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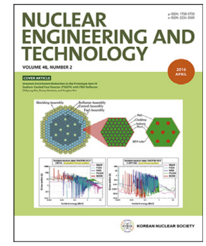

Original Article

Application of Best Estimate Approach for Modelling of QUENCH-03 and QUENCH-06 Experiments

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ABSTRACT

One of the important severe accident management measures in the Light Water Reactors is water injection to the reactor core. The related phenomena are investigated by performing experiments and computer simulations. One of the most widely known is the QUENCH test-program. A number of analyses on QUENCH tests have also been performed by different computer codes for code validation and improvements. Unfortunately, any deterministic computer simulation is not free from the uncertainties. To receive the realistic calculation results, the best estimate computer codes should be used for the calculation with combination of uncertainty and sensitivity analysis of calculation results.

In this article, the QUENCH-03 and QUENCH-06 experiments are modelled using ASTEC and RELAP/SCDAPSIM codes. For the uncertainty and sensitivity analysis, SUSA3.5 and SUNSET tools were used. The article demonstrates that applying the best estimate approach, it is possible to develop basic QUENCH input deck and to develop the two sets of input parameters, covering maximal and minimal ranges of uncertainties. These allow simulating different (but with the same nature) tests, receiving calculation results with the evaluated range of uncertainties.

1. Introduction

The phenomena, related to the flooding of an overheated core, were comprehensively investigated in a QUENCH test program realized by Karlsruhe Institute of Technology, (Karlsruhe, Germany). Within the frame of this program, loss of coolant accidents in a light water reactor was analyzed using an experimental facility to determine the amount of hydrogen produced, the so-called hydrogen source term. Up to now (since 1996), a total of 17 QUENCH tests were performed with different fuel/cladding materials and different boundary conditions in each test [1]. Based on the post-test calculations of the QUENCH experiments, the capability of the best estimate codes [Reactor Excursions and Leak Analysis Program/Severe Core Damage analysis Package Innovative Systems Software (RELAP/SCDAPSIM), Accident Source Term Evaluation Code (ASTEC), ATHLET CD, etc.] can be established and evaluated.

In this article, the QUENCH experiments regarding the oxidation of zircaloy cladding in the steam environment

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(QUENCH-03 and QUENCH-06 tests) were analyzed. The QUENCH-03 test was chosen for modelling because this test reflects one of the most serious losses of coolant accident scenarios, as it generates a large amount of hydrogen after reflooding. In this test, the reflood of imitators of the fuel bundle starts with a thin oxidation layer, which is similar to the condition of comparably fresh fuel in the reactor. The imitators of the fuel rod assemblies in both tests have the same cladding alloys, same quenching agent, control rods, etc. However, in the QUENCH-06 test, the reflooding of the imitators of the fuel assembly begins when the claddings are oxidized (~220-μm thickness of oxide) in a steam environment. The maximal temperature reached in the QUENCH-06 test bundle is lower than that in QUENCH-03. Thus, together these two QUENCH tests envelop a large range of loss of coolant accidents.

A literature review [2–7] showed that different researchers modelling QUENCH tests that are based on the zircaloy cladding oxidation in the steam environment use different approaches and methods. Moreover, different researchers used different values of initial parameters for modelling of the same QUENCH tests [2–4], where QUENCH-03 test is modelled using RELAP/SCDAPSIM and ASTEC codes. This difference in initial parameters is partly associated with the code differences and correlations used for modelling of the a steam–zirconium reaction. However, where the QUENCH-06 test is modelled using RELAP/SCDAPSIM [5–7], one can see that in each publication the initial parameters are slightly different. One of the reasons is that providing post-test calculations, studies focus on the result (experimental measurements, which also have uncertainties) and on how to approximate the calculation results to the experiment measurements.

The idea of this article is to propose an approach for the basic RELAP/SCDAPSIM and ASTEC input decks for simulation of QUENCH experiments using the estimation codes. Later, these developed input decks, could be used for the simulation of different QUENCH tests of the same nature without any significant changes. However, for the implementation of this idea, the possible uncertainties must be taken into account, and a best estimate approach should be implemented. In order to verify the possibility of the basic input decks development, input decks for the QUENCH tests employing the ASTEC and RELAP/SCDAPSIM computer codes were developed (Chapter 3), the uncertain input parameters were defined (Section 4.1), and calculations were provided for two similar QUENCH tests (i.e., QUENCH-03 and QUENCH-06). The uncertainty analysis of QUENCH-03 was provided using the SUNSET computer tool, while the uncertainty analysis of QUENCH-06 was provided using the SUSA computer tool (Section 4.2). The results of sensitivity analysis for the calculation results of the QUENCH-03 and QUENCH-06 tests are presented in Section 4.3. Based on the uncertainty and sensitivity analysis, the two sets of parameters were developed (Section 4.4). The ASTEC and RELAP/SCDAPSIM simulation results of these two sets of parameters bounded the experimental data from the QUENCH-03 and QUENCH-06 tests, (Sections 4.5 and 4.6), which demonstrated the appropriateness of the developed basic input decks.

2. Brief description of QUENCH-03 and QUENCH-06 tests

The main focus of the QUENCH tests lies on the analyses of hydrogen generation, especially, during the reflood, because in the CORA tests, temperature escalations together with a high hydrogen production were detected and the mechanisms therefore were not fully understood at the time [2]. A general description of the QUENCH facility is available on the Karlsruhe Institute of Technology website [8]. In this section, the QUENCH-03 and QUENCH-06 tests are presented.

Generally, each QUENCH test consists of different phases: heat-up, preoxidation, transient (test bundle is cooled by saturated steam), and a quenching phase (the bundle is reflooded by water). Before the quench phase, superheated steam and argon are injected at the bottom of the facility as a carrier gas in order to transport and measure the reaction products from the test section. In the QUENCH-03 test, the preoxidation phase can be neglected, because at the beginning of the transient phase, the claddings should only be slightly oxidized with an oxide layer of approximately 30 μm, as it is in the normal operation state of a pressurized water reactor. The progression of the QUENCH-03 test can be seen in Fig. 1 [2].

The first phase of QUENCH-03 is the heat-up phase, where the bundle was heated from room temperature to approximately 900 K in an atmosphere of flowing argon (3 g/s) and steam (3 g/s) by increasing electrical power. In order to stabilize the test set-up, the reached temperature was held for about 900 seconds with an electrical power input of 3.75 kW [2]. The transient phase followed which began at about 900 seconds and lasted roughly until 2,600 seconds. During this phase, the bundle power was ramped from 3.75 kW to 18.4 kW. Afterwards, the thermocouples in the upper area of the shroud and upper bundle elevations showed the same behavior due to the exothermal zircon–steam reaction that runs faster at higher temperature levels. The thermocouples at the 750-mm bundle elevation detected a maximum temperature over 2,400 K causing a thermocouple failure at that elevation and higher [2]. The achievement of the defined temperature of 2,400 K inside the bundle at 2,600 seconds led to the initiation of the final quench phase, in which the reflood water was injected first at a high rate of 90 g/s for 25 seconds to

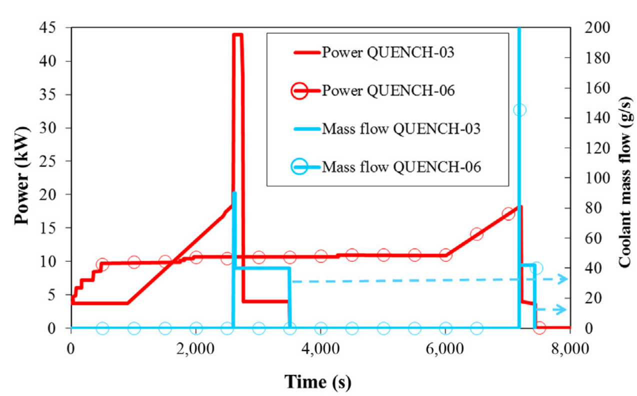

Fig. 1 – Progression of the QUENCH-03 and QUECH-06 tests.

fill the lower plenum. With the initiation of reflooding, the electrical power was increased from 18.4 kW to 44 kW to compensate the convective heat losses occurring due to the boiling of the inserted water at the hot structure material. At 2,625 seconds, the water injection rate was reduced to 40 g/s. After reaching the maximum bundle temperature ~2,460 K at 2,627 seconds, the electric power was reduced to 37.5 kW until 2,747 seconds. During this period, substantial temperature escalations occurred in the upper bundle area so that the claddings and the shroud collapsed at about 2,627 seconds. Due to this collapse, melt formation and relocation resulted, which then resulted in an increase of the surface available for oxidation and subsequently resulted in an additional massive hydrogen production. In the period from 2,747 seconds to 2,762 seconds, the electrical power was reduced from 37.5 kW to 4 kW to simulate the typical decay heat of a light water reactor [2]. The main events and phases of the QUENCH-03 test during the time are presented in Table 1.

