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Sensitivity And Uncertainty Analysis For The Thorium Molten Salt Reactor Using The SCALE And ERANOS Code Systems

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1 Introduction

1.1 Goal of the project

Extensive research on the Non-Moderated Thorium Molten Salt Reactor (TMSR-NM) is performed at the 'Physique des Réacteurs Nucléaires' research group of the 'Laboratoire Physique Subatomique et de Cosmologie' in Grenoble [1]. Among this research is the Sensitivity & Uncertainty (S&U) analysis of the TMSR-NM, which focusses on the impact of the nuclide composition and the available nuclear data to the reactor operation and its uncertainties.

The goal of this project is to explore the possibilities to perform S&U analysis of the TMSR-NM by using both the ERANOS and the SCALE code system (separately), and perform this analysis for the most relevant nuclides. The sensitivity results will provide insight in the importance of each nuclide to the overall reactor operation. The uncertainty results indicate the accuracy by which the simulations can be performed. The project focusses mainly on the capabilities of both code systems for performing S&U analysis, rather than going into details about the calculation results. Various calculation configurations will be tested and their results will be compared.

This report also serves as a good reference or starting point for people who want to continue the S&U analysis with the ERANOS and/or SCALE code system performed in this project¹.

ERANOS At the start of the project, the ERANOS code system was not in use at the research group 'Physique des Réacteurs Nucléaires' of LPSC Grenoble. Therefore, a copy of the ERANOS2.1 release, obtained from Cadarache, had to be installed on the network. Due to some compilation errors it took a few days to succeed the installation. Since there was no experience with ERANOS within the group staff, including myself, two weeks of practicing with the code system were required to commence the sensitivity and uncertainty calculations. A lack of (English) documentation also hardened the process of getting acquainted with the code system.

SCALE The SCALE code system was already installed on the network at the start of the project. The SCALE modules are well documented and easier to program with respect to ERANOS, so sensitivity and uncertainty calculations could readily be started.

¹For the ERANOS and SCALE input files and visualization tools used in this project, contact Michiel Hoogmoed, michielhoogmoed@hotmail.com.

1.2 Motivation of the project

This project is performed as part of the MSc programme of Applied Physics at the Delft University of Technology. The course code is 'AP3911 Work Placement (Internship)' and constitutes 18 ECTS, which equals 3 months of full-time work. The project has been performed between september 23rd 2009 and december 24th 2009.

2 Theory

In this section the physics will be introduced that is essential for a basic understanding of the Sensitivity & Uncertainty analysis applied in this project. Section 2.1 introduces the concept of Generalized Perturbation Theory. A derivation of the sensitivity coefficients of k_{eff} and the breeding ratio is given in 2.2 and 2.3 respectively. Section 2.4 discusses implicit- and explicit sensitivity coefficients, and 2.5 explains how covariance data is used to calculate uncertainties. Section 2.6 discusses the relation between sensitivity coefficients of nuclide densities and sensitivity coefficients of nuclide cross sections.

2.1 Generalized Perturbation Theory

Sensitivity analysis in nuclear reactor physics investigates how strong reactor operation is influenced by the perturbation of one of the reactor parameters. This is done by using the Generalized Perturbation Theory (GPT). The content of this section is strongly based on Williams [2], and should be used as a quick introduction to the basic aspects of the calculations performed. Consult Williams for a more thorough derivation and discussion of the content of this section.

Two reactor operation aspects are analyzed in this project: the thorium breeding ratio and the effective multiplication factor, k_{eff} , which are called 'responses'. In Williams the response is indicated as

$$R = R[H(x), Y(x)] \quad (2.1)$$

where the response R depends on some response function $H(x)$ and a solution function $Y(x)$. The independent variable 'x' stands for all variables over which the functions $H(x)$ and $Y(x)$ are defined.

Next an expression should be found for a perturbation of the response. For this, the first order Taylor series expansion of a perturbation in R is written as

$$R' = R_0 + \frac{dR}{d\alpha} \Delta\alpha \quad (2.2)$$

where α represents a perturbed variable from the set of variables x . This can also be written as

$$\Delta R = \frac{dR}{d\alpha} \Delta\alpha. \quad (2.3)$$

In perturbation theory it is common to work with relative changes when expressing sensitivities,

$$\frac{\Delta R}{R} = \frac{dR}{d\alpha} \frac{\Delta\alpha}{\alpha} = S_\alpha \frac{\Delta\alpha}{\alpha}. \quad (2.4)$$

The proportionality constant S_α is called the 'relative sensitivity coefficient of R with respect to α ', but is normally shortened to just the sensitivity

coefficient. An increase of 1% in α will result in a change of S_α in R. The net effect on R due to changes in a set of variables α_i results in a linear combination of the individual effects

$$\frac{\Delta R}{R} = \sum_i S_{\alpha_i} \frac{\Delta \alpha_i}{\alpha_i} \quad (2.5)$$

2.2 Perturbation theory for k_{eff}

The main goal of this project is to determine sensitivity coefficients with respect to k_{eff} . In this case, the response function is found by first considering the neutron balance equation

$$L\phi(x) - \lambda P\phi(x) = 0 \quad (2.6)$$

where L and P represent the neutron loss and production mechanisms respectively, and $\phi(x)$ is the neutron flux distribution. The relation between the eigenvalue λ and the effective multiplication factor is $k_{\text{eff}} = 1/\lambda$. Taking the inner product over (2.6) with an arbitrary weight function $w(x)$, the response function is written as

$$\lambda = \frac{\langle w(x)L\phi(x) \rangle}{\langle w(x)P\phi(x) \rangle}. \quad (2.7)$$

A perturbation in system (2.6) will result in a perturbation in the eigenvalue, given by

$$(L + \Delta L)(\phi + \Delta\phi) = (\lambda + \Delta\lambda)(P + \Delta P)(\phi + \Delta\phi). \quad (2.8)$$

Neglecting products of perturbations this can be written as

$$(L - \lambda P)\Delta\phi = -(\Delta L - \lambda\Delta P) + \Delta\lambda P\phi. \quad (2.9)$$

Solving this equation for $\Delta\lambda$ and taking the inner product with the weight function $w(x)$ results in

$$\Delta\lambda = \frac{\langle w(\Delta L - \lambda\Delta P)\phi \rangle + \langle w(L - \lambda P)\Delta\phi \rangle}{\langle wP\phi \rangle}. \quad (2.10)$$

The presence of the perturbation of the neutron flux field $\Delta\phi$ is undesirable, and can be avoided by a specific choice for the weight function $w(x)$. The λ -mode adjoint neutron flux is chosen as the weight function, satisfying

$$L^*\phi^*(x) - \lambda P^*\phi^*(x) = 0. \quad (2.11)$$

A motivation for this particular choice and its physical meaning can be found in Williams. Applying this weight function in equation (2.10) will cause its second term to vanish,

$$\langle \phi^*(L - \lambda P)\Delta\phi \rangle = \langle \Delta\phi(L^* - \lambda P^*)\phi^* \rangle = 0 \quad (2.12)$$

using the property of adjoints $\langle fAg \rangle = \langle gA^*f \rangle$ and equation (2.11). Dividing the remainder of (2.10) by λ provides the relative perturbation in the eigenvalue as a function of the forward- and adjoint neutron flux field,

$$\frac{\Delta\lambda}{\lambda} = \frac{\langle \phi^*(\Delta L - \lambda\Delta P)\phi \rangle}{\lambda \langle \phi^*P\phi \rangle}. \quad (2.13)$$

The relation between relative perturbations in λ and k_{eff} is given by

$$\frac{\Delta\lambda}{\lambda} = \frac{k}{k'} - 1 = -\frac{\Delta k}{k'} = -\frac{\Delta k}{k} + O(\Delta^2) \quad (2.14)$$

to obtain the final equation

$$\frac{\Delta k}{k} = \frac{\langle \phi^*(\frac{1}{k}\Delta P - \Delta L)\phi \rangle}{\langle \phi^*\frac{P}{k}\phi \rangle}. \quad (2.15)$$

