AN UNCERTAINTY ASSESSMENT METHODOLOGY FOR MATERIALS BEHAVIOUR IN ADVANCED FAST REACTORS

D. Blanchet, K. Mikityuk, P. Coddington and R. Chawla
Paul Scherrer Institut, Switzerland

Abstract

The current study represents a first important step towards the extension of the FAST code system to perform a statistically based uncertainty analysis of fast reactor fuel behaviour under base-irradiation conditions. The principal input parameters related to the physical models and to the system description (geometry, material properties, etc.) are characterized by their uncertainty ranges and probability distributions based on state-of-the-art knowledge. These input parameters are then randomly sampled with the use of a Monte-Carlo method. The basic procedure has currently been implemented in the context of a statistical analysis of the thermal-mechanical behaviour of ETDR helium-cooled fast reactor fuel (MOX pins in stainless steel cladding) under base-irradiation conditions.

Introduction

The FAST code system [1], which is under development at Paul Scherrer Institut, is devoted to the steady-state and transient analysis of advanced fast-spectrum reactor concepts in multi-domains including different coolants, fuel types, structural materials, reactor designs, etc. The stand-alone neutron kinetics, thermal-hydraulics and fuel behaviour codes are coupled together and being qualified for analysis of different advanced fast-spectrum reactor systems. In particular, the FRED code [2] is used in the frame of the FAST code system for simulating fuel element thermal-mechanics under both base-irradiation and transient conditions, taking into account the evolution of fuel and cladding temperatures, fuel-clad gap heat conductance, inner gas content and pressure, fuel and clad stress-strain conditions (considering thermal-elastic-viscous-plastic deformation), fission gas release (FGR) and fuel swelling, etc.

The current study represents a first important step towards the extension of the FAST code system to perform a statistically based uncertainty analysis of fast reactor fuel behaviour under base-irradiation conditions. The principal input parameters related to the physical models and to the system description (geometry, material properties, etc.) are characterized by their uncertainty ranges and probability distributions based on state-of-the-art knowledge. These input parameters are then randomly sampled with the use of a Monte-Carlo method. The basic procedure has currently been implemented in the context of a statistical analysis of the thermal-mechanical behaviour of the ETDR helium-cooled fast reactor fuel [3] (MOX pins in stainless steel cladding) under base-irradiation conditions.

The assessment of uncertainties in the calculational results of the FAST code system is based on the statistical approach originally proposed at Los Alamos by McKay et al.[4], and further developed and expanded at the Gesellschaft für Reaktor Sicherheit (GRS) in Germany [5] with the use of the Wilks' formula [6] and the quantification of uncertainty by means of tolerance limits. This methodology has already been successfully applied at PSI in the context of the BEMUSE project [7], as also for the objective quantification of prediction uncertainty for specific code physical models [7].

Main parameters of the ETDR start-up core

The European Technological Demonstration Reactor (ETDR) [3] aims at providing a vehicle for the demonstration of Gas-cooled Fast Reactor (GFR) technology. It will provide a "first-of-a-kind" demonstration of this new technology and provide qualification of the innovative GFR fuel concepts and materials under prototypic fast neutron spectrum irradiation. The evolutionary approach of two successive core configurations will be considered, through a "start-up core", based on conventional LMFBR pin bundle subassembly containing $(U,Pu)O_2$ fuel in stainless steel cladding, with inlet/outlet He temperature of 260/560°C and a "demonstration core", based on GFR plate type subassembly (U,Pu)C-SiC, with inlet/outlet He temperature of 480/850°C. Although the ETDR MOX fuel pin design relies on existing technology, questions still remain on material structures for clad that will be submitted to fast neutron fluence and relatively high temperatures. The main characteristics of ETDR startup core are summarized in Table 1. A fuel pin with an average linear heating rate of 85 W/cm is used for the analysis.

