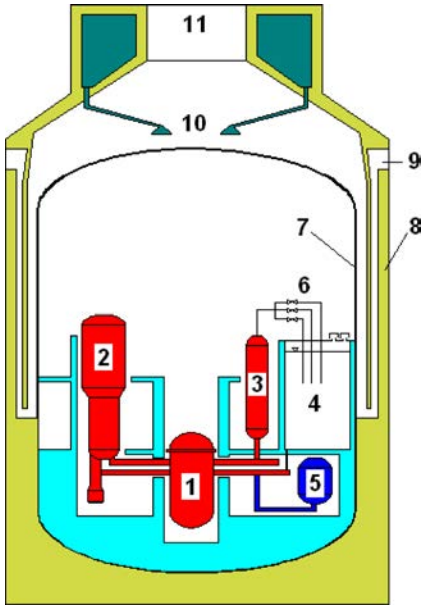

Fig. 1. Containment structure of the AP-600 reactor: 1 – reactor pressure vessel, 2 – steam generator, 3 – pressurizer, 4 – in-containment refueling water storage tank, 5 – hydro-accumulator, 6 – automatic depressurization system valves, 7 – steel containment vessel, 8 – shield building, 9 – air intake, 10 – external spraying system, 11 – air discharge.

3. Numerical tools

3.1. Lumped parameter code HEPCAL

The obtained results are an outcome of simulations performed using the HEPCAL-AD code. This code has been developed at the Institute of Thermal Technology of the Silesian University of Technology [6]. The code, which is of the lumped parameter type, is designed to predict changes of thermodynamic parameters within containment during LOCA. The whole containment is simulated

by a couple of zones (volumes), connected to each other in a given way. Usually the geometry and dimensions of a control volume correspond to the real dimensions of the specified compartment of the accident localization system. The control volumes are connected through open channels, orifices, valves, membranes or siphon closures. For each zone homogeneous conditions (perfect mixing) are assumed. Considering this, one may note that the applied model is a discrete one in reference to space and time also. Its base are the energy balance equations written for each specified control volume in a given time span (time step) $\Delta\tau$. Energy streams flowing in and out of the control volume are associated primarily with heat transfer to walls and structures and intercompartment flows of media. A very important issue in modeling is taking into account operation of safety systems. Mass and energy streams resulting from operation of pumps, fans and other devices should be considered in the energy balance. These quantities as well as the initial internal energy U_1 are determined based on the values of thermodynamic parameters at the beginning of time step. Transforming general relationship for energy balance in a control zone one obtains:

$$U_2 = (\dot{E}_{in} - \dot{E}_{out})\Delta\tau + U_1. \tag{1}$$

The right-hand side components of Eq. (1) are known, so the internal energy at the end of the time step can be calculated. Unknown thermodynamic parameters at the end of the time step are functions of the internal energy U_2.

Such an approach allows for one-dimensional analysis and determination of time-dependent changes of basic thermodynamic parameters (temperature, pressure)within the containment building. It should be clearly stated that the model does not include processes taking place within the primary cooling circuit. Data considering the coolant leakage (mass flow rates and specific enthalpy) are the boundary conditions for HEPCAL code. These informations are obtained from external programs.

The mathematical basis of the model describing changes of thermodynamic parameters consist of the equations of mass and energy balance for specified phases and equations of state [6–8]. The equations of mass and energy balance apply to the time step; however, the equations of state concern to the end of each time step. All the equations are nonlinear and their form depend on the state of the 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 the walls and structures, operation of safety systems.

As thermodynamic nonequilibrium between states is assumed the basic equations mentioned earlier may have different form, depending on an actual state of water and steam within the control zone. The model includes six possible cases:

a) lack of water, superheated steam;

b) subcooled water, superheated steam;

c) subcooled water, saturated steam;

d) saturated water, superheated steam;

e) saturated water, saturated steam;

f) lack of water, saturated steam.

