

# PROPAGATION OF NUCLEAR DATA UNCERTAINTY FOR A CONTROL ROD EJECTION ACCIDENT USING THE TOTAL MONTE-CARLO METHOD

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## ABSTRACT

The Total Monte-Carlo method was applied to a full 3-D core of a typical pressurized water reactor (PWR) for the uncertainty analysis of key reactor parameters as result of uncertainties in nuclear data of the isotopes  $^{235,238}\text{U}$ ,  $^{239}\text{Pu}$ , and thermal scattering data for H in  $\text{H}_2\text{O}$ . Both steady-state and transient reactor states were considered. Uncertainty evaluation of key physical quantities is of importance in the safety assessment during licensing of new nuclear power plants (NPP), and upgrading of operating conditions of NPP already in operation. This work focus on the uncertainties in important reactor parameters followed during the evolution of a control rod ejection accident, where the control rod with the highest worth is supposed to be ejected from the core within 0.1 seconds. Among other parameters studied, the clad-to-coolant heat flux (and the associated uncertainty) was considered, which is an important parameter in relation with the departure of nucleate boiling (DNBR) safety criteria used for this type of reactivity insertion accident scenarios.

*Key Words:* Uncertainty, Total Monte-Carlo, RIA, Rod ejection, Safety

## 1. INTRODUCTION

The Total Monte-Carlo method (TMC) was developed in 2008 (see [1, 2]) as an alternative method to the more traditional deterministic methods (see [3]) used to perform uncertainty analysis using perturbation theory. This relatively new method takes advantage of the increasing computational power of nowadays computers. Basically the method entails in performing the same type of calculation a large number of times, and randomly varying each time certain input parameters sampled within a pre-determined interval. In the last years the method has been extensively applied to several nuclear systems (from light water reactors to accelerator-driven systems and Generation IV systems) with different degrees of complexity to perform uncertainty analysis due to variations in nuclear data. Both Monte-Carlo (see [4]) and deterministic codes (see [5]) have been used in these studies.

This work extends on those studies by applying the TMC method to a full 3-D core model of a PWR with thermal-hydraulic feedback for both steady-state and transient conditions. One

of the transient scenarios considered during safety analysis is the reactivity insertion accidents (RIA). We considered in this study a control rod ejection scenario, which is identified by the regulators as a design basis accident. For these accident scenarios, as well as for other scenarios in general, an uncertainty analysis of the results is of importance to determine with confidence the margins to the regulatory acceptance criteria (see [6]). The uncertainty in the calculated physical parameters have to be evaluated, and their sources identified. The study of the sources of these uncertainties and their importance can be used to start actions to reduce the uncertainties, and possibly as a consequence either to increase the margin to the acceptance criteria or to relax the specifications of some of the key safety components. The quantification of the uncertainties due to variations in nuclear data is the subject of this paper.

The paper is organized in the following way. Section 2 describes the assembly and core models used. Sections 3 and 4 present the calculational tools and the methodology applied. Section 5 discusses the details of the calculations at steady-state and transient conditions. Section 6 presents the main results of the control rod ejection calculations, and the conclusions are summarized in Section 6 together with the prospects for future work.

## 2. ASSEMBLY AND CORE MODEL

The model used in the assembly and core calculations are based on a Westinghouse 3-loop PWR loaded with UO<sub>2</sub> fuel with 4.8% enrichment. The main data used for this reactor model are included in Table I (see [5]).

**Table I.** Main data for the Westinghouse reactor model.

| Parameter                     |       |
|-------------------------------|-------|
| Nominal thermal power [MWth]  | 2800  |
| Power density [W/gHM]         | 39    |
| Nr. of loops                  | 3     |
| Number of Assemblies          | 157   |
| Pin configuration             | 17x17 |
| Assembly pitch [cm]           | 21.5  |
| Core intet temperature [°C]   | 286   |
| Core outlet temperature [°C]  | 323   |
| Core average temperature [°C] | 305   |
| Mass flow through core [kg/s] | 13250 |
| Pressure [bar]                | 155   |

The reactor is loaded with assemblies filled with fuel rods arranged in a 17x17 square lattice configuration with 25 guide tubes. Table II includes the main parameters used for the fuel assemblies. As a simplification of this study the assemblies do not contain burnable absorbers in order to decrease the excess reactivity at the beginning of the cycle (BOC). A 4-batch loading

scheme is adopted where the fresh fuel assemblies are placed mostly at the outer boundaries of the core.