Table 1: Main characteristics of the ETDR start-up core

Core thermal power (MW)	50
Cycle length (EFPD)	1705
Fuel pellet material	(U,Pu)O2 (+A.M.)
Fuel cladding material	AIM1 austenitic stainless steel alloy
Fissile length (mm)	860
Pellet diameter (mm)	5.42
Clad inner diameter (mm)	5.65
Clad outer diameter (mm)	6.65
Operating coolant (He) pressure (bar)	70
Coolant flow rate (kg/s)	32
Core inlet temperature (°C)	260
Core outlet temperature (°C)	560

Sources of uncertainties considered

The effects of uncertainties on the most important input parameters, such as material properties, initial and boundary conditions related to the system description and physical models are considered as part of this analysis. Uncertainty ranges and distributions assumed in this study for the different variables under consideration are given in Table 2 as multipliers for the corresponding values.

Table 2: Input uncertainty ranges and distributions for the parameters considered

Variable	Law	Min	Max	Mean	Std dev
Initial gap width	Uniform	0.88	1.12	—	—
Fission gas release	Normal	0.0	—	1.0	0.3
Fuel swelling	Uniform	0.6	1.0	—	—
Fuel thermal conductivity	Normal	0.0	—	1.0	0.1
Inner gas conductivity	Normal	0.0	—	1.0	0.11

The following sections address, in more detail, the justification of the choice of these uncertainties.

Uncertainties in the initial gap width

The uncertainty in the initial fuel-clad gap width is relatively small because the fabrication tolerances for fuel pellet and cladding are very low (~0.1%). However, during the initial stages of irradiation (burnup lower than 5 MWd/kgHM), there is a number of effects which significantly increase the uncertainty in the gas gap size. These effects include, first of all, fuel pellet cracking and relocation caused by thermal stresses as well as fuel densification as a result of a sintering process. Analytical examination of uncertainties in prediction of these effects with simple engineering models used in the FRED code showed that they could result in uncertainty in the fuel outer radius of up to 0.5%. Therefore, to take into account the uncertainties introduced by the relocation and densification models, we consider a uniform variation of

± 0.5% of the initial fuel outer radius, which approximately corresponds to a uniform conservative variation of ± 12% in the initial fuel-clad gap size. This uncertainty appears to be consistent with the specifications given in [9].

Uncertainties in fission gas release model

The fission gas atoms produced in the fuel either remain in the pellets and contribute to the swelling, or are released from the pellets and increase the rod inner gas pressure while reducing the heat transfer in the gap by degradation of the inner gas thermal conductivity (fission gases have a much lower conductivity than helium). The fission gas release model implemented in FRED is an empirical function of local fuel temperature, burnup and linear heat generation rate, which is a modification of the engineering zone fission gas release model [10].

If one considers the wide spread of measured values and predictions of available models for FGR (see for example FUMEX-II code benchmark results in Fig. 19 in [11] which show that FGR predictions by the different codes vary in the range from 5 to 35%), it appears that there is a rather large uncertainty in this important parameter. We assumed that the predicted gas release fractions are normally distributed with an approximate relative standard deviation of 30%. This assumption seems quite reasonable in regard to the FRAPCON-3 [12] recommendations on the modified Massih-Forsberg model (σ~100% for FGR < 1%, σ~50% for FGR < 0.1, and σ~15% for FGR > 0.3).

Uncertainties in the fuel swelling model

The fuel swelling, resulting from the progressive buildup of fission products, has two components:

- the solid fission products swelling which is linearly dependent on burnup and has an averaged rate ranging from 0.6% to 1.0% ($\Delta V/V$) per 10 MWd/kgHM (according to [12]);
- the gaseous fission product swelling which occurs at high temperature and is related to the gas pressure in fuel pores.

The fuel swelling is assumed to be isotropic. Due to a relatively low linear heat generation rate in the ETDR core, a low temperature (<1000°C) swelling, i.e. mainly due to the solid fission products, dominates under ETDR conditions. In this case, the linear swelling rate is assumed to be uniformly distributed from 0.6% to 1.0% ($\Delta V/V$) per 10 MWd/kgHM.

Uncertainties in the fuel thermal conductivity

The degradation of fuel thermal conductivity with irradiation was predicted by the model of Philipponeau [13], which has been implemented in FRED. This model correlates a range of experimental data and accounts for the effects of temperature, fuel burnup, stoichometry and porosity. On the basis of examining the spread of the test data which were used for deriving the correlation [13], we assumed a normal distribution for the predicted values of conductivity with a relative standard deviation of 10%. This value is consistent with the FRAPCON code recommendation [12] to use a relative standard deviation of 7% for burnups lower than 40 MWd/kgHM and 10% for burnups in the range from 40 to 60 MWd/kgHM [14].