2.3 Perturbation theory for the breeding ratio

In this project also sensitivity calculations are performed with the breeding ratio as response, which is given by

$$\text{BR} = \frac{\Sigma_c^{\text{Th}} - \Sigma_c^{\text{Pa}}}{\Sigma_c^{\text{U}} + \Sigma_f^{\text{U}}}. \quad (2.16)$$

In this section a derivation is given for the sensitivity of the breeding ratio, with the modification that the capture of protactinium will not be considered here, since this element was not taken into consideration in the reactor model. Then the response of the breeding ratio takes the general form

$$R = \frac{\langle \Sigma_1\phi \rangle}{\langle \Sigma_{2a}\phi \rangle + \langle \Sigma_{2b}\phi \rangle}. \quad (2.17)$$

For the first order GPT, as described in (2.2), the derivatives are required to all variables in the equation,

$$\frac{\partial R}{\partial \Sigma_1} = R \frac{\phi}{\langle \Sigma_1\phi \rangle} \quad (2.18)$$

$$\frac{\partial R}{\partial \Sigma_{2a}} = -R \frac{\phi}{\langle \Sigma_{2a}\phi \rangle + \langle \Sigma_{2b}\phi \rangle} \quad (2.19)$$

$$\frac{\partial R}{\partial \Sigma_{2b}} = -R \frac{\phi}{\langle \Sigma_{2a}\phi \rangle + \langle \Sigma_{2b}\phi \rangle} \quad (2.20)$$

$$\frac{\partial R}{\partial \phi} = R \left[\frac{\Sigma_1}{\langle \Sigma_1\phi \rangle} - \frac{(\Sigma_{2a} + \Sigma_{2b})}{\langle \Sigma_{2a}\phi \rangle + \langle \Sigma_{2b}\phi \rangle} \right]. \quad (2.21)$$

Substituting the derivatives in (2.2) gives

$$\begin{aligned} \frac{\Delta R}{R} = & \frac{\langle \Delta \Sigma_1\phi \rangle}{\langle \Sigma_1\phi \rangle} - \frac{\langle \Delta \Sigma_{2a}\phi \rangle + \langle \Delta \Sigma_{2b}\phi \rangle}{\langle \Sigma_{2a}\phi \rangle + \langle \Sigma_{2b}\phi \rangle} + \\ & \left\langle \left(\frac{\Sigma_1}{\langle \Sigma_1\phi \rangle} - \frac{(\Sigma_{2a} + \Sigma_{2b})}{\langle \Sigma_{2a}\phi \rangle + \langle \Sigma_{2b}\phi \rangle} \right) \Delta\phi \right\rangle \end{aligned} \quad (2.22)$$

The first two terms of the RHS form the direct effect of the perturbation and the last term represents the indirect effect. Just as in section 2.2, the next step is to find an alternative expression for the indirect term which contains the perturbation of the flux field. In this case, the following generalized adjoint equation is chosen

$$(L^* - \lambda P^*)\Gamma^* = \frac{1}{R} \frac{dR}{d\phi} = \frac{\Sigma_1}{\langle \Sigma_1 \phi \rangle} - \frac{(\Sigma_{2a} + \Sigma_{2b})}{\langle \Sigma_{2a} \phi \rangle + \langle \Sigma_{2b} \phi \rangle} \equiv S^* \quad (2.23)$$

in which Γ^* is called the generalized importance. Taking the inner product of Γ^* with (2.9), $\Delta\phi$ with (2.23), and subtracting the results one obtains

$$\left\langle \left(\frac{\Sigma_1}{\langle \Sigma_1 \phi \rangle} - \frac{(\Sigma_{2a} + \Sigma_{2b})}{\langle \Sigma_{2a} \phi \rangle + \langle \Sigma_{2b} \phi \rangle} \right) \Delta\phi \right\rangle = \langle \Gamma^*(\Delta L - \lambda \Delta P)\phi \rangle - \Delta\lambda \langle \Gamma^* P \phi \rangle. \quad (2.24)$$

Using this relation in (2.22) avoids the need for $\Delta\phi$, but now the perturbation in the eigenvalue $\Delta\lambda$ is required. In Williams[2] the concept of 'fundamental mode contamination' is introduced, which explains that under suitable conditions the relation $\langle \Gamma^* P \phi \rangle = 0$ holds, to finally obtain

$$\frac{\Delta R}{R} = \frac{\langle \Delta \Sigma_1 \phi \rangle}{\langle \Sigma_1 \phi \rangle} - \frac{\langle \Delta \Sigma_{2a} \phi \rangle + \langle \Delta \Sigma_{2b} \phi \rangle}{\langle \Sigma_{2a} \phi \rangle + \langle \Sigma_{2b} \phi \rangle} - \langle \Gamma^*(\Delta L - \lambda \Delta P)\phi \rangle. \quad (2.25)$$

Thus, by first calculating the generalized importance from equation (2.23), the breeding ratio sensitivities can be calculated with equation (2.25).

2.4 Implicit- and explicit sensitivity coefficients

This section discusses the difference between implicit- and explicit sensitivity coefficients. This section is an abstract of Williams and Rearden [3], which can be consulted for more details.

Evaluated data from an ENDF/B library is processed into continuous-energy nuclear data indicated by $x_r^{(j)}(E)$, with nuclide j and reaction r . This data is averaged with a smooth weighing function $w(E)$ to obtain generic multigroup (MG) data,

$$\alpha_{r,g}^{(j)} = \frac{\langle x_r^{(j)}(E)w(E) \rangle}{\langle w(E) \rangle} \quad (2.26)$$

where the brackets indicate an inner product over the energy interval g . Changes in the evaluated data due to uncertainties are indicated as $\Delta x_r^{(j)}(E)$, which propagates in the generic MG data as

$$\Delta \alpha_{r,g}^{(j)} = \left\langle \frac{\partial \alpha_{r,g}^{(j)}}{\partial x_r^{(j)}(E)} \Delta x_r^{(j)}(E) \right\rangle = \frac{\langle w(E) \Delta x_r^{(j)}(E) \rangle}{\langle w(E) \rangle} \quad (2.27)$$

Problem-specific data is weighted with an energy spectrum representative of the application of interest,

$$\sigma_{r,g}^{(j)} = \frac{\langle x_r^{(j)}(E)\phi_w(E) \rangle}{\langle \phi_w(E) \rangle} \quad (2.28)$$

in which ϕ_w approximates the problem-specific flux spectrum. The flux, and thus $\sigma_{r,g}^{(j)}$, depends on library data of the nuclide considered, j , as well as on the other nuclides, indicated by j' . Thus we should write

$$\sigma_{r,g}^{(j)} \left[x_r^{(j)}(E); x_{r'}^{(j')}(E) \right]. \quad (2.29)$$

Variations in the evaluated data cause changes in $\sigma_{r,g}^{(j)}$ given by

$$\Delta\sigma_{r,g}^{(j)} = \left\langle \frac{\partial\sigma_{r,g}^{(j)}}{\partial x_{r'}^{(j')}} \Delta x_{r'}^{(j')}(E) \right\rangle + \sum_{j',r'} \left\langle \frac{\partial\sigma_{r,g}^{(j)}}{\partial\phi_w} \frac{\partial\phi_w}{\partial x_{r'}^{(j')}} \Delta x_{r'}^{(j')}(E) \right\rangle. \quad (2.30)$$

If the changes in processed data are approximated by

$$\Delta x_{r'}^{(j')}(E) \rightarrow \Delta\alpha_{r',g}^{(j')} \quad (2.31)$$

then equation (2.30) can be written as

$$\Delta\sigma_{r,g}^{(j)} = \Delta\alpha_{r,g}^{(j)} + \sum_{j',r'} S_{\sigma_{r,g}^{(j)};\alpha_{r',g}^{(j')}} \Delta\alpha_{r',g}^{(j')} \quad (2.32)$$

in which a sensitivity coefficient has been defined that indicates how sensitive changes in the generic cross-section data are to the changes in the self-shielded cross-section data,

$$S_{\sigma_{r,g}^{(j)};\alpha_{r',g}^{(j')}} = \sum_{j',r'} \left\langle \frac{\partial\sigma_{r,g}^{(j)}}{\partial\phi_w(E)} \frac{\partial\phi_w(E)}{\partial x_{r'}^{(j')}(E)} \right\rangle. \quad (2.33)$$