The QUENCH-06 experiment [5] was similar to the QUENCH-03 experiment. The main difference between these experiments is that the QUENCH-06 experiment had a preparatory and a "real" preoxidation phase. The progression of the QUENCH-06 test can be seen in Fig. 1 [5] and Table 1.

In the preparatory phase in the QUENCH-03 experiment, the bundle was heated by a series of stepwise increases of electrical power from room temperature to nearly 900 K in an atmosphere of flowing argon (3 g/s) and steam (3 g/s). The bundle was stabilized at that temperature for about 2 hours with the electrical power being about 4 kW. At the end of the stabilization period, the heat-up and preoxidation phases began. In the heat-up phase, the bundle was ramped by stepwise increases in power up to about 10.5 kW to reach an appropriate temperature for preoxidation (~1,400 K). In the preoxidation phase, ~1,400 K temperature was maintained for 4,050 seconds by controlling the electrical power to reach the desired oxide layer thickness (~220 μm). At the end of the preoxidation period (which lasted from 1,960 seconds to 6,010 seconds), the bundle was ramped at 0.32 W/s per rod to start the transient phase. A corner rod was withdrawn during the transient to check the amount of oxidation at that time (6,620 seconds). During heat-up, preoxidation, and transient phase, the bundle was cooled with flowing steam and argon both having an inlet mass flow rate of approximately 3 g/s and an inlet temperature that varied between 607 K and 650 K [5]. In QUENCH-06 (differently than in QUENCH-03), the quenching was initiated after a long time (4050 s) preoxidation phase and after a transient phase when two rod thermocouples showed temperatures higher than 2,000 K. The quench phase began at 7,179 seconds by shutting down the steam supply and with the initiation of quench water injection. Within 5 seconds, 4 kg of water were injected to fill the lower parts of the facility (fast water injection system). At the same time, the quench pump starts to inject water from the bottom of the test section at a rate of approximately 42 g/s. The water used for quenching was at room temperature. About 25 seconds later, the electrical power was reduced from 18 kW to 4 kW within 17 seconds to simulate the decay heat level. Quenching of the test section was completed within 260 seconds. Quench water injection and electrical power were then shut off terminating the experiment. During the quench phase, argon injection was switched to the upper plenum to continue providing carrier gas for quantitative hydrogen detection [5].

The general accuracy of temperature measurements was ± 50 K the temperatures in the QUENCH fuel rods bundle and shroud were measured using thermocouples. The concentration of H_2 was measured using a quadruple mass spectrometer with an accuracy of 5% [9].

The experimental phases (heat-up, preoxidation, transient, quenching, and postreflood) of the QUENCH-03 and QUENCH-06 tests are presented in Table 1. This table also contains the main events within the phases. As already mentioned, the preoxidation phase was omitted in the QUENCH-03 test.

3. ASTEC and RELAP/SCDAPSIM models of the QUENCH test

ASTEC [9] was jointly developed several years ago by the French Institut de Radioprotection et de Sûreté Nucléaire IRSN (Paris, France) and the German Gesellschaft für Anlagen und Reaktorsicherheit mbH GRS (Cologne, Germany) to simulate all the phenomena that occur during a severe accident in a water-cooled nuclear reactor. For modelling of a QUENCH experimental facility, a simple nodalization scheme for ASTEC V2.0r3 code ICARE module has been developed (Fig. 2A).

The QUENCH-03 and QUENCH-06 experiment fuel bundle model includes models of an unheated central rod ROD1, two rings of electrically heated rods (the inner ring with eight rods ROD2 and the outer with 12 rods ROD3), and corner rods. The shroud is modelled as manufactured with all layers. Flow rate through the core is modelled by employing two fluid channels VAP1 for steam and argon and LIQ1 for water. Also, grids are modelled. In the axial direction, the QUENCH facility core was divided into 32 nodes.

The RELAP/SCDAPSIM computer code is designed to describe the overall reactor coolant system thermal hydraulic response and core behavior under normal operating conditions or under design basis or severe accident conditions [10]. RELAP/SCDAPSIM uses the publicly available RELAP/MOD3.3 and SCDAP/RELAP5/MOD3.2 models developed by the US Nuclear Regulatory Commission in combination with proprietary advanced programming and numerical methods, user options, and models developed in the frame of the International SCDAP Development and Training Program (SDTP). The administrator for the SDTP program and main developer of specific models for the RELAP/SCDAPSIM is the private, limited liability company Innovative Systems Software (Idaho Falls, USA). The QUENCH experimental facility was modelled using RELAP/SCDAPSIM code version Mod3.5 [11]. The QUENCH nodalization scheme is presented in Fig. 2. The space between the heated rods and the outer cooling loop of the QUENCH facility was modelled using RELAP5 components: pipe, time-dependent volumes and junctions, single junctions, and others. Imitators of fuel rods and the surrounding shroud are modelled using the components of the SCDAP package: "fuel", "cora", and "shroud". A total of five components are described using the SCDAP package. Component 1, one central rod (not heated) modelled as a "fuel" element is composed of ZrO_2 pellets in the Centre, a gas-

Table 1 – Events and phases of the QUENCH-03 and QUENCH-06 tests.

Phase	QUENCH-03		QUENCH-06	
	Time (s)	Event	Time (s)	Event
Heat-up	0	Start of data acquisition	0	Start of data acquisition
	20	Heat up to ~900 K. Power 3.75 kW.	20	Power 4 kW. Power stepwise increase started
	900	Transient phase initiation	1,960	Reached power 10.5 kW. Max temp. 1,400 K
Preoxidation		–	1,960	Beginning of bundle oxidation at about 1,400 K
			6,010	Transient phase initiation
Transient	900	Initiation of power increase	6,010	Initiation of power transient
	2,455	Begin of temperature escalation of the shroud at the 1,250 mm level up to ~987 K	6,620	Initiation of pull-out of corner rod
	2,590	Begin of temperature escalation at the 1,150-mm level up to ~1,372 K	6,640	End of pull-out of corner rod transient
	2,600	Power reached 18.4 kW Quench phase initiation	7,179	Power reached ~18.2 kW. Quench phase initiation
Quenching/reflood	2,600	Power increase from 18.4 kW to 44 kW	7,179	Shut down of steam supply
	2,600	Onset of fast water injection	7,179	Onset of fast water injection
	2,602	Electric bundle power 44 kW	7,179	Onset of quench water injection
	2,606	Steam flow shut off, argon flow switched to upper bundle head	7,181	Steam mass flow rate zero
	2,616	Maximum quench water flow 90 g/s	7,204	Onset of electric power reduction from ~18.2 kW down to ~4 kW
	2,627	Shroud failure, starting between 750 mm & 950 mm	7,222	Decay heat level reached
	2,630	Quench water flow of 40 g/s	7,429	Onset of final power reduction quench/reflood
	2,747	Start of electric power reduction from 37.5 kW to 4 kW	7,431	Shut down of quench water injection
Postreflood	2,762	Electric power 4 kW	7,435	Quench water mass flow zero
	3,501	Electric power shut off < 0.5 kW	7,437	Electric power < 0.5 kW
	3,508	Quench water mass flow zero	11,420	End of data acquisition

Max, maximum; temp, temperature.