Uncertainties in the inner gas thermal conductivity

The uncertainty in the gas-gap conductance depends on uncertainties in both the gas conductivity and gap width (in particular in case of swelling and cracking): as the initial gap size uncertainty is already taken into account, only the gas conductivity uncertainty is considered here.

In the open gap regime (ETDR conditions), the gap conductance due to the inner gas conductivity is calculated in FRED according to the classical Ross and Stoute model [15]:

$$h_{gas} = \frac{k_{gas}}{\Delta r_{gap} + \delta r}$$

where Δr_{gap} is the fuel-cladding radial gas-gap (m), δr the temperature jump distance to account for the imperfect heat transport across the solid-gas interface (m), and k_{gas} the thermal conductivity of the gas mixture (W/mK) which is calculated in FRED by the following equation:

$$k_{gas} = \prod_i k_i^{\,w_i}$$

where w_i stands for the gas component mass fractions (He, Ar, Kr, and Xe) and k_i are the individual gas conductivities given by the general temperature-dependent correlation: $k_i = k_0 * T^n$, using the fixed parameter k_0 and n given in Table 3 [16].

Table 3: Gas conductivity correlations

	k_0	n	Std dev on k at T=900 °C
He	2.639E-3	0.7085	6.6%
Ar	2.986E-4	0.7224	5.4%
Kr	8.247E-5	0.8363	4.8%
Xe	4.351E-5	0.8616	4.9%

These uncertainties were averaged to estimate the uncertainty on k_{gas} as equal to 11% (1σ). As different gases have similar uncertainties in their conductivities, the resulting standard deviation is assumed independent of the gas composition (and therefore of the burnup).

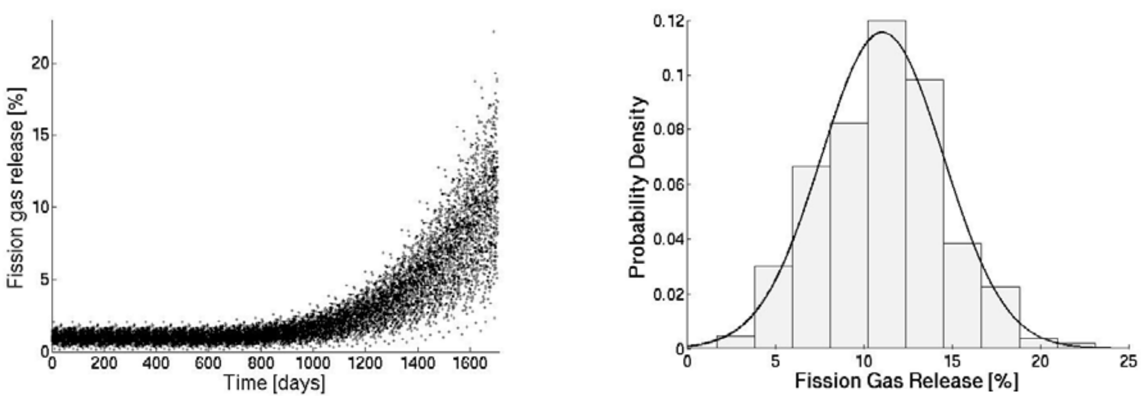
Propagation of uncertainties

The statistical analysis has been performed using the GRS (Gesellschaft fur Anlagen und Reaktorsicherheit) methodology, implemented in the code package SUSA [7]. A Monte-Carlo method is used to generate N random samples of the input parameters, taking into account their ranges and probability distributions. These inputs are then processed by N code executions. The analysis of the output samples allows a determination of statistical tolerance intervals for the output parameters, with a certain probability content and a certain confidence level. The determination of this two-sided tolerance interval, including for example a fraction of at least $\beta = 95\%$ of the output population with a confidence level of $\gamma = 95\%$, requires a minimum number of N=93 samples, with regard to the application of the Wilks formula [6]. However, to improve the statistical output results we used 500 samples.

The main statistical results concerning the fission gas release, gap size, inner gas pressure and peak fuel temperature are presented in Table 4 and in Figs. 1-4. For each output variable, the table shows the mean and standard deviation, minimum and maximum values, as well as the confidence intervals including 95% of the population with a 95% confidence level.