**Table II.** Main data for the Westinghouse fuel assemblies.

| Parameter                |               |
|--------------------------|---------------|
| Configuration            | 17x17 lattice |
| Nr. of guide tubes       | 25            |
| Clad material            | Zirconium     |
| Clad outer diameter [cm] | 0.95          |
| Clad thickness [cm]      | 0.06          |
| Pellet diameter [cm]     | 0.82          |
| Active stack [cm]        | 365           |
| Pin pitch [cm]           | 1.26          |

### 3. CALCULATION TOOLS

This section describes the calculation codes and procedures of the modelling used in the study.

#### 3.1. PANTHER

The simulation of a control rod ejection accident requires a full 3-D core calculation considering thermal-hydraulic feedback. The calculations were performed with the neutronic code PANTHER (see [7]). PANTHER is a 3D nodal code for steady-state, fuel management and core transient analyses, and includes an internal therma-hydraulics module. No modelling is available in this module for the azimuthal and axial conduction. The user has full control over the material data, including the conductivity and specific heat capacity, which can be provided as function of temperature, irradiation and rating. Each channel is treated separately and no account is made for flow redistribution between the channels. The model used cannot predict the propagation of shock waves or choking. Boiling of the coolant is allowed and the code treats it as a vapour/liquid mixture with the possibility to account for sub-cooled boiling and steam-water slip. The conductivity data used originates from an expression for UO<sub>2</sub> used in the ENIGMA fuel performance code (see [8]).

In PANTHER each assembly is considered homogenized, and represented as a block (with possible sub-divisions in all three cartesian directions). At the input PANTHER reads a nuclear database for one (or several) fuel type, and for each of the reflector types (radial, axial top, and axial bottom). The nuclear database contains mainly macroscopic cross sections (like absorption, fission, scattering and power cross sections), kinetic parameters, isotope concentrations and microscopic cross sections for important fission products. These data are given in a broadband energy structure (2 energy groups), and are tabulated as a function of the fuel burn-up and important reactor parameters like: fuel and coolant temperature, coolant density, boric acid

concentration, and control rod state. The code DRAGON version 4.0.6 is used to generate this nuclear database.

### 3.2. DRAGON

DRAGON (see [9, 10]) is a lattice cell code developed to simulate a large diversity of thermal and fast spectrum systems, in several types of geometry (1-D up to 3-D). It can solve the neutron transport equation in a unit cell or fuel assembly using diverse algorithms like: method of collision probabilities, interface-current method, or the long characteristics method. Other modules are also available for interpolation of microscopic cross sections, resonance shielding calculations, editing of condensed and homogenized nuclear quantities, depletion calculations, and sensitivity analysis. It supports different formats for the microscopic library, apart from its native DRAGLIB format.

For the nuclear data base generation several DRAGON runs are required, in order to deplete the fuel up to a maximum burn-up level and at different reactor conditions. The automation of these runs is achieved by means of UNIX shell scripts. An octant of a fuel assembly is modelled, and using a microscopic cross section library in 172 energy groups (XMAS energy structure) based on JEFF3.1 data. More details on the modelling in DRAGON were described in a previous publication (see [5]).

### 3.3. NJOY

The microscopic cross section library read by DRAGON are generated by the code NJOY (see [11]). NJOY is a modular code for nuclear data processing. It basically reads the evaluation nuclear data files (ENDF), processes them at different temperatures and dilution levels, collapses the nuclear data in a few-groups energy grid, and writes the data into a format recognized by DRAGON. In this study the DRAGLIB format was chosen. The standard version of NJOY (version 99.125) is compiled with an external module (DRAGR) which takes care of writing the necessary information in the DRAGLIB format. The automation of the generation of nuclear data in DRAGLIB format for the different isotopes is taken care by a script written in the PYTHON language. This script is also included in the DRAGON code package.