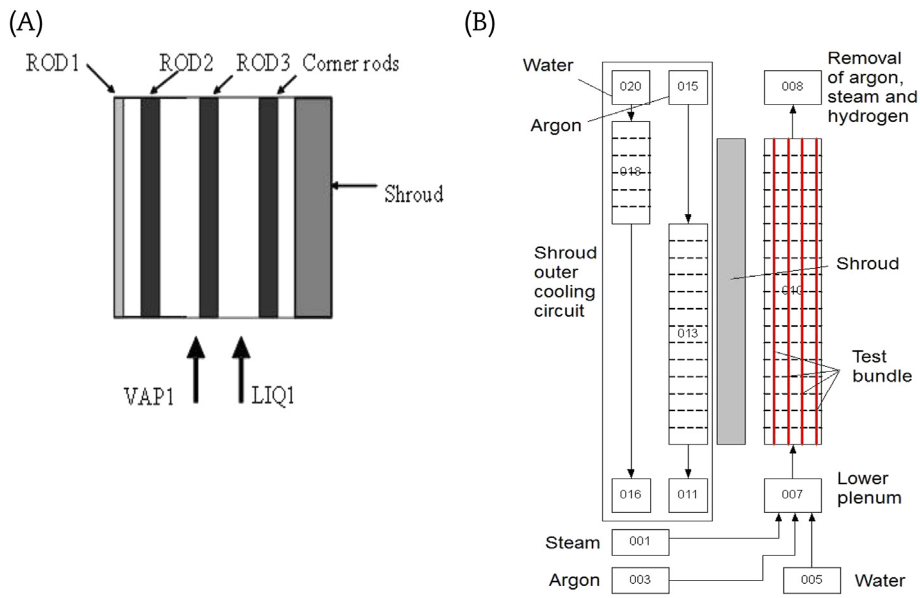

Fig. 2 – Nodalization scheme of QUENCH test developed. (A) Accident Source Term Evaluation Code ICARE module. (B) RELAP/SCDAPSIM computer code.

filled gap, and cladding of zircaloy; Component 2, eight heated rods (around the central rod), which simulate heated fuel rods, modelled using "cora" component composed of tungsten heating elements in the center, ZrO_2 pellets, gas-filled gap, and cladding of zircaloy; Component 3, 12 heated rods modelled using "cora" component; Component 4, the four rods in the corners, modelled as the "fuel" components; and Component 5, shroud of the bundle modelled as the "shroud" component, which consists of the inner zircaloy layer, an insulating layer of ZrO_2, and an inconel layer (using properties of stainless steel).

The first four components are connected to the RELAP5 structure, which describes the space between heated rods and pipe element "010" (Fig. 2). Element "010" is divided in an axial direction into 18 nodes of 3.009×10^{-3} m length each. In order to have heat exchange at the wall, the fifth component (shroud of the bundle) is connected to the hydrodynamic structures of RELAP5. This structure and pipe elements "013" and "018" are modelling the outer cooling circuit of the shroud. The layer thickness of the shroud component heat structure is 1.2×10^{-3} m and it has five radial mesh points. Element "013" is divided into 13 nodes in the axial direction, and element "018" is divided into five nodes that are 3.684×10^{-3} m length each.

The process of Zr oxidation in RELAP/SCDAPSIM is represented by parabolic rate correlations. Using the RELAP/SCDAPSIM code Mod3.5 version, the calculations were performed using two options: (A) with shattering oxidation model enabled; and (B) with shattering oxidation model disabled. These models strongly influence the temperature and, especially, hydrogen generation rate calculation results (Section 4.5).

The ASTEC V2.0r3 code uses the same Zr oxidation correlation for the whole range of temperatures (no Zr oxide layer shattering model is applied). In the QUENCH input deck developed using ASTEC, the shroud outer cooling circuit was not modelled. Instead, the outer shroud surface temperature changes in the time were prescribed as boundary conditions. The behavior of outer shroud temperatures was taken from RELAP5/SCDAPSIM calculations.

4. Implementation of best estimate methodology for QUENCH-03 and QUENCH-06 tests analysis

For the analysis of accidents in nuclear reactors, the best-estimate approach, which is free of deliberate pessimism regarding selected acceptance criteria, has been used for many years. This approach uses a best-estimate code and includes uncertainty analysis [12]. There are a few types of methodologies of uncertainty analysis: developed at Pisa University (Italy) [13–17], GRS (Germany) [18–20], Nuclear Regulatory Commission (USA) [21,22], Institute for Protection and Nuclear Safety (France) [23,24]. According the joint work of experts from different scientific centers [25], three main types can be selected: (1) Uncertainty Method based on Accuracy Extrapolation is based on the accuracy extrapolation of modelling of thermal hydraulic experiments towards the modelling of postulated accidents; (2) Method developed by the United Kingdom Atomic Energy Authority and AEA Technology is based on definition by experts of initial uncertainties in some confidence boundaries, and the impact of these uncertainties is further investigated in terms of calculations with variations of limiting parameters; and (3) GRS, Institute for Protection and Nuclear Safety, and ENUSA (Spain) uncertainty and sensitivity analysis methodologies are based on statistical (probabilistic) uncertainty extrapolations, when uncertainties are assumed in terms of random values with selected distributions.

At the Lithuanian Energy Institute, the propagation of code input uncertainty method developed in the GRS [19,20] is used. The selected parameter values for the best estimate code runs are generated using the computer tool Software System for Uncertainty and Sensitivity Analysis (SUSA) [18]. The computer tool SUSA is developed in GRS mbH (Munich, Germany). The GRS method considers the effect of uncertainties of input parameters, the options of modelling, and the parameters of solution algorithms on the simulation results. The method is based on a systematic identification of relevant physical processes and on a probabilistic quantification of the uncertainty of corresponding parameters. The computer code ASTEC has a special option that allows it to link with the Sensitivity and Uncertainty Statistical Evaluation Tool (SUNSET) computer tool. The SUNSET computer tool is a statistical tool providing a collection of methods for information treatment in risk analysis studies [26]. Both SUSA and SUNSET computer tools are based on statistical methods.

The uncertainty and sensitivity analysis of calculation results of the QUENCH-03 and QUENCH-06 tests using different tools is presented in this section. For the QUENCH-03 test, the uncertainty and sensitivity analysis was provided using the ASTEC code and SUNSET computer tool, while for the QUENCH-06 test analysis was provided using RELAP/SCDAPSIM code and SUSA computer tool. Because the phenomena occurring in the QUENCH-03 and QUENCH-06 tests are similar, the sensitivity analysis for QUENCH-03 and QUENCH-06 were compared together.

According to the GRS methodology [19], at the beginning, the list of uncertain parameters (range of input parameters and probability distribution function of the parameters) must be specified (Section 4.1). It must be assumed that the uncertain parameters, which may impact the calculation uncertainty, are independent. Using GRS methodology, the number of calculation runs necessary for one-side or two-side tolerance intervals depends only on the required probability and confidence level of the statistical tolerance limits. The relationship between these parameters is described by Wilks' formula [27]. In calculated cases, the uncertainty analysis is performed using a two-side tolerance limit with 0.95 of probability and 0.95 confidences. For this case, according to Wilks' formula, the number of calculation runs necessary for two-side tolerance intervals is 93. However, in practice, it is usually necessary to have 100 collections of input parameters taking into account the possibility of computer code failure of calculation of some collections of input parameters. Therefore, using SUNSET and SUSA computer tools, 100 collections of input parameters were composed.

For each collection of parameters, the input files for the ASTEC and RELAP/SCDAPSIM codes were composed, calculations were performed, and uncertainty analysis was done (Section 4.2). Based on the results of the performed calculations, the impact of input parameters on the calculation results of the QUENCH-03 (SUNSET) and QUENCH-06 (SUSA) tests was analyzed (Section 4.3).

Table 2 – Uncertain input parameters used in the best estimate analysis.

