
Dose rate calculation at transport and storage casks for spent nuclear fuel

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Abstract:

Interim storage of irradiated fuel assemblies in transport and storage casks (TSC) is part of the German approach of waste management. Some features of modern fuel assemblies are increasing enrichment, burn-up and irradiation time in the reactor core. During irradiation in the core about one thousand radioactive nuclides, fission products, higher actinides and activated structure material isotopes are generated in the fuel assembly and structure materials, emitting neutron and gamma radiation. These different kinds of radiation have to be shielded effectively by the cask. Since 1981 GRS is involved in dose calculations for TSCs using own developments of burn-up and shielding calculation systems. The paper shows the actual state-of-art of dose calculation in GRS considering axial burn-up profiles and n- γ -sources in more dimensional shielding procedures in the environment of transport codes.

1 INTERIM STORAGE OF TRANSPORT AND STORAGE CASKS

Part of the German waste management concept is to store irradiated fuel assemblies in interim facilities until a final storage facility becomes available. In Germany there are currently twelve interim storage facilities at NPP sites and three central interim storage facilities. The central storage facilities at Ahaus and Gorleben for example have a capacity of 420 storing positions for TSCs each capable of holding 19 PWR or 52 BWR fuel elements. Figure 1 shows two well known TSC types, the CASTOR V/52 of GNS and the TN 24 BH of AREVA.

2 COMPUTATIONAL STEPS TO DETERMINE THE DOSE RATE OF A TSC

The specifications of the TSC are designed to meet four main criteria: maintaining sub criticality, proper residual heat transfer, containment of the radioactive inventory and proper shielding of radiation. At present the TSCs are constructed to host fuel elements with burn-ups up to 55 GWd/tSM and initial enrichment up to 4.6 wt% ^{235}U . In the future increasing burn-up as well as an increasing enrichment of the fuel will have to be handled.

The present work aims at the last criterion for the design specifications: shielding of n- γ radiation and determination of the corresponding dose rate at the surface of the TSC as well as in the surrounding area. The computation takes four sequential steps in order to compute the dose rate: the burn-up calculation, the n- γ source term determination, the radiation transport and finally the dose computation at different space points as well as on the surface of the cask.

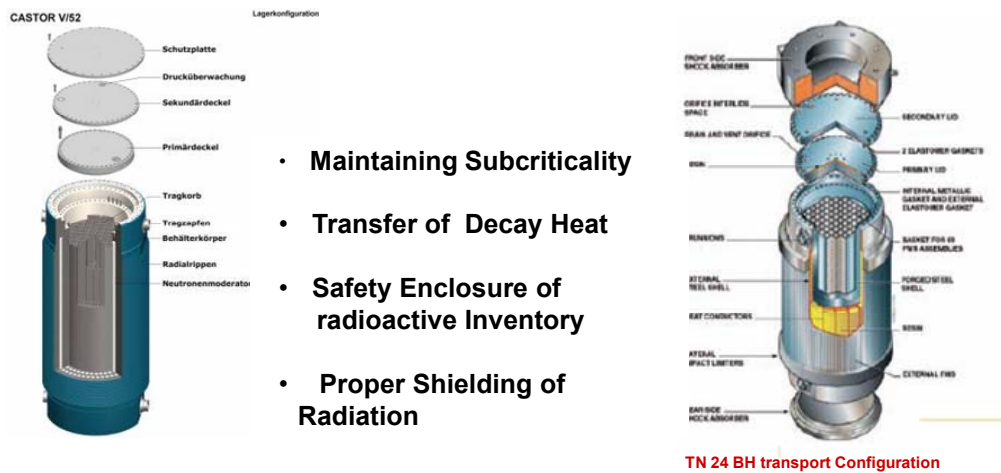


Figure 1: Profile of the transport and storage casks CASTOR V/52 and TN 24 BH.