Table 4: Uncertainty results at EOC

values	fission gas release, %	gap size, μm	peak fuel temperature, °C	inner gas pressure, bar
mean ± 1 σ	11 ± 4	19 ± 8	872 ± 38	28 ± 2
minimum — maximum	2 — 23	1 — 36	780 — 989	23 — 35
lower — upper limit for β= 0.95, γ= 0.95	4 — 18	3 — 34	798 — 952	24 — 32



a) b)

Figure 1: Fission gas release: a) time history, and b) probability density at EOC

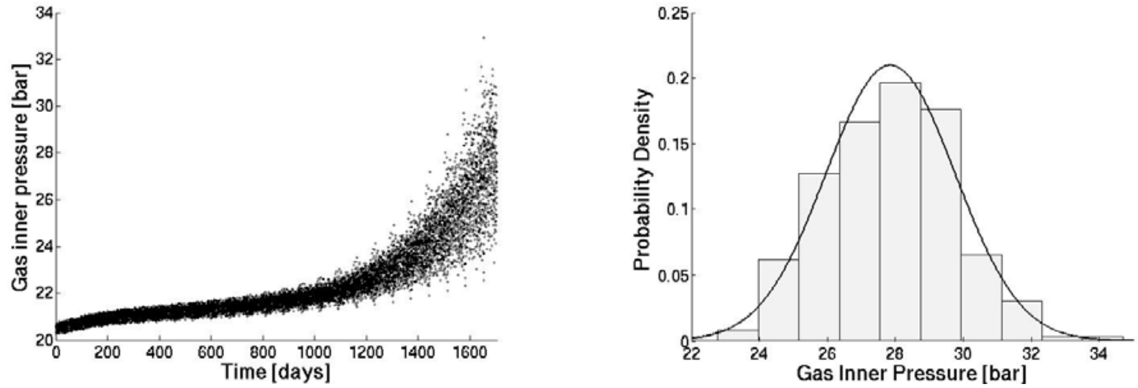


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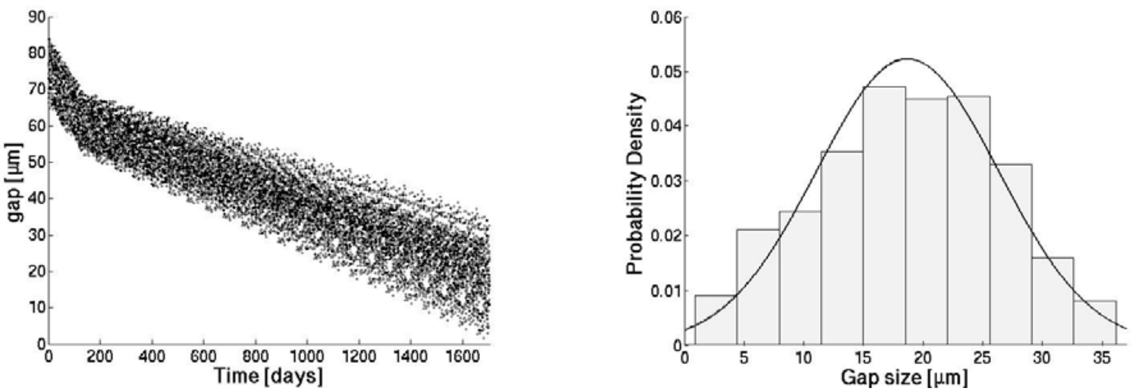
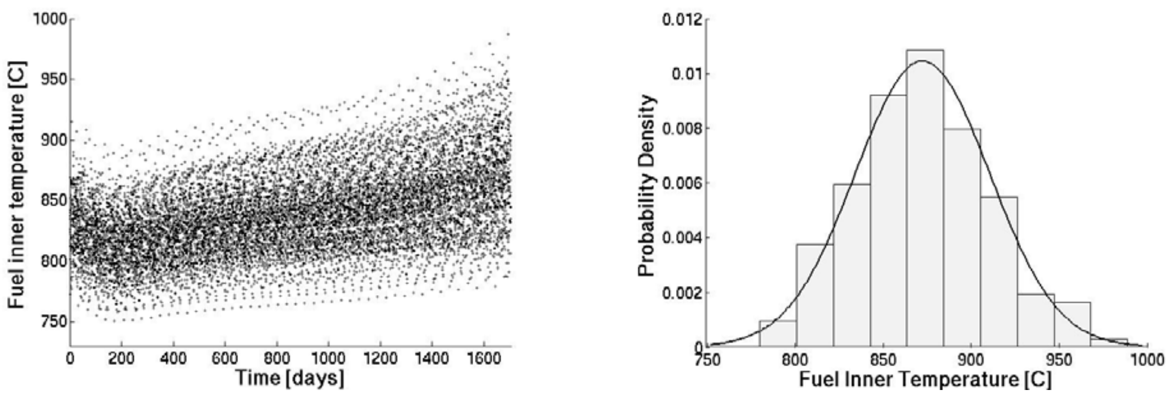
Figure 2: Inner gas pressure: a) time history and b) probability density at EOC