The basic equations for cases a–e, in general form, can be written as follow [6]:

- energy balance equation for gaseous phase in time step

$$F_1 = (m_s + m_{we} - m_{sc})h_s - p_s V_g + (m_a c_{va} + m_h c_{vh})t_g + m_{sc}h'_s(t_g) - m_{we}h''_s(t_w) - U_{g1} - \Delta E_g = 0; \quad (2)$$

- energy balance equation for liquid phase in time step

$$F_2 = \delta_1[(m_w - m_{we} + m_{sc})c_w \cdot t_w + m_{we} \cdot h''_s(t_w) - m_{sc} \cdot h'_s(t_g) - U_{w1} - \Delta E_w] = 0; \quad (3)$$

- equation expressing the sum of volumes of the phases at the end of time step

$$F_3 = v_w(m_w - m_{we} + m_{sc}) + v_s(m_s + m_{we} - m_{sc}) - V_{tot} = 0; \quad (4)$$

- equation expressing the sum of partial pressures (Dalton's law) at the end of time step

$$F_4 = \delta_2[p_a + p_h + p_s(t_g) - p_s(t_w)] = 0. \quad (5)$$

Relationships (2)–(4) are valid for cases a–d. Equation (5) is valid only for the case e. Values of constants δ_1 and δ_2 are

$\delta_1 = 1$ for cases b, c, d, e,
$\delta_1 = 0$ for case a,
$\delta_2 = 1$ for case e,
$\delta_2 = 0$ for cases a, b, c, d.

Some numerical problems, leading to unreal values of thermodynamic parameters, may appear in the case of very little amount of water in a control zone. Due to this reason after crossing the minimum, limiting amount of water in the control zone the model assumes thermal equilibrium between phases. So, in the case f it is considered that $t_g = t_w$. In such a case the unknown parameters are: gas temperature t_g and mass of condensed steam m_{sc}. These quantities are determined using the energy balance equation for both phases:

$$F_1 = (m_s - m_{sc})h''_s(t_g) - p_s(t_g) \cdot V_g + (m_a \cdot c_{va} + m_h \cdot c_{vh})t_g + (m_w + m_{sc})c_w \cdot t_w - U_{g1} - U_{w1} - \Delta E_g - \Delta E_w = 0 \quad (6)$$

and Eq. (4).

Determination of unknown parameters is a gradual process. In the first step, mass and energy streams are determined, i.e., leak of coolant from the primary circuit, media flows through the intercompartment junctions, mass flow rate of water from the spraying system and accumulation of heat in walls and structures. Heat transfer between phases is also calculated in this step. All these quantities regard to the beginning of time step and allow for determining the internal energy of gas and liquid.

Taking this into account, the amounts of media as well as the internal energy at the end of time step are computed in the second step. The amounts of steam and water and their internal energies initially are determined neglecting the phase changes during the time step.

The values of the basic thermal parameters are determined in the third step. For calculation of these parameters from equations (2)–(6) are chosen these ones which are valid for actual state of media within the control volume. Eventually, one obtains a system of n nonlinear equations, which is solved using the Newton-Raphson's method. This system can be noted in general form as:

$$F_i(x_1, x_2, \ldots, x_n) = 0, \quad (7)$$

where x_i stands for an unknown parameter. A number of equations in the system depend on current state of agents in the control zone. The calculating process is repeated in each time step for every control zone until the desired accuracy is achieved.

Values of remaining unknown parameters (pressures, volumes and final masses of agents) are computed in the last step from basic thermodynamic laws and geometrical relationships.

The model applied in the HEPCAL code allows to determine the thermal parameters (temperature, pressure, density) in the specified volumes and the mass flow rates as well as the energy transfer rates between the control zones. The spraying system work is taken into account as well as the heat transfer between phases and heat accumulation in the structures of the containment.

Considering the spraying system operation is an important issue. The HEPCAL code uses a spraying efficiency parameter in order to simulate spraying system work. This efficiency is defined as the ratio between the real heat transfer rate between gaseous atmosphere and water droplets to the maximum heat transfer rate at given temperature difference.

3.2. CFD model

There have been several numerical models built for a detailed simulations using the commercial CFD software ANSYS-Fluent. The CFD models have been elaborated for the modeling of natural circulation phenomena taking place between the steel vessel and the shield building for the AP-600 reactor. All models worked out up to date are two-dimensional and their geometries have been created using Gambit preprocessor. The first model has been elaborated for the purpose of determination of the heat transfer coefficient from the steel vessel outer wall to the flowing air. This 2D model assumes axial symmetry and consists of only a part of the considered system. This model, as well as the second one (see Fig. 2), has been used for simulations in coupling with the HEPCAL code.