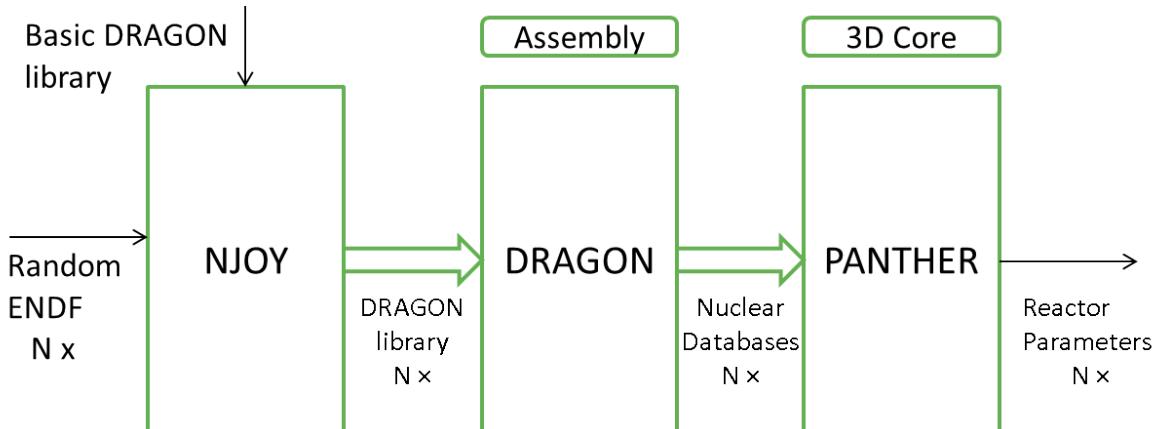
## 4. METHODOLOGY

The TMC method has been selected to simulate the uncertainty in key reactor parameters that describe the control rod ejection accident scenario due to variations in nuclear data. The method has been developed at NRG as an alternative to the more cumbersome perturbation methods used so far extensively over the world. This method takes advantage of the large computational power available nowadays. Basically the TMC method involves the repetition of the same calculation (in our case the same control rod ejection scenario) a large number of times, varying in each

calculation the basic nuclear data used. In this study the different nuclear data libraries are obtained by changing randomly nuclear model parameters within some pre-defined boundaries. In our case the chosen parameters to be randomized are nuclear data parameters for the isotopes  $^{235,238}\text{U}$ ,  $^{239}\text{Pu}$ , and thermal scattering data for H in  $\text{H}_2\text{O}$ . The following parameters were included: cross sections,  $\bar{\nu}$ , energy per fission, angular and energy distributions, resonance information, etc. The evaluation data files in ENDF format contain all these parameters, and are generated in our case by the TALYS nuclear reaction code system (see [12]), according to a procedure described in dedicated references (see [1, 13]). A total of 20-30 theoretical parameters are varied within pre-determined ranges to create the TALYS input. With the addition of random resonance parameters, nuclear reactions from thermal energy up to 20 MeV are covered. The TALYS system creates random ENDF nuclear data files based on these random inputs, according to a procedure described in (see [2]).

Around 450 random nuclear data evaluation files were used to create the same number of DRAGON libraries. One basic DRAGON library is used in the process to create the large number of DRAGON libraries, and it is fully based on JEFF3.1 data. To this basic library the random data for the chosen isotopes ( $^{235,238}\text{U}$ ,  $^{239}\text{Pu}$ , and thermal scattering data for H in  $\text{H}_2\text{O}$ ) were appended. The random data are taken from the nuclear data library TENDL-2011. The generation of the random data files for thermal scattering for H in  $\text{H}_2\text{O}$  are discussed in a dedicated paper (see Ref. [14]).

The same number of nuclear databases for PANTHER are generated with DRAGON, as described in the previous section. These PANTHER databases are finally used for the PANTHER runs, both for the steady-state calculations and the transient analyses. Figure 1 shows schematically the total calculation flow. By performing statistical analysis of the final results (parameters which characterize the steady-state and the transient calculations), the different moments can be determined and thus infer the final uncertainties in the studied parameters, as a first approximation to the solution of the likelihood equations.



**Figure 1.** Calculation scheme for the determination of the uncertainties in the main reactor parameters due to nuclear data uncertainties.

## 5. STEADY-STATE AND TRANSIENT CALCULATIONS

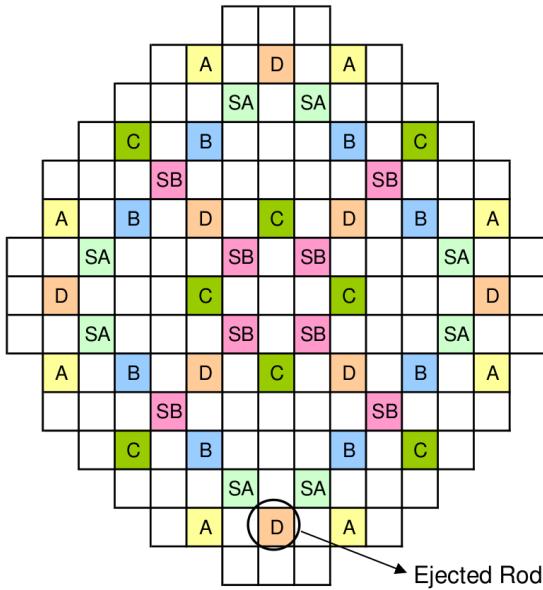
In this section the procedure followed in PANTHER to simulate the steady-state and the control rod ejection transient scenario are described in detail.

