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Thermodynamic consequences of hydrogen combustion within a containment of pressurized water reactor

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Abstract Gaseous hydrogen may be generated in a nuclear reactor system as an effect of the core overheating. This creates a risk of its uncontrolled combustion which may have a destructive consequences, as it could be observed during the Fukushima nuclear power plant accident. Favorable conditions for hydrogen production occur during heavy loss-of-coolant accidents. The author used an own computer code, called HEPCAL, of the lumped parameter type to realize a set of simulations of a large scale loss-of-coolant accidents scenarios within containment of second generation pressurized water reactor. Some simulations resulted in high pressure peaks, seemed to be irrational. A more detailed analysis and comparison with Three Mile Island and Fukushima accidents consequences allowed for withdrawing interesting conclusions.

Keywords: Nuclear reactor; LOCA; Hydrogen; Combustion; Containment

1 Introduction

An accident initiated by a rupture of one of the primary circuit pipes constitutes a serious challenge for a water cooled reactor safety systems. This is the loss-of-coolant accident – LOCA, in brief. The primary circuit break is followed by a rapid coolant leakage and this may lead to the core overheating and the fuel melt when unmitigated. There is also another serious problem. During such transients gaseous hydrogen can be produced in the

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reaction of steam with fuel cladding at elevated temperature. Hydrogen is then released through the cracks into the containment building and may create flammable mixture with the internal atmosphere. If the consequences of the event are limited, that means the accident is in the frame of the design, the amount of hydrogen released into the containment is low. Beyond the design basis accidents may lead to overheating of the core, up to a partial or complete core melting. In such cases oxidation of metallic components of the core produces significant quantities of hydrogen. To avoid a severe damage of the containment and the release of fission products to the environment uncontrolled combustion of hydrogen must be prevented. A sufficient method of hydrogen mitigation technique had to be chosen. For safety reasons it is crucial to get knowledge about the amount of hydrogen produced and released into the containment interior and about its distribution within compartments of the containment building. An expensive experimental analysis of this problem can be partly replaced by a precise computational analysis with a validated code [1,2].

The mathematical modeling and numerical simulations are widely used for thermal-hydraulic analyses of LOCA. Lumped parameter codes based on zero dimensional models of physical processes are commonly used for such purposes. These codes have reached a high degree of maturity so far and they are approved by nuclear authority bodies. It is however obvious that most of phenomena taking place within containment during a LOCA are clearly three dimensional. It seems that application of rapidly developing computational fluid dynamics (CFD) tools is a natural choice for the next step thermal-hydraulic analyses of LOCA. There are two main problems limiting CFD codes use in nuclear reactors safety assessment, namely size of systems under consideration and lack of experimental database for results validation and uncertainty determination.

This work deals with numerical analysis of thermal-hydraulic containment response to a LOCA. The problem investigated is hydrogen distribution within containment building during a heavy LOCA case and thermodynamic consequences of its combustion. The problem has been simulated by means of an in-door lumped parameter code called HEPCAL. Simulations have been realized for a standard containment configuration of the second generation pressurized water reactor. Mathematical models of such code assume perfect mixing of gaseous agents within a specified volume, so one can only get an average fraction of that gas within this volume and its mass. Therefore, it is also not possible to obtain detailed information about the hydrogen distribution and its local combustion. Additional estimating computations have been carried out assuming that the latest phenomena may significantly affect the thermodynamic parameters inside the containment building. The own results have been also compared with outcomes of computations accomplished by using a dedicated simulator of the considered reactor.

2 Hydrogen generation during loss-of-coolant accidents

The rates and quantities of hydrogen produced and the location of its release into the containment depend on a variety of conditions largely independent of each other (accident scenarios, the core degradation progress, the unavailability of engineered safeguards, etc.) and also independent of the reactor type. Hydrogen is generated by radiolysis of the reactor coolant, by the zirconium-water reaction and by chemical reactions of material in the post-accident containment environment [3]. The first two sources are briefly described further.

Following the postulated accident a major source of hydrogen production would result from the decomposition of water by radiolysis. Such decomposition of water is caused by the complex interaction of ionising radiation and water or dilute aqueous solutions. For pure water the maximum rate of production of the species, H_2, as a result of beta and gamma radiation is 0.44 molecules per 100 eV absorbed [4,5]. This value is a representative maximum value to describe the net hydrogen yield immediately following the loss of coolant accident, and is expected to decrease as the coolant temperature decreases. The energy source of radiolysis derives from the decay of fission products originally located within the fuel rods. Following a severe LOCA some cladding damage is expected and consequently a fraction of the more volatile fission products contained in the fuel rod gas gap would be released and will be distributed throughout the water and atmosphere within the containment, so hydrogen may also be produced out of the core.