No.	Parameter	Reference value	Deviation range (%)
1	Quenching water flow (g/s)	Presented in Fig. 1	±3
2	Steam flow (g/s)	3	±3
3	Argon flow (g/s)	3	±3
4	Quenching water temperature (K)	370	±2
5	Steam temperature (K)	840	±2
6	Argon temperature (K)	840	±2
7	Thermal conductivity of ZrO_2 (W/m·K)	Depending on temp. varying in interval: 0–0.45 [30]	±20
8	Specific heat of ZrO_2 (J/kg·K)	Depending on temp. varying in interval: 400–850 [30]	±20
9	In RELAP/SCDAPSIM code: contact resistance of sliding contacts (mΩ)	4	±10
	In ASTEC code: additional resistance outside the bundle (OCR) (mΩ)	0.22	±10
10	Quencing water pressure (bar)	2	±2
11	Steam pressure (bar)	2	±2
12	Argon pressure (bar)	2	±2

ASTEC, Accident Source Term Evaluation Code.

4.1. *Uncertain parameters for QUENCH-03 and QUENCH-06 calculations*

For the uncertainty and sensitivity analysis of QUENCH-03 and QUENCH-06 test modelling results, the following input parameters were selected: flow rate of water steam and argon used for the experimental fuel bundle cooling during heat-up and transient phases; quenching water flow rate; the temperatures of steam, argon, and quenching water; the pressure of steam, argon, and quenching water; the parameter influencing the power generation in the experimental bundle of fuel imitators; and the thermal properties of shroud (the thermal conductivity and specific heat of ZrO_2). The uncertainty of the investigated parameters is described by their ranges and subjective probability distributions. The uncertain input parameters, reference value, and deviation range are presented in Table 2. The deviation range was assumed based on experience and possible measurements errors: for the flow rate values ± 3% and ± 2% for the temperature and pressure values. The influence of thermal conductivity and specific heat is significant on the heat transfer processes in the radial direction, but not so significant on the behavior of the temperature of the fuel rod imitator cladding. To investigate the influence of the thermal conductivity and specific heat of the shroud material, a ± 20% deviation range for these parameters was assumed.

It is necessary to mention that depending on the code used for the calculation, there are two parameters that influence power generation in the experimental fuel bundle: (1) in RELAP/SCDAPSIM code: contact resistance of sliding contacts, mΩ; and (2) in ASTEC code: additional resistance outside the bundle (OCR), mΩ.

These resistances have slightly different meaning in both computer codes, and reference values with a ± 10% deviation range were assumed based on the investigations, performed by other authors [28,29].

It was assumed that the uncertain parameters presented in Table 2 could vary in the entire deviation range with the same probability. In this case, the uniform distribution was used for all 12 parameters. However, the function of probability distribution of the uncertain parameters does not affect the minimal and maximal values of calculation results and does not influence the agreement between experiments and results of uncertainty analysis. More information about the uncertain input parameters used for the calculation is presented in reference [30].

4.2. *Analysis of uncertainty*

As has already been presented, according to Wilks' formula, the number of calculation runs necessary for two-side tolerance intervals is 93. However, using the SUNSET computer tool and ASTEC code, 100 different collections of uncertain input parameters were composed according to the data presented in Table 1. After this, all these inputs were calculated using the ASTEC code.

The results of computational modelling of the QUENCH-03 test using the ASTEC code are presented in Figs. 3 and 4. The behavior of fuel rod imitator temperatures (outer ring) and the total amount of generated hydrogen are presented. The calculation results using two bounding cases (bounding upper limit and bounding lower limit) are compared with the experiment measurements. The calculated temperatures are in reasonable agreement with the measurements. The possible deviations of measured temperatures and generated hydrogen are labelled (±50 K for temperature measurements and 5% accuracy for hydrogen) [29]. However, the calculated amount of generated hydrogen is below the measured values. In the ASTEC calculations, the "Urbanic" correlation for the steam–zirconium reaction was used. The selection of this correlation was based on the investigations presented in [29].

It is necessary to mention that other authors also observed the discrepancy between calculation results and QUENCH-03 test measurements when the standard ASTEC options are used [31]. It is due to the fact that the use of the same correlation for the whole range of temperatures is not in agreement with the experimental results. In the ASTEC case, the standard options, adapted to the slow oxidation case, were used. Use of correlations combining the steam–zirconium oxidation at low temperature and high temperature is necessary in the investigation of the reflooding phenomena.

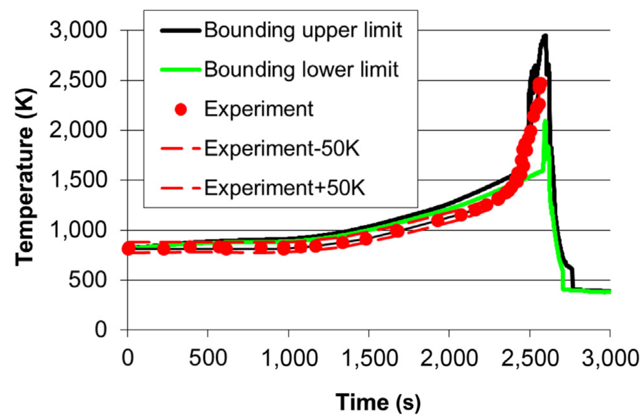

Fig. 3 – Results of ASTEC calculation of QUENCH-03 test, behavior of cladding temperatures of the fuel rod imitator from the outer rod ring at 750 mm-height. Max, maximum; min, minimum.

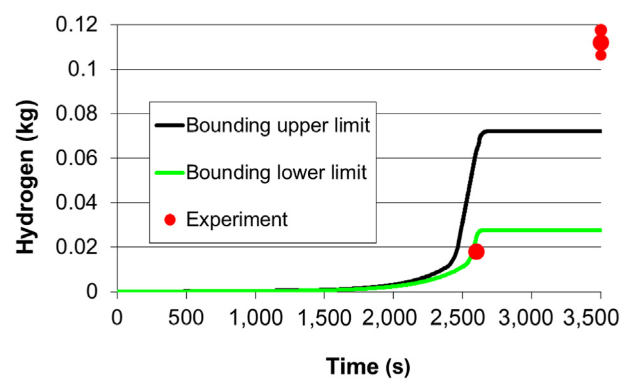

Fig. 4 – Result of Accident Source Term Evaluation Code calculation of QUENCH-03 test, amount of generated hydrogen.

Using the RELAP/SCDAPSIM code and SUSA computer tool, uncertainty analysis is provided for the calculation results of the QUENCH-06 test. Uncertain parameters, their deviation range, and distribution function were chosen the same as those for QUENCH-03 test (Table 2).

Using the SUSA computer tool, 100 different collections of uncertain input parameters were composed. All these inputs were calculated using the RELAP/SCDAPSIM code. The option with disabled shattering oxidation model was applied. The results of computational modelling of the QUENCH-06 test are presented in Figs. 5 and 6. The behavior of the fuel rod imitator temperatures (outer ring) is presented in Fig. 5. The calculation results of all 100 different input files are compared with the experiment measurements (square dots). As shown in the figure, the calculation results are in good agreement with the experimental data during heat-up phase. During the preoxidation phase, the calculation results overestimate the experimental data. However, during transient phase, the calculation results become similar to the experimental data, but during quench phase, the experiment instrumentation recorded ~400 K higher temperature than RELAP/SCDAP calculates.

Calculation results of generated hydrogen from all 100 different inputs are presented in Fig. 6. The total amount of generated hydrogen in the experiment is bounded by 100 calculation results. However, total hydrogen generated during the preoxidation and transient phases are overestimated in the calculation results (even taking into account the accuracy of measurements). The quantity of generated hydrogen is related to the temperature of the rods. Fig. 5 shows what calculated temperatures in the rods are overestimated during preoxidation phase and it reflects the hydrogen generation. These discrepancies are discussed in Section 4.6.

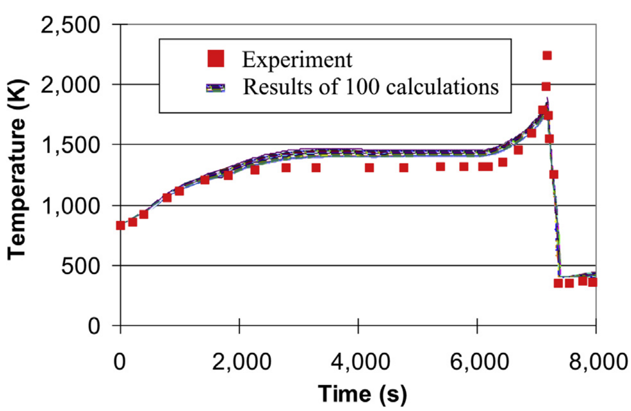

Fig. 5 – Results of RELAP/SCDAPSIM calculation of QUENCH-06 test. Behavior of cladding temperatures of the fuel rod imitator from the inner rod ring at 750 mm-height.