### 5.1. Steady-State Calculation

The first core implemented in the PANTHER model is loaded with fuel of different compositions and enrichment dependent on the batch number. The equilibrium core for the 4.8% enriched fuel considered in this study was achieved after 12 cycles, where fresh assemblies are loaded at the begining of each cycle, and resident assemblies are shuffled according to a defined loading scheme. The burn-up of the core is followed at small time steps with all control rod banks removed from the core. The core is kept critical at each time step by adjusting the boric acid concentration in the coolant. After simulation of 12 cycles the equilibrium is achieved, as could be verified by comparing the boron letdown curve obtained for the last three cycles. From the results of cycle 12 the parameters characterizing the equilibrium cycle were analysed. From the statistical analysis of the results for all 450 random nuclear databases, the uncertainty on these parameters due to uncertainties in nuclear data were obtained.

### 5.2. Control Rod Ejection Calculation

The simulation of the control rod ejection accident was initiated at the beginning of the cycle (BOC) of cycle 12. The reactor state at the end of cycle (EOC) of cycle 11 (from the steady-state calculations) is stored in data files for all 450 nuclear databases. These files are used to start the PANTHER run for the transient analyses, after reloading of the core for cycle 12. A control rod ejection scenario at full reactor power (FP) was investigated. The following sequence of events was considered, that leads to the control rod ejection: (1) reactor is at full power (FP) state and at BOC; (2) one single control rod (with the highest worth) inadvertently gets stuck in the core; (3) the reactor is made critical by adjusting the soluble boron concentration; (4) due to failure of the control rod mechanism housing, the stuck control rod (CR) is ejected from the core within 100 ms. After ejection it is supposed that the reactor scram system fails. The boron concentration is kept unchanged and equal to the critical value before the onset of the accident. Figure 2 shows a mapping of the core with the position of the control rod banks and the position of the ejected rod. This accident leads to a loss of primary coolant because of the failed control rod mechanism housing. Since a loss of coolant accident (LOCA) develops within a longer time scale than the actual control rod ejection accident, this aspect is normally treated in a LOCA analysis and therefore not considered in our study. We should point out that for licensing purposes the inclusion of the effect of the loss of primary system integrity is required by the regulatory authorities (see Ref. [15]). The control rod ejection initiated at FP and BOC conditions is generally not the most limiting case, however it illustrates well the potential of using the TMC method for transient analyses.



**Figure 2.** Scheme of Westinghouse core with distribution of control rod banks and position of the ejected control rod.

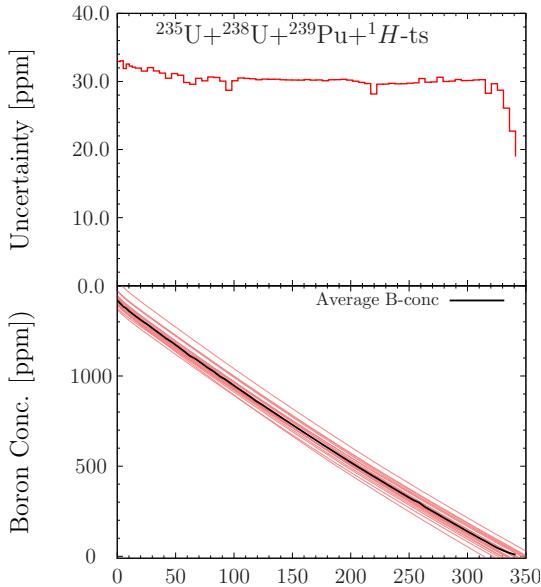
## 6. RESULTS OF CONTROL ROD EJECTION CALCULATIONS

### 6.1. Steady-State conditions before control rod ejection

Figure 3 shows the boron letdown curve obtained for cycle 12. The average cycle length is around 338 effective full power days (efpd), with a standard deviation of 8 days. To illustrate the variation of the letdown curve due to uncertainties in nuclear data, a series of other curves correspondent to several random nuclear databases are also shown. The convergence of the result after 450 runs is satisfactory and the skewness is close to zero. In the top graph the uncertainty in critical boron concentration is given as function of time. The absolute uncertainty is virtually constant during the cycle and amounts to 30 ppm ( $1\sigma$ ). The sharp decrease in uncertainty close to the EOC is an artifact caused by the interruption of the burn-up procedure when the critical boron concentration gets negative.