Implicit- and explicit sensitivity in responses Let the functional $k(\Phi)$ be a response calculated by SCALE. The explicit sensitivity coefficient of k with respect to a data parameter $\sigma_{r,g}^{(j)}$ is

$$S_{k,\sigma_{r,g}^{(j)}}^{[\text{exp}]} = \frac{\partial k}{\partial\sigma_{r,g}^{(j)}} \Delta\sigma_{r,g}^{(j)}. \quad (2.34)$$

The response change due to changes in the problem-specific MG data is calculated by

$$\Delta k = \sum_g \sum_{j,r} S_{k,\sigma_{r,g}^{(j)}}^{[\text{exp}]} \Delta\sigma_{r,g}^{(j)}. \quad (2.35)$$

It is useful to relate the response perturbations to changes in the generic data rather than to changes in the problem-specific data. This can be done by substituting (2.32) in equation (2.35),

$$\Delta k = \sum_g \sum_{j,r} \left\{ S_{k,\sigma_{r,g}^{(j)}} + \sum_{j',r'} S_{k,\sigma_{r',g}^{(j')}} S_{\sigma_{r',g}^{(j')}}; \alpha_{r,g}^{(j)} \right\} \Delta \alpha_{r,g}^{(j)}. \quad (2.36)$$

The second term of the RHS indicates the implicit sensitivity coefficient, so that we can write

$$S_{k,\alpha_{r,g}^{(j)}}^{[\text{com}]} = S_{k,\alpha_{r,g}^{(j)}}^{[\text{exp}]} + S_{k,\alpha_{r,g}^{(j)}}^{[\text{imp}]} \quad (2.37)$$

and finally

$$\Delta k = \sum_g \sum_{j,r} S_{k,\alpha_{r,g}^{(j)}}^{[\text{com}]} \Delta \alpha_{r,g}^{(j)}. \quad (2.38)$$

The implicit sensitivity coefficients accounts for the fact that changes in a cross section may affect other problem-specific MG cross sections via self-shielding perturbations, and the latter data variations cause additional response changes.

2.5 Response uncertainty

Williams and Rearden [3] also discuss how the response uncertainty is calculated. The variance of a response k can be written as

$$Var(k) = \sum_{g,g'} \sum_{j,j';r,r'} S_{k,\alpha_{r',g'}^{(j')}}^{[\text{com}]} Cov(\alpha_{r',g'}^{(j')}; \alpha_{r,g}^{(j)}) S_{k,\alpha_{r,g}^{(j)}}^{[\text{com}]} \quad (2.39)$$

in which the covariance is defined as

$$Cov(\alpha_{r',g'}^{(j')}; \alpha_{r,g}^{(j)}) = E(\Delta \alpha_{r',g'}^{(j')}; \Delta \alpha_{r,g}^{(j)}). \quad (2.40)$$

So the response variance is related to the covariance of generic MG data by using the complete sensitivity coefficients.

2.6 Relation between cross-section and nuclide density perturbation

This project considers mainly sensitivity coefficients of neutron cross sections. One might also want to obtain the sensitivity coefficients of the nuclide densities used in the reactor. In this section it is shown that the sensitivity coefficients of the nuclide densities are equal to the sensitivity coefficients of the total cross section of that particular nuclide.

The sensitivity of k_{eff} to perturbations in the nuclide cross-sections can be stated as

$$\frac{\Delta k}{k} = \sum_n \sum_r S_{\Sigma}(n, r) \frac{\Delta \Sigma(n, r)}{\Sigma(n, r)} \quad (2.41)$$

where r and n indicate reactions and nuclides respectively. The sensitivity of k_{eff} to perturbations in the nuclide density can be stated as

$$\frac{\Delta k}{k} = \sum_n S_N(n) \frac{\Delta N(n)}{N(n)}. \quad (2.42)$$

The macroscopic cross-section is related to the nuclide density and the microscopic cross-section as

$$\Sigma(n, r) = N(n)\sigma(n, r). \quad (2.43)$$

A perturbation in the nuclide density causes a perturbation in the macroscopic cross-section

$$\Delta \Sigma(n, r) = \Delta N(n)\sigma(n, r). \quad (2.44)$$

Combining equations (2.41), (2.43) and (2.44) gives

$$\frac{\Delta k}{k} = \sum_n \sum_r S_{\Sigma}(n, r) \frac{\Delta N(n)\sigma(n, r)}{N(n)\sigma(n, r)} \quad (2.45)$$

from which the microscopic cross-sections cancel, and the nuclide densities are independent on the reaction. Now the relation becomes

$$\frac{\Delta k}{k} = \sum_n \sum_r S_{\Sigma}(n, r) \frac{\Delta N(n)}{N(n)} \quad (2.46)$$

Comparing equations (2.42) and (2.46) the following relation is obtained between S_{Σ} and S_N

$$S_N(n) = \sum_r S_{\Sigma}(n, r). \quad (2.47)$$

In other words, the sensitivity of k_{eff} to perturbations in the nuclide density is equal to the sum of the sensitivities of the reactions involved of that nuclide. Since the total cross-section is in fact this summation, the final result is

$$S_N(n) = S_{\Sigma_t}(n). \quad (2.48)$$

3 Calculation methods and reactor configuration

This section discusses the calculation methods and how the reactor is modeled in the code systems. Section 3.1 discusses the reactor model configuration. Section 3.2 provides an overview of the output capabilities of the code systems, and 3.3 introduces their calculation methods.

3.1 Reactor configuration

The nuclear reactor considered in this project is the Non-Moderated Thorium Molten Salt Reactor. In this section, only the parameters will be provided that are of interest for the S&U analysis. For additional details about this reactor concept, see Delpech [5].

Reactor materials Here the density and nuclide composition of the used materials are provided. The complete atomic composition of these three materials can be found in section B of the appendix.

- The reactor core is a molten salt, which consists of the elements U-233, Th-232, F-19 and Li-7. The density of the salt is 4.3 g/cm^3 .
- The breeder blanket consists of the elements Th-232, F-19, Li-7 and Li-6. It's density is also 4.3 g/cm^3 .
- The reflector is a NiWCr alloy, also containing several other elements in minor quantities. The density of the reflector is 10.0 g/cm^3 .

Reactor geometry The reactor geometry used is very simple. The core is a cylinder with radius 1.25m and height 2.60m, surrounded by a cylindrical layer of the breeder blanket, with a thickness of 0.40m and the same height as the core. The reflector is also a cylindrical layer around the breeder blanket, with thickness 0.25m and also with height 2.60m.

3.2 Overview of sensitivity coefficients

The SCALE 5.1 code system and the ERANOS 2.1 code system have been utilized to perform sensitivity and uncertainty calculations for the Non-Moderated Thorium Molten Salt Reactor. Both code systems have been applied to perform the calculations on the same reactor configuration in order to be able to compare the results. The analysis presented in this report has been confined to the most important nuclides in the system²: U-233, Th-232, F-19 and Li-7.

²S&U data of the other nuclides present in the system is available in the data corresponding to this project.

ERANOS Table 1 lists the components for which ERANOS can compute sensitivity values. In ERANOS sensitivity analysis, the 'total' component does not represent the total cross section³, so the total cross section sensitivity has been composed of the individual components 'fission', 'capture', 'elastic', 'inelastic' and 'n,xn'.

capture	fission	elastic	inelastic
nu	transport	total	n,xn

Table 1: Sensitivity components available in ERANOS.

SCALE Table 2 lists the components for which SCALE can compute sensitivity values. These components are not all unique, some are simply combinations of other components. The following relations between the components hold:

$$\begin{aligned} \text{capture} &= \text{n,alpha} + \text{n,d} + \text{n,gamma} + \text{n,p} + \text{n,t} \\ \text{nubar} &= \text{chi} \\ \text{scatter} &= \text{elastic} + \text{n,n}' \\ \text{total} &= \text{elastic} + \text{n,n}' + \text{fission} + \text{capture}. \end{aligned}$$

capture	fission	elastic	n,n'
nubar	total	n,2n	scatter
n,gamma	n,p	n,t	n,d
n,alpha	chi		

Table 2: Sensitivity components available in SCALE.

