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Application of the ASYST Code in Estimating Uncertainty of the QUENCH-03 Experiment Calculation

Petra Strmečki, Siniša Šadek, Davor Grgić

Summary **— Core quenching is the main safety measure for mitigation of the consequences of a severe accident in a light water reactor (LWR), but it results in cladding oxidation with a large release of heat and hydrogen. Produced hydrogen presents a new potential problem for containment integrity since hydrogen mixed with air creates an easily flammable containment atmosphere. Therefore, it is important to accurately estimate the amount of hydrogen released during core quenching. Hydrogen production and other physical-chemical phenomena in the reflooded core are modeled using specialized severe accident computer codes, but due to the complexity of those phenomena, it is difficult to create precise and accurate computer models. In order to deliver experimental and analytical data to support the development of quench-related models in severe accident computer codes, QUENCH experimental program has been launched in 1996 at the Karlsruhe Institute of Technology (KIT). The QUENCH-03 experiment was conducted in January 1999 with the aim of investigating the reflood behavior of PWR fuel rods with low oxidation. Although QUENCH experiments have given new insight into severe LWR accidents, there are many sources of uncertainty in quench-related calculations, e.g. modeling of physical phenomena or numerical models of the plant. Those uncertainties are taken into account by the ASYST code, a severe accident code that uses probabilistic methodology based on propagation of input uncertainties. For the observed QUENCH-03 experiment, the calculation and uncertainty analysis were carried out in the ASYST code, and the results obtained by simulation were compared with the experimental values.**

Keywords **— QUENCH-03, ASYST, severe accident progression, uncertainty analysis**

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I. Introduction

Loss of coolant accident in a nuclear reactor can result in a severe reactor overheating leading to a possible core meltdown. In order to avoid such a scenario, one of the main actions in light-water reactors (LWR) is core quenching, i.e. reflooding of the uncovered degraded core [1]. Although quenching prevents further core overheating, it causes a new safety concern, which is hydrogen production [2]. At high temperatures, steam reacts with zirconium, which is present in the fuel cladding. Zirconium oxidation is highly exothermic, producing large amounts of heat and hydrogen, as shown in Eq. (1). Hydrogen and air create a flammable mixture, meaning there is a high risk of explosion, containment damage and radioactive material release to the environment.

$$Zr + 2H_2O \rightarrow ZrO_2 + 2H_2 + 6400\,\frac{kJ}{kg}\,Zr \qquad (1)$$

QUENCH experimental program, launched in Karlsruhe Institute of Technology (KIT, formerly FZK) in 1996, aims to investigate hydrogen production that results from the water or steam interaction with overheated elements of the fuel assembly and to identify the limits, e.g. temperature, for successful core reflood and quenching [3]. QUENCH program is still active and 20 experiments have been conducted to date, providing researchers with important findings about physical-chemical phenomena occurring in the reflooded core. Since the number of experimental facilities and conducted experiments is very limited, existing databases are extremely valuable sources of data for severe accident code development and verification.

Although there are ongoing efforts in severe accident research and experimental database expansion, severe accident phenomena and related models still contain numerous uncertainties. Those uncertainties can have a significant influence on simulation results and therefore should be included in safety analyses of nuclear power plants [4, 5].

This paper shows a comparison of experimental and simulation results for the QUENCH-03 experiment, where experimental facility nodalization is adapted from [6, 7, 8]. Calculation and uncertainty quantification was carried out in the ASYST code [9].

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II. Quench Experimental Program

A. QUENCH Experimental Facility

QUENCH experiments are conducted in the QUENCH experimental facility at the Karlsruhe Institute of Technology (KIT), Germany. The main component of the facility is the test bundle, which consists of 21, 24 or 31 fuel rod simulators, depending on the configuration for the specific experiment. Other systems include a DC power supply for tungsten heaters, steam, water and argon supply systems for cooling, hydrogen measurement devices, process control and data acquisition systems [2]. Components of the QUENCH experimental facility are shown in Figure 1.