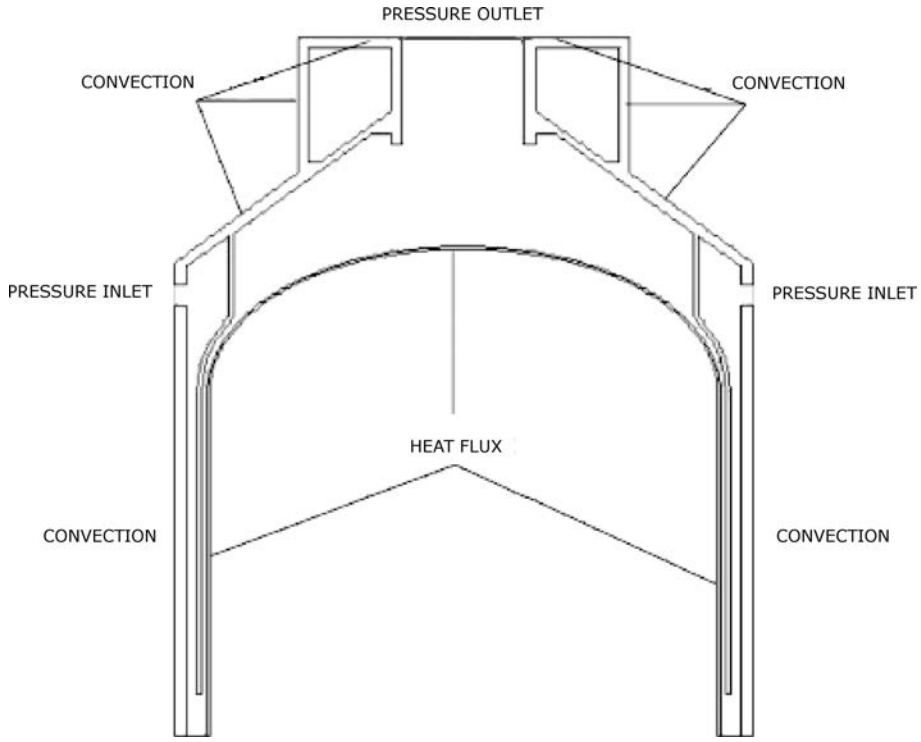

Fig. 2. Geometry of the containment CFD model and boundary conditions set.

The numerical mesh for all the models is created by the quad type elements which number ranges from about 60 to 430 thousands. The CFD model of the analyzed system has been completed by

applying energy balance equation, continuity equation and momentum balance equation to the numerical mesh. These equations have been supplemented by equations of state and turbulence model. Testing computations performed in the first step allow also to choose a turbulence model. The k-turbulence model has been used for basic computations.

4. Codes coupling and its verification

The HEPCAL code cannot accurately simulate natural circulation of fluids. To be more precise, only thermal processes regarding natural convection are modeled using this code. The first attempt to apply the HEPCAL code for the considered AP-600 containment system gave non-physical results. The general idea of coupling the HECPAL code with commercial CFD package, taking into account the AP-600 reactor containment structure, is as follows: the processes taking place within the steel containment vessel are simulated by the HEPCAL code and the space between the vessel and the shield building is modeled by the CFD model. The coupling of both codes takes place on the outer walls of the steel vessel. The pressure inlet and pressure outlet boundary condition type were used for the external air intake and outflow respectively. The natural convection conditions have been assumed for the outer walls of the shield building (see Fig. 2).

4.1. Method No. 1

The first method of coupling has been applied for reproduction of the heat transfer coefficient from the steel vessel outer wall to the flowing air. The simulations have been realized as follows. First, the HEPCAL code has been started with assumed constant value of the heat transfer coefficient from the walls to the air in the considered area. After computations are converged in time step (0.001 s) the HEPCAL code is stopped. Heat fluxes from internal atmosphere to the containment walls are then put into Fluent code as the boundary conditions and the CFD simulation is started assuming steady state conditions. The heat transfer coefficient from external containment wall to the air flowing through gaps is then calculated based on known fluid and walls temperatures and the heat fluxes. The computed value is then used for the next time step simulations with the HEPCAL code. The heat transfer coefficient taken from the CFD model is applied as the constant value along the air gap to the lumped parameter code.

4.2. Method No. 2

Previous method of coupling has been used for simulations without considering the spraying system operation. The CFD models described earlier did not include the spraying system model. Thus, in the second method the HEPCAL code was used to simulate LOCA course in the whole analyzed object, including the gas gap and external spraying system work.