a) b)

Figure 3: Gas gap size: a) time history and b) probability density at EOC



a) b)

Figure 4: Peak fuel temperature: a) time history and b) probability density at EOC

The Lilliefor's test of normality is passed successfully (with a significance level of 5%) for the different predictions: the histograms can indeed be fitted by normal distributions (Fig. 1b-4b). The fission gas release (Fig. 1) is in fact one of the input parameters, so that the close-to-normal distribution obtained at EOC in this case (Fig. 1b) serves to demonstrate the validity of the procedure for random sampling of the input parameters. The inner gas pressure increases due to the fission gas release (Fig. 2), but remains lower than the coolant pressure. Therefore, the cladding hoop stress remains negative and the cladding undergoes no plastic deformation. Among the relatively small number of input variables currently considered for the propagation of uncertainties, the gap size at EOC (Fig. 3) has the largest uncertainty (~ 41%). The tolerance limits obtained for the gap size reveals that, under the used assumptions, no pellet-clad mechanical interaction occurs during the entire base irradiation. The peak fuel temperature has a standard deviation of 4.4%, which is comparable with other analysis: For example, the corresponding value presented in [11], and reproduced in Figure 5, is close to 6.5%. The difference may be explained by the fact that we did not take into account the uncertainty in the linear heat generation rate taken into account in [11].

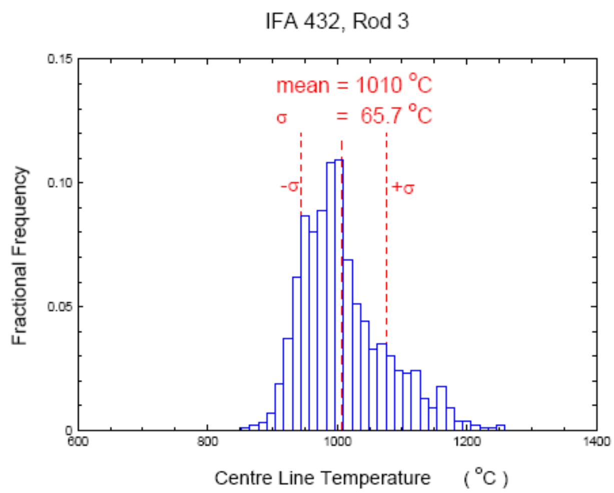


Figure 5: Fractional frequency of centreline temperature predictions when varying only three input parameters (q`, h_{gap}, λ) (Fig. from [12])

Sensitivity studies

The Monte-Carlo uncertainty propagation method determines the tolerance limits for the output, as a global measure of the output variability with respect to the uncertainties in the inputs. However, it is also possible to supplement this uncertainty information by performing a sensitivity study, which is based on a regression analysis of the input and output samples, so as to separate and quantify the contribution of individual input parameters to the global output variability. Indeed, a regression coefficient such as the simple correlation coefficient of Pearson provides a good measure of the strength and direction of a linear relationship between two random variables, which is of particular interest in our case to measure the linear sensitivity of the output to an input variable. A better measure of the linear association, between two variables from a set of variables, would be the partial correlation coefficient of Pearson. One can also obtain sensitivity coefficients from the least square solution of a multi-linear regression. Finally, the partial rank correlation coefficient of Spearman offers the possibility of measuring a non-linear, but monotonic, relation between two variables. These various sensitivity measures provide statistical criteria to select and rank the input variables by importance, with respect to their respective contributions to the output uncertainty. For example, Fig. 7 shows the ranking of relative sensitivity of the gas gap size at EOC, and of the peak fuel temperature at EOC, to the considered input variables. The final gap size is evidently most sensitive to fuel swelling and initial gap size uncertainties (with different sign). Increases in fuel conductivity, fuel swelling and gas conductance result in better cooling of the fuel and hence to the reduction of the peak fuel temperature (Fig. 7b), while increases in values of the fission gas release and initial gap have reverse effects.