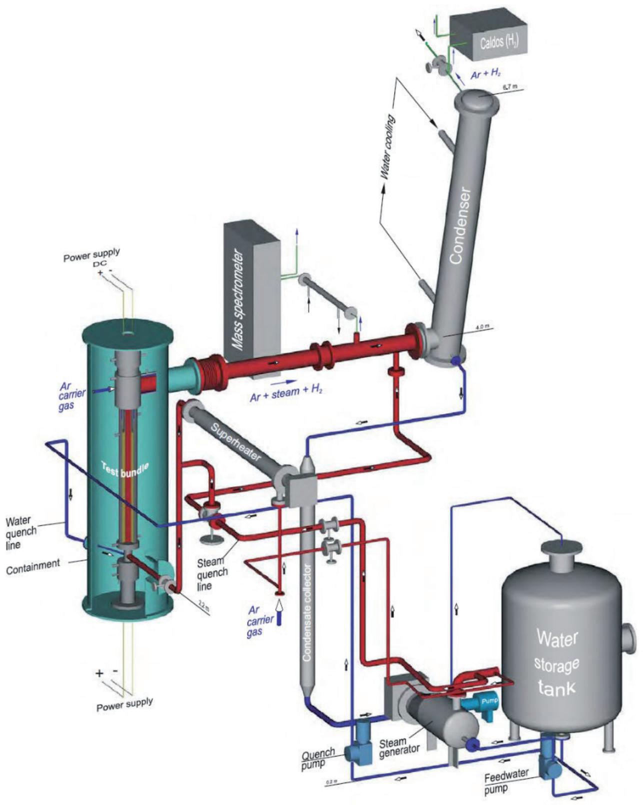

Fig. 1. QUENCH experimental facility

For the QUENCH-03 experiment, the test bundle consisted of 20 electrically heated fuel rod simulators and one central unheated fuel rod simulator. There were four additional corner rods positioned to achieve a uniform radial temperature profile in the bundle.

The unheated fuel rod simulator is filled with ZrO_2. Heated fuel rod simulators consist of tungsten heaters surrounded by annular ZrO_2 pellets. The rods are filled with a mixture of 95% argon and 5% krypton, where argon facilitates cooling and krypton is used for easier fuel rod damage detection. Fuel rod cladding is made of Zircaloy, a material normally used for fuel rod cladding in LWRs. The described test bundle is enclosed in a containment.

Axial cross-section of the test bundle is shown in Figure 2 (left). Fuel rod simulators are heated over the length of 1024 mm. Radial cross-section of the bundle is shown in Figure 2 (right), displaying the layout of fuel rod simulators and four corner rods.