The calculations were stopped after every time step. Applying the same CFD model as in previous method the mass flow rates of the air flowing into the gap and discharging to the atmosphere were computed and put into the HEPCAL code.

4.3. Verification of coupling methods

Both proposed methods, of coupling have been verified against the experimental results obtained from two specially designed test stations. These test facilities are similar and the reason for using them for verification of coupling methods was availability of experimental data.

4.3.1. Westinghouse large-scale test facility No. 1

The first AP-600 passive containment cooling large-scale test facility includes a steel pressure vessel (cross-section shown in Fig. 3), 6 m high by 4.5 m in diameter. The vessel initially contains air at 101.325 kPa of absolute pressure. The vessel is surrounded by an acrylic cylinder which forms a 75 mm air cooling annulus [9].

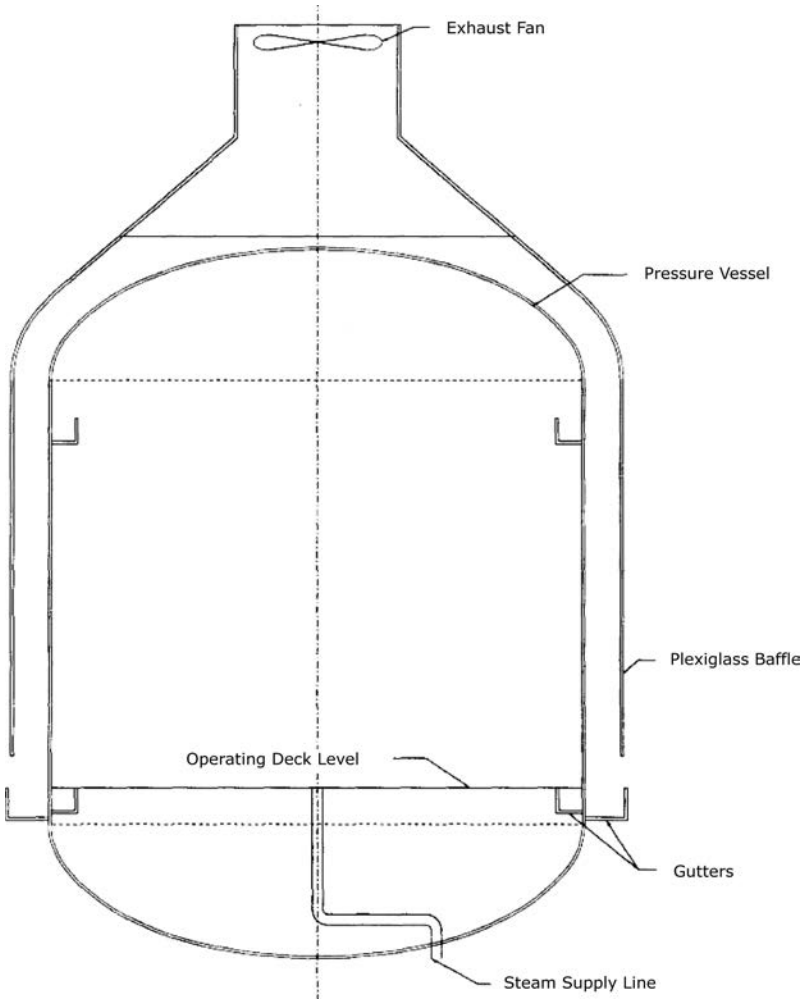

Fig. 3. Cross-section of the large-scale test facility No. 1 [9].

Superheated steam from a boiler is throttled to a variable but controlled pressure and is supplied to the center of the vessel through a 75 mm pipe as shown in Fig. 3. An axial fan at the top of the annular shell provides the ability to run tests at higher air velocities than can be achieved during natural convection. The tests used for verification were performed with the fan operating. Air flowing up the annulus cools the vessel surface, resulting in condensation of the steam inside the vessel. The tests discussed in this paper are from the initial AP-600 large scale test series which has no representation of the full scale plant internals. The vessel only contains an operating deck grating approximately 1.45 m from the bottom of the vessel. The tests are constant pressure tests, i.e., a pressure is specified and the steam flow is adjusted to achieve that pressure. All test results given in [9] and used for verification are at steady state conditions at ambient atmospheric conditions. To establish the total heat transfer from the test vessel, measurements are recorded for steam inlet pressure, temperature, and condensate flow and temperature from the vessel. Eighty thermocouples located on both the outer and inner surfaces of the vessel wall indicate the temperature distribution

over the height and circumference of the vessel. Thermocouples placed approximately 25 mm inside the pressure vessel provide a measurement of the vessel bulk steam temperature as a function of position.

