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TOTAL MONTE-CARLO METHOD APPLIED TO THE ASSESSMENT OF UNCERTAINTIES IN A REACTIVITY-INITIATED ACCIDENT

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Abstract

The Total Monte-Carlo (TMC) method has been applied extensively since 2008 to propagate the uncertainties in nuclear data for reactor parameters and fuel inventory, and for several types of advanced nuclear systems. The analyses have been performed considering different levels of complexity, ranging from a single fuel rod to a full 3-D reactor core at steady-state. The current work applies the TMC method for a full 3-D pressurized water reactor core model under steady-state and transient conditions, considering thermal-hydraulic feedback. As a transient scenario the study focused on a reactivity-initiated accident, namely a control rod ejection accident initiated by a mechanical failure of the control rod drive mechanism. The uncertainties on the main reactor parameters due to variations in nuclear data for the isotopes $^{235,238}U$, ^{239}Pu and thermal scattering data for ^{1}H in water were quantified.

Introduction

In licensing process an increasing attention is being directed to the development of safety assessment procedures based on the use of best estimate (BE) methods combined to uncertainty analysis of the output safety parameters [1]. This will relax some of the conservative procedures, which are responsible for the large margins between conservative values and the actual values. The great motivation behind the more accurate prediction of the outcome of some limiting transients is the maximization of plant efficiencies and power. The utilities can consequently reduce the cost of plant operation.

The uncertainty analysis methods in use nowadays are either based on propagation of input uncertainties or on the extrapolation of output uncertainties observed for relevant experiments. In its turn the propagation of input uncertainties are performed either by deterministic or statistical methods. The Total Monte-Carlo method (TMC) developed in 2008 [2] [3] is a statistical method, which takes advantage of the increasing computational power nowadays. 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. 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 [4] and deterministic codes [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 pressurized water reactor (PWR) with thermal-hydraulic feedback for both steady-state and transient conditions. As transient a control rod ejection scenario has been selected for this study, which is considered by the regulators as a design basis accident. The paper is organized as follows.

Section 1 describes the model of the PWR considered. Section 2 discusses the methodology and the code systems used. Section 3 and 4 presents the main results for steady-state and transient conditions, respectively. Finally in Section 5 the conclusions are summarized and prospects for further studies discussed.

1. PWR model

As subject of the study a model of the Westinghouse 3-loop PWR was selected. The reactor was assumed to be loaded with the UO_2 fuel assemblies and without using any burnable absorbers either integrated in the fuel or in the 25 guide tube positions. Therefore a relatively short fuel cycle is obtained for the adopted enrichment of 4.8%. The assemblies are composed of fuel rods distributed in a 17x17 rectangular lattice with pitch of 1.26 cm, and zirconium being used as cladding material. The core is filled with 157 fuel assemblies with an assembly pitch of 21.5 cm. A four batch loading scheme was adopted according to a strategy where the fresh assemblies are loaded mostly at the edge of the core (low-leakage configuration). Representative axial and radial reflectors were modelled. Table 1 shows the main assembly and reactor parameters used in the model [6].

Table 1 - General parameters for the Westinghouse reactor model.

A. Fuel Assembly	
Configuration	17x17
Nr of guide tubes	25
Assembly pitch	21.5 cm
UO_2 weight per assembly	519 kg
B. Fuel Rod	
Clad material	Zirconium
Clad outer diameter	0.95 cm
Clad thickness	0.06 cm
Pellet diameter	0.82 cm
Active stack	365 cm
Pin pitch	1.26 cm
C. Core Parameters	
No of loops	3
Number of assemblies	157
Nominal power produced by the core (MWth)	2800
Power density (W/gHM)	39
Boron-10 content	19.8 at %
D. Coolant info	
Core inlet (^oC)	286
Core outlet (^oC)	323
Core average (^oC)	305
Mass flow through core (kg/s)	13250
Pressure (bars)	155

2. Methodology and code systems

The TMC method was applied to determine the uncertainty due to variations in nuclear data in key reactor parameters that describe the core at steady-state and during the control rod ejection accident scenario. The method entails the repetition of the same calculation (in this case a core simulation with the nodal code PANTHER) a large number of times varying in each calculation the basic nuclear data used. In this study the different nuclear data files are obtained by changing randomly nuclear model parameters within some pre-defined boundaries. The chosen parameters to be randomized are nuclear data parameters for the isotopes $^{235,238}U$, ^{239}Pu, and thermal scattering data for ^{1}H in H_2O. The following parameters were included: cross sections, ν-bar, energy per fission, angular and energy distributions, resonance information, etc. The evaluated nuclear data files in ENDF format contain all these parameters, and are generated by the TALYS nuclear reaction code system [3][7], according to a procedure described in dedicated references [2][8]. 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 [3]. Around 450 random nuclear data evaluation files (for each considered isotope) were used to create the same number of microscopic cross section libraries for the lattice code DRAGON. The microscopic cross sections were generated with the processing code NJOY.