Hydrogen generated in a large break loss of coolant accident from the Zircaloy-steam reaction is the most significant quantity of hydrogen produced in the first few hours. The amount of hydrogen released when the fuel cladding is oxidised in steam is directly proportional to oxygen consumed or Zircaloy reacted. Thus, for each mol of zirconium reacted two moles of hydrogen gas are produced, hence for each kilogram of zirconium reacted 0.044 kg of hydrogen are generated. The reaction rate becomes significant at a temperature of 900 ^{o}C and increases rapidly with increasing temperature [4,5]. However, in the case of controlled LOCA the action of the emergency core cooling system will limit temperature attained by the reactor core such that only a small fraction of the zirconium in the core will react.

As it has been mentioned earlier a serious problem for the containment integrity may result from hydrogen combustion. The flammability limit in gaseous mixtures such as steam, air and hydrogen, is defined as the minimum concentration of hydrogen required to propagate the flame in the environment where oxygen is present in excess. The experimentally determined flammability limits in steam-saturated air at room temperature and pressure are [3]:

- 4.1% vol. for upward propagation,
- 6.0% vol. for horizontal propagation,
- 9.0% vol. for downward propagation.

Significant hydrogen concentration could be reached locally in a short time, leading to a flammable gas mixture, but because of the presence of high steam concentrations, hydrogen burn may be prevented. If the atmosphere is undergoing rapid condensation – e.g. by spray initiation – a potentially detonable mixture could form rapidly in case of a high concentration of hydrogen.

3 The HEPCAL computer code

The results received here are an effect of simulations performed using the code HEPCAL, worked out at the Institute of Thermal Technology of the Silesian University of Technology [6–8]. This is a lumped parameter system code using the so-called control volume method to reproduce physical phenomena. The whole containment is simulated by a couple of zones (volumes), connected to each other in the 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. The mathematical basics of the model describing changes of thermodynamic parameters present equations of mass and energy balance for specified phases and equations of state [6,8]. All the equations are nonlinear and their form depend on the actual state of the specified media in the control volume.

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, and also heat transfer between phases and heat accumulation in the structures of the containment. The calculations of the 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 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.

4 Results of simulations

4.1 Containment model and analyzed accident scenario

The choice of the analyzed object has been influenced by possibilities of further comparisons between own and other results of the same unit. Therefore analyses consider a standard western design of a pressurized water reactor (PWR) with two vertical steam generators and dry containment structure. This created the possibility of comparison with the PCTRAN PWR simulator results [9], which has been also used to obtain the coolant leak data as well as hydrogen mass flow rate.

The reactor thermal power is 1800 MW (600 MWe) and the design refers to many units constructed by Westinghouse, Framatome or KWU. The containment building for this plant is presented in Fig. 1 [10]. This is the steel lined, prestressed concrete structure which houses the primary circuit and safety systems. The pressure suppression system is constituted by an active spraying system and the fan air cooling system.

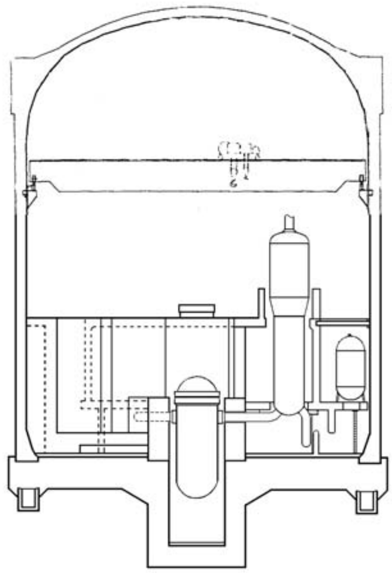

Figure 1. Sketch of the standard second generation PWR containment [10].

According to the requirements of the HEPCAL code the free volume of the analyzed containment has been defined as one control volume (40000 m^3). There were 5 LOCA scenarios simulated: cold leg and hot leg LOCA at full and zero power, and finally the pressurized safety relief valve (PSRV) failure. The last scenario was an attempt to reproduce the Three Mile Island accident and is presented further in the paper.