Comparing ERANOS and SCALE Table 3 shows which reactions are suitable for direct comparison between ERANOS and SCALE. The difference in definition between 'n,xn' and 'n,2n' will be allowed⁴, and will be considered comparable.

3.3 Calculation methods

3.3.1 ERANOS

Sensitivity coefficients Sensitivity analysis with ERANOS can be performed in several ways. In this project, the following design parameters have been used:

³Consult ERANOS documentation for the definition of the various reactions.

⁴The component 'n,xn' contains 'n,2n', 'n,3n' etc..

ERANOS		SCALE
capture	↔	capture
fission	↔	fission
elastic	↔	elastic
inelastic	↔	n,n'
nu	↔	nubar
n,xn	↔	n,xn

Table 3: Components suitable for direct comparison between ERANOS and SCALE.

- Flux calculation performed by diffusion solver or by transport solver:
 - `fd_rectangular_diffusion_iteration` module (FRDI)
 - `rectangular_sn_transport_iteration` module (RSTI)
- Choice of neutron cross-section library:
 - ENDF/B-VI library
 - JEFF-3.1 library
- Choice of energy group discretization:
 - 172-group
 - 33-group discretization

These options allow eight different configurations for the sensitivity calculations. In the next section the results of these configurations will be presented and compared.

Uncertainty The ERANOS code system is delivered with covariance data for nuclides present in 'classical' fast breeder reactors, i.e. U238 fuel cycle, solid (oxide) fuel, steel structures and sodium coolant. This covariance data set could thus not be applied for TMSR uncertainty calculations. Instead, the BOLNA⁵ [4] covariance matrix has been applied. This matrix contains covariance data of three of the most important nuclides, U-233, Th-232 and F-19, but unfortunately not for Li-7.

3.3.2 SCALE

Sensitivity coefficients The S&U calculations by SCALE are performed by the TSUNAMI-3D module, which applies a 238-group transport solver and uses the ENDF/B-VI library⁶. First it performs a forward- and an

⁵BOLNA is a combination of the first letters of BNL, ORNL, LANL, NRG and ANL, the laboratories wherein the covariances were produced.

⁶SCALE 5.1 uses the ENDF/B-VI release 7 library, while ERANOS 2.1 uses the ENDF/B-VI release 8 library.

adjoint flux calculation with the KENO-Va module, followed by sensitivity and uncertainty calculations with the SAMS module.

Uncertainty SCALE includes four cross-section covariance matrices by which uncertainty values can be calculated, '44 GROUP V5 COV' and '44 GROUP V5 REC' to be used with the ENDF/B-V library, and '44 GROUP V6 COV' and '44 GROUP V6 REC' to be used with the ENDF/B-VI library. The recommended ('REC') matrices are extended with integral uncertainty information of a number of nuclides. In this project the '44 GROUP V6 REC' library has been applied for the uncertainty analysis.

4 Results

Section 4.1 presents the results of the direct- and adjoint k_{eff} calculations for SCALE and ERANOS. The calculated sensitivity coefficients and their comparisons are discussed in 4.2. The relative contributions of the explicit- and implicit components of the sensitivity coefficients are presented in 4.3. Uncertainty results can be found in 4.4. Section 4.5 presents the results of 'manual' nuclide density perturbation, as a method of verifying the sensitivity coefficients of the nuclide cross sections. The results regarding sensitivity coefficients of the breeding ratio are discussed in 4.6.

4.1 Forward- and adjoint k_{eff} calculations

Table 4 shows the direct and adjoint k_{eff} values obtained by with the ERANOS and SCALE code systems for the various configurations. For ERANOS, the difference between the direct and adjoint k_{eff} is well below 1%, which is considered as a upper limit for a trustworthy sensitivity calculation. One exception is the 172-group JEFF-3.1 transport calculation, for which no converging solution could be obtained. In SCALE the difference between the direct- and adjoint k_{eff} calculation is considerably higher, nearly 2%. It must be noted that this decreases the quality of the sensitivity coefficient calculation performed by SCALE.

	33-group			172-group		
	$k_{\text{eff-direct}}$	$k_{\text{eff-adjoint}}$	$\Delta\%$	$k_{\text{eff-direct}}$	$k_{\text{eff-adjoint}}$	$\Delta\%$
ENDF-FRDI	1.05635	1.05635	0	1.05339	1.05339	0
ENDF-RSTI	1.05563	1.05562	0	1.05262	1.05253	0.009
JEFF-FRDI	1.03374	1.03374	0	1.04702	1.04702	0
JEFF-RSTI	1.03320	1.03317	0.003	1.03729	-	-
	238-group					
SCALE	1.0357	1.0165	1.89			

Table 4: Direct and adjoint k_{eff} values obtained by ERANOS and SCALE calculations, and their percentual difference.

4.2 Sensitivity coefficients

4.2.1 ERANOS

Sensitivity coefficients in ERANOS have been calculated with eight different configurations, so eight sets of coefficients are obtained. Since their results are more or less equal, one set of sensitivity coefficients is presented, and for the other sets it will be discussed how much they differ from this reference

calculation. In section A of the appendix a complete overview can be found of the sensitivity coefficients from all calculations.

Table 5 shows the sensitivity coefficients obtained by applying a calculation with 33 energy groups, using the ENDF/B-V library and the diffusion neutron flux solver.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	-5.359E-02	5.419E-01	1.379E-03	-1.403E-04	4.533E-05	9.840E-01
th-232	-4.746E-01	8.872E-03	1.358E-02	-2.723E-03	1.002E-03	1.596E-02
f-19	-1.524E-02	0.000E+00	8.730E-02	-4.902E-03	3.975E-06	0.000E+00
li-7	-2.635E-04	0.000E+00	2.285E-02	-2.488E-04	1.042E-05	0.000E+00

Table 5: Sensitivity coefficients for 33-group ENDF/B-V diffusion calculation.

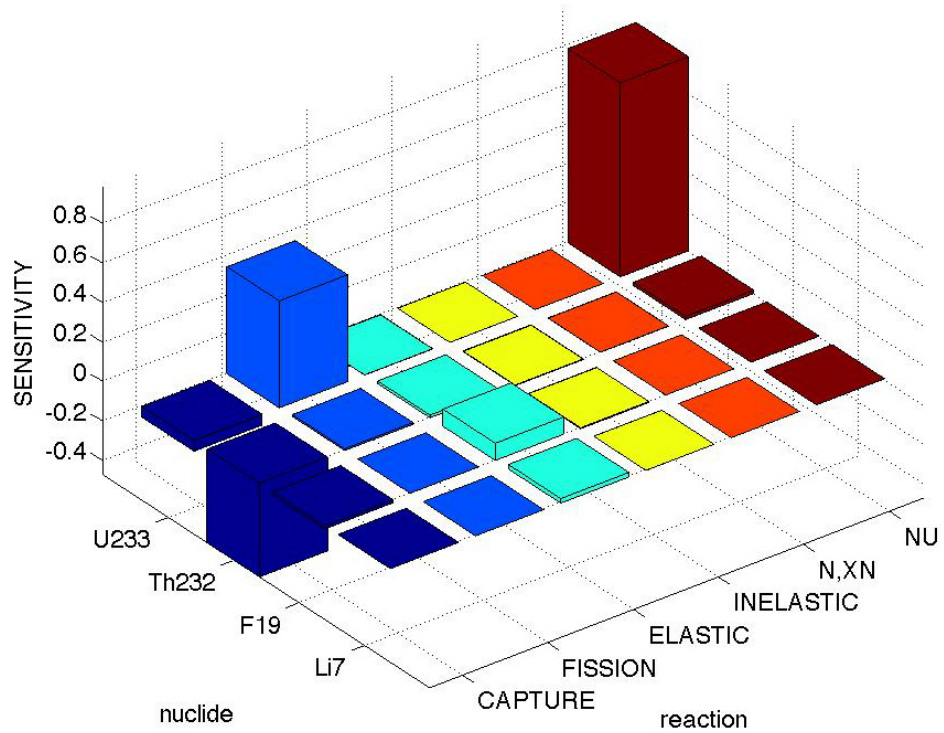


Figure 1: Sensitivity coefficients for 33-group ENDF/B-V diffusion calculation.

