Criticality Assessment of Fuel Assemblies with Missing Fuel Rods
An intractable Problem?

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1. Introduction

In current certificates of package approval the arrangement of water and guide tubes within the array of fuel rods of a fuel assembly is specified in detail. Fuel assemblies with deviating water and guide tube arrangements or missing rods are not allowed to be loaded into the casks. The reason behind is that the reactivity of a standard fuel assembly increases if some rods are removed. For a certain number and arrangement of missing rods a maximum of reactivity is reached. Due to the missing fissile material the reactivity will decrease again if further rods are then removed.

For the comprehensive assessment of the maximum of reactivity all possible configurations of fuel rods and missing rods have to be investigated. The paper describes the problem at hand in detail giving estimates for the complexity of the analysis.

A complete analysis is only possible for cases with a very small number of fuel rods. Fuel assemblies which are used in reality can only be treated with approximation methods. The paper describes two such methods. With the first method up to 8 x 8 fuel assemblies can be analyzed in detail by using reasonable simplifications and assumptions. For fuel assemblies with a higher number of fuel rods a Monte Carlo approach is used. This second method can be applied to all fuel assemblies currently in use.

The accuracy of both approximation methods is compared for a 8 x 8 fuel assembly. The paper describes the statistical uncertainties and the influence of the parameters used for the individual calculations. Results are given for some of the mostly used fuel assembly types.

Finally, a procedure for the proof of criticality safety of fuel assemblies with missing fuel rods is defined. The application of this procedure will allow more flexibility in the definition of the licensed contents with respect to number and arrangement of missing rods in the fuel assemblies.

2. The Problem

Fig. 1 shows the cross section of a 4 x 4 assembly consisting of maximal 16 fuel rods. The fuel (red) consists of uranium with an enrichment of 5% U-235. The pellet diameter is 9.14 mm. The cladding (green) consists of Zirkaloy-2 with an outer diameter of 10.7 mm and an inner diameter of 9.7 mm. Between pellet and cladding void is assumed, between the fuel rods water (light blue) of density 1 g/cm^3. The fuel assembly is surrounded by a 20 cm water reflector (dark blue), which is shown only partially. Axially, the model is infinite.

It would be natural to assume that the completely filled fuel assembly is the most reactive configuration. However, removal of fuel pins leads to a slightly larger reactivity. The configuration shown in Fig. 2 with two missing fuel rods is actually the most reactive configuration.

The problem is to find the most reactive configuration. For the comprehensive assessment of the maximum of reactivity all possible configurations of fuel rods and missing rods have to be investigated. Unfortunately, the number of possible configurations for a given fuel assembly increases exponentially with the number of the grid positions. Assuming *n* to be the number of grid positions on one side of the assembly – the assembly such having *n x n* grid positions if completely filled – the number of possible configurations is

$$N_{conf} = C \times 2^{n^2}$$

where $C \approx 1/6$ takes into account that rotated or mirrored configurations need only be analyzed once.

This is a NP-hard problem and considered to be intractable but for very small *n*. Tab. 1 lists the possible configurations and the required time for the complete analysis for some fuel assembly types. For this table it is assumed that an individual criticality calculation takes 1 minute which would apply for a fast modern PC. The table shows that even for simple fuel assembly types a complete analysis is impossible.

assembly	configurations to be analyzed	required calculation time
4 x 4	10222	1 week
5 x 5	6×10^{6}	11 years
6 x 6	1×10^{10}	22000 years
7 x 7	1×10^{14}	200 Million years
8 x 8	3×10^{18}	6 000 billion years (approx. 400 times the age of the universe)
16 x 16	2×10^{76} (approx. the number of atoms in the universe)	infinite