2.1 NJOY

NJOY [9] 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. 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. The random data for the chosen isotopes ($^{235,238}U$, ^{239}Pu, and thermal scattering data for ^{1}H in H_2O) were appended to this basic library. The libraries contain data in 172 energy groups (XMAS energy structure). The random data are taken from the nuclear data library TENDL-2011. The generation of the random data files for thermal scattering for ^{1}H in H_2O are discussed in a dedicated paper [10].

2.2 DRAGON

DRAGON [11] 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 solves 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, besides its native DRAGLIB format. For the nuclear data base generation required by the neutronic code PANTHER, several DRAGON runs were required, to deplete the fuel up to a maximum burn-up level and at different reactor conditions. UNIX shell scripts were used to automate these runs. The code DRAGON version 4.0.6 was used in this work. An octant of a fuel assembly is modelled. More details on the modelling in DRAGON were described in a previous publication [12].

2.3 PANTHER

The steady-state and transient calculations were performed with the neutronic code PANTHER [13]. PANTHER is a 3D nodal code for steady-state, fuel management and core transient analyses, and includes an internal thermal-hydraulics module. 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. No modelling is available in this module for the azimuthal and axial conduction. 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 originates from an expression for UO_2 used in the ENIGMA fuel performance code.

Each assembly is represented in PANTHER as a homogenized block (with possible sub-divisions in all three Cartesian directions). PANTHER reads as input a nuclear database for one (or several) fuel type(s), 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, with group boundary at 0.625 eV), and are tabulated as a function of the fuel burn-up and reactor parameters like: fuel and coolant temperature, coolant density, boric acid concentration, and control rod state.

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) obtained separately for each of the available 450 nuclear databases, the different moments (average, standard deviation, and skewness) can be determined and thus infer the final uncertainties in the studied parameters, as a first approximation to the solution of the likelihood equations.

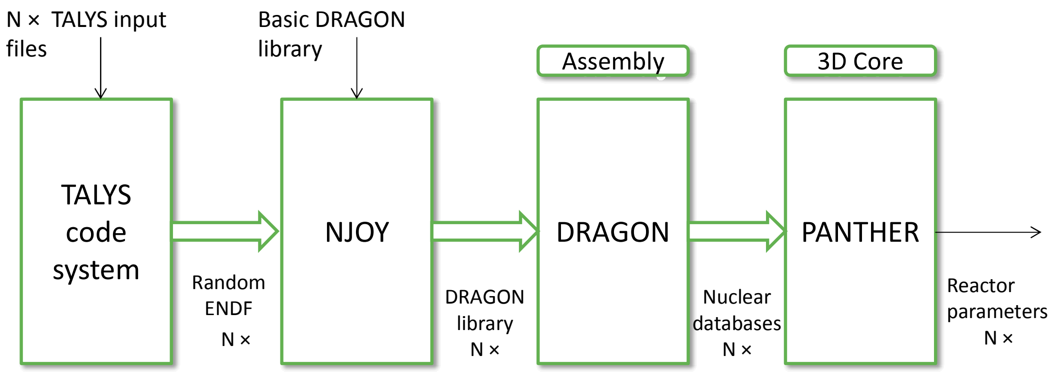

Figure 1 Calculation scheme for the determination of the uncertainties in the main reactor parameters due to nuclear data uncertainties

3. Steady-state calculations

The equilibrium core was obtained by simulating the first 12 cycles, where fresh assemblies are loaded at the beginning of each cycle, and resident assemblies are shuffled according to the loading scheme discussed in Section 1. The first core implemented in the PANTHER model is loaded with fuel of different compositions and enrichment dependent on the batch number. With all control rod banks removed from the core the burn-up of the core is followed at small time steps. The boric acid concentration (with natural boron isotopic composition) in the coolant is adjusted at each time step to keep the core critical, until the end of the natural cycle. From the results of cycle 12 the parameters characterizing the equilibrium cycle were analyzed. After 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.