Comparison of flux solvers Table 6 shows the percentual differences between the sensitivity coefficients obtained with the diffusion- and the transport neutron flux solver. These cases have been performed by a 33-group ENDF/B-VI calculation. It can be observed that only minor differences

occur, and that the significant percentual differences correspond to cross sections with a very low sensitivity coefficient.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	-0.01	0.00	2.10	1.90	-0.02	0.00
th-232	0.05	-0.02	0.73	1.07	0.24	0.05
f-19	0.14	0.00	-0.07	-4.48	0.58	0.00
li-7	-0.05	0.00	-0.14	-13.50	0.93	0.00

Table 6: Percentual differences between diffusion and transport sensitivity coefficients in 33-group ENDF/B-VI calculation.

Comparison of neutron cross-section library Table 7 shows the percentual differences between sensitivity coefficients obtained with the ENDF/B-VI and the JEFF-3.1 library. These cases have been performed by a 33-group calculation with diffusion flux solver. Large differences occur for nearly all sensitivity coefficients, up to 793% for the Li-7 capture sensitivity coefficient.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	11.4	1.9	1.4	-56.5	30.3	0.1
th-232	-2.7	-4.4	1.6	97.7	-10.9	-4.1
f-19	128.0	0.0	-1.2	-87.9	-11.6	0.0
li-7	793.1	0.0	-5.0	-185.6	-3.6	0.0

Table 7: Percentual differences between ENDF/B-VI and JEFF-3.1 sensitivity coefficients in 33-group diffusion calculation.

Comparison of energy group discretization Table 8 shows the percentual differences between sensitivity coefficients obtained with 33-group and 172-group calculations. These cases have been performed with the ENDF/B-VI library and the diffusion flux solver. Large percentual differences only occur for the minor sensitivity coefficients.

4.2.2 SCALE

This section presents the sensitivity coefficients obtained by the SCALE 5.1 code system. Table 9 and figure 2 show the resulting sensitivity coefficients.

4.2.3 Comparison ERANOS and SCALE

Table 10 shows the percentual differences between the sensitivity coefficients of the 238-group ENDF/B-VI (SCALE) transport calculation and

	capture	fission	elastic	inelastic	n,xn	nu
u-233	-1.0	0.8	-5.5	-8.9	-0.5	0.0
th-232	-0.6	-2.2	-6.1	-11.6	0.6	-2.2
f-19	-10.3	0.0	-7.4	-3.8	33.2	0.0
li-7	2.2	0.0	-11.3	-12.2	7.4	0.0

Table 8: Percentual differences between 33-group and 172-group sensitivity coefficients in ENDF/B-VI diffusion calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	-5.223E-02	5.489E-01	1.560E-03	-1.519E-04	4.588E-05	9.833E-01
th-232	-4.804E-01	9.436E-03	1.654E-02	-3.031E-03	9.981E-04	1.669E-02
f-19	-1.465E-02	0.000E+00	9.040E-02	-5.981E-03	4.475E-06	0.000E+00
li-7	-2.662E-04	0.000E+00	2.454E-02	-3.527E-04	1.024E-05	0.000E+00

Table 9: Sensitivity coefficients for 238-group SCALE (ENDF/B-VI) transport calculation.

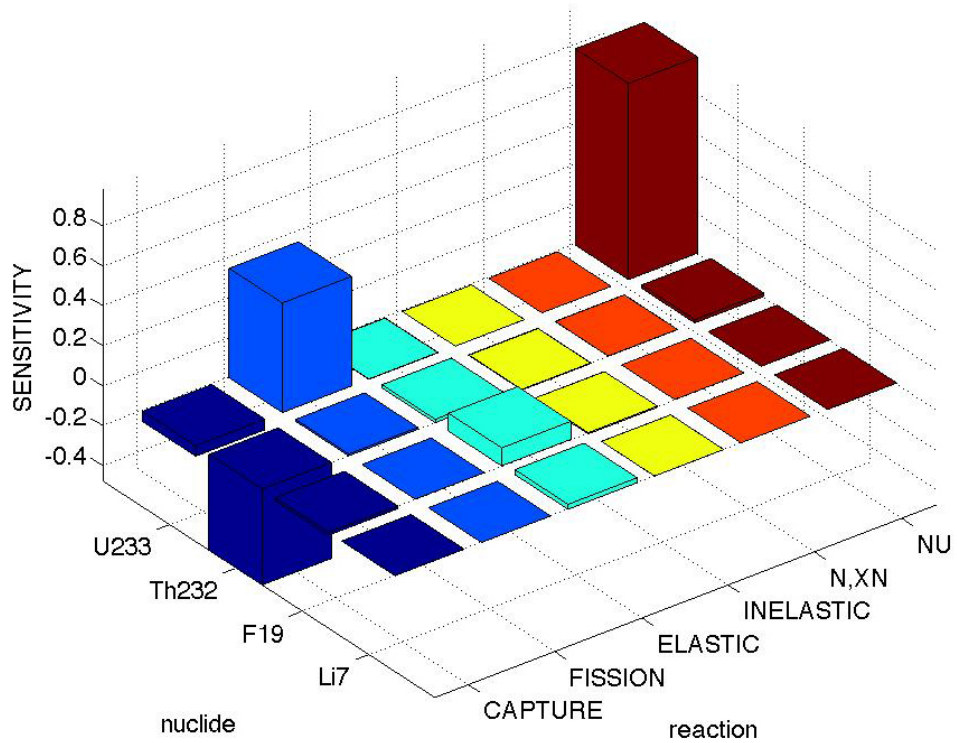


Figure 2: Sensitivity coefficients obtained with 238-group SCALE (ENDF/B-VI) transport calculation.

the 33-group ENDF/B-VI diffusion calculation with ERANOS. It shows that the percentual differences for the most important sensitivity coefficients are small. The results of the elastic- and inelastic components are considerably different.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	2.5	-1.3	-13.1	-8.2	-1.2	0.1
th-232	-1.2	-6.3	-21.8	-11.3	0.4	-4.5
f-19	3.9	0.0	-3.6	-22.0	-12.6	0.0
li-7	-1.0	0.0	-7.4	-41.7	1.7	0.0

Table 10: Percentual differences between the sensitivity coefficients of the 238-group ENDF/B-VI (SCALE) transport calculation and the 33-group ENDF/B-VI diffusion calculation with ERANOS

4.2.4 Sensitivity coefficients per neutron group

All sensitivity coefficients mentioned in the report are integrated over their energy groups. It might be of interest to consult the sensitivity coefficients per energy group, rather than the total sensitivity coefficients. SCALE contains a module called JAVAPENO to visualize this data, but for ERANOS such a module was not present. Therefore a Matlab module has been created which enables group-wise plotting of the sensitivity coefficients calculated by ERANOS as well as by SCALE. Figure 3 shows an example of such a plot⁷.

4.3 Explicit- and implicit sensitivity coefficients

In section 2.4 it has been shown that sensitivity coefficients are constituted from explicit- and implicit components. SCALE calculates both components, while ERANOS is only capable of calculating the explicit components. To enable comparison between the code systems, only the explicit components of the SCALE results are mentioned in this report. To visualize the contribution of the implicit components to the total sensitivity coefficients, table 11 shows the size of the implicit component relative to the explicit component, e.g. a value of 200% means that the implicit component is twice as large as the explicit component, and 0.0% means that the component is negligible. The table shows that only the elastic reaction has a large implicit component.