2.1 Burn-up calculation

Applying burn-up credit the generation of heat in the TSC, the shielding as well as sub-criticality depends significantly on the nuclear inventory inside the cask. Thus, three of the four design criteria strongly depend on the burn-up calculation. For this reason, the GRS methode treats the burn-up with a simultaneous build-up of more than a thousand radioactive isotopes in PWR and BWR systems as close to reality as possible. Here we apply self-developed tools, which can be applied to two- and even three-dimensional problems [2]. With these tools we can compute the neutron spectrum during burn-up in radial and axial direction by taking into account the geometrical and neutron moderated environment. We consider (amongst others):

- Coolant pressure and coolant temperature
- Boron poisoning and void fraction in the coolant
- Rod temperature depending on actual reactor power
- Fuel element design and rod geometry
- Rodwise power output history
- Influence of surrounding fuel elements and BWR baskets

Thus, we already can meet the recommendation of the draft IAEA Safety Guide on spent fuel storage [6]. The results can be stored in a custom-build burn-up data base [1] and can be retrieved at any time. In a further decay step we determine the inventory after a desired decay time from the inventory of the fuel assembly. Afterwards the inventory is fed into a source-term generator (described below) which yields the energy and local spectra of the neutrons and gammas.

2.2 n-γ spectrum

The approximately 1000 radioactive isotopes, generated by fission and activation are fed into the so called source-term generator, which produces the desired n-γ spectra. Here we use our own developed code NGSRC [2], which incorporates all relevant emission channels:

- γ-spectrum using complete γ-line libraries (e.g. for $^{137}\text{Cs}/^{137\text{m}}\text{Ba}$)
- Bremsstrahlung from beta decay in the nuclear environment (e.g. for $^{90}\text{Sr}/^{90}\text{Y}$)
- Neutron spectra from spontaneous fission of higher actinides (e.g. ^{244}Cm)
- Neutron spectra from collisions of α-particles (e.g. from ^{238}Pu) and light nuclides (e.g. ^{18}O) by using α- line libraries and semi-quantum-mechanical models
- Optionally additive n-γ spectra from induced fission because of remaining reactivity of the fuel (e.g. ^{235}U and ^{239}Pu)
- Automatic condensation of the computed n-γ spectra to the chosen cross-section transport library taking into account rate and/or power conservation for the subsequent radiation transport calculation

2.3 Radiation transport and shielding

In the subsequent transport calculation the geometry and material of the cask under consideration is modelled as realistic as possible. After the inventory, which was determined before, is inserted into the cask model and connected to the chosen transport library, the shielding calculation starts with the n-γ-spectra calculated in the previous section.

Concerning the transport calculation several codes are available. The following list contains codes based on stochastic methods as well as deterministic codes.

- The 3d Code MCNP [4], which is suitable for a variety of problems, is based on statistical methods and “point data” cross sections.
- The deterministic ORNL-Codes 1d ANISN, 2d DORT und 3d TORT [3] are also suited for a variety of transport problems and run with “broad group data” cross sections. Three different production libraries are available with up to 175 neutron and 42 γ groups employing data from JEF2.2 and ENDF/B-VI. The cross section data are updated for each isotope taking into account the resonance corrections.

At the same time the sub-critical neutron multiplication and the radiative capture of neutrons with γ-emission is taken into account during the shielding calculation, which induces another neutron source as well as secondary gamma source.

2.4 Calculation of the local dose rate (LDR)

Choosing the Monte-Carlo Code MCNP it is suggestive to determine the LDR already during the run at certain space points on the surface of the TSC and the surrounding area. For the deterministic models, however, it is favourable to determine the dose in two steps. First we calculate the neutron and γ fluxes in the shielding calculation and afterwards we consider the radiation transport from the container to the surrounding area with separate analysis tools. The space points at which the dose shall be determined can be chosen independent from the first part. The fluxes are connected to the dose by applying dose conversion factors taken from ANSI-77, ICRP-74 or ICRP-2005. The following analysis tools are available at GRS.

- 2d SURF [2] calculates the LDR in the vicinity of finite ANISN-cylinders. The radiation transport is determined by solving the transport equation in vacuum based on 1d boundary fluxes from ANISN in 2d geometry (here R-Z, also available X-Y).

- 2d FALSTF [3] calculates the LDR in the vicinity of the DORT cask model. Here the radiation transport is determined by solving the integral Boltzmann equation into the vacuum, based on fluxes for each space cell and flux-weighted cross sections from DORT in 2d geometry (R-Z).

A further module is 2d FLXDOSD, which calculates the LDR in all cells of the TSC model by simply connecting the DORT results and the LDR conversion coefficients.