Tab. 1. Number of Assembly Configurations and required Calculation Time

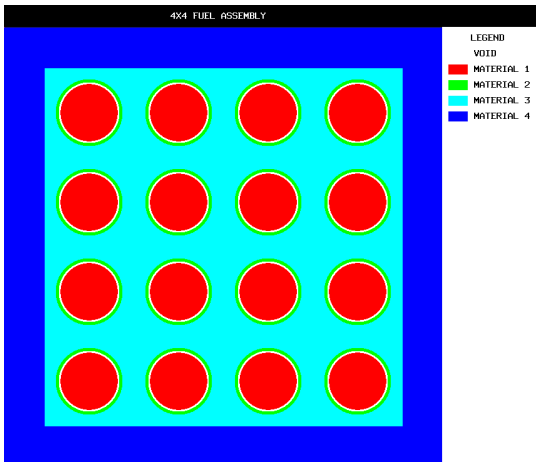

Fig. 1. A simple 4 x 4 fuel assembly

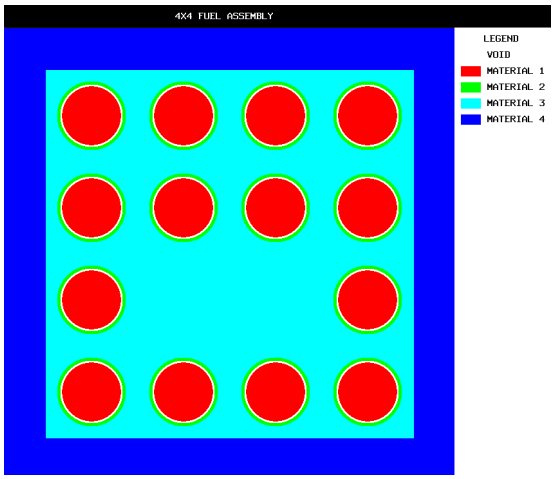

Fig. 2. The most reactive arrangement

3. Criticality Safety Analysis Code

For the criticality safety analysis the calculation sequence CSAS25/KENO V of the SCALE4.4A package [1] was used. The fuel was treated as homogeneous and the Dancoff factor was specified by using the MORE DATA option. For the calculations 203 generations were used in each run unless specified otherwise in the paper. By using these options the processing time for one calculation was approx. 1 minute. The standard deviation of the KENO V calculations is designated as σ_{KENO} in the following.

4. General Assumptions for the Approximation Methods

For the approximation methods is assumed that for every most reactive configuration all outer grid positions contain fuel rods. Missing rods are assumed only in inner grid positions. This is a reasonable assumption as missing rods in outer grid positions would inevitable lead to higher neutron leakage and hence to reduced reactivity of the configuration.

5. Approximation Method 1

The problem defined above can only be solved with approximation methods. Approximation method 1 assumes that a subset of all possible configurations can be constructed which contains the most reactive configurations. This subset is much smaller than the total set of all possible configurations. The algorithm is given below.

definitions:	
n x n	the number of grid positions of the complete fuel assembly
k = (n – 2) x (n – 2)	the analyzed part of the grid positions
conf(i, j)	configuration j of fuel rods with i missing rods
set(i)	set of all configurations conf(i, j), j = 1, ..., m with i missing rods
calculate k_{eff} for the one configuration in set(0) set kmax(0) = k_{eff}	
calculate k_{eff} for all configurations in set(1) set kmax(1) = MAX[k_{eff} of all configurations in set(1)]	
calculate k_{eff} for all configurations in set(2)	
discard all configurations from set(2) where k_{eff} + f σ_{KENO} < kmax(1) giving red(2) set kmax(2) = MAX[k_{eff} of all configurations in red(2)]	
repeat until red(i) is empty	
	construct set(i) from set(i-1) by removing in each possible position one fuel rod from every configuration in red(i - 1)
	calculate k_{eff} for all configurations in set(i)
	discard all configurations from set(i) where k_{eff} + f σ_{KENO} < kmax(i - 1) giving red(i) if red(i) is not empty then set kmax(i) = MAX[k_{eff} of all configurations in red(i)]
set kmax(total) = MAX[kmax(1) ... kmax(i - 1)]	

Algorithm 1. Approximation Method 1

The processing time and the accuracy of Algorithm 1 depends only on the factor f which is relevant for constructing the subset of configurations to be considered in the next calculation step. If this factor is chosen too large then the number of configurations in the subset remains large. This leads to a long processing time. If this factor is chosen too small then the number of configurations in the subset is reduced to a few configurations. It may happen then that the most reactive configuration is not found.

Algorithm 1 is applicable for fuel assemblies with up to 8 x 8 fuel rods. Tab. 2 lists the configurations calculated and compares the required processing time with the complete analysis. The table takes into account that the outer positions are always set with fuel rods. Therefore the analyzed part is smaller than the complete fuel assembly. The factor f was set to 1.