⁷For help or information about this module, contact Michiel Hoogmoed, michielhoogmoed@hotmail.com

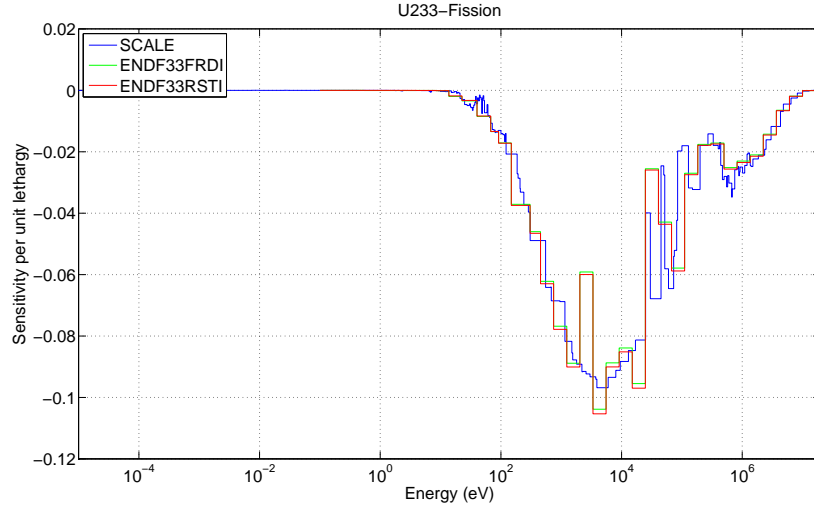


Figure 3: By group sensitivity coefficients of the U-233 fission cross-section. Data is shown for the 238-group SCALE calculation as well as for the 33-group ERANOS calculation with diffusion- and with transport flux solver.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	0.0	0.0	206.8	0.0	0.0	0.0
th-232	-2.3	0.0	227.6	0.0	0.0	0.0
f-19	0.0	0.0	-50.5	0.6	0.0	0.0
li-7	0.7	0.0	-25.6	0.0	0.0	0.0

Table 11: Relative size (percentage) of the implicit component with respect to the explicit component of the sensitivity coefficients calculated by SCALE.

4.4 Uncertainty

Both the SCALE and the ERANOS code system are capable of calculating the contribution to the uncertainty in k_{eff} by using the sensitivity data and covariance data of the nuclides involved. The relative differences between the other uncertainty calculations obtained with ERANOS will not be discussed since their calculation method is not different, except that they use other sensitivity coefficients. In section A of the appendix, a complete overview can be found of the uncertainties from all calculations.

ERANOS Table 12 and figure 4 show the uncertainties ($\% \Delta k/k$) for 33-group ENDF/B-V diffusion calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	3.561E-01	2.880E+00	5.021E-03	2.886E-03	8.195E-04	1.607E-01
th-232	6.188E-01	1.858E-02	5.545E-03	7.417E-03	1.002E-02	0.000E+00
f-19	1.398E-01	0.000E+00	1.574E-01	7.991E-02	2.862E-05	0.000E+00
li-7	-	-	-	-	-	-

Table 12: Uncertainties ($\% \Delta k/k$) for 33-group ENDF/B-V diffusion calculation.

SCALE Table 13 and figure 5 show the uncertainties ($\% \Delta k/k$) for 238-group SCALE (ENDF/B-VI) transport calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	3.507E-01	3.907E+00	1.187E-02	0.000E+00	0.000E+00	1.382E-01
th-232	3.323E-01	7.410E-03	1.350E-02	0.000E+00	0.000E+00	1.149E-02
f-19	2.466E-01	0.000E+00	1.231E-01	4.557E-02	3.626E-05	0.000E+00
li-7	5.978E-03	0.000E+00	9.410E-02	1.511E-03	0.000E+00	0.000E+00

Table 13: Uncertainties ($\% \Delta k/k$) for 238-group SCALE (ENDF/B-VI) transport calculation.

4.5 Nuclide density perturbation

In section 2.6 it has been stated that the sum of the sensitivities of k_{eff} to perturbations in the nuclide cross-sections is equal to the sensitivity of k_{eff} to perturbations in the nuclide density. So, if all nuclide densities would be increased with 1%, the new k_{eff} is expected to have changed by this amount.

This 'manual' check has been performed for the ERANOS sensitivity calculations. Table 14 shows the direct- and adjoint k_{eff} results before and

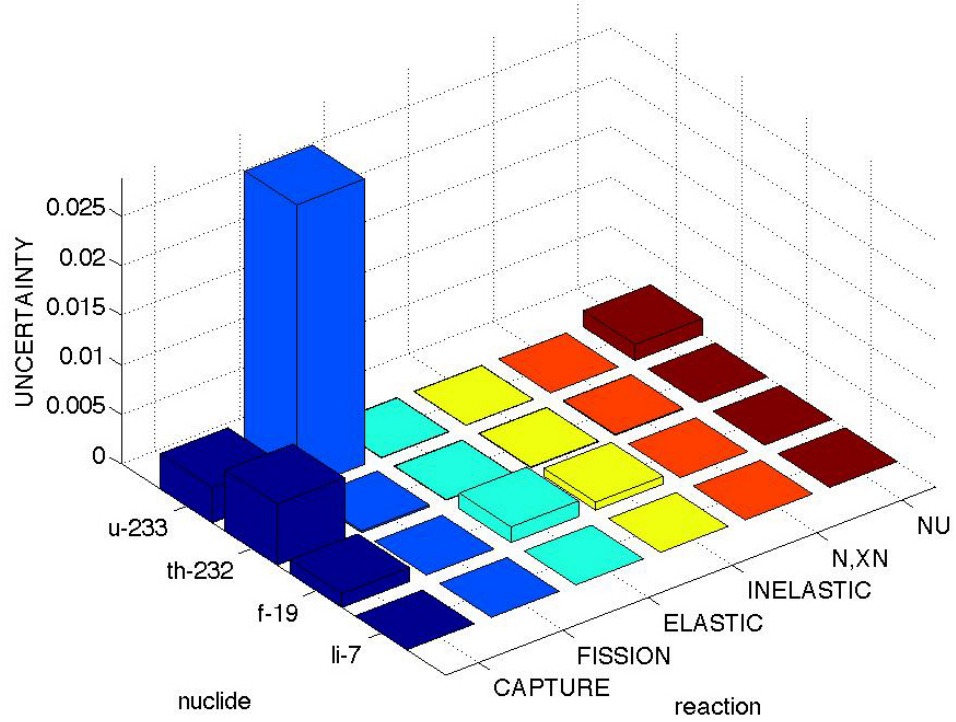


Figure 4: Uncertainties ($\% \Delta k/k$) for 33-group ENDF/B-V diffusion calculation.

after adding 1% to the nuclide densities. In the second and third column of table 15 the percentual difference between these k_{eff} values are stated. The fourth column shows the expected percentual change by adding up the total cross section sensitivities of all nuclides in the system. Finally, the last two columns represent the percentual difference between the manually calculated change in k_{eff} and the expected change in k_{eff} caused by the sensitivities.

It can be concluded that the sensitivities calculated with ERANOS generally satisfy the relation posed in section 2.6, except for the 172-group JEFF-3.1 calculations.

4.6 Breeding Ratio sensitivity coefficients

The ERANOS code system contains a module that facilitates calculation of the sensitivity coefficients of a reaction rate ratio of the form

$$R = \frac{\langle \Sigma_1 \phi \rangle}{\langle \Sigma_2 \phi \rangle}. \quad (4.1)$$

It has been attempted to use this module to calculate sensitivity coefficients of the breeding ratio, which has a slightly different form as can be seen in equation (2.16) in section 2.3. For testing purposes, the sensitivity coefficients of the reaction rate ratio as in equation (4.1) have successfully been