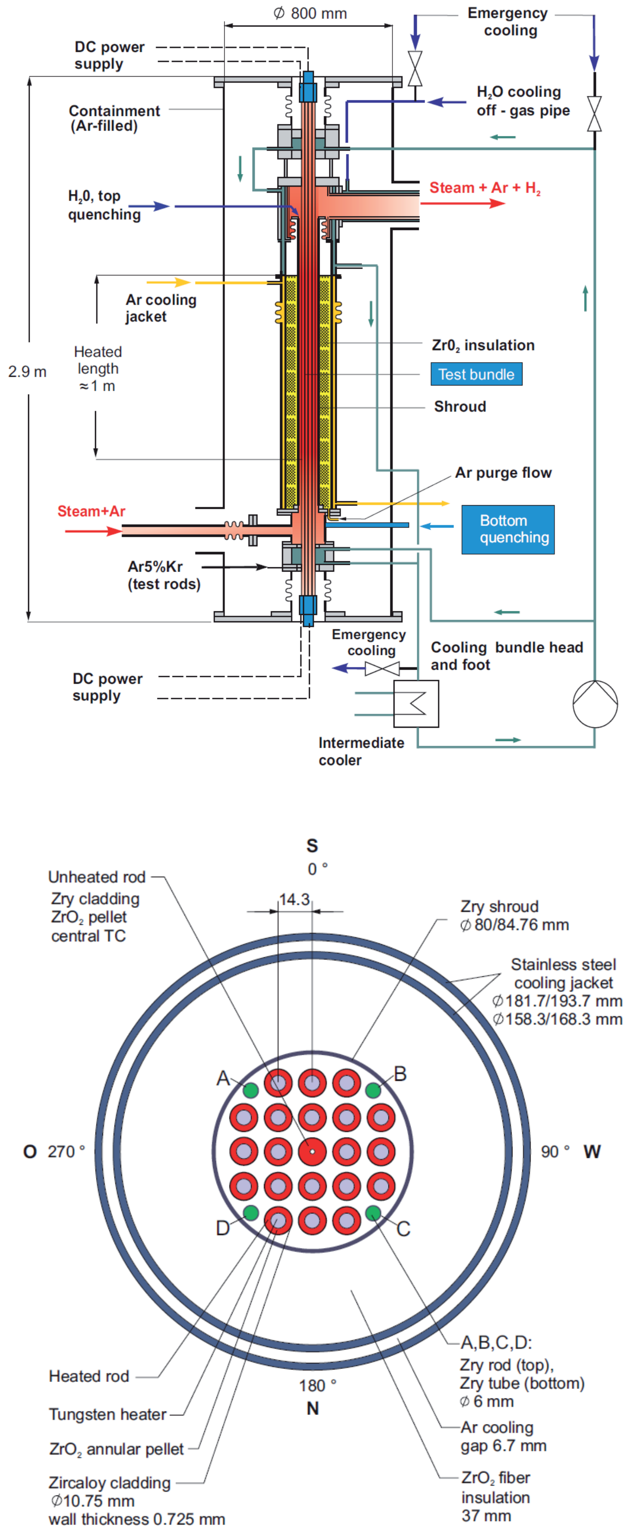

Fig. 2. QUENCH facility and rod layout

B. QUENCH-03 Experiment

Objective of the QUENCH-02 and QUENCH-03 experiments was the investigation of the behavior of PWR fuel rods without pre-oxidation phase during the core reflood. The two experiments differed in electrical power profile, where QUENCH-03 had a steeper power transient. Pre-test calculations were conducted for both experiments. Obtained experimental data was planned to be

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used for developing a database for severe accident models and computer codes [2].

The QUENCH-03 experiment consisted of three phases: the heatup phase, during which the bundle was heated from room temperature to ~900 K, the transient phase and the quenching phase. During the transient phase, electrical power was increased from 3.75 kW to 18.4 kW. When the temperature in the bundle reached ~2400 K, quenching was initiated, and a total amount of 38 liters of water was injected in the test bundle by the end of the experiment. The total amount of electrical energy used in the bundle was 30.3 MJ. Table 1 shows the detailed sequence of events.

According to the pre-test calculations, temperature escalation was supposed to begin at the end of the heated zone, at 950 mm. However, temperature escalation started at a different location, at 750 mm, and therefore went unnoticed by the operators who expected and monitored the temperature excursion at 950 mm. Due to the late response by the operators, the flooding of the test bundle was delayed and bundle damage was more severe than predicted in the pre-test calculations.

Table I:
QUENCH-03 sequence of events [2]

Time [s]	Event
0	Start of data recording
900	Start of electric power transient
2379	The beginning of temperature escalation at the 750 mm level ~ 1402 K
2600	Quenching program initiated, electric power increase, onset of quenching water injection (90 g/s)
2602	44 kW of electric bundle power reached
2606	Steam flow shut off, argon flow switched to the upper bundle head
2619	Onset of cooling, the beginning of significant H_2 production
2627	Shroud failure starting between 750 and 950 mm
2630	Quench water flow of 40 g/s reached
2734	Temperature drop at 550 mm
2747	Start of electric power reduction
2762	4 kW of electric bundle power reached
3501	Electric power shut off
3508	Quench water flow at 0 g/s
3894	End of data recording

III. ASYST model

ASYST model of the QUENCH experiment consists of nodalization of the facility, boundary conditions and uncertainty calculation. Boundary conditions are experimentally measured data that describe mass flows, temperatures and pressure drops in the facility. Uncertainty calculation contains parameters to be varied, their base case values and probability density functions.

A. Nodalization and Boundary Conditions

The QUENCH facility nodalization was adapted from [6], where it was used for the calculation of the QUENCH-06 experiment. Figure 3 (left) shows the axial nodalization of the facility with two types of components used in the model. RELAP5 components are used to model argon cooling of the cooling jacket, water cooling in the upper and lower cooling chamber and fluid flow in the test bundle. SCDAP components are used to model the shroud along with four different types of rods in the test bundle.

Rod layout is shown in Figure 3 (right). There is one central unheated rod, 20 heated rod simulators, and four unheated corner rods positioned to maintain a uniform radial temperature profile in the bundle. Shroud component includes a Zircaloy liner, fiber insulation and a cooling jacket inner tube [6].

Boundary conditions used in the model are argon, steam and quench water flow rates, electric power released in the heaters, temperature of the fluid at the test bundle inlet and outlet, pressure at the test bundle inlet and outlet, temperature at the outer surface of the cooling jacket and temperature of argon used for cooling at the bundle inlet and outlet. Volume 024 represents fluid flow in the test bundle, and therefore gives boundary conditions for the rods. Volumes 034 and 040 represent argon and water cooling, and therefore give boundary conditions for the outer surface of the cooling jacket.