Tab. 2 shows a significant reduction of processing time. Nevertheless, the processing time increases also for algorithm 1 exponentially. Compared with the full analysis more fuel types can be analyzed, but important fuel types are still out of reach.

assembly	inner part	configurations for full assembly analysis	configurations for full analysis of inner part	configurations analysed with algorithm 1	reduction factor compared to full analysis	reduction factor compared to partial analysis
4 x 4	2 x 2	10222	6	5	5×10^4	1.2
5 x 5	3 x 3	6×10^6	102	68	8×10^4	1.5
6 x 6	4 x 4	1×10^{10}	10222	1562	6×10^6	6.5
7 x 7	5 x 5	1×10^{14}	6×10^6	7641	1×10^{10}	785
8 x 8	6 x 6	3×10^{18}	1×10^{10}	58345	5×10^{13}	2×10^5

Tab. 2. Configurations analyzed with algorithm 1

6. Approximation Method 2

Approximation method 2 uses a Monte Carlo approach to construct a subset of all possible configurations. For this subset a statistical evaluation is carried out to define the band where the most reactive configuration is to be expected. This subset is calculated in linear time. The algorithm is given below.

definitions:	
n x n	the number of grid positions of the complete fuel assembly
k = (n – 2) x (n – 2)	the analyzed part of the grid positions
conf(i, j)	configuration j of fuel rods with i missing rods
set(i)	set of all configurations conf(i, j), j = 1, ..., m with i missing rods
calculate k_{eff} for the one configuration in set(0) set kmax(0) = k_{eff}	
calculate k_{eff} for all configurations in set(1) set kmax(1) = MAX[k_{eff} of all configurations in set(1)]	
repeat for set(2) to set(k – 2)	
	select randomly N1 configurations from set(i) giving set rand1(i)
	calculate k_{eff} for all configurations in rand1(i) set kmax(i) = MAX[k_{eff} of all configurations in rand1(i)]
calculate k_{eff} for all configurations in set(k - 1) set kmax(k - 1) = MAX[k_{eff} of all configurations in set(k - 1)]	
calculate k_{eff} for the one configuration in set(k) set kmax(k) = k_{eff}	
set kmax(total) = MAX[kmax(0) ... kmax(k)]	
define p and q such that for all p ≤ i ≤ q kmax(i) + f σ_{KENO} > kmax(total)	
repeat for set(p) to set(q)	
	select randomly N2 configurations from set(i) giving set rand2(i)
	calculate k_{eff} for all configurations in rand2(i) set kmax(i) = MAX[k_{eff} of all configurations in rand2(i)]
calculate statistical values for all k_{eff} of rand2(p), ..., rand2(q)	

Algorithm 2. Approximation Method 2

The processing time and the accuracy of Algorithm 2 depends only on the numbers N1 and N2 which are relevant for constructing the subset of configurations to be considered in the calculation. N1 should be not too large as it is used for the initial calculations to narrow down the relevant configurations. N2 is used for the final calculations and has direct influence on statistics and accuracy.

Algorithm 2 is applicable for all fuel assemblies currently in use with up to 18 x 18 fuel rods or even more. Tab. 3 lists the configurations calculated and compares the required processing time with the complete analysis. The table takes into account that the outer positions are always set with fuel rods. Therefore the analyzed part is smaller than the complete fuel assembly. N1 was set to 100 configurations for the initial calculations and N2 was set to 500 configurations for the final calculations. Tab. 3 shows that the processing time for algorithm 2 increases linearly.

assembly	inner part	configurations for full assembly analysis	configurations for full analysis of inner part	configurations analysed with algorithm 2	reduction factor compared to full analysis	reduction factor compared to partial analysis
8 x 8	6 x 6	3E+18	1E+10	8734	4E+14	1E+06
9 x 9	9 x 9	4E+23	9E+13	11368	4E+19	8E+09
10 x 10	8 x 8	2E+29	3E+18	15283	1E+25	2E+14
11 x 11	9 x 9	4E+35	4E+23	17410	3E+31	2E+19
12 x 12	10 x 10	4E+42	2E+29	21329	2E+38	1E+25
13 x 13	11 x 11	1E+50	4E+35	22662	6E+45	2E+31
14 x 14	12 x 12	2E+58	4E+42	24985	7E+53	1E+38
15 x 15	13 x 13	9E+66	1E+50	32723	3E+62	3E+45
16 x 16	14 x 14	2E+76	2E+58	38251	5E+71	4E+53

Tab. 3. Configurations analyzed with algorithm 2

7. Accuracy of the Approximation Methods

A complete analysis was carried out for 3 x 3 and 4 x 4 fuel assemblies. For 5 x 5 fuel assemblies only configurations up to 5 missing fuel rods were fully analyzed. The results achieved with Algorithm 1 and the full analysis were identical.