Figure 2 shows the boron letdown curve obtained at equilibrium. The average cycle length is around 338 effective full power days (efpd), with a standard deviation of 8 days. The variation in the letdown curve due to uncertainties in nuclear data is also illustrated in the same figure (bottom graph), where a series of curves correspondent to several random nuclear databases are shown. The convergence of the result after 450 runs is satisfactory (for all time steps) and the skewness is close to zero. The absolute uncertainty in critical boron concentration (top graph) is virtually constant during the cycle and amounts to 30 ppm (1σ). The sharp decrease in uncertainty close to the end of cycle (EOC) is an artefact caused by the interruption of the burn-up procedure when the critical boron concentration gets negative.

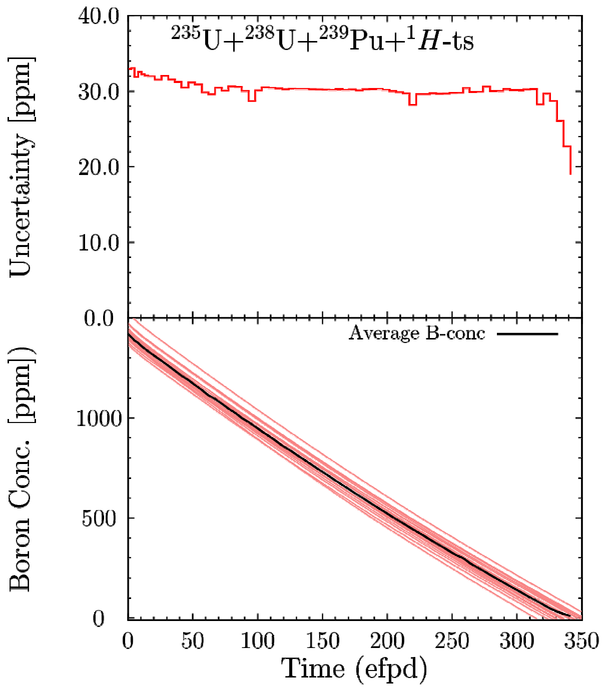

Figure 2 Boron letdown curve for the equilibrium core (bottom) and uncertainty in boron concentration due to nuclear data variations (top).

The uncertainty in other important parameters were also studied like: fuel and clad temperatures, power density, peaking factors, fuel burn-up, control rod bank worth's, reactivity feedback coefficients, and kinetic parameters. **Figure 3** shows the time evolution of some of these parameters and their corresponding uncertainties in absolute unities. The values for the power density, fuel temperature and fuel burn-up are the maximum values over the core. For most of these parameters the uncertainties due to nuclear data are small and in the order of 1-2% relative, except for the boron concentration as discussed in the previous paragraph.

Other parameters like the control rod bank worths, reactivity feedback coefficients, and kinetic parameters have also been studied and the corresponding uncertainty due to nuclear data. Table 2 includes these results at three instants during the equilibrium cycle. The relative uncertainty in the control rod bank worth varies in the range 1%-3%, and the bank with the largest reactivity worth is Bank D. A single control rod cluster (the one closest to the core edge) of this bank was also selected for the control rod ejection scenario described in the next section. The relative uncertainties for the reactivity coefficients amounts to 1-6%. The largest uncertainty is observed for the moderator temperature coefficient (MTC) at beginning of cycle (BOC), 6%, which decreases to about 2% at the EOC. The boron coefficient has the smallest uncertainty throughout the entire cycle, ~ 1%. Regarding the kinetic parameters we should remark that the uncertainty in delayed neutron fraction (β_0) is an underestimation of the actual value and caused solely by changes in neutron energy spectrum. Changes in the actual six-groups delayed neutron fractions calculated by DRAGON are not imported into the PANTHER databases. This explains the very low uncertainties (~ 0.2% relative) found. The relative uncertainty on the prompt neutron lifetime is about 1%, and virtually constant throughout the cycle.