B. Uncertain Parameters

Uncertainty analysis is needed in case there are uncertain parameters in the model, i.e. there are parameters to be defined for which the author does not have exactly determined information. When it comes to severe accidents, there are many processes for which there is a lack of experimental data and, therefore, not enough knowledge about their progression [4].

Sources of uncertainty can be classified as:

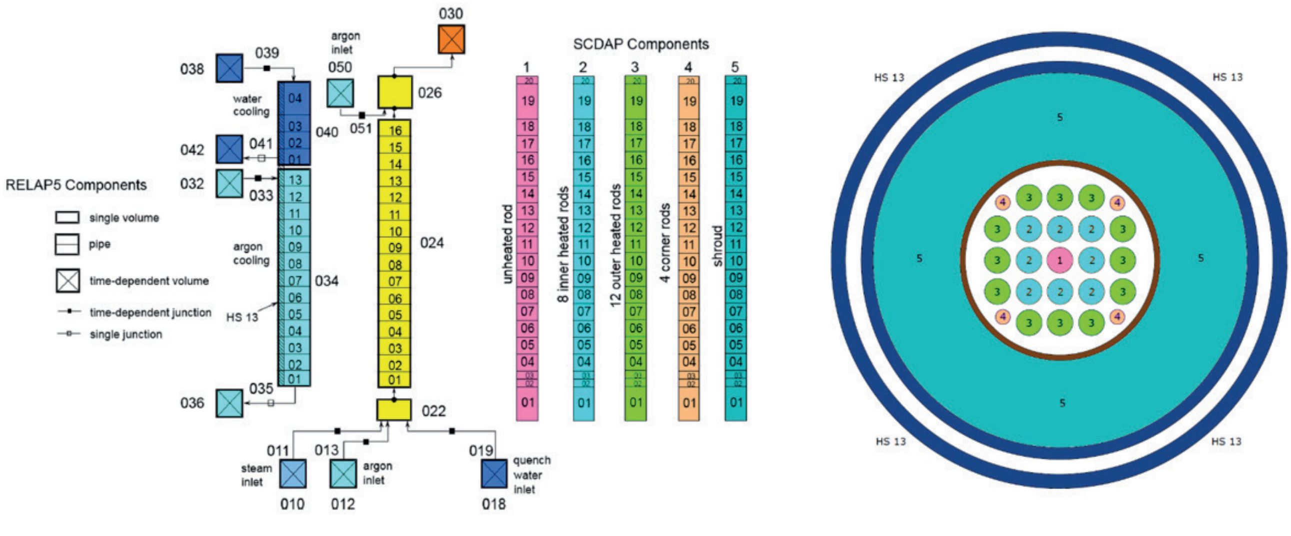

Fig. 3. Nodalization of the QUENCH facility for the QUENCH-03 experiment

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- uncertain parameters related to experimental measurements (e.g. pressure and temperature)
- uncertain parameters related to material properties (e.g. thermal conductivity)
- uncertain parameters related to code modeling (e.g. nodalization, coefficients and correlations used in the codes).

Uncertain parameters varied in the analysis include boundary conditions such as steam flow rate, quench water flow rate, temperature of the outer stainless steel tube and electric power, parameters for cladding oxidation and parameters related to melting and structural behavior. Variations in parameters are described by either a normal distribution or a uniform distribution. Selection of the uncertain parameters is subjective to some point, and depends on the author's knowledge of the problem. Total of 16 parameters have been included in this analysis, with variations up to 2%, depending on the parameter.

For conducting the uncertainty analysis on the RELAP/SCDAPSIM input model from [6], the ASYST program was used. ASYST (Adaptive SYStem Thermal-hydraulics) is an advanced software for nuclear safety analyses with an integrated uncertainty analysis option. The program determines a required number of calculations with uncertain parameters, using the Wilks formula. Wilks formula, Eq. (2), gives the number of calculations N to be performed in order to obtain the desired confidence based on three parameters. Parameters in the formula are confidence level β, cumulative probability γ and order m. In case of the first-order Wilks formula, the general expression is greatly simplified, Eq. (3).

$$\beta = 1 - \sum_{i=N-m+1}^{N} \frac{N!}{i!(N-i)!} \gamma^i (1-\gamma)^{N-i} \quad (2)$$

$$\beta = 1 - \gamma^N \quad (3)$$

For the first-order Wilks formula and standard values of confidence level and cumulative probability, both being 0.95, number of calculations needed to be performed is 59. Number of calculations to be performed does not grow with the number of uncertain parameters.