An 8 x 8 fuel assembly was used to compare the accuracy of Algorithm 1 and Algorithm 2. Tab. 4 shows that the two algorithms give the same results taking into account statistical uncertainties.

Algorithm 1					Algorithm 2				
generat.	water holes	k_{eff}	σ_{KENO}	calculations	generat.	water holes	keff	σ_{KENO}	calculations
203	11	0.6571	0.0019	58345	203	15	0.6562	0.0016	8734
					1203	13	0.6529	0.0007	7289

Tab. 4. Comparison of Algorithm 1 and Algorithm 2 for 8 x 8 fuel assemblies

In Fig. 3 and 4 the distribution of calculated k_{eff} values in a band of configurations around the most reactive configuration is shown. For this all configurations in rand2[i], i = h1, ..., h2 were taken into account, where kmax(i) + g σ_{KENO} > kmax(total). For Fig. 3 following applies: h1 = 10, h2 = 21 and g = 3; for Fig. 4 applies: h1 = 10, h2 = 19 and g = 3. Fig. 3 is based on 5847 and Fig. 4 on 4764 different configurations.

Fig. 3 and 4 show that the distribution (calculated) complies rather good with a normal distribution (normal). The statistical values of both figures are given in Tab. 5. This table shows that the average k_{eff} for the considered band of configurations does not depend on the number of generations run for each configuration. The standard deviation $\sigma_{Algorithm2}$ of all configurations is the sum of the standard deviation σ_{KENO} of the KENO calculations and the standard deviation of the reactivity of the individual configurations which can be seen by comparing the columns average σ_{KENO} and $\sigma_{Algorithm2}$. The maximal k_{eff} is for the statistical values listed in Tab. 5 within 3 standard deviations from the average k_{eff}.