3 GRS-SYSTEMS FOR DETERMINATION OF THE LDR AT TRANSPORT AND STORAGE CASKS CONTAINING SPENT FUEL ELEMENTS

Due to the complexity of the sequence of the four computational steps, all steps have to be integrated in one complete system. Since 1981 the GRS has been involved in the development of own systems for combined burn-up and shielding calculations. These systems determine the dose rate for TSCs containing burned PWR and BWR fuel. Here we employ statistical and deterministic models from available well known code packages [3], [4], which constitute the basis of our user systems. All other tools are for providing necessary problem specific input data or analysing of results. The coupling of the base modules is realised by relatively simple I/O routines and interface programs. The systems are supposed to support the user and to avoid mistakes, which might occur by coupling the modules by hand. In the following we give a short chronological overview of the GRS developments

- 2d CASYST [5] (1984-1988) based on an OREST pre-run, on 1d ANISN (R-geometry) and 2d-DOT3.5 (R-Z-geometry) specialised for design studies of CASTOR TSCs; not further maintained
- 1d ANITABLE [2] (since 1988) based on an OREST pre-run and on ORIGEN to take into account variable decay times. Further tools incorporated are NGSRC, ANISN und SURF
- 3d MCNP, coupled to ANITABLE-NGSRC and SRCMCNP to convert results to MCNP-format (since 1993)
- 2d DORTABLE [2] (since 2005) with OREST, ANITABLE, DORT and the 2d-LDR-analysing tools FALSTF und FLXDOSD.
- Planned for 2009: RZ Φ -TORTABLE with TORT [3]

3.1 Computation with using DORTABLE

Figure 2 shows the simplified setup of RZ-DORTABLE. In the following, seven main steps of the calculation route are commented briefly.

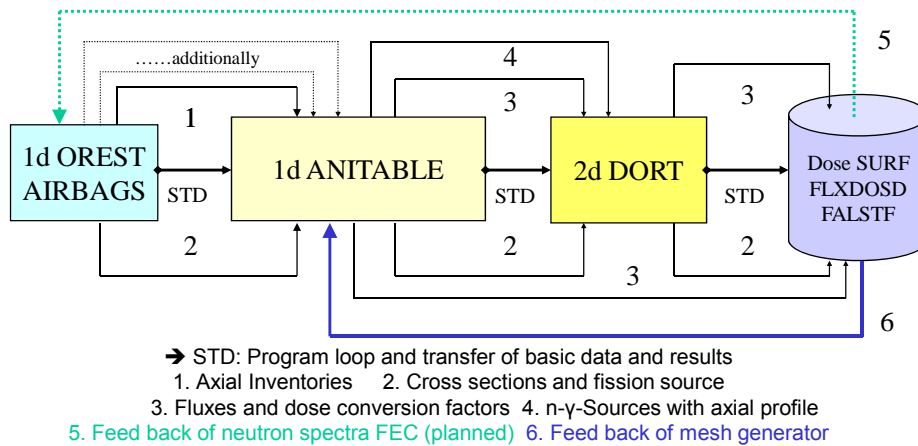


Figure 2: Coupling diagram of DORTABLE supported by ANITABLE

- As a first step AIRBAGS/OREST calculates the axial burn-up profile for a variety of axial positions considering varying coolant properties. The inventory yield is feed into path 1 of ANITABLE, which further processes them to axial-dependent cross sections for DORT.
- In path 2 OREST transfers updated resonance-corrected microscopic cross-sections for each isotope to ANITABLE, which passes the resonance-corrected macroscopic cross sections to the modules DORT and FALSTF.
- The 1d fluxes (together with the LDR conversion coefficients), calculated by ANITABLE, are used as start “first guess” fluxes in the DORT iteration. After the 2d calculation of DORT the resulting fluxes are further processed by the analysing tools FLXDOSD and FALSTF.
- In path 4 ANITABLE-NGSRC calculates the axial-dependent n-γ sources, which are afterwards fed into DORT. At present this transfer of the n-γ-sources is realised by employing an axial form factor to account for the axial dependence. The direct transfer per energy group and cell is currently under development.
- Path 5 shows a (planned) automatic back coupling of the spectrum according to the FEC (*flux equivalent cell*) method as it is presently realised in the startup-loop of KENOREST for guaranteeing spectral equilibrium in the last burnup step of OREST and the DORT model of a TSC. The purpose is to adjust the last resonance treatment including the cross section determination in OREST to the real spectrum in the storage container (path 2) in order to achieve consistent cross section data for each isotope.
- A further analysing tool GRSMESH, which is not shown in Figure 2, receives the data from path 3 and computes a new mesh, which the user is supposed to use in a subsequent iteration step (path 6). The mesh is determined by using the flux gradient method, which means the changes of the (so far calculated) flux from one cell to another shall not exceed or fall below a certain value. This start-up repeated until the change in the flux meets the above criteria. This is an additional convergence criterium on top of the usual convergence which is present in ANISN and DORT. The flux gradient method considers the problem dependent flux in the mesh generation