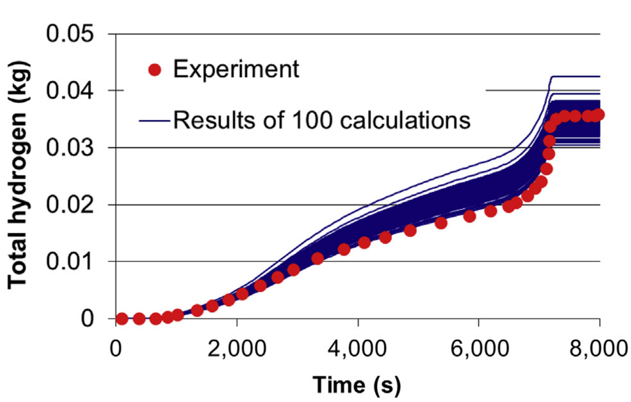

Fig. 6 – Result of RELAP/SCDAPSIM calculation of QUENCH-06 test, amount of generated hydrogen.

4.3. *Sensitivity analysis*

The analysis of sensitivity of uncertain parameters on the calculation results was performed using the SUNSET computer tool for QUENCH-3 and the SUSA computer tool for QUENCH-6. Spearman's rank correlation coefficient method was chosen. At first, Spearman's method sorts all parameters according to the impact to calculation results and gives them a rank. Then, the correlation is provided for these ranks, which shows the magnitude of impact in relative units. The coefficient of determination (R^2) with respect to Spearman's rank correlation is very important. In statistics, R^2 is used in the context of statistical models, the main purpose of which is the prediction of future outcomes on the basis of other related information. In practice, it is often required that the linear model determination ratio should be no less than 0.6. If the R^2 value is less, then the standardized regression coefficient of the sensitivity ranking of parameters may be incorrect because of too many unexplained parameter variations.

As seen from Fig. 7, the linear model determination ratio value is higher than 0.6, thus the usage of the SUSA computer tool is appropriate.

The influence of uncertain parameters on the calculated temperatures of the cladding of the fuel rod imitator (in the outer ring) for QUENCH-03 and QUENCH-06 is presented in Fig. 8. The sensitivity of uncertain parameters, presented in Table 1, with respect to the calculation results was analyzed for two phases. For QUENCH-03: (1) for the experimental bundle heat-up phase; and (2) at the quenching phase (at time moment > 2,600 seconds, when the maximal temperatures are reached). For QUENCH-06: (1) for the experimental

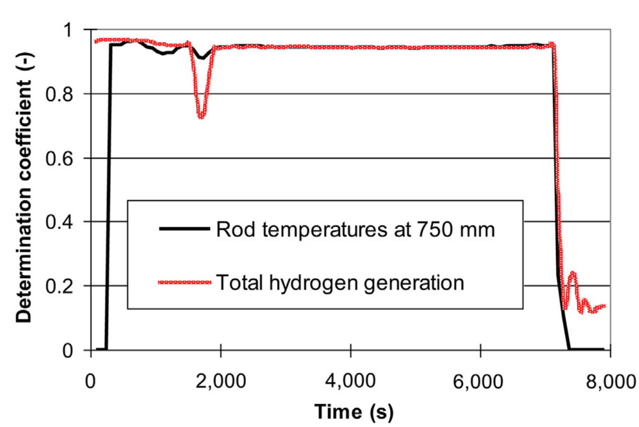

Fig. 7 – Input parameters determination coefficient for the calculated fuel rod cladding temperature at 750 mm-height and total hydrogen generation.

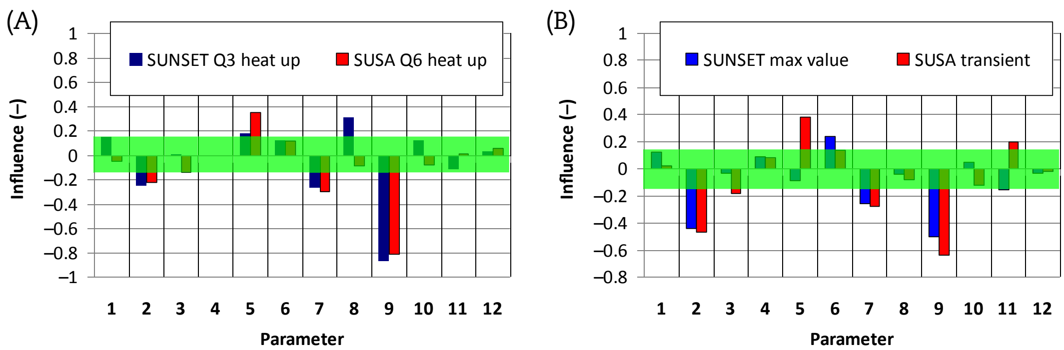

Fig. 8 – Influence of uncertain parameters to the calculated cladding temperature of the fuel rod imitators the in outer ring at 750 mm-height. (A) Heat-up phase. (B) Quenching (SUNSET) and transient (SUSA) phases. Max, maximum; SUNSET, Sensitivity and Uncertainty Statistical Evaluation Tool; SUSA, System for Uncertainty and Sensitivity Analysis.

bundle heat-up phase; and (2) at the transient phase. The sensitivity of uncertain parameters with respect to the calculation results of QUENCH-06 was analyzed at transient phases instead of the quench phase, because the SUSA computer tool calculated the a low determination coefficient in the quenching phase (Fig. 7).

Using the SUNSET computer tool in the ranking of the parameters influence on the calculation results, a cut-off region equal to 0.17 was applied. This a cut-off region corresponds to the 95% confidence threshold of the Spearman coefficient. In Fig. 8 the cut-off region is marked by the green zone.

The influences of uncertain parameters on the calculated cladding temperature of fuel rod imitators in the outer ring at 750-mm height (QUENCH-03 and QUENCH-06 tests) slightly differ for two selected time phases. As seen from Fig. 8, at the heat-up phase, the biggest influence on the temperature of the cladding of fuel rod imitator calculation results for QUENCH-03 and QUENCH-06 have: additional/contact resistance (parameter number 9), thermal conductivity of ZrO_2 (parameter number 7), and steam-flow rate and temperature (parameter numbers 2 and 5).

Parameter numbers 2, 7, and 9 have negative influence to the calculation results; this means the decrease of these parameters leads to an increase of temperature. Conversely, parameter number 5 has a positive influence—increase of the temperature of the supplied steam increases the temperature of the fuel rod imitators. The sensitivity evaluation by the SUNSET computer tool for the QUENCH-03 test calculation showed that parameter number 8 (specific heat) is also important for the fuel rod temperature calculation results, and this parameter has a positive influence. This is due to the fact that the increase of specific heat of zirconium oxide in the shroud leads to a lower heat transfer from the fuel assemblies to the shroud and higher temperature of the cladding of the fuel rod imitators.

At the quench phase in QUENCH-03 and transient phase in QUENCH-06, the parameters mainly influencing the calculation results of fuel rod imitators' temperature are similar at the "heat-up" phase: additional/contact resistance (parameter number 9), steam flow rate (parameter number 2), and thermal conductivity of ZrO_2 (parameter number 7).

Contrary to the QUENCH-03 test, in the QUENCH-06, parameter 5 (steam temperature) and parameter 11 (steam pressure) exhibit an influence on the calculation results. According to the SUSA computer tool calculation, the steam temperature has 0.4 and the steam pressure has 0.2 influence according to Spearman's correlation coefficient to the temperature of the cladding of the fuel rod imitator calculation results. This could be explained by the specifics of this test. The QUENCH-06 test has a long preoxidation phase, and the initial parameters of supplied steam and argon are very important. A higher temperature of steam and argon at the entrance of the test bundle will lead to a higher temperature of the fuel rod imitator cladding. For the QUENCH-06 test at the quenching phase, the steam temperature did not have any influence, because no steam was injected to the bundle. But for the QUENCH-03 test calculations at the quenching phase, the argon temperature had little influence, because during the quenching phase, the injection of argon gases is switched to the upper plenum to continue providing carrier gas for quantitative hydrogen detection.