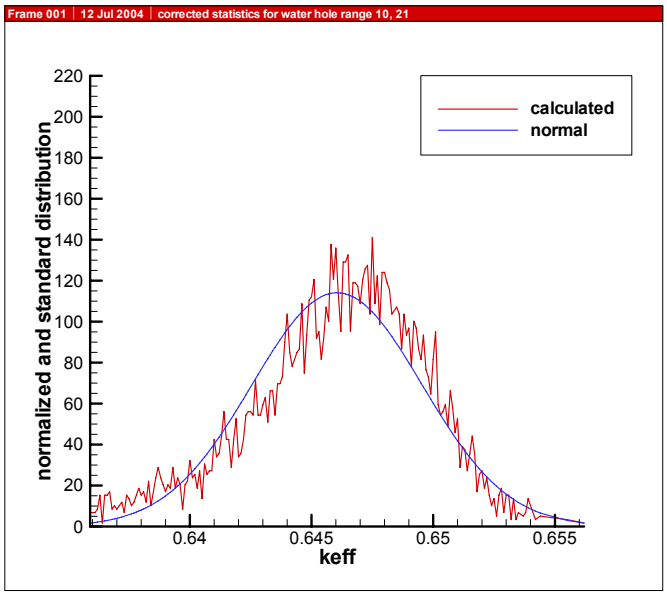

Fig. 3. Statistics for Algorithm2, 8 x 8 fuel assembly, 203 generations per run

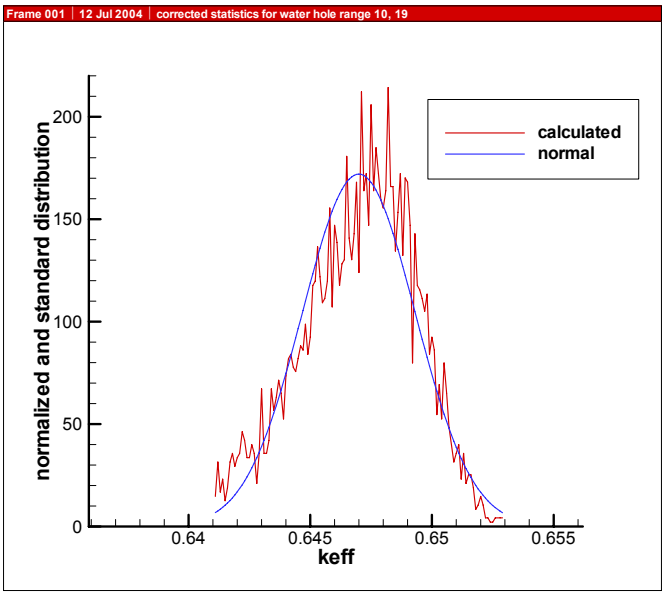

Fig. 4. Statistics for Algorithm2, 8 x 8 fuel assembly, 1203 generations per run

number of generations	average k_{eff}	average σ_{KENO}	$\sigma_{Algorithm2}$	calculated maximal k_{eff}
203	0.6460	0.0017	0.0035	0.6562
1203	0.6470	0.0007	0.0023	0.6529

Tab. 5. Statistical values for Fig. 3 and 4

8. Results

Results are shown for all fuel assemblies from 3 x 3 to 16 x 16 in Fig. 5 for the full configurations with fuel rods in all positions and for the most reactive configuration. Fig. 6 shows the reactivity difference between the full configuration and the most reactive configuration.

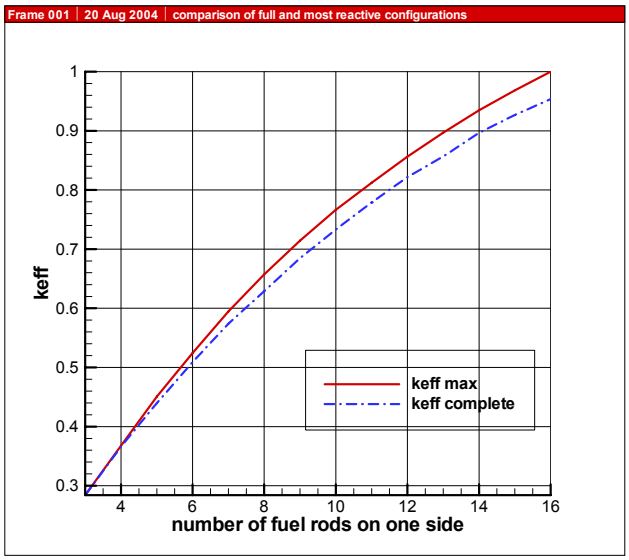

Fig. 5. k_{eff} values for 3 x 3 to 16 x 16 fuel assemblies, full (lower curve) and most reactive (upper curve) configurations