In Table III the main parameters describing the core conditions at the onset of the transient is shown, and a comparison with the normal reactor state where no control rod bank is inserted into the core.

Due to the insertion of one of the control rods into the core, an assymetry in the power profile is introduced. The maximum local power density ( $P''_{\max}$ ) increases by about 10% and consequently the two peaking factors ( $F_{\Delta H}$  and  $F_Q$ ). This reflects as well on the maximum local fuel temperature and the maximum heat flux. With an increase in the maximum clad-to-coolant heat flux the minimum coolant density decreases (by about 6%). With the insertion of a neutron absorber into the core (the stuck control rod) the critical boron concentration decreases. We should remark that the values for the two peaking factors ( $F_{\Delta H}$  and  $F_Q$ ) are relatively high. This is because of



**Figure 3.** Boron letdown curve (bottom) and uncertainty (top) in boron concentration due to nuclear data variations.

the non-optimized shuffling scheme adopted for the 4-batch core. This is however not expected to influence the conclusions regarding the uncertainties due to nuclear data.

## 6.2. Control rod ejection results

Several reactor parameters were followed during the evolution of the control rod ejection accident, including: multiplication factor, total power, fuel, clad and coolant temperatures, peaking factors ( $F_{\Delta H}$  and  $F_Q$ ), coolant void fraction and heat flux. For each of these quantities the uncertainty due to nuclear data was obtained at each time step. The accident was followed for 16 minutes, with varying time steps from 0.001 to 0.5 seconds depending on the time during the accident simulation. Figure 4 displays the time evolution of these parameters. The fuel temperature ( $T_{pin}$ ) shown is the maximum value observed over the entire core, and determined at the center of the fuel pellet. The clad temperature, void fraction and heat flux are also the maximum values over the entire core.

We assumed that the control rod is ejected from the core at  $t = 2\text{sec}$  from the beginning of the PANTHER simulation. The reactivity insertion amounts to 0.42\$, where a delayed neutron fraction at BOL of 745 pcm was considered. The rapid reactivity insertion causes a power excursion (75% above the nominal power), and a distortion of the power distribution. Due to the distortion of the power distribution there is a fast increase in the hot spot peaking factors, with a maximum increase of 68%. At the same instant the maximum heat flux to the coolant peaks at a value about 20% above the value observed before the start of the accident. This increase in maximum heat flux will decrease the DNBR (departure of nucleate boiling ratio), which could trigger the onset of boiling crisis and consequent failure of a certain number of

**Table III.** Main reactor parameters at steady-state and BOC with unrodded core and with one stuck control rod.  $T_{\text{fuel-max}}$ : max. fuel temperature,  $T_{\text{cool-max}}$ : max. coolant temperature,  $\rho_{\text{cool-min}}$ : minimum coolant density,  $P''_{\text{max}}$ : max. power density,  $\phi_{\text{source-max}}$ : max. clad-to-coolant heat flux,  $F_{\Delta H}$  and  $F_Q$ : peaking factors.

| Parameter                                       | Unrodded State | Stuck-Rod State |
|-------------------------------------------------|----------------|-----------------|
| Critical Boron [ppm]                            | 1465           | 1435            |
| $T_{\text{fuel-max}}$ [K]                       | 1123.94        | 1162.40         |
| $T_{\text{cool-max}}$ [K]                       | 617.45         | 618.32          |
| $\rho_{\text{cool-min}}$ [kg/m <sup>3</sup> ]   | 573.4          | 541.3           |
| $P''_{\text{max}}$ [MW/m <sup>3</sup> ]         | 215.7          | 232.6           |
| $\phi_{\text{source-max}}$ [W/cm <sup>2</sup> ] | 126.5          | 136.6           |
| $F_{\Delta H}$                                  | 1.71           | 1.79            |
| $F_Q$                                           | 2.04           | 2.16            |