IV. Calculation And Results

A. Base Case Results

Before uncertainty analysis, a base case calculation is needed in order to confirm the validity of the model. Therefore, first part of the results refers to the comparison of base case results with data measured in the experiment. Base case results were obtained using the boundary conditions, e.g. quench water flow rate and pressure at the test bundle inlet and outlet, given in the experiment.

The base case calculation lasted 3894.5 seconds, which is in agreement with the duration of the experiment. The main observed variables are temperatures reached at different elevations in the test bundle, collapsed water level in the bundle and total hydrogen production. Results of the base case calculation are shown in Figure 4 and Figure 5.

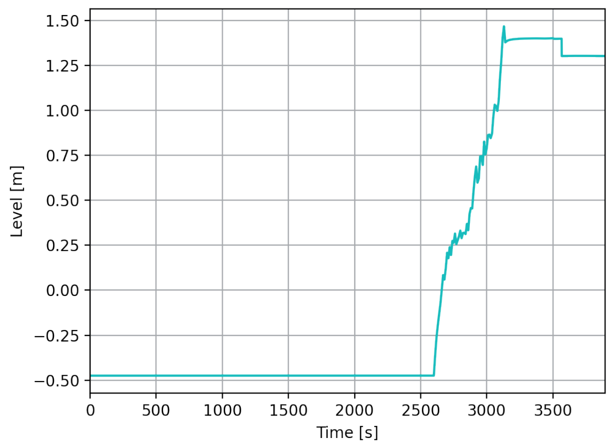

Fig. 4. Collapsed water level in the bundle (base case)

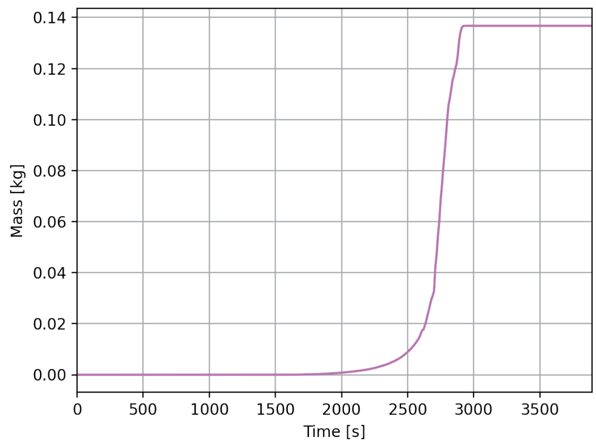

Fig. 5. Total hydrogen production (base case)

Total base case hydrogen production was 136 g, which is in satisfactory agreement with 123 g measured in the experiment. However, shape of the curve for the collapsed water level from the simulation, Figure 4, differs considerably from the curve containing experimentally measured values, marked EXP in Figure 6. Since there was a similar problem with some measurements obtained from QUENCH-02 experiment, after which there was a conclusion that some equipment did not work properly during the experiment, authors of this article considered the possibility that measurement of the collapsed water level for QUENCH-03 was not correct. Additional reason for considering the above possibility is similarity between QUENCH-02 and QUENCH-03 experiments, shown in Table 2. Since both experiments had the same objective and very similar conditions in the bundle, their results were also expected to be similar. For instance, both experiments had similar power profiles and quenching water injection rates. Comparing curve shapes for QUENCH-02 and QUENCH-03 experiments also indicates that QUENCH-03 measurements of the collapsed water level could be wrong.

Table II:
QUENCH test matrix [10]

Test	QUENCH medium injection rate [g/s]	Temp. at onset of flooding (at 950 mm) [K]	Post-test average ZrO2 thickness (at 950 mm) [µm]	H_2 prod. before/ during cooldown [g]
QUENCH-02 Jul 7, 98	water 47	2400	completely oxidized	20/140
QUENCH-03 Jan 20, 99	water 40	2350	completely oxidized	18/120

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However, an additional calculation was carried out with an adjusted collapsed water level that matches the measurement, marked SIM in Figure 6. Total hydrogen production in the additional calculation was around 15 g, which differs considerably from experimentally measured 123 g. Therefore, the input used for all further uncertainty calculations was the original base case input, with the results for collapsed water level shown in Figure 4.