The total amount of generated hydrogen is one of the most important parameters of the QUENCH experiment. The input parameters, affecting the calculated (during QUENCH-03 and QUENCH-06 tests) amount of generated hydrogen are given in Fig. 9. SUNSET calculated the influence at the point where the maximal value of hydrogen generation is received in the QUENCH-03 test (at the end of the quench phase). SUSA calculated the influence in the transient phase of the QUENCH-06 test.

The parameters having the biggest influences on the hydrogen calculation results are the same for QUENCH-03 and QUENCH-06 test calculations. They are: additional/ contact resistance (parameter number 9), thermal conductivity of ZrO_2 (parameter number 7), steam flow at the heat-up phase (parameter number 2), specific heat of ZrO_2 (parameter number 8), flow rate of argon (parameter number 3), temperature of steam (parameter number 5), and temperature of argon (parameter number 6).

Only the last two parameters (numbers 5 and 6) have positive influence to calculation results, while the remaining have negative influence. As shown in the Fig. 9, the

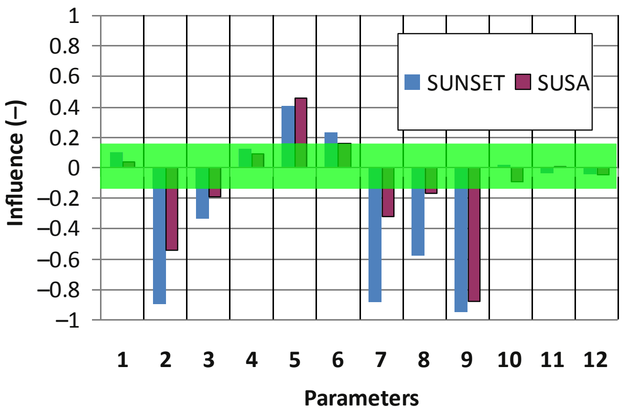

Fig. 9 – Influence of uncertain parameters to the generated hydrogen calculation results. SUNSET, Sensitivity and Uncertainty Statistical Evaluation Tool; SUSA, System for Uncertainty and Sensitivity Analysis.

parameters affecting the results of the fuel rod imitator cladding temperature also influence the results of hydrogen generation. This is evidently because the higher temperatures promote the steam–zirconium reaction and generation of hydrogen.

4.4. *Development of sets of parameters for the minimal and maximal calculations*

Based on the uncertainty and sensitivity analysis, performed with the SUNSET and SUSA computer tools (evaluating the influence of input parameters to the calculation results), two sets of parameters (parameters that give the highest and lowest hydrogen generation value) were developed. In the set, where the goal was to obtain a larger amount of generated hydrogen, all parameters which have a positive influence on hydrogen generation were maximized within their variation range. Conversely, the parameters which have a negative influence to calculation results were minimized within their variation range. The set of parameters for the minimal amount of hydrogen was created in the opposite manner (Table 3). Maximal and minimal values of parameters were determined according to the reference values presented in Table 2 and marked as "Ref." in Table 3. However, the parameters that directly affect the simulation of steam and zirconium oxidation phenomena (the oxidation models used in the ASTEC and RELAP/SCDAPSIM computer codes) are not included in the list of uncertain parameters.

The developed sets of input parameters were used for the calculation of the QUENCH-03 and QUENCH-06 tests by employing the RELAP/SCDAPSIM and ASTEC computer codes using models presented in Fig. 2. The same input models were used for the calculation of QUENCH-03 and QUENCH-06 tests. The maximal and minimal values of parameters (Table 3) where entered in the same input files for the QUENCH-03 and QUENCH-06 test calculations.

4.5. *Results of bounding calculations of QUENCH-03 test*

As already mentioned, when using the RELAP/SCDAPSIM code Mod3.5 version, it is possible to model the steam–zirconium oxidation with enabled shattering and with disabled shattering oxidation models. The general material oxidation model used in RELAP/SCDAPSIM calculates the generation of heat, production of hydrogen, and reduction of steam. This model uses oxidation rate equations with material temperatures defined by the component heat conduction model. Material oxidation is assumed to behave according the parabolic rate equation:

$$\frac{d\delta}{dt} = \frac{A}{\delta} e^{\left(\frac{-B}{T}\right)}, \tag{1}$$

where δ is weight gain or layer thickness (kg/m^2 or m); T is temperature (K); t is time (s); A and B are parabolic rate constants taken from MATPRO [32]. This general model for slow steam–zirconium oxidation cases and the shattering oxidation model is disabled.

Coryell et al. [32], when performing the modelling of reflood oxidation using SCDAP/RELAP5, proposed to use the model of enhanced oxidation when the outer oxide layer of a fuel rod component is considered to shatter. This will occur when the following criteria are met: β phase thickness is

Table 3 – Input parameters for the calculation of maximal and minimal values.

No.	Parameter	Maximal calc. (%)	Minimal calc. (%)
1	Quenching water flow	Ref. −3	Ref. +3
2	Steam flow (g/s)	Ref. −3	Ref. +3
3	Argon flow (g/s)	Ref. −3	Ref. +3
4	Quenching water temperature (K)	Ref. +2	Ref. −2
5	Steam temperature (K)	Ref. +2	Ref. −2
6	Argon temperature (K)	Ref. +2	Ref. −2
7	Thermal conductivity of ZrO_2	Ref. −20	Ref. +20
8	Specific heat of ZrO_2	Ref. −20	Ref. +20
9	Contact resistance of sliding contacts (in RELAP/SCDAPSIM code); Additional resistance outside the bundle (in ASTEC code) (mΩ)	Ref. −10	Ref. +10
10	Quenching water pressure (bar)	Ref. −2	Ref. +2
11	Steam pressure (bar)	Ref. −2	Ref. +2
12	Argon pressure (bar)	Ref. −2	Ref. +2

ASTEC, Accident Source Term Evaluation Code; Calc., calculation; Ref., reference.

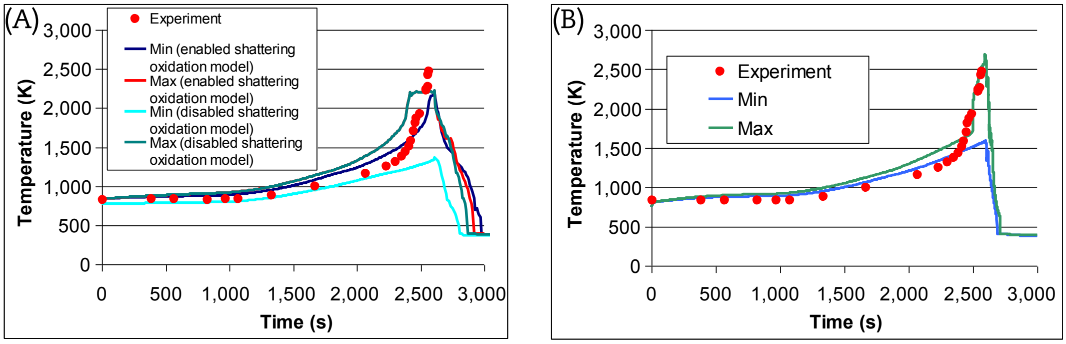

Fig. 10 – Calculation results of QUENCH-03 test, temperature of cladding of the fuel rod imitator from the outer rod ring at 750-mm height. (A) RELAP/SCDAPSIM. (B) Accident Source Term Evaluation Code. Max, maximum; Min, minimum.

≤ 0.1 mm and cooling rate is > 0 for four consecutive time steps within the temperature range of 1,150–1,560 K.

In addition to the shattering criteria, a Boolean variable has been introduced which, when true, will shatter the oxide layer on all components at all axial nodes. This Boolean variable is linked to a RELAP5 logical trip which is specified on input. It should be noted that this Boolean variable is intended to be drastically conservative, since all in-core oxide is shattered, and should dramatically over predict the rate of hydrogen production. This part of the model has been implemented to allow the user to estimate the maximum oxidation rate that could be experienced for a given transient [32].