The analyzed accident scenario assumes hydrogen generation in the core region as an effect of the steam-zirconium reaction and is summarized in Tab. 1. The accident is initiated by a malfunction of the main condensate pump which stops. Next, the feedwater pumps are also stopped by the automatic control system. The primary circuit pressure rises as the effect of the heat removal loss. The primary coolant flows into the pressurizer in order to compensate the rising pressure. This in turn causes the increase in the level of liquid in the tank and increase of steam pressure at the top of the pressurizer. Despite the sprinkling system the steam pressure still rises to a level at which the PSRV opens. After several openings and closings this valve eventually gets stuck in the open position, thus allowing a constant flow of evaporating coolant to the letdown condenser tank first, and after the membrane break also to the containment. Pressure in the primary circuit then begins to fall to a level at which the emergency core cooling system

Table 1. Chronology of the most important events of the analyzed scenario (according to simulation made using the PCTRAN).

Time, s	Event
10	feedwater pumps stopped
69.5	reactor scram
71	turbine trip
1256	first opening of the PSRV
1501	breaking the membrane in the letdown condenser
1927	high pressure injection pumps (HPIP) turned on
3700	operator turns of the HPIP
3760	operator turns of the main coolant pumps
4680	hydrogen leakage into the containment starts
5527	first hydrogen ignition

is activated. In response to vibrations caused by local evaporation of the coolant operators turn off first the emergency coolant injection, and then the main coolant pumps. From this moment begins the gradual emptying of the reactor pressure vessel, which eventually leads to the core exposure and its overheating.

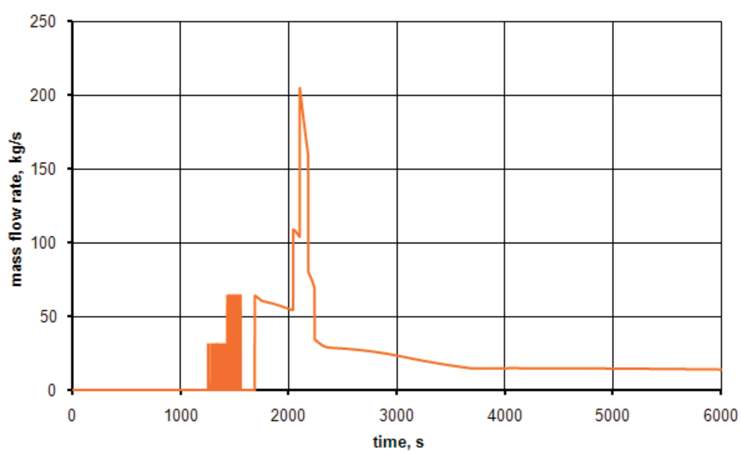

Figure 2. Mass flow rate of the coolant leakage (according to simulation made using the PCTRAN).

The mass flow rate of the coolant leaking from the primary circuit is shown in Fig. 2. As it can be observed the leak is not very big but it lasts a long time. This accident is a non-typical LOCA (there is no break in the primary piping system) but finally it turns into a severe accident.

4.2 Results of simulations

First simulations have been accomplished using the standard version of the HEPCAL-AU code and PCTRAN PWR simulator. The mentioned version of the HEPCAL code does not consider the hydrogen combustion, while PCTRAN is equipped with a simple model of hydrogen generation and distribution as well as its combustion. This allows to simulate the course of serious accidents leading to the uncontrolled burning of hydrogen [9]. The applied model assumes that ignition of hydrogen occurs at the concentration equal to 5% by volume. About 60% of hydrogen contained in the control zone is considered to be burned out.

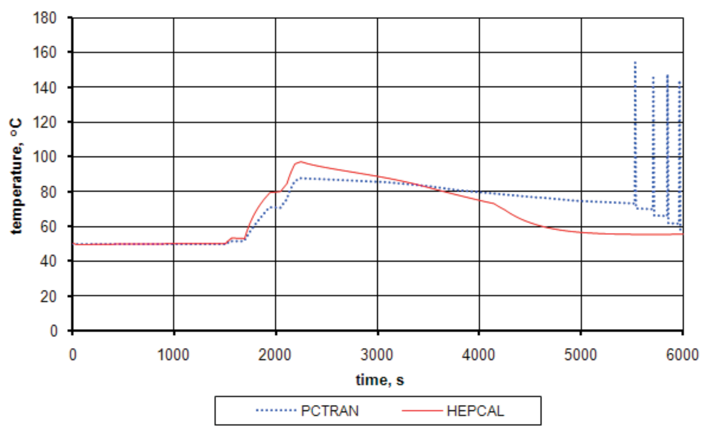

Figure 3. Temperature trend inside the containment during analyzed accident.