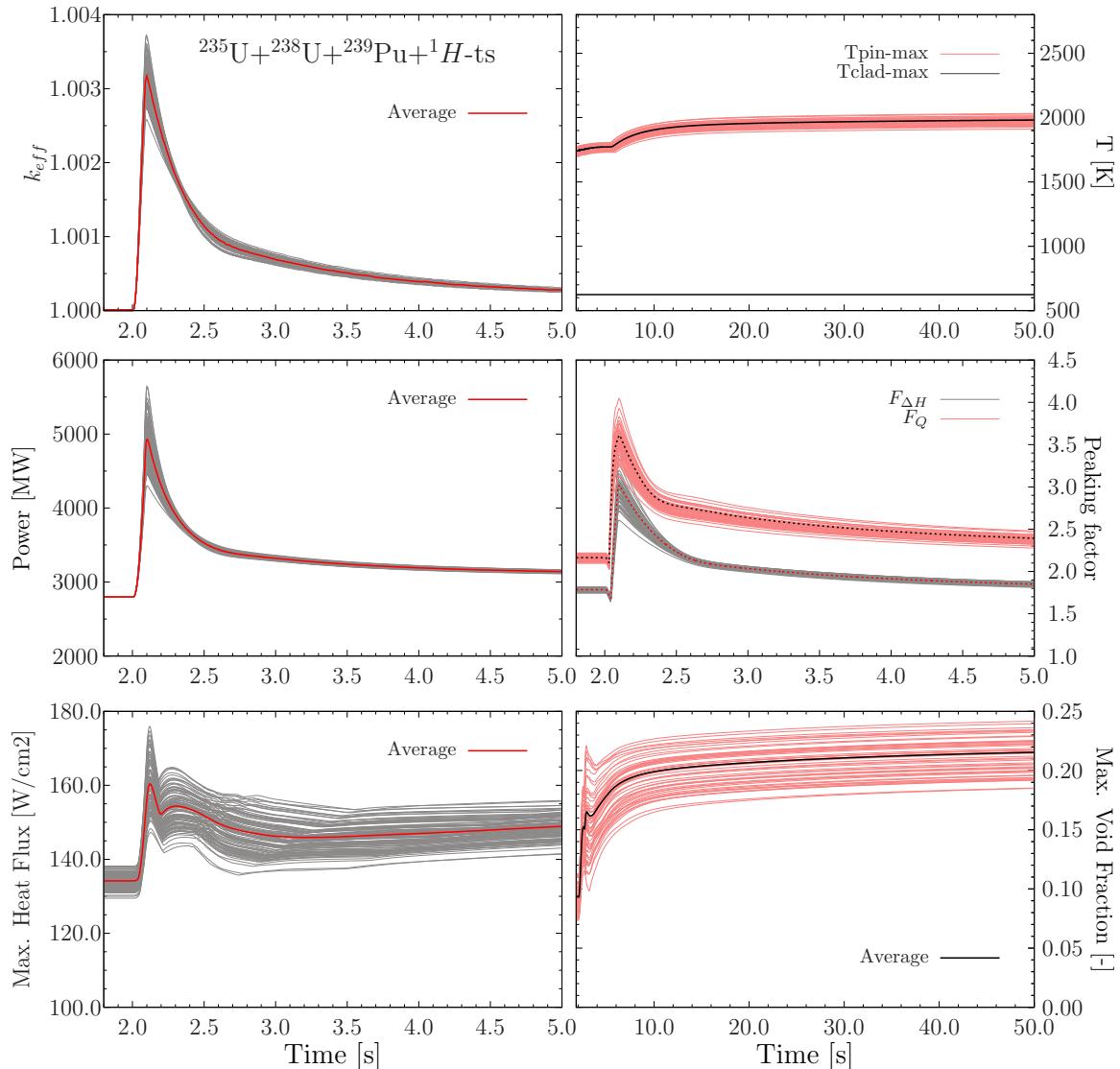
fuel pins. The code system used for this study so far does not have the capability of performing a DNB analyses necessary to take conclusions on the number of fuel rods experiencing clad failure and on the fission products inventory release to the coolant. Notice that the fuel and clad temperatures graph in Figure 4 are given in a different time scale, since the fuel temperature reacts slower to the power excursion and reaches a value about 300 Kelvin above the value observed before the onset of the transient.

Following the fast peak in reactivity and power, the transient is mitigated by the negative Doppler feedback coefficient (around -2.32 pcm/K at BOC), and in a long time scale the reactor power reaches a new equilibrium at a higher level (around 3135 MW thermal) than the nominal power. In this new equilibrium the key reactor parameters show a notable increase, as displayed in Table IV. Within the safety analysis required for reactor licensing the control rod ejection scenario would be interrupted by initiation of automatic reactor trip, triggered by an increase in neutron flux. This aspect of the accident was not considered in the study.