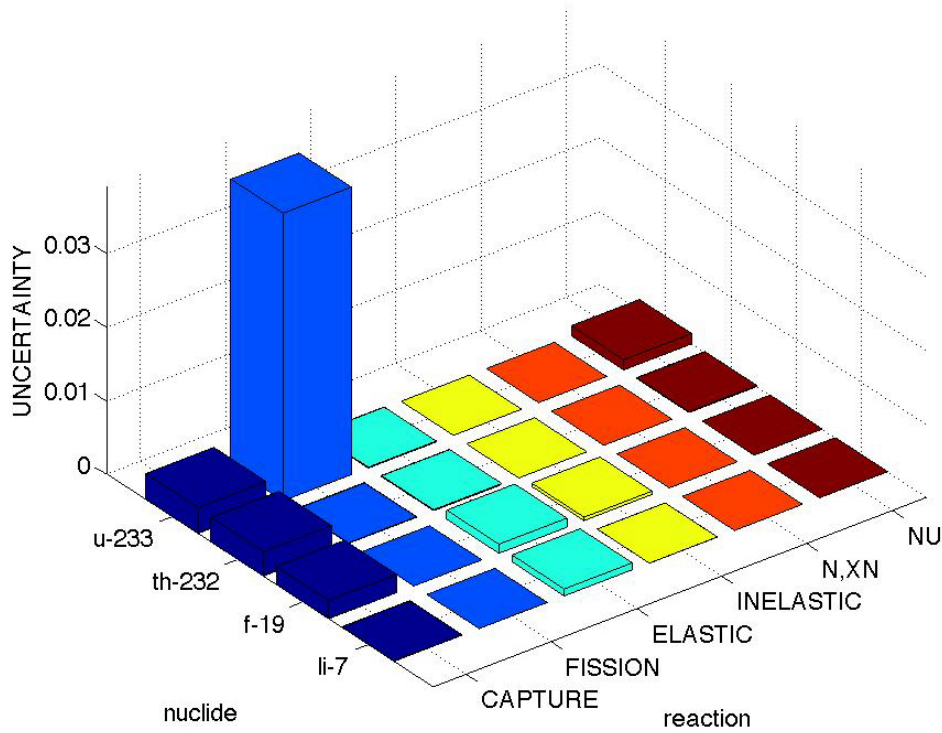


Figure 5: Uncertainties ($\% \Delta k/k$) for 238-group SCALE (ENDF/B-VI) transport calculation.

No.	Library	NG	Solver	$k_{\text{eff_dir}}$	$k_{\text{eff_adj}}$	$k_{\text{eff_dir_1\%}}$	$k_{\text{eff_adj_1\%}}$
1	ENDF/B	172	FRDI	1.05339	1.05339	1.05469	1.05469
2	ENDF/B	172	RSTI	1.05262	1.05253	1.05396	1.05384
3	ENDF/B	33	FRDI	1.05635	1.05635	1.05765	1.05765
4	ENDF/B	33	RSTI	1.05562	1.05562	1.05693	1.05693
5	JEFF	172	FRDI	1.04702	1.04702	1.04793	1.04793
6	JEFF	172	RSTI	1.02958	-	1.04112	-
7	JEFF	33	FRDI	1.03374	1.03374	1.03504	1.03504
8	JEFF	33	RSTI	1.03319	1.03321	1.03451	1.03444

Table 14: Calculated k_{eff} values with and without a 1% change in nuclide densities.

No.	$\% \Delta k_{\text{eff_dir}}$	$\% \Delta k_{\text{eff_adj}}$	ΣS_N	$\% \Delta$ columns 2-4	$\% \Delta$ columns 3-4
1	0.1234	0.1234	0.1245	0.84	0.84
2	0.1273	0.1245	0.1245	2.26	0.02
3	0.1231	0.1231	0.1242	0.88	0.88
4	0.1241	0.1241	0.1242	0.06	0.06
5	0.0869	0.0869	0.3460	74.8	74.9
6	1.1208	-	0.1045	972	-
7	0.1258	0.1258	0.1285	2.12	2.12
8	0.1278	0.1190	0.1267	0.88	6.00

Table 15: The percentual changes in $k_{\text{eff_dir}}$ and $k_{\text{eff_adj}}$ caused by a 1% change in nuclide density are stated in the second and third column. Column four is the summation of the sensitivities of the total cross sections for all nuclides in the system. The last two columns are the percentual difference between column four and five with respect to column 6, respectively.

calculated. Adjusting the ERANOS modules to calculate sensitivity coefficients of the breeding ratio form has proven to be a rather difficult process, and could not be finished within this project.

5 Conclusions & Recommendations

5.1 Conclusions

- Sensitivity and uncertainty analysis for the Non-Moderated Thorium Molten Salt Reactor has been performed using the SCALE 5.1 and ERANOS 2.1 code systems.
- Various configurations have been performed and compared for ERANOS sensitivity coefficient calculations, regarding the choice for neutron flux solver, neutron data library and energy discretization.
- SCALE is capable of calculating the implicit- and explicit components of the sensitivity coefficients, while ERANOS is only able to calculate the explicit components. Comparison of results from both code systems has therefore only been applied for the explicit components.
- Both code systems yield roughly the same results regarding sensitivity coefficients and uncertainty results.
- Attempts have been made to calculate sensitivity coefficients of the breeding ratio with ERANOS, but this has proven to require in-depth knowledge of the code system and was not feasible within this project.

5.2 Recommendations

- Both code systems yield roughly the same results regarding sensitivity coefficients and uncertainty results, but significant differences do occur for various configurations of ERANOS. For a better understanding of the results, the cause of these differences should be investigated.
- The forward- and adjoint flux calculations in SCALE differ by almost 2%, and the standard deviations in the obtained sensitivity coefficients are also rather large. This should be improved to have more reliable results with the SCALE code system.
- Sensitivity coefficient and flux calculations with ERANOS are unstable to configuration changes when using the JEFF-3.1 library.
- Continue attempts to calculate sensitivity coefficients of the breeding ratio with ERANOS. The documentation of the code system does not provide information how to do this, so experienced ERANOS users should be consulted⁸.

⁸Contact Jean Tommasi, CEA, jean.tommasi@cea.fr.

Part I
Appendix

A Sensitivity and uncertainty data

A.1 Complete overview of sensitivity coefficients

	capture	fission	elastic	inelastic	n,xn	nu
u-233	-5.411E-02	5.376E-01	1.454E-03	-1.528E-04	4.555E-05	9.837E-01
th-232	-4.776E-01	9.072E-03	1.441E-02	-3.039E-03	9.962E-04	1.631E-02
f-19	-1.681E-02	0.000E+00	9.378E-02	-5.088E-03	2.654E-06	0.000E+00
li-7	-2.577E-04	0.000E+00	2.543E-02	-2.791E-04	9.640E-06	0.000E+00

Table 16: Sensitivity coefficients for 172-group ENDF/B-V diffusion calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	-5.412E-02	5.376E-01	1.435E-03	-1.498E-04	4.555E-05	9.837E-01
th-232	-4.772E-01	9.074E-03	1.436E-02	-3.011E-03	9.932E-04	1.630E-02
f-19	-1.674E-02	0.000E+00	9.370E-02	-5.280E-03	2.623E-06	0.000E+00
li-7	-2.540E-04	0.000E+00	2.547E-02	-3.154E-04	9.537E-06	0.000E+00

Table 17: Sensitivity coefficients for 172-group ENDF/B-V transport calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	-5.359E-02	5.419E-01	1.379E-03	-1.403E-04	4.533E-05	9.840E-01
th-232	-4.746E-01	8.872E-03	1.358E-02	-2.723E-03	1.002E-03	1.596E-02
f-19	-1.524E-02	0.000E+00	8.730E-02	-4.902E-03	3.975E-06	0.000E+00
li-7	-2.635E-04	0.000E+00	2.285E-02	-2.488E-04	1.042E-05	0.000E+00

Table 18: Sensitivity coefficients for 33-group ENDF/B-V diffusion calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	-5.360E-02	5.418E-01	1.350E-03	-1.377E-04	4.533E-05	9.840E-01
th-232	-4.743E-01	8.874E-03	1.348E-02	-2.694E-03	9.999E-04	1.596E-02
f-19	-1.522E-02	0.000E+00	8.736E-02	-5.121E-03	3.951E-06	0.000E+00
li-7	-2.636E-04	0.000E+00	2.288E-02	-2.825E-04	1.032E-05	0.000E+00

Table 19: Sensitivity coefficients for 33-group ENDF/B-V transport calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	-6.950E-02	1.926E-01	-1.702E-03	-2.615E-04	3.093E-05	9.834E-01
th-232	-4.786E-01	9.137E-03	-1.278E-02	-2.432E-04	1.087E-03	1.660E-02
f-19	6.087E-01	0.000E+00	-5.540E-02	-1.049E-02	3.543E-06	0.000E+00
li-7	1.567E-01	0.000E+00	9.429E-03	-8.302E-04	1.010E-05	0.000E+00