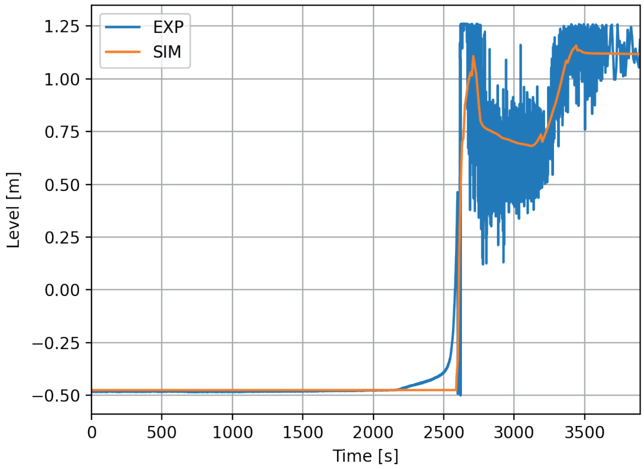

Fig. 6. Experimental and simulated (adjusted) collapsed water level in the bundle

B. Uncertainty Quantification

In accordance with the Wilks formula, Eq. (3), there was one base case calculation and 59 calculations with uncertainties. Results for all 60 calculations are shown in Figures 7 – 10.

Although the parameters were varied within narrow intervals, big variations could be observed in the results. All cases have shown a steady continuous increase in temperature until ~2250 s. After that point, some cases show local oxidation of the cladding, resulting in hydrogen production and temperature peaks. Highest achieved values of temperature and hydrogen production vary greatly depending on the case.

Figure 7 shows collapsed water level in the bundle. Quenching program was initiated at 2600 s, after which there is a sharp increase in collapsed water level in the bundle. Figure 8 shows the total, i.e. cumulative hydrogen production. Total hydrogen production varies from 20 to 267 grams. Although there is some oxidation visible between 2250 and 2600 s, it is quite weak and not noticeable in Figure 10. Rapid oxidation and hydrogen production start after 2600 s. At the same time, there is a noticeable temperature escalation, in some cases exceeding 3000 K, Figure 9. Depending on the case, maximum cladding temperature reached from 2422 to 3134 K. Since total reflooding of the heated part of the bundle occurs after 3000 s in most cases, there is almost no production of hydrogen after that. Accordingly, Figure 10 shows a very low hydrogen production rate after 3000 s and Figure 8 shows that total hydrogen production stays almost constant after 3000 s. There is a significant temperature decrease after 3000 s, with temperature in most cases reaching below 1000 K.