In the implementation of the enhanced oxidation model (the model with enabled shattering), the oxidation model was modified to track two oxide histories, a physical oxide history, and an effective oxide history. The physical oxide history was unchanged and is used for all the mass balance and heat conduction modelling. An effective oxide history was represented as two independent variables, the effective oxide thickness, and the effective oxygen weight gain. These variables are tracked for each axial node of each component and represent δ in Eq. (1). When the reflood criteria are met, the effective oxide thickness is reset to model fresh unoxidized zircaloy, and the oxygen weight gain is reset to the difference between the physical oxygen weight gain and the oxygen in the removed oxide layer.

In the ASTEC V2.0r3 code ICARE module [33], the same parabolic rate equation as in the SCDAP is used to define oxidation. The upper temperature that can possibly activate the shattering process is 1,560 K. The oxide shattering is activated in the ICARE component when the following criteria are locally fulfilled for the sudden quenching case: the component temperature is > 1,150 K and < 1,560 K, the cooling rate is > 2 K/s during two consecutive time steps, the thickness of the Zr layer is ≤ 0.1 mm (100 microns), and the ZrO_2 layer thickness is > 2 microns.

For the strong heat-up case: the component temperature is > 1,150 K and < 1,560 K, the heating rate is > 2 K/s during two consecutive time steps, the thickness of the Zr layer is ≤ 0.1 mm (100 microns), and the ZrO_2 layer thickness is > 2 microns.

In this section, the results of two RELAP/SCDAPSIM code calculations for the maximal and minimal values of parameters were performed. One pair calculation was provided with the shattering oxidation model enabled, another with the shattering oxidation model disabled. The RELAP/SCDAPSIM and ASTEC computer code calculation results are presented in Figs. 10–14. In Fig. 10, the QUNCH-03 test temperature of the cladding of the fuel rod imitator from the outer rod ring at 750 mm calculated by the RELAP/SCDAPSIM and ASTEC computer codes is presented. The ASTEC calculations using input with a "maximal" set of parameters gives good agreement with the experimental data. However, the minimal temperature values calculated using ASTEC are much lower than the experimental data. The maximal and minimal values of the temperatures calculated using RELAP/SCDAPSIM in

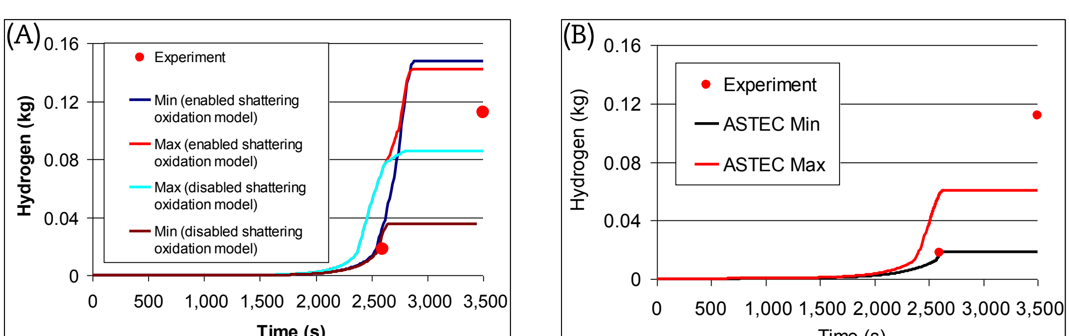

Fig. 11 – Total hydrogen generation calculation results of QUENCH-03 test. (A) RELAP/SCDAPSIM. (B) Accident Source Term Evaluation Code (ASTEC). Max, maximum; Min, minimum.

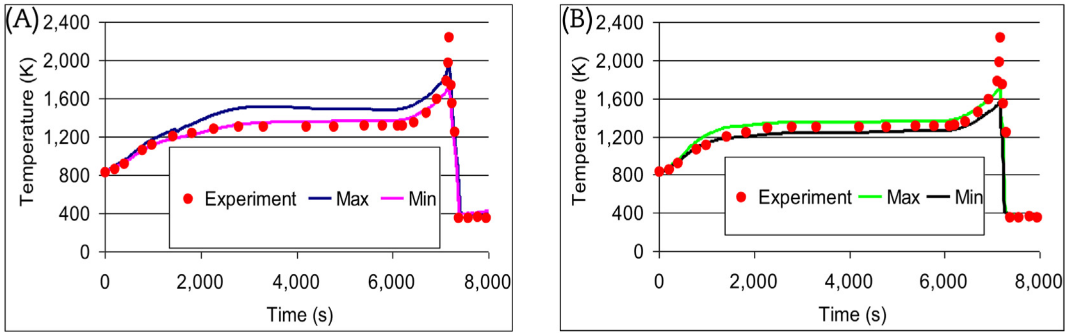

Fig. 12 – Calculation results of QUENCH-06 test, temperature of cladding of the fuel rod imitator from the outer rod ring at 750 mm-height. (A) RELAP/SCDAPSIM. (B) Accident Source Term Evaluation Code. Max, maximum; Min, minimum.

both calculations (with enabled shattering and with disabled shattering oxidation models) are similar. Both maximal and minimal (with enabled shattering oxidation model) calculation results overestimate the temperatures during the transient phase, but the peak of the temperature during the quench phase is lower than the experimental data. Using the minimal values of the temperature with then the shattering oxidation model is disabled, the temperatures in all phases are lower than the experimental data.

The total hydrogen generation of the QUENCH-03 test is presented in Fig. 11. The total amount of generated hydrogen, calculated by the ASTEC code, is only ~50% of the experimental data. Using the RELAP/SCDAPSIM code with the shattering oxidation model enabled, the calculated total amount of generated hydrogen is ~30% higher than the experimental data. The input parameters, which give minimal values for the temperatures of the fuel rod imitator cladding, give the highest total hydrogen generation values. This is because one of the input parameters is mass flow rate of quenching water. In the "minimal" set, more water is injected in the QUENCH bundle during the quenching phase, and that provides better cooling of the test bundle. This assumption works well for ASTEC and RELAP/SCDAPSIM calculations when the shattering oxidation model is disabled. Using shattering oxidation model, this water provides more reactions of zirconium oxidation and more hydrogen is generated. In the opposite case, using the "maximal" set of parameters (with the decreased flow rate of water for the quenching), the total amount of generated hydrogen is lower than when the shattering oxidation model was enabled.

As visible from Figs. 10 and 11, the described RELAP/SCDAPSIM shattering oxidation model has limitations. Using this model, the calculated cladding surface temperature during the shattering process is lower than the experimentally measured value. Moreover, because of the parabolic rate equations to define oxidation, the code does not calculate the profile of oxygen content through the cladding. The proposed shattering criterion deviates from the experiment of Chung and Kassner [34] when the maximum cladding temperature exceeds 1,560 K, and will under-predict the enhanced oxidation. In order to improve the model, the reaction–diffusion equations must be implemented [35].

4.6. *Results of bounding calculations of QUENCH-06 test*

The ASTEC and RELAP/SCDAPSIM code calculation results for the QUENCH-06 test are presented in Figs. 12–14. The calculation results of cladding temperature in the fuel rod imitator from the outer rod ring at 750 mm are presented in Fig. 12. It is shown that during preoxidation and transient phases, the RELAP/SCDAPSIM code in the maximal case overestimates the temperatures of fuel rod imitators. In the minimal case, the calculated temperatures are similar to the experimental data. In the QUENCH-06 test, the heating rate of the fuel rod imitators is slower and the maximum heating power is lower compared those in the QUENCH-03 test. Therefore, the temperature rises slower, and the maximum value of the imitator

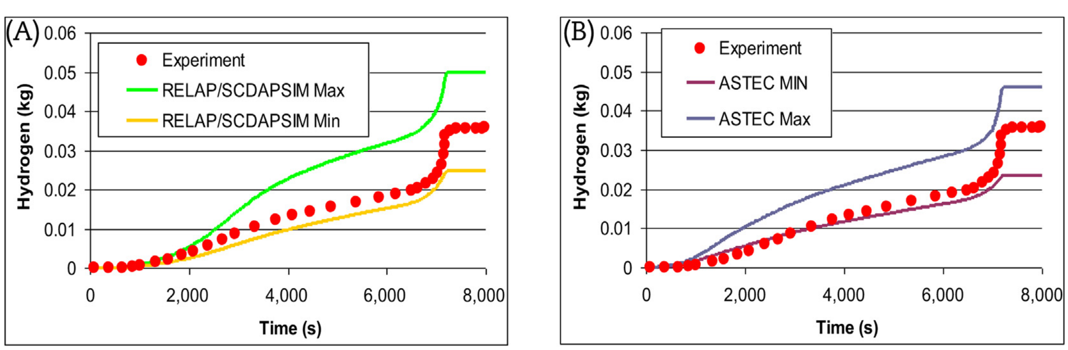

Fig. 13 – Calculation results of QUENCH-06 test, total hydrogen generation. (A) RELAP/SCDAPSIM. (B) Accident Source Term Evaluation Code (ASTEC). Max, maximum; Min, minimum.