**Table IV.** Main reactor parameters before and after the control rod ejection accident.  $T_{\text{pin}}^0$ -max: max. center-line fuel temperature,  $f_{\text{void}}$ : max coolant void fraction,  $\phi_{\text{source-max}}$ : max. heat flux,  $P''_{\text{max}}$ : max. power density.

| Parameter                                       | Before CR Ejection | After CR Ejection |
|-------------------------------------------------|--------------------|-------------------|
| Total Power [MW]                                | 2800               | 3135              |
| $T_{\text{pin}}^0$ -max [K]                     | 1748               | 2060              |
| $T_{\text{clad-max}}$ [K]                       | 621.5              | 621.8             |
| $P''_{\text{max}}$ [MW/m <sup>3</sup> ]         | 232.6              | 285.7             |
| $\phi_{\text{source-max}}$ [W/cm <sup>2</sup> ] | 170.1              | 136.6             |
| $F_{\Delta H}$                                  | 1.79               | 1.79              |
| $F_Q$                                           | 2.16               | 2.41              |
| $f_{\text{void-max}}$ [%]                       | 0.96               | 24                |

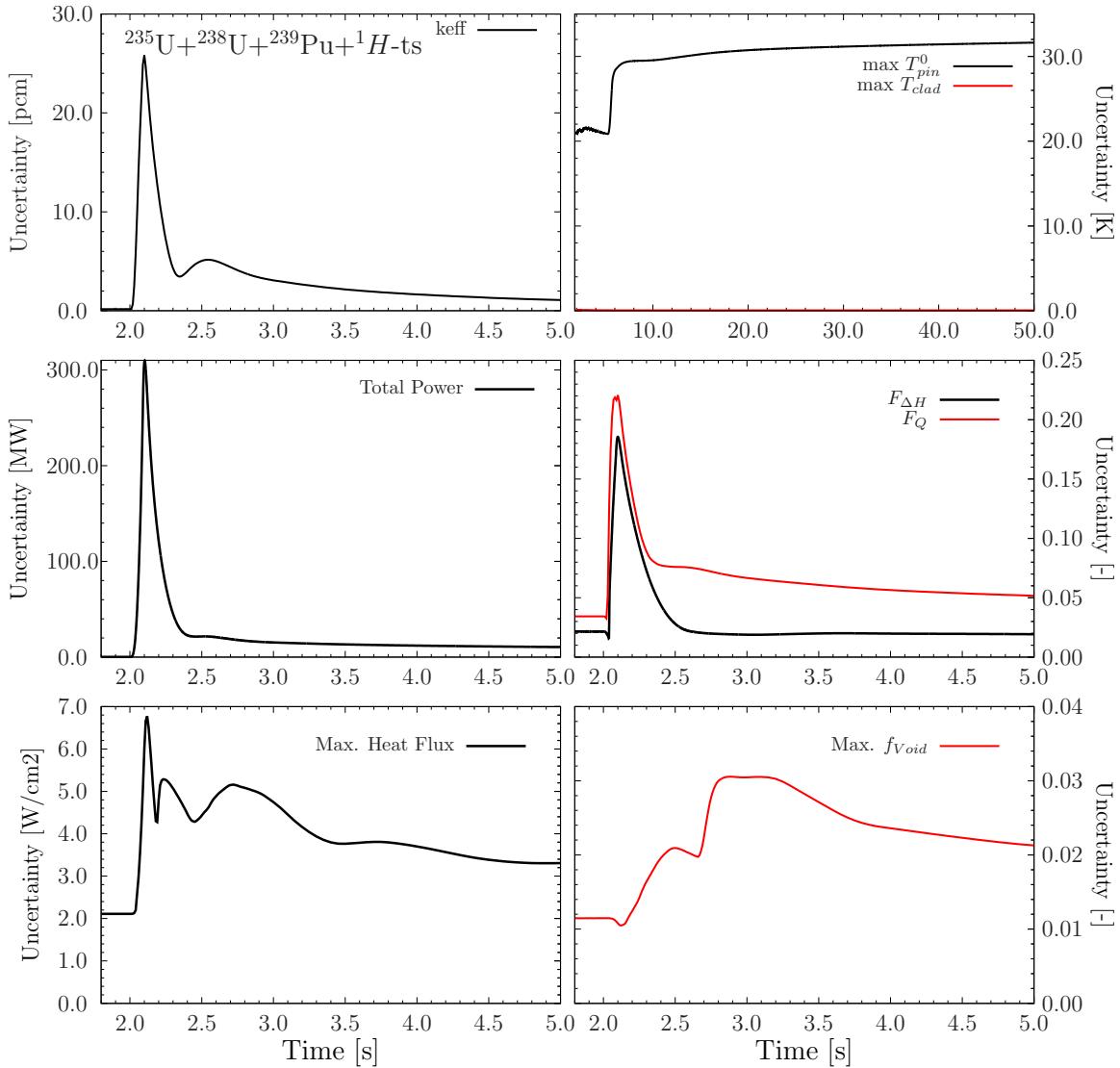
Also shown for all parameters in Figure 4 are a large number of curves correspondent to the