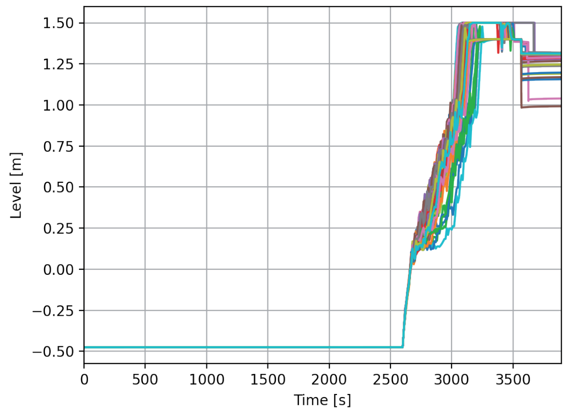

Fig. 7. Collapsed water level in the bundle

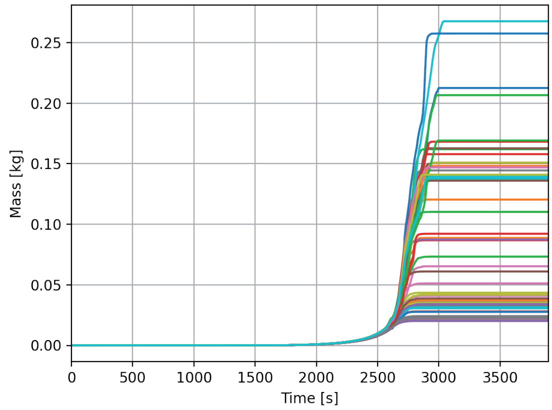

Fig. 8. Total hydrogen production

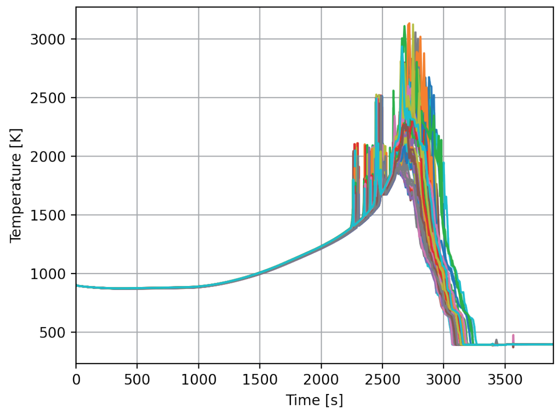

Fig. 9. Maximum cladding temperature

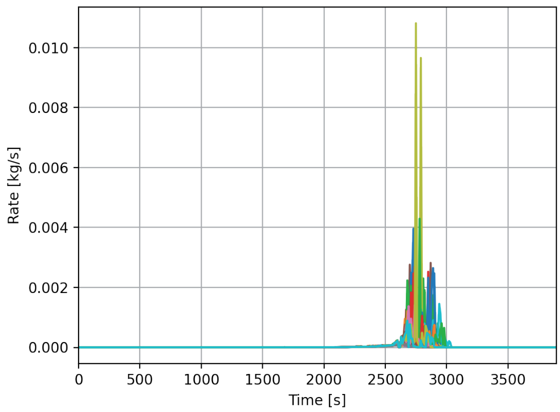

Fig. 10. Hydrogen production rate

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C. Statistical analysis

Standard deviation represents the mean square deviation of numerical values from their mean. Relative standard deviation, i.e. a normalized standard deviation, is calculated as the ratio of the standard deviation to the mean, Eq. (4).

$$RSD = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\frac{x_i}{\bar{x}} - 1\right)^2} \tag{4}$$

Relative standard deviation for selected output data is shown in Figure 11. As can be seen, large deviation appears for hydrogen production rate (BGTH) and total hydrogen production (HYDMASS) at ~1500 s, when local oxidation occurred in some cases. Although the oxidation was very weak, its occurrence in only a few cases caused a large relative standard deviation.

After the quenching phase started at 2600 s, an increase in relative standard deviation is noticeable for all selected output data. The largest deviation appears in hydrogen production rate, with maximum values being reached from 3000 to 3100 s. During that period, the bundle is completely covered with water for most of the cases. However, that small number of cases with uncovered bundle, producing hydrogen, significantly increases the relative standard deviation.

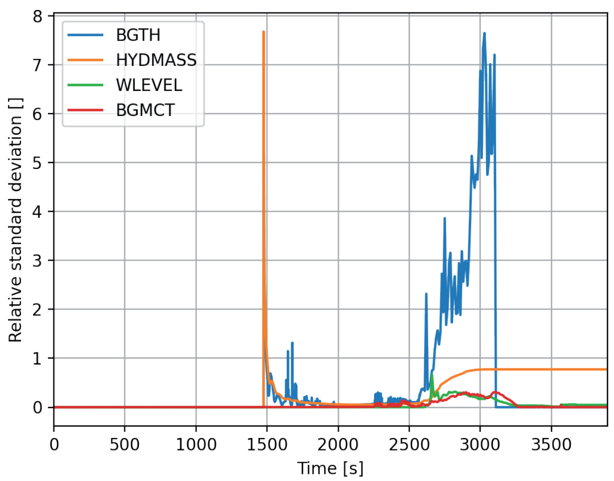

Fig. 11. RSD for selected output data

Correlation coefficient is a value between –1 and 1, used for quantifying the relationship between two sets of variables. In this case, correlation coefficient is used for quantifying the relationship between input variables, such as electrical power profile, and output data. Pearson correlation coefficient, usually represented by r, Eq. (5), is the most commonly used correlation coefficient. It is used for measuring linear correlation between two sets of data. N is the data set size, x_i and y_i are single values from analyzed data sets for each of N calculations, and $\bar{x}$ and $\bar{y}$ are mean values for both data sets. Positive value of the coefficient indicates a positive correlation between the data sets, meaning that increase in the first variable tends to lead to increase in the second variable. Absolute value of the coefficient shows the strength of correlation, with absolute values higher than 0.7 indicating a strong correlation.

$$r = \frac{\sum_{i=1}^{N}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{N}(x_i - \bar{x})^2 \sum_{i=1}^{N}(y_i - \bar{y})^2}} \tag{5}$$

The highest absolute value of the correlation was obtained between the electric power of the heaters and the production of hydrogen, due to the relationship between temperature and the zirconium oxidation process that produces hydrogen. A positive correlation coefficient shows that a higher temperature in the bundle should result in increased hydrogen production.