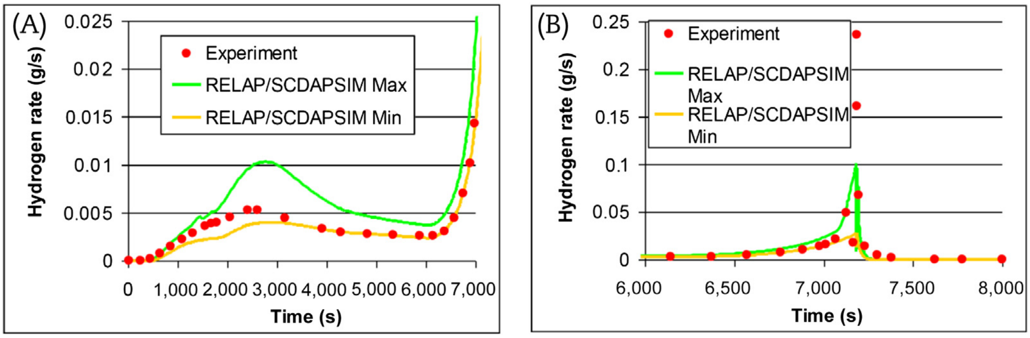

Fig. 14 – RELAP/SCDAPSIM calculation results of hydrogen generation rate. (A) Time interval from 0 seconds to 7,000 seconds. (B) Time interval from 6,000 seconds to 8,000 seconds. Max, maximum; Min, minimum.

cladding temperature is lower. The zirconium oxide layer grows slowly, and the shattering of the oxide layer does not occur. Therefore, during the QUENCH-06 test modelling using the developed input deck for the RELAP/SCDAPSIM code, only the steam–zirconium model with disabled shattering oxidation was applied. The results calculated by the ASTEC code demonstrated better agreement with experimental data (minimal and maximal calculations bounding the experimental data) in the preoxidation and transient phases. However, during the quenching phase, both codes calculated lower temperatures and than measured during the experiment: the maximal temperature using RELAP/SCDAPSIM reaches ~2,000 K, while ASTEC reaches ~1,650 K.

The calculations of total hydrogen generation during the QUENCH-06 test are presented in Fig. 13. The minimal and maximal values calculated by the RELAP/SCDAPSIM code bound the experimental data. Similar calculation results were also received using the ASTEC code but the minimal calculation values in the heat-up phase are a little bit overestimated. However, the peak of hydrogen generation rate during quenching phase (Fig. 14B) using the RELAP/SCDAPSIM code in the "maximal case" is 2.5 times lower than the experimental data. In the "maximal case," the small peak of hydrogen generation rate during preoxidation phase has been observed. This peak occurred because the temperatures in the maximal case were higher than the experimental data.

5. Conclusions and Discussion

The analysis and simulation of the QUENCH experiments allowed us to achieve two goals to be achieved. Firstly, it provided a better understanding of the processes in the reactor cores during a severe accident—the overheating of the core and further injection of water (quenching). Secondly, it revealed the limitations of computer codes when calculating zirconium oxidation, oxide layer formation, and shattering.

The QUENCH-03 and QUENCH-06 tests with oxidation of fuel rod imitators in the steam environment were selected as the main object of investigation in this article. The main purpose of the article is to propose an approach for how to develop a basic input deck for simulation of QUENCH experiments using best estimation codes. This approach evaluates possible uncertainties of calculations. The developed nodalization (input deck), without any significant changes, could be used later for simulation of different QUENCH tests of the same nature. In order to achieve the scope, basic input decks were developed using the ASTEC and RELAP/SCDAPSIM computer codes. The analysis of sensitivity of uncertain parameters of calculation results, obtained using the best-estimate computer code ASTEC, was performed using the SUNSET tool, while the results of the RELAP5/SCDAPSIM computer code calculations were analyzed using the SUSA tool. This allowed evaluating the influence of uncertain input parameters on the tests modelling results.

Despite differences between the QUENCH-03 and QUENCH-06 tests, the sensitivity analysis showed that the influence of initial parameters on calculation results of the temperatures of fuel rod imitators and total hydrogen generation is similar for both tests: at the heat-up phase, the biggest influence on the temperature of the cladding of fuel rod imitator calculation results were exhibited by the contact resistance of electrical heaters, thermal conductivity of ZrO_2, steam flow rate and coolant temperature; during the quenching and transient phases, the biggest influence on the temperature of the cladding of the fuel rod imitator calculation results were exhibited by contact resistance, steam flow rate, and thermal conductivity of ZrO_2; and the parameters, with the biggest influences on the hydrogen calculation results, are: contact resistance, thermal conductivity of ZrO_2, steam flow at the heat-up phase, and specific heat of ZrO_2.

Taking into account the results of uncertainty and sensitivity analysis, two sets of parameters which give the highest and lowest values of hydrogen generation were developed. However, the parameters that directly affect the steam and zirconium oxidation phenomena (the oxidation models, used in ASTEC and RELAP/SCDAPSIM computer codes) were not included in the list of uncertain parameters. This is because more effort is needed to validate the available and newly developed oxidation models in these computer codes. The results of the calculations, performed using both computer codes and both sets, showed that the calculation results of the maximal and minimal sets bounded the experimental data. Thus, it could be concluded that the RELAP/SCDAPSIM and ASTEC computer codes sufficiently reflect the main phenomena that occurred during these two tests and it is possible to develop a basic input deck for similar QUENCH tests. This input deck, developed using the RELAP/SCDAPSIM and ASTEC codes, can represent QUENCH-03 and QUENCH-06 experiments with the present range of uncertainties.

For similar analyses, where the initial, boundary conditions, and the main occurring phenomena are similar, the influence of uncertain input parameters on the calculation results will be very similar too. The results of analyses, performed in the current article, demonstrated that it is possible to use the experience gained from the comprehensive uncertainty analysis and to evaluate only those parameters which have the biggest influence (by developing only 2 sets of minimal and maximal parameters). In such a case, it is necessary to perform only two calculations instead of 59–100.

The RELAP/SCDAPSIM and ASTEC computer codes have limitations related to Zr oxidation modelling. The shattering of the oxide layer model in the RELAP/SCDAPSIM code Mod3.5 version cannot reveal the relations of the cladding surface temperature before cooldown with the cladding conditions after shattering. Because of the parabolic rate equations that define oxidation, the code does not calculate the profile of oxygen content through the cladding. The calculations using the ASTEC V2.0r3 code and the same correlation for the entire range of temperatures showed bad agreement with the experimental results. On the other hand, a correlation combining the steam–zirconium oxidation at low and high temperatures should be created to perform the reliable simulation of the reflooding, melting, and relocation of the cladding and fuel material phenomena.

Gained experience will be used in the future for the modelling of other QUENCH experiments. This will enable one to have a better understanding of computer code specifics and limitations. The adequate modelling of the phenomena related to the flooding of an overheated reactor core is very important when performing the safety analysis of nuclear power plants and developing severe accident management guidelines. The lessons learned from the performed work will be used in the modelling of severe accidents in different light water reactors and spent fuel pools.

Conflicts of interest

The authors have no conflicts of interest to disclose.

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