The simulation results presented in Figs. 3–5 show a very strong influence of the hydrogen combustion on the thermodynamic parameters inside the containment. In the case of temperature (Fig. 3) the maximum value slightly exceeds 150 °C for a few moment, which is an acceptable result for safety reasons. However, in the case of pressure (Fig. 4) peaks are much more visible: the changes are of the order of 450% of the initial value and far exceed the limit value of about 450 kPa.

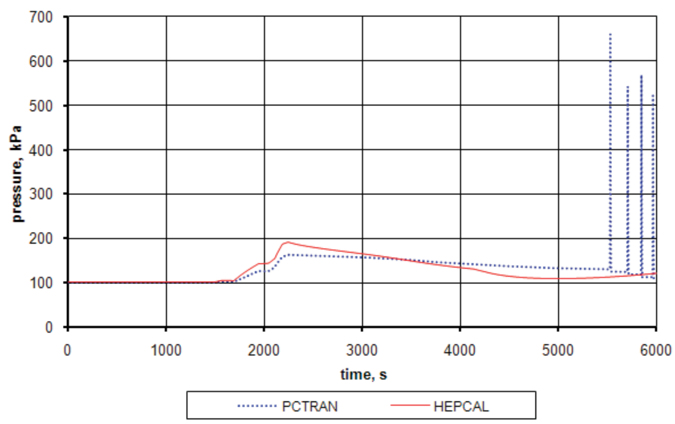

Figure 4. Pressure trend inside the containment during the analyzed accident.

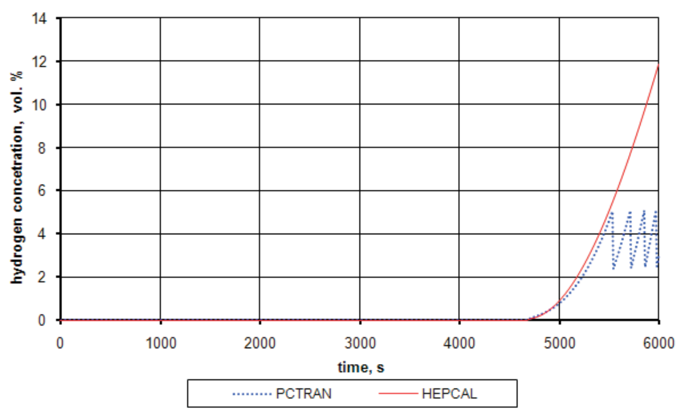

Figure 5. Hydrogen concentration inside the containment during the analyzed accident.

4.3 Additional computations

The lumped parameter codes, as previously mentioned, assume perfect mixing of the components of the phase in the entire volume of the control zone occupied by this phase. The resulting parameter values can thus be regarded as average in the present volume. This assumption makes it impossible to reflect the local differences in the concentrations of ingredients, e.g. by stratification. Previous experience with modeling the behavior of hydrogen during LOCA [11] and the calculations made using three-dimensional models [8] show that the flammability limits are exceeded locally much earlier than it is predicted by the lumped parameter codes. It can be assumed that the local effects of combustion of hydrogen will have much less influence on the global changes in pressure and temperature than those forecasted using the PCTRAN simulator. Due to the adopted in the lumped parameter codes representation of geometry of considered systems the account of these processes is not possible. One can solve this problem by using three-dimensional models, which, however, dramatically increases the time required for the analysis [8].

Considering the above observations, additional, completely estimating simulations have been performed using the code HEPCAL, whose purpose was to assess the local impact of the combustion of hydrogen on the course of changes in thermodynamic parameters. First of all a more detailed nodalization has been applied – according to data taken from [10] and [12] the containment has been divided into 5 control volumes. Next, it was assumed that the same leakage as described earlier takes place within the main coolant pumps and isolation valves compartment of 3500 m^3 volume. Moreover, an additional numerical procedure has been created for taking into account hydrogen combustion. The model assumes that hydrogen ignition occurs at its volumetric fraction equal to 5% and that 80% of the mass of the gas present in the control zone is burnt.