**Figure 4.** Time evolution of the main parameters for a control rod ejection accident at HFP:  $k_{eff}$  - multiplication factor,  $T_{pin}$ ,  $T_{clad}$ : center-line fuel temperature and clad temperature, Power - total reactor power,  $F_{\Delta H}$  and  $F_Q$  - peaking factors, heat flux, and void fraction .

PANTHER runs for different random databases. This illustrates the spread in the results due to combined variations in nuclear data. For each of the parameters an average curve is displayed (curve in a different color in each graph), obtained from the statistical analysis of the results from the 450 PANTHER runs. Figure 5 displays for all parameters the absolute uncertainties ( $1\sigma$ ) as function of time. For most quantities the uncertainties show a peak that coincides with the peaking behaviour on the respective quantity (also when displayed as relative uncertainty). The convergence of each parameter (and as a function of time) was verified by statistical analysis of the results where the running average of the different momenta were analysed. Some of the quantities show a skewed distribution, although within the range -0.6 to 0.6. The uncertainties in Figure 5 should be judged in combination with the safety criteria which apply to this particular accident scenario. For a control rod ejection scenarios for a PWR, the DNBR and the radially-

average fuel pellet specific enthalpy criteria applies in most countries. However, results from RIA tests showed that for irradiated fuels the pellet-clad mechanical interaction (PCMI) mechanism might be the most important mechanism that leads to cladding failure rather than the critical heat flux (see [16]). Therefore, changes in the safety criteria for RIA are under way in most countries to include these new findings in the current regulations. In the current study the obtained uncertainties were not analysed in relation to these criteria, an aspect which will be reserved for a follow-up study.



**Figure 5.** Absolute uncertainty ( $1\sigma$ ) for parameters followed during control rod ejection accident: keff - multiplication factor,  $T_{pin}^0$ ,  $T_{clad}$ : center-line fuel temperature and clad temperature, Total Power - total reactor power,  $F_{\Delta H}$  and  $F_Q$  - peaking factors, clad-to-coolant heat flux, and  $f_{Void}$ : void fraction.

## 7. CONCLUSION AND PROSPECTS

The Total Monte-Carlo (TMC) method was applied for a control rod ejection accident scenario in a typical PWR in order to perform uncertainty analysis as result of uncertainties in nuclear data. Nuclear data for  $^{235,238}\text{U}$ ,  $^{239}\text{Pu}$ , and thermal scattering data for H in  $\text{H}_2\text{O}$  were varied simultaneously. The total calculational scheme was presented where the combination of the TALYS code system, and the codes NJOY, DRAGON and PANTHER were used. In the control rod ejection scenario selected for the study the control rod with the highest worth is supposed to be ejected completely from the core within 0.1 seconds. The core is originally at full power and at beginning of the cycle (BOC) conditions. The time evolution of several key parameters characterizing the accident was analysed, and by statistical analysis the uncertainties on these parameters due to nuclear data were quantified. The following conclusions could be taken from the results:

- During the equilibrium cycle the absolute uncertainty in critical boron concentration is rather flat and amounts to 30 ppm ( $1\sigma$ ), with a maximum boron concentration of 1450 ppm at BOC.
- During the control rod ejection the sharp peak in reactivity coincides with a simultaneous peaking in total power, peaking factors ( $F_{\Delta H}$  and  $F_Q$ ) and maximum clad-to-coolant heat flux. The uncertainty in these quantities also show a peak behaviour, and the relative uncertainty comes to a maximum of 6% (in total power and peaking factors) and 4% (in clad-to-coolant heat flux). The uncertainty for the maximum fuel temperature shows a more smooth behaviour (with a larger time constant), with a maximum relative uncertainty of about 1.5%.

Although the uncertainties in some key parameters were quantified, this work did not evaluate the implications to the margins to the regulatory acceptance criteria that apply to this type of accidents, like the departure of nucleate boiling ratio (DNBR) and the radially-averaged fuel pellet specific enthalpy criteria. Moreover the separate contributions (of each of the considered isotopes) to the total uncertainties were not determined, which could be of importance to identify areas of improvement in nuclear data available in the main libraries. These aspects will be part of follow-up studies.

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