Only two tests without active spraying system have been analyzed using the CFD model of the first large-scale test facility. The CFD model has been prepared analogically to the previous case. Due to the limited data available pressure has been compared and the maximum ratios of numerical to experimental pressure values are 1.06 and 1.09 for two considered cases. This agreement between numerical and experimental results is good/satisfactory.

4.3.2. Westinghouse large-scale test facility No. 2

More experimental data is available for the second AP-600 containment model. This system, illustrated in Fig. 4, consists of ellipsoidal upper and lower domes and a cylindrical shell between the domes. The domes have a horizontal major axis of 1.5 m and a vertical minor axis of 0.8 m. The cylinder has a height of 3 m. A cylindrical air baffle is placed outside of the cylindrical containment vessel with an air gap of 0.2 m. The whole system is initially stagnant at 25°C and 1 atm. To simulate a design basis accident (DBA), steam is introduced into the containment vessel by a jet at the bottom of the lower dome. The inlet steam has a temperature of 140°C and a flow rate of 0.1 kg/s. At the same time, water of a temperature 25°C starts to spray on the outside surface of the upper dome at a constant rate of 0.5 kg/s. Air enters the bottom of the annulus at a velocity 2 m/s, carrying heat and moisture as it flows out at the top chimney [10].

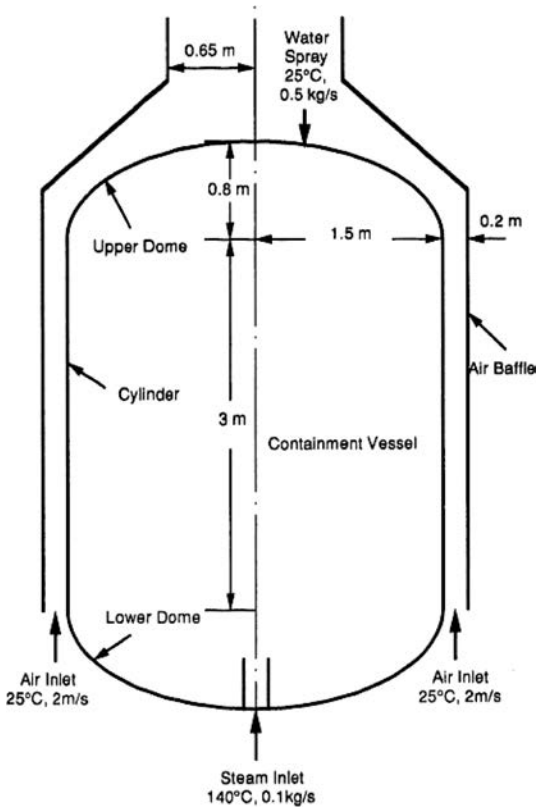

Fig. 4. Cross-section of the large-scale test facility No. 2 [10].

The CFD models of described test facility have been elaborated (as shown in Fig. 5), next, boundary conditions as presented in Fig. 2 have been applied to the models. These models have been next coupled with the HEPCAL code model consisting of three control zones: lower and upper domes and cylindrical part.