Pearson correlation coefficients calculated for different combinations of input and output parameters in the described model are shown in Figure 12 and Figure 13. Figure 12 shows Pearson correlation coefficient between selected input parameters and total hydrogen production. Figure 13 shows Pearson correlation coefficient between selected input parameters and maximum cladding temperature. Once again, results have shown that electric power of the heaters tends to have the strongest influence on the observed output parameter.

All the other selected parameters show a negative correlation with total hydrogen production. Steam flow actually cools the bundle, since steam temperature is low compared to the temperatures reached by the rod cladding. Therefore, increased steam flow rate results in decreased hydrogen production, meaning there is a negative correlation between the two. Increase in water flow rate also results in decreased hydrogen production, cooling the bundle. Influence of the water flow rate is visible from 2600 s, when the quenching phase started, to 3500 s, when heated length of the rods was fully covered. Thermal conductivity of ZrO_2 influences the hydrogen production negatively from the moment oxidation and hydrogen production start to the end of the simulation. Higher thermal conductivity means there is a better heat transfer and, therefore, easier cooling of the bundle. That is why there is a negative correlation between ZrO_2 thermal conductivity and hydrogen production. Since higher ZrO_2 conductivity enhances cooling of the bundle, it negatively influences the hydrogen production.

The results related to the maximum cladding temperature show higher amplitudes of the correlation coefficients, but very variable values in time, which, unfortunately, do not give clear and unambiguous results.

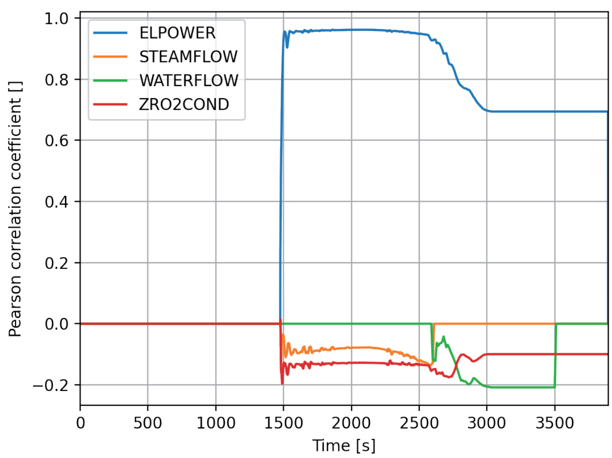

Fig. 12. Pearson correlation coefficient between input parameters and total hydrogen production

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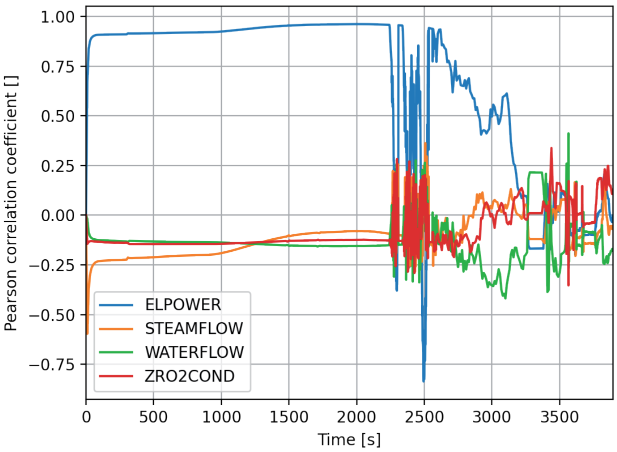

Fig. 13. Pearson correlation coefficient between input parameters and maximum cladding temperature

V. Conclusion

In the QUENCH-03 experiment analysis 16 parameters have been varied within narrow intervals, up to +/−2%, depending on the parameter. Due to the complexity of physical processes present during the core quenching, even very small changes in input parameters caused significant changes in output data.

Maximum cladding temperatures reached from 2422 to 3134 K, while the base case maximum cladding temperature was 2626 K, proving that input uncertainty introduction leads to significant dispersion of output data. Noticeable differences in total hydrogen production are a clear indicator of different hydrogen production rates for individual cases. Total hydrogen production varied from 20 to 267 grams, while the base case production was 136 g. The biggest differences in output data occurred after the quenching phase started, although the differences in temperature are visible before that phase, caused by difference in electrical power profiles. Input uncertainty with the clearest influence on output data is related to thermal power. Other input parameters also show a correlation with output data like maximum cladding temperature, but those correlations, due to the complexity of physical-chemical phenomena during core quenching, are not unambiguous.

It is evident that even small variations of input parameters cause a significant dispersion of output data, which shows that relatively small uncertainties considerably affect simulation results and determine the further experiment or NPP accident course.

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