Table 20: Sensitivity coefficients for 172-group JEFF-3.1 diffusion calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	-1.160E-01	-5.522E-01	-2.180E-02	-3.013E-04	3.056E-05	9.829E-01
th-232	-5.077E-01	9.513E-03	-2.643E-01	-1.332E-03	1.096E-03	1.707E-02
f-19	1.920E+00	0.000E+00	-8.167E-01	-1.135E-02	3.545E-06	0.000E+00
li-7	5.193E-01	0.000E+00	-4.960E-02	-9.653E-04	1.015E-05	0.000E+00

Table 21: Sensitivity coefficients for 172-group JEFF-3.1 transport calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	-4.748E-02	5.313E-01	1.360E-03	-2.195E-04	3.161E-05	9.834E-01
th-232	-4.876E-01	9.265E-03	1.336E-02	-6.154E-05	1.112E-03	1.662E-02
f-19	4.264E-03	0.000E+00	8.836E-02	-9.211E-03	4.434E-06	0.000E+00
li-7	1.826E-03	0.000E+00	2.400E-02	-7.107E-04	1.079E-05	0.000E+00

Table 22: Sensitivity coefficients for 33-group JEFF-3.1 diffusion calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	-4.780E-02	5.271E-01	1.294E-03	-2.195E-04	3.165E-05	9.834E-01
th-232	-4.869E-01	9.270E-03	1.291E-02	-2.815E-05	1.112E-03	1.662E-02
f-19	9.078E-03	0.000E+00	8.605E-02	-9.417E-03	4.423E-06	0.000E+00
li-7	2.379E-03	0.000E+00	2.366E-02	-7.512E-04	1.072E-05	0.000E+00

Table 23: Sensitivity coefficients for 33-group JEFF-3.1 transport calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	-5.223E-02	5.489E-01	1.560E-03	-1.519E-04	4.588E-05	9.833E-01
th-232	-4.804E-01	9.436E-03	1.654E-02	-3.031E-03	9.981E-04	1.669E-02
f-19	-1.465E-02	0.000E+00	9.040E-02	-5.981E-03	4.475E-06	0.000E+00
li-7	-2.662E-04	0.000E+00	2.454E-02	-3.527E-04	1.024E-05	0.000E+00

Table 24: Sensitivity coefficients for 238-group SCALE (ENDF/B-VI) transport calculation.

A.2 Complete overview of uncertainty data

	capture	fission	elastic	inelastic	n,xn	nu
u-233	3.691E-01	2.894E+00	5.407E-03	3.094E-03	8.225E-04	1.590E-01
th-232	6.335E-01	1.900E-02	5.860E-03	8.356E-03	9.962E-03	0.000E+00
f-19	1.375E-01	0.000E+00	1.678E-01	8.939E-02	1.911E-05	0.000E+00
li-7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

Table 25: Uncertainties ($\% \Delta k/k$) for 172-group ENDF/B-V diffusion calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	3.689E-01	2.894E+00	5.287E-03	3.038E-03	8.225E-04	1.589E-01
th-232	6.330E-01	1.900E-02	5.827E-03	8.277E-03	9.932E-03	0.000E+00
f-19	1.373E-01	0.000E+00	1.671E-01	9.159E-02	1.888E-05	0.000E+00
li-7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

Table 26: Uncertainties ($\% \Delta k/k$) for 172-group ENDF/B-V transport calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	3.561E-01	2.880E+00	5.021E-03	2.886E-03	8.195E-04	1.608E-01
th-232	6.188E-01	1.858E-02	5.545E-03	7.417E-03	1.002E-02	0.000E+00
f-19	1.398E-01	0.000E+00	1.574E-01	7.991E-02	2.862E-05	0.000E+00
li-7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

Table 27: Uncertainties ($\% \Delta k/k$) for 33-group ENDF/B-V diffusion calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	3.559E-01	2.880E+00	4.887E-03	2.828E-03	8.196E-04	1.607E-01
th-232	6.183E-01	1.858E-02	5.459E-03	7.336E-03	9.999E-03	0.000E+00
f-19	1.396E-01	0.000E+00	1.570E-01	8.202E-02	2.845E-05	0.000E+00
li-7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

Table 28: Uncertainties ($\% \Delta k/k$) for 33-group ENDF/B-V transport calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	2.828E-01	2.904E+00	6.196E-03	5.014E-03	5.616E-04	1.532E-01
th-232	6.843E-01	1.911E-02	2.745E-02	1.482E-02	1.087E-02	0.000E+00
f-19	3.806E+00	0.000E+00	1.318E-01	1.301E-01	2.551E-05	0.000E+00
li-7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

Table 29: Uncertainties ($\% \Delta k/k$) for 172-group JEFF-3.1 diffusion calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	4.891E-01	4.474E+00	6.524E-02	5.858E-03	5.550E-04	1.531E-01
th-232	9.300E-01	1.990E-02	2.459E-01	1.123E-02	1.096E-02	0.000E+00
f-19	1.182E+01	0.000E+00	1.688E+00	1.416E-01	2.552E-05	0.000E+00
li-7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

Table 30: Uncertainties ($\% \Delta k/k$) for 172-group JEFF-3.1 transport calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	2.660E-01	2.923E+00	4.902E-03	4.193E-03	5.744E-04	1.566E-01
th-232	6.266E-01	1.937E-02	5.698E-03	2.330E-02	1.112E-02	0.000E+00
f-19	1.722E-01	0.000E+00	1.638E-01	1.105E-01	3.193E-05	0.000E+00
li-7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

Table 31: Uncertainties ($\% \Delta k/k$) for 33-group JEFF-3.1 diffusion calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	2.660E-01	2.923E+00	4.717E-03	4.165E-03	5.751E-04	1.566E-01
th-232	6.263E-01	1.939E-02	5.742E-03	2.306E-02	1.112E-02	0.000E+00
f-19	1.918E-01	0.000E+00	1.586E-01	1.124E-01	3.185E-05	0.000E+00
li-7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

Table 32: Uncertainties ($\% \Delta k/k$) for 33-group JEFF-3.1 transport calculation.

	capture	fission	elastic	inelastic	n,xn	nu
u-233	3.507E-01	3.907E+00	1.187E-02	0.000E+00	0.000E+00	1.382E-01
th-232	3.323E-01	7.410E-03	1.350E-02	0.000E+00	0.000E+00	1.149E-02
f-19	2.466E-01	0.000E+00	1.231E-01	4.557E-02	3.626E-05	0.000E+00
li-7	5.978E-03	0.000E+00	9.410E-02	1.511E-03	0.000E+00	0.000E+00

Table 33: Uncertainties ($\% \Delta k/k$) for 238-group SCALE (ENDF/B-VI) transport calculation.

B Material composition

In tables 34, 35 and 36, the percentual atomic isotope composition of the materials used in the reactor is provided.

U-233	0.94	Th-232	7.47	F-19	62.62	Li-7	28.97
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Table 34: Percentual atomic isotope composition of the core salt.

Th-232	8.41	F-19	62.62	Li-7	28.97	Li-6	0.0014
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Table 35: Percentual atomic isotope composition of the breeder blanket.

Ni-58	54.068	Ni-60	20.827	Ni-61	0.9053	Ni-62	2.8866
Ni-64	0.7351	Cr-50	0.3481	Cr-52	6.7138	Cr-53	0.7613
Cr-54	0.1895	Fe-54	0.0370	Fe-56	0.5801	Fe-57	0.0133
Fe58	0.0001	Mn-55	0.2570	W-182	2.6465	W-183	1.4291
W-184	3.0600	W-186	2.8392	Al-27	0.0523	Si-28	0.2319
Si-29	0.0118	Si-30	0.0008	P-31	0.0228	B-10	0.0006
B-11	0.0262						

Table 36: Percentual atomic isotope composition of the reflector.

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