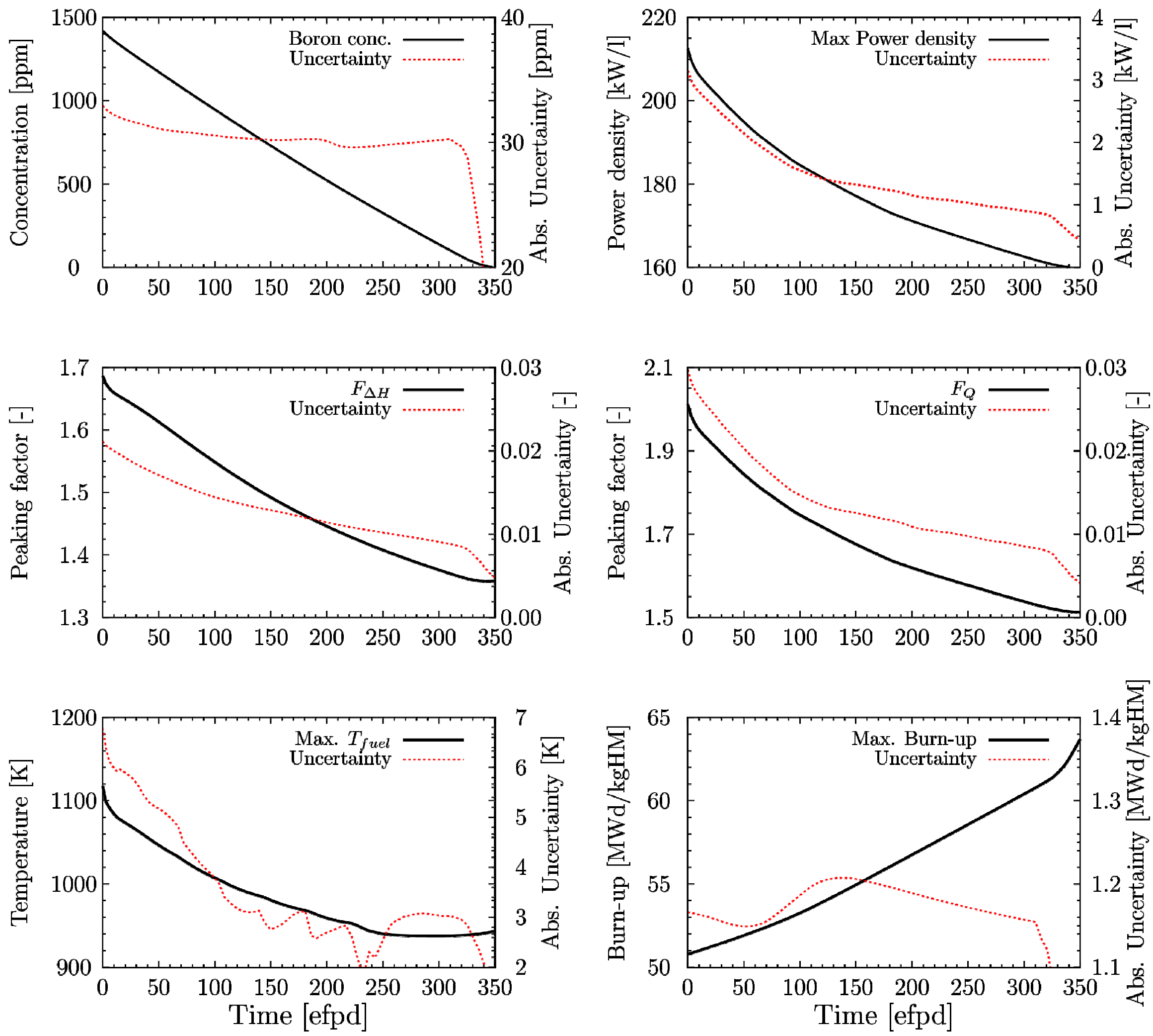

Figure 3 Time evolution of reactor parameters (left scale) and corresponding uncertainties (right scale) due to nuclear data for the equilibrium core: critical boron concentration, maximum power density, peaking factors $F_{\Delta H}$ and F_Q, maximum fuel temperature, and maximum fuel burn-up.

4. Control rod ejection calculations

The simulation of the control rod ejection accident was initiated at BOC of cycle 12, and therefore the steady-state conditions before the onset of the transient are different for each of the 450 PANTHER nuclear databases. 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 (from bank D, with the highest reactivity 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. It is assumed that the reactor scram system fails. The boron concentration is kept unchanged and equal to the critical value before the onset of the accident. 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. For licensing purposes the inclusion of the effect of the loss of primary system integrity is required by the regulatory authorities [14].