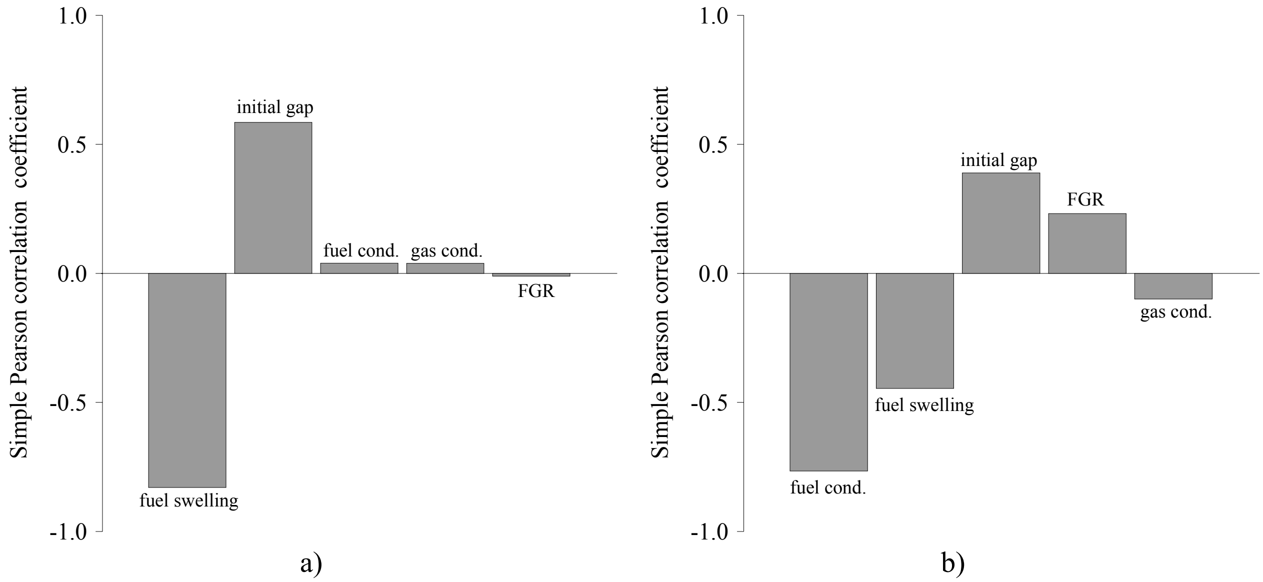


Figure 6: Sensitivity of a) the gas gap size at EOC, and b) peak fuel temperature at EOC, to considered input variables

Conclusions

This study initiates the development and application of a robust uncertainty and sensitivity calculation methodology in the context of the FAST code system, which couples the neutronic, thermal-hydraulic and thermal-mechanical calculations for a wide range of Generation IV reactors concepts. A working framework has been developed and successfully tested for the application of the statistical methodology, which propagates uncertainties in input and physical model variables to output results. As a demonstration, the thermal-mechanical behavior of the pin-type MOX fuel foreseen for the ETDR gas-cooled fast reactor has been investigated during base irradiation. Within the limitations of the present study (small number of input variables considered), it has been shown that the fuel rod design yields an open-gap regime during the entire cycle. Further variables need to be included in the analysis, and work is under way to investigate the possibility of considering the effects of other types of uncertainty, e.g. in the coupled neutronic (cross sections, kinetic parameters, etc.) and thermal-hydraulic (heat transfer correlations, physical properties, etc.) calculations. This is clearly a major challenge, a key aspect being the identification of reliable uncertainty information on the different parameters and models involved.

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