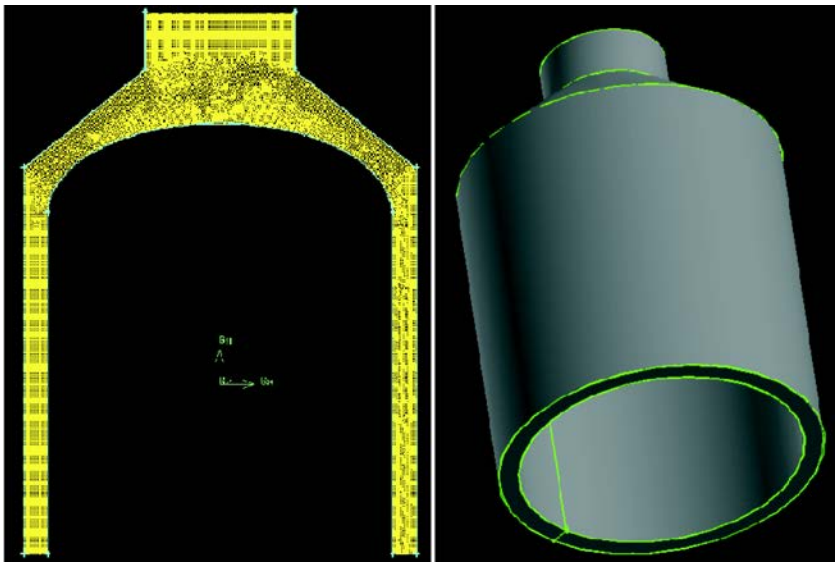

Fig. 5. Geometries of two- and three-dimensional CFD models of the large-scale test facility No. 2.

Several experiments have been then simulated using both coupling methods. The second coupling method has been applied as the wet tests were analyzed. The time-dependent pressure trend for selected test is shown in Fig. 6. The transient pressures are normalized to the steady-state measured pressures. This is done with the available data [11].

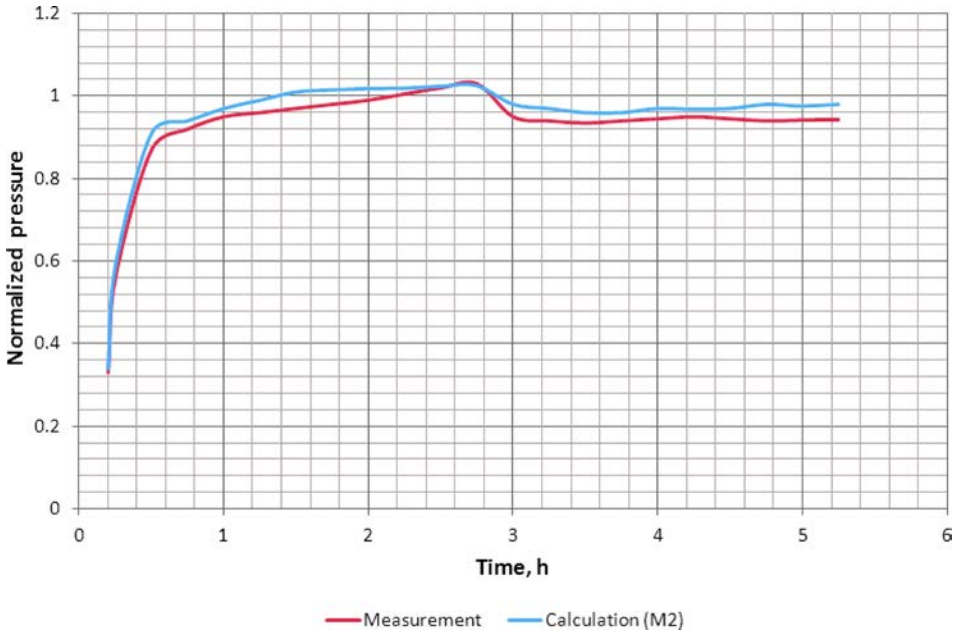

Fig. 6. Comparison of experimental and computational normalized pressure values.

4.4. Results of simulations for the AP-600 reactor containment

The accident scenario used for this analysis is a small break LOCA which assumes a rupture of the primary circuit hot leg. The break diameter is about 75 mm. The break appears near to the reactor outlet nozzle.

It has been assumed that all safety and emergency systems work properly. The initial containment temperature is 30°C and the initial pressure value is 100.0 kPa. The external steel containment dousing in the AP-600 system is actuated at the internal pressure of 115 kPa.

The HEPCAL code computational domain consists of three control zones:

- reactor shaft;
- steam generator box;
- operational deck compartment (whole space under the containment dome).

As it can be seen in Fig. 1 only the last space has a direct contact with steel containment walls. Due to this the heat flux calculated for this control zone has been applied as the boundary condition to the CFD model.

The time-dependent pressure and temperature trends obtained from simulations are presented in Figs. 7 and 8. The results seem to be rational and the observed parameters behave as expected. These results also remain in quite good compliance with outcomes of the AP-600 reactor simulator [12] for the analyzed scenario – see dotted lines in Figs. 7 and 8.