Table 2 - Control rod bank worths, feedback reactivity coefficients and kinetic parameters determined at beginning (BOC), middle (MOC) and end of equilibrium cycle (EOC). Doppler - Doppler temperature coefficient, MTC - total moderator temperature coefficient, TPC – total power coefficient, Boron – boron coefficient, β_0 – delayed neutron fraction, t_{prompt} – prompt neutron lifetime.

	BOC	MOC	EOC
Control Rod Bank Worth:			
Bank-A	869 ± 27	972 ± 15	1065 ± 12
Bank-B	1279 ± 17	1384 ± 16	1475 ± 15
Bank-C	882 ± 22	1067 ± 17	1218 ± 12
Bank-D	1576 ± 17	1534 ± 16	1535 ± 16
Bank-SA	1430 ± 17	1397 ± 14	1426 ± 15
Bank-SB	997 ± 28	1162 ± 20	1286 ± 15
Feedback Reactivity Coefficients:			
Doppler [pcm/K]	-2.33 ± 0.07	-2.52 ± 0.08	-2.62 ± 0.08
MTC [pcm/K]	-27.3 ± 1.7	-46.5 ± 1.7	-66.5 ± 1.4
TPC [pcm/%]	-17.05 ± 0.59	-22.08 ± 0.57	-28.46 ± 0.54
Boron [pcm/ppm]	-6.363 ± 0.054	-6.702 ± 0.065	-7.357 ± 0.078
Kinetic Parameters:			
β_0 [pcm]	744.8 ± 1.7	739.6 ± 1.5	735.1 ± 1.4
t_{prompt} [μs]	12.17 ± 0.12	12.80 ± 0.14	13.75 ± 0.17

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. Several reactor parameters were followed, including: multiplication factor (k_{eff}), total power, fuel, clad and coolant temperatures, peaking factors ($F_{\Delta H}$ and F_Q), coolant void fraction and clad-to-coolant heat flux. **Figure 4** displays the time evolution of these parameters. The fuel temperature (Tpin) shown represents the maximum value observed over the entire core, and determined at the center of the fuel pellet. The clad temperature, void fraction and clad-to-coolant heat flux are also the maximum values over the entire core.