The course of changes in the concentration of hydrogen in the leakage control zone is shown in Fig. 6. As expected, the flammability limit in this control zone is reached earlier than for the previous case.

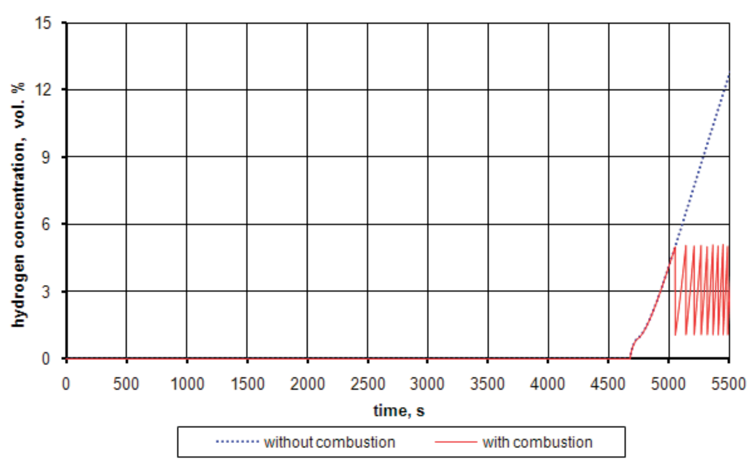

Figure 6. Hydrogen concentration within the leakage zone.

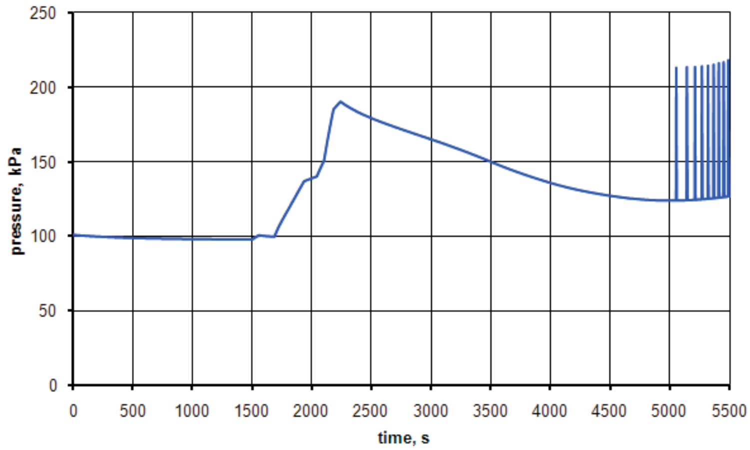

Figure 7. Pressure trend under the containment dome considering the local combustion effects.

Global effects of combustion are determined by the code HEPCAL by including additional components in the balance of mass (steam formed from the combustion of hydrogen) and energy balance (the heat generated during combustion). The results of calculations of the pressure under the containment dome (the largest control zone and the most important for the containment integrity) for this case are presented in Fig. 7. The local hydrogen combustion impact on the global pressure change is much smaller than the global burning. It should be noted that the calculations were purely an estimate, so the results presented may be subject to considerable uncertainty.

5 Conclusions

The calculations show a strong influence of the selected method of hydrogen combustion on the course of changes in the basic thermodynamic parameters. The assumption of the perfect mixing of ingredients in the control zones seems to blur the results – the effects of global hydrogen burning very strongly influence the course of changes in pressure or temperature. Probability of local hydrogen burning after reaching the limits of flammability is very high, and the effects of such an event far less impact on the global values of thermodynamic parameters. The most reasonable, therefore, appears to modeling the hydrogen behavior during a LOCA with spatial codes, which, however, significantly prolongs the time of analysis.

The results obtained from estimate calculations suggest that the pressure limit is not exceeded for this type of containment. Analysis of Three Mile Island accident confirms this observation. Note, however, that the combustion of hydrogen in the cases under consideration may have an explosive character and as a result of these local explosions may cause damage to components responsible for the proper operation of safety systems or even to containment structure as observed during the Fukushima plant accident.

An additional problem when analyzing the behavior of hydrogen during accidents are random events that can cause ignition of the gas, such as sparks from electrical installation, hit the gas stream with a hot surface.

In conclusion it should be noted that the analysis of the behavior of hydrogen during LOCA is a very complex task. Available models that consider the distribution and combustion are usually simplified, and the results derived from them are subject to significant uncertainty. A very important factor increasing the uncertainty of numerical simulations is the lack of experimental verification of the results.

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