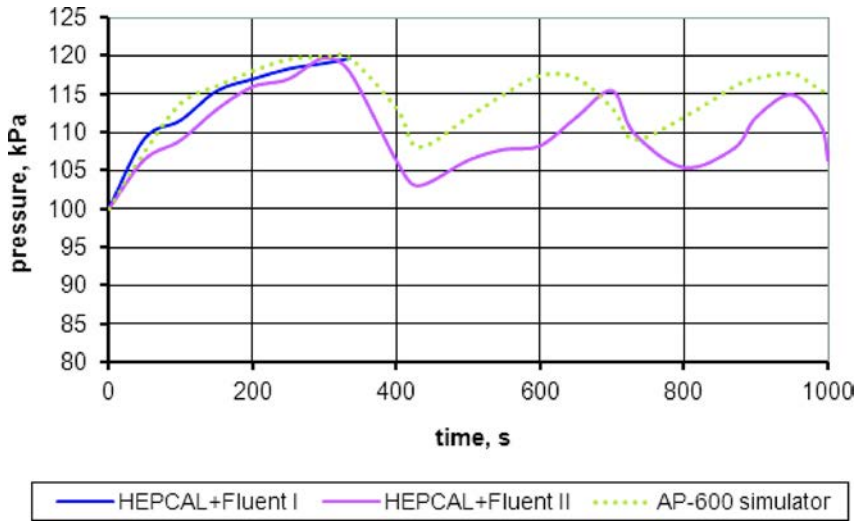

Fig. 7. Pressure trend within steel containment vessel.

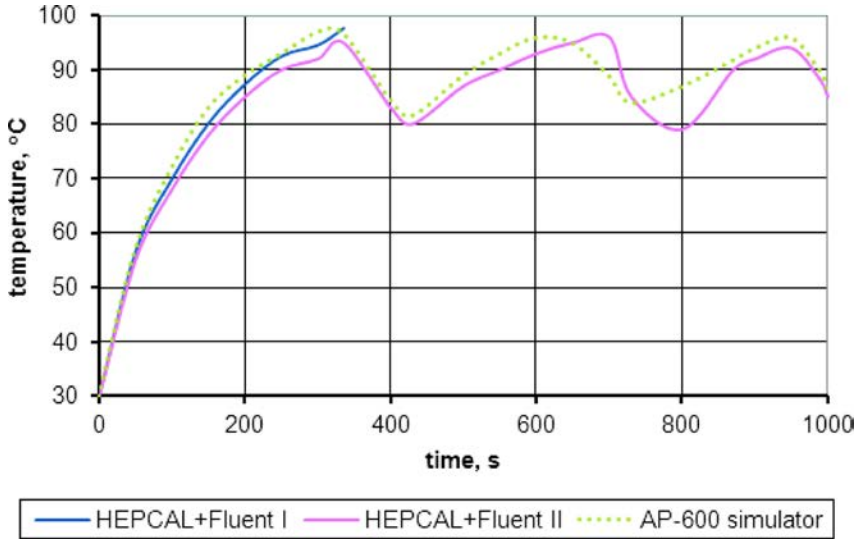

Fig. 8. Temperature trend within steel containment vessel.

5. Final remarks and conclusions

Lumped parameter codes have proven that valuable results can be obtained for containment thermal-hydraulics. As stated earlier, these codes will always require less CPU time than CFD, and thus are suitable for sensitivity calculations. Such sensitivity computations are required for nuclear reactor safety analyses that have to deal with the stochastic nature of initial and boundary conditions. It is impossible to perform such analyses by means of CFD codes. Therefore, it is evident that lumped parameter codes will always remain the main "workhorse" for analyzing containment thermal-hydraulic accident scenarios. Due to some inherent limitations of lumped parameter codes resulting from the applied simplified models of physical phenomena a large user influence on lumped parameter code results can be observed. Therefore, combined use of both lumped parameter codes and CFD codes is recommended.

According to the conducted analysis, the coupling of a lumped parameter code with a CFD code seems to be a good solution for simulations of thermal-hydraulic processes within containments of water reactors.

The two applied ways of such a coupling have given results qualitatively comparable with outcomes of the AP-600 reactor simulator.

The main problem in establishing the coupling is to find an interface where the coupling should occur. The first applied method probably has better physical basis due to the fact that there is a wall between computational domains analyzed by means of lumped parameter and CFD code respectively.

The presented solution should be treated as the first trial of this kind approach. Proposed combined approach requires some further development of both codes and conducting the verification of coupling methods is necessary.

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