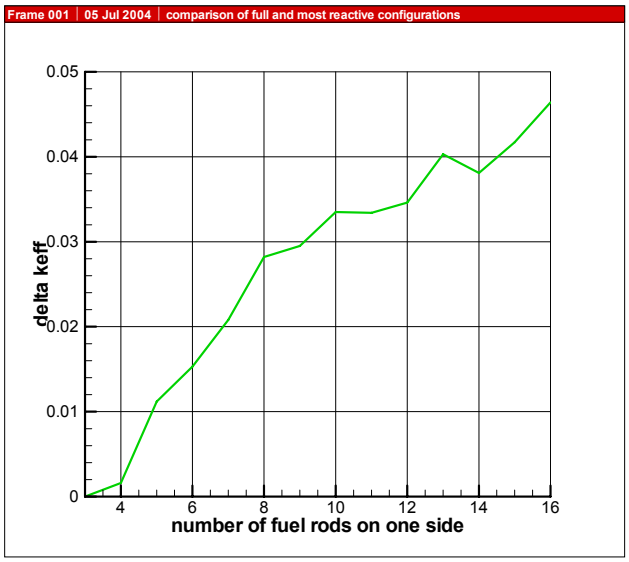

Fig. 6. k_{eff}-difference between full and most reactive configurations

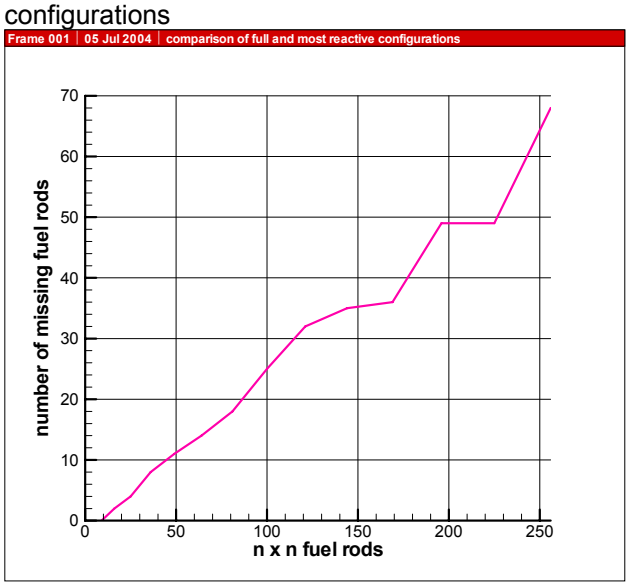

Fig. 7. Number of missing fuel rods in the most reactive configuration

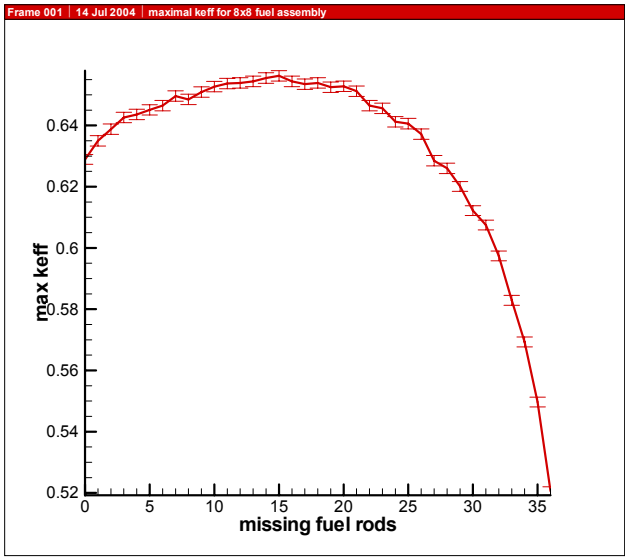

Fig. 8. Maximal k_{eff} in relation to the number of missing fuel rods for a 8 x 8 fuel assembly

The number of missing fuel rods in the most reactive configurations is shown in Fig. 7. The typical relation between the maximal k_{eff} and the number of missing fuel rods is shown in Fig. 8 for a 8 x 8 fuel assembly.

Fig. 5 shows that k_{eff} exceeds 0.95 for a 15 x 15 fuel assembly. For a 16 x 16 fuel assembly with approx. 70 missing fuel rods k_{eff} reaches 1.0. From Fig. 6 a linear relation between number of fuel rods on one side and difference of k_{eff} for the full and most reactive configuration can be assumed. The number of missing fuel rods increases linearly with the total number of fuel rod positions in the assembly. Fig. 8 shows a wide maximum of the reactivity in relation to the number of missing fuel rods.

Fig. 9 and 10 show the two most reactive configurations calculated with Algorithm 1 (Fig. 9) and Algorithm 2 (Fig. 10).

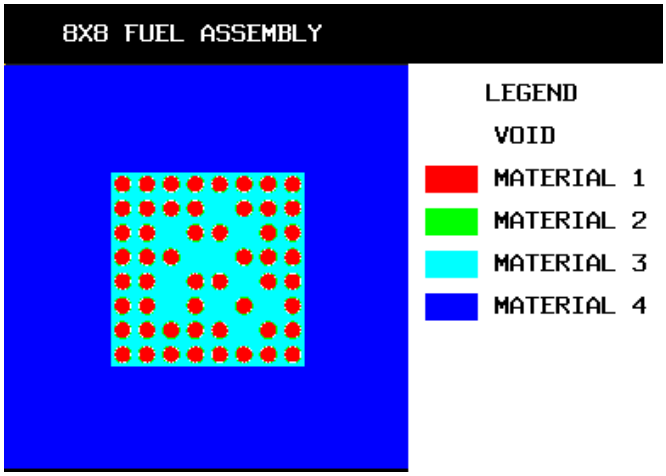

Fig. 9. Most reactive configuration for a 8 x 8 fuel assembly, 11 missing rods, k_{eff} = 0.6571 ± 0.0019, calculated with Algorithm 1