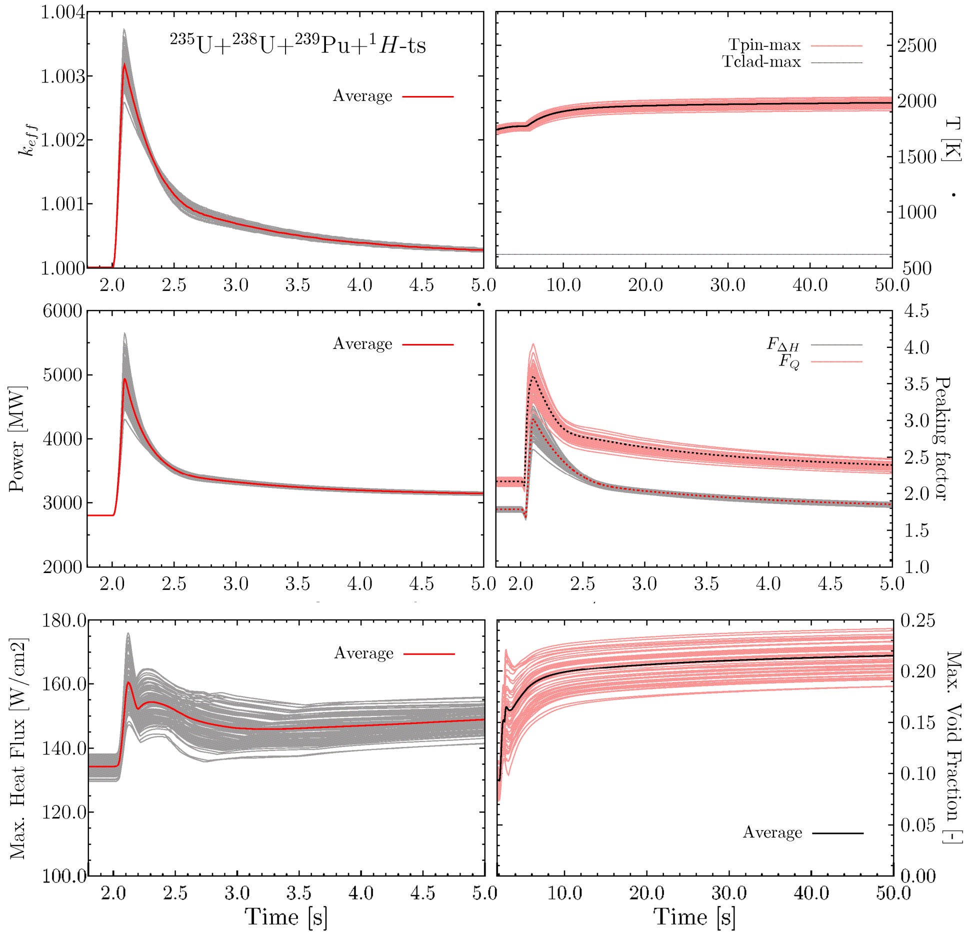

Figure 4 Time evolution of the main parameters for a control rod ejection accident at HFP: k_{eff}-multiplication factor, *T*pin, *T*clad: center-line fuel temperature and clad temperature, Power - total reactor power, $F_{\Delta H}$ and F_{Q} - peaking factors, clad-to-coolant heat flux, and void fraction.

The control rod cluster is assumed to be ejected from the core at t = 2sec from the beginning of the transient simulation. The rapid reactivity insertion (0.42$) 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 clad-to-coolant heat flux peaks at about 20% above the value observed before the start of the accident. This increase in maximum heat flux will decrease the departure of nucleate boiling ratio (DNBR), which could trigger the onset of boiling crisis and consequent failure of a certain number of fuel pins. The PANTHER code does not have the capability of performing a DNBR 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 graph for the fuel and clad temperatures in **Figure 4** are given in a different time scale. 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, power and peaking factors, the transient is mitigated by the negative Doppler feedback coefficient and in a long time scale the reactor power reaches a new equilibrium at a higher level (around 3135 MWth) than the nominal power. 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.

Figure 4 also shows a large number of curves correspondent to the PANTHER simulations using different random databases. It illustrates the spread in the results due to combined uncertainties in nuclear data. An average curve is displayed (curve in a different color in each graph) for each parameter, obtained from the statistical analysis of the results from the 450 PANTHER runs. **Figure 5** displays the absolute uncertainties (1σ) as function of time for all parameters. For most quantities the uncertainties show a peak that coincides with the peaking behavior on the respective absolute quantity (also when displayed as relative uncertainty). The convergence of each parameter was verified by analyses of the running average of the different momenta. 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 [15]. 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 analyzed in relation to these criteria, an aspect which will be reserved for a follow-up study.

5. Conclusions

The application of the Total Monte-Carlo (TMC) method for the determination of uncertainty due to nuclear data was demonstrated for a full 3-D core model of a Westinghouse 3-loop reactor. The uncertainties in nuclear data for $^{235,238}U$ and ^{239}Pu were considered, together with uncertainties in thermal scattering data for ^{1}H in water. Uncertainty analysis was performed for both steady-state and transient conditions, using the reactor code PANTHER. As transient a control rod ejection scenario was selected, with the ejection of the most reactive control rod cluster at beginning of cycle (BOC) conditions and at full reactor power. The uncertainties in key reactor parameters were quantified and the conclusions can be summarized as follows:

- During steady-state conditions the uncertainty in critical boron concentration is virtually constant during the equilibrium cycle and equals about 30 ppm (with a maximum concentration of 1450 ppm at BOC). The relative uncertainties in other parameters like: fuel and clad temperatures, peaking factors, fuel burn-up, power density are relatively small and are in the order of 1-2%. For the considered reactivity coefficients the relative uncertainties vary in the range 1-6%, with the moderator temperature coefficient showing the largest value: 6% at BOC.
- During the control rod ejection scenario the uncertainties due to nuclear data show a sharp peaking behaviour in the parameters: reactivity, peaking factors, total power and clad-to-coolant heat flux. The behaviour coincides with that of the respective absolute quantities. The relative uncertainties amount to a maximum of 6% (in total power and peaking factors) and 4% (in clad-to-coolant heat flux). The maximum fuel temperature shows a different behaviour with a monotonically increasing behaviour towards the end of the transient, and with a maximum uncertainty of 30 Kelvin (1.5% relative).