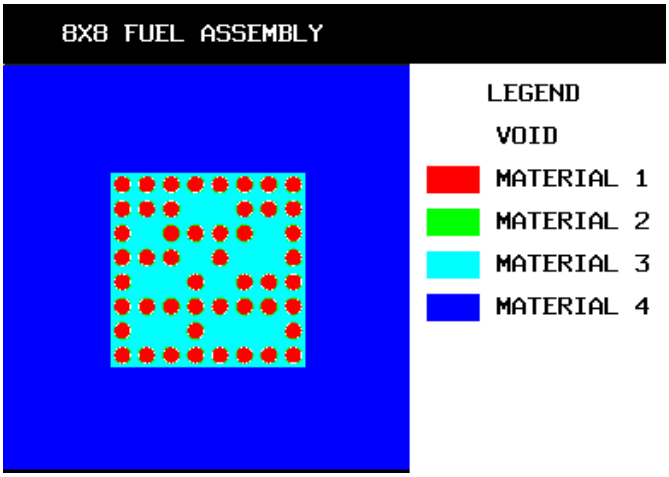

Fig. 10. Most reactive configuration for a 8 x 8 fuel assembly, 15 missing rods, k_{eff} = 0.6562 ± 0.0016, calculated with Algorithm 2

Finally, for some of the mostly used fuel assemblies the most reactive configurations calculated with Algorithm 2 are shown in Fig. 11 to Fig. 14.

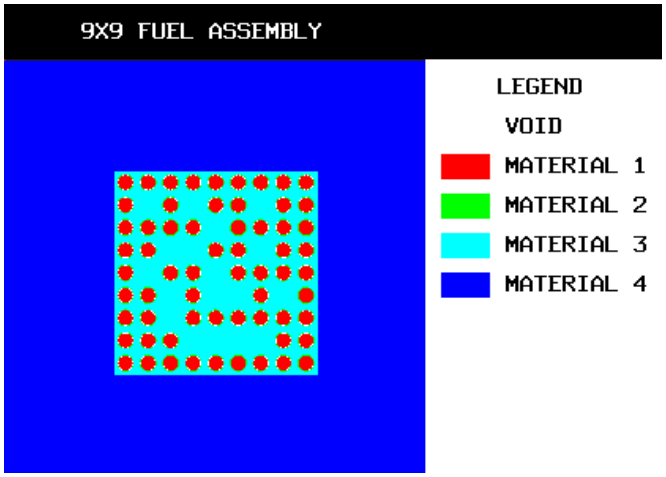

Fig. 11. Most reactive configuration for a 9 x 9 fuel assembly, 18 missing rods, k_{eff} = 0.7143 ± 0.0018

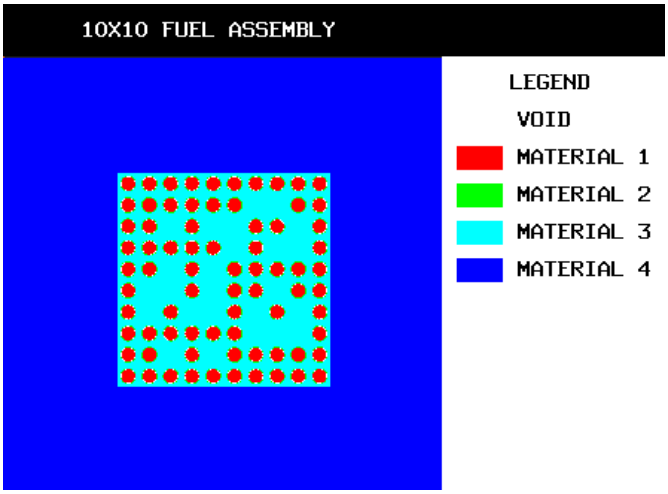

Fig. 12. Most reactive configuration for a 10 x 10 fuel assembly, 25 missing rods, k_{eff} = 0.7266 ± 0.0018

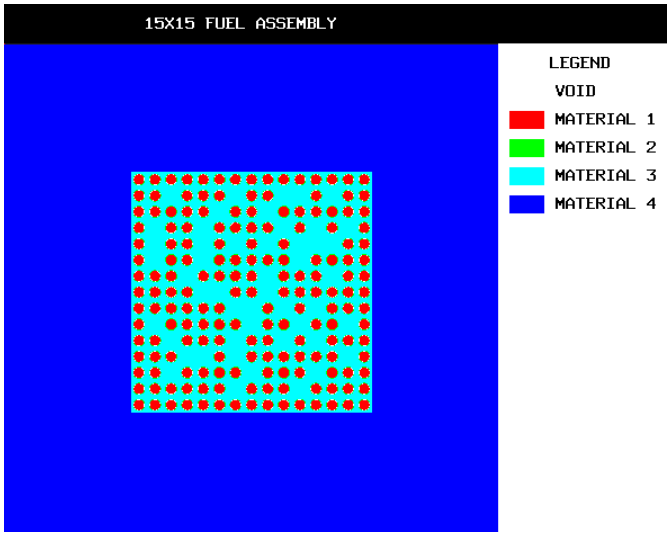

Fig. 13. Most reactive configuration for a 15 x 15 fuel assembly, 49 missing rods, k_{eff} = 0.9684 ± 0.0019

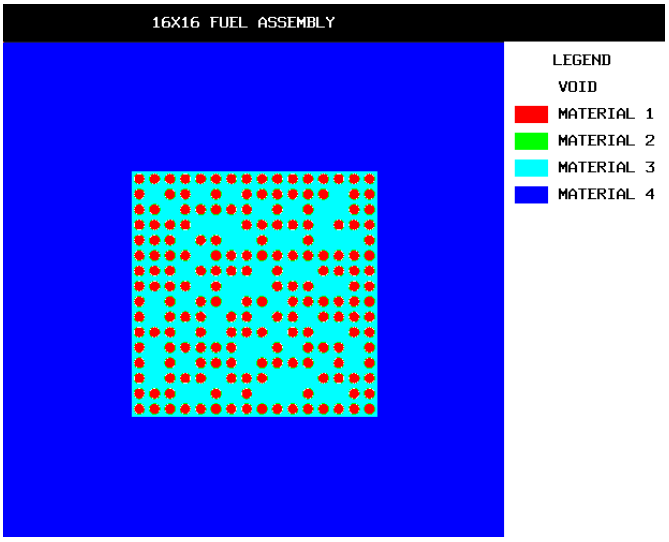

Fig. 14. Most reactive configuration for a 16 x 16 fuel assembly, 68 missing rods, k_{eff} = 1.0000 ± 0.0020

9. Proposed Guideline for Proof of Criticality Safety

Given problem: analysis of a n x n fuel assembly

Step 1: define W = ¼ x n x n the probable number of missing fuel rods which leads to maximal reactivity (derived from Fig. 7); define a range of 0.75 x W – 1.25 x W of missing fuel rods and calculate k_{eff} for a sufficiently large number of randomly chosen configurations with all numbers of missing fuel rods in the range defined above.

Step 2: Check if the calculated values of k_{eff} comply with a normal distribution (see Fig. 3 and 4); if this can be proved, assume the value of $k_{eff, max}$ which must comply with the limit given in the Regulations to be defined by

$k_{eff, max}$ = MAX[k_{eff} of all configurations with missing rods in the range 0.75 x W – 1.25 W] + 2 x $\sigma_{Algorithm2}$

Example: assume a 8 x 8 fuel assembly

- W = ¼ x 8 x 8 = 16
- calculate k_{eff} for a sufficiently large number of configurations with 12 to 20 missing fuel rods
- the distribution of calculated values complies with a normal distribution (Fig. 3), hence
- $k_{eff, max}$ = 0.6562 + 2 x 0.035 = 0.6632

10. Summary

The paper shows that the criticality assessment of fuel assemblies with missing fuel rods is feasible. Algorithm 2 is applicable to all fuel assemblies currently in use in commercial BWR and PWR nuclear facilities.

The required computer time for all fuel assembly types presently in use is in the range of several days to one month with a state of the art desktop computer. For the more complex analysis of a complete transport cask only several of the most reactive configurations need to be chosen as relevant cases, then.

11. Literature

[1] SCALE4.4A, A Modular Code System for Performing Standardized Computer Analysis for Licensing Evaluation, NUREG/CR-0200, Rev. 6, ORNL/NUREG/CSD-2/R6