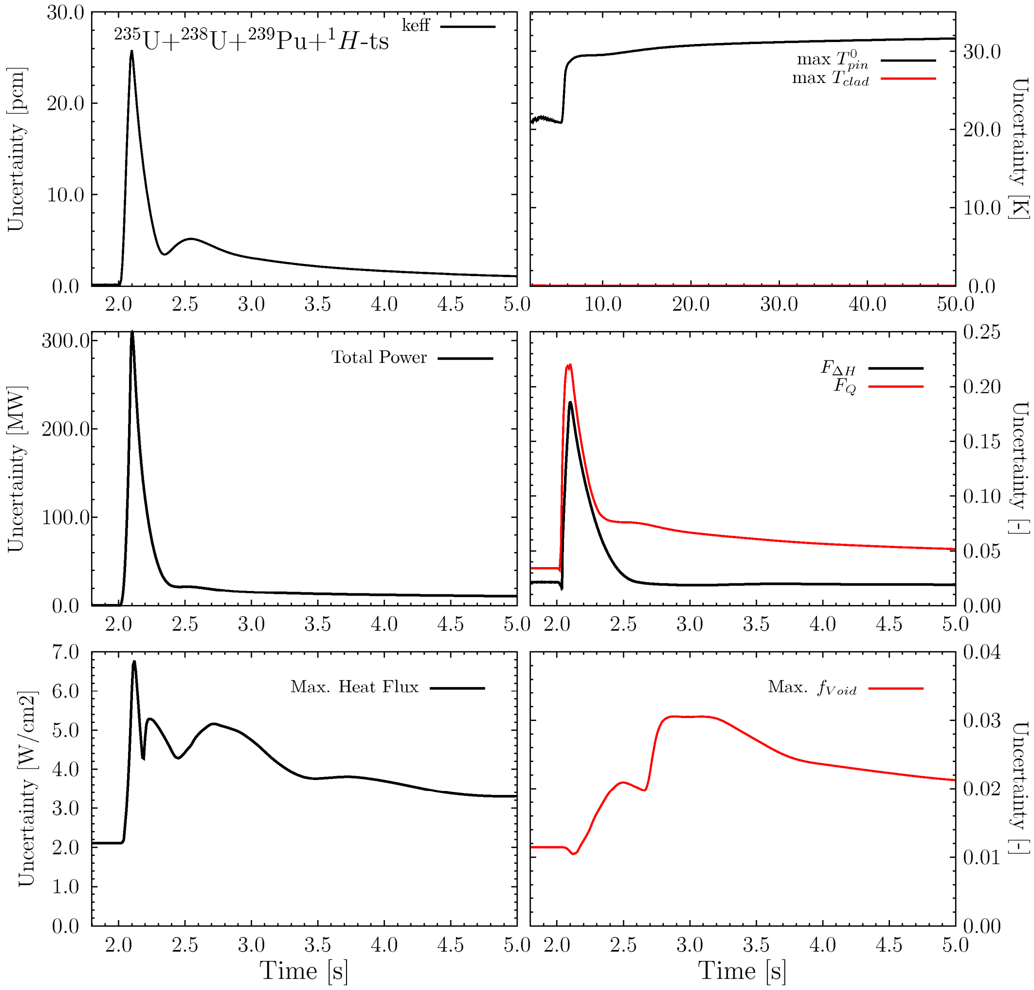

Figure 5 Absolute uncertainty (1σ) for parameters followed during control rod ejection accident: k_{eff} - multiplication factor, $T^0{}_{\text{pin}}$, T_{clad}: center-line fuel temperature and clad temperature, Total Power - total reactor power, $F_{\Delta H}$ and F_{Q} - peaking factors, clad-to-coolant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

Although uncertainties in important reactor parameters were quantified, the consequences to the margin to the safety limits that apply to this type of transients has still to be assessed, like the departure of nuclear boiling ratio (DNBR) and the radially-averaged fuel pellet specific enthalpy criteria. Moreover, the uncertainties due to nuclear data should also be analysed in relation with other sources of uncertainties (tolerances in plant parameters, geometry uncertainties, fuel specifications, etc.). These aspects should be considered in a follow-up study.

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