and therefore constitutes an improvement comparing to standard procedures considering only the cross-sections. Before the startup-convergence in the mesh sizing is achieved we use smaller transport libraries (e.g 13 neutron and 9 γ groups) to save CPU time.

7. In the path <STD> the common structure material data and basic results are handed over from step to step.

All steps starting from the burnup calculation up to the final dose results are fully automatic, such that the user only has to work up one single input card. The input cards for DORT and all other codes are determined internally during the calculation.

3.2 Calculation using MCNP and auxiliary programs

Figure 3 shows the simplified setup of 3d MCNP supported by AIRBAGS, OREST, ANITABLE and SRCMCNP. At present the construction of the input file is not yet done automatical by using the input from the previous section. The transfer of the material data, source data and conversion coefficients in the same energy group are connected by the following scheme: In Figure 3 it can be seen that - similar to the process in Figure 2 - one starts by calculating the axial-dependent inventory by using AIRBAGS, which determines the axial burn-up profile considering axially changing coolant properties.

1. Path 1: The axially varying inventories are fed into the MCNP input file. In addition, the inventories are further processed by NGSRC, which yields the axial-dependent spectral n- γ source terms.
2. The transfer of the n- γ source in path 2 is realised by applying an axial form factor as it has been done already in DORTABLE. The one-to-one transfer of the sources in this case is also part of present developments.
3. In path 3 the module SRCMCNP converts the chosen dose conversion factors from ANITABLE to MCNP format and hands it over to MCNP.

The dose results at different space points are determined directly by MCNP.

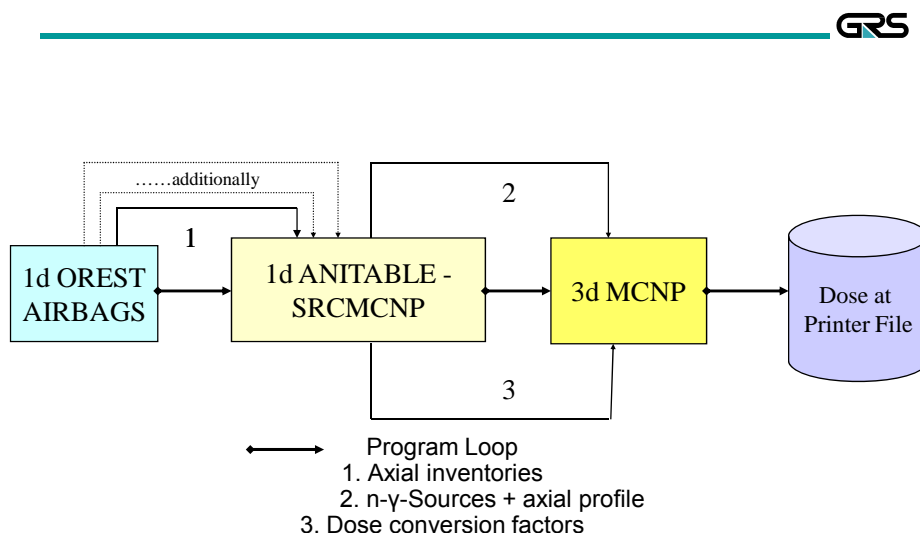


Figure 3: Coupling diagram of MCNP with ANITABLE-SRCMCNP acting as support.

3.3 Comparison of the deterministic and statistical methods

Since many years the GRS applies statistical as well as deterministic methods in criticality, inventory and shielding calculations. The burn-up system KENOREST [2], for example, employs both methods at the same time, the statistical 3d KENO and the deterministic 1d OREST, which are directly coupled.

Both methods have advantages and disadvantages. In Table 1 the our experiences with the two methods (here MCNP and DORT/TORT) for the example of dose calculations in the vicinity of TSCs are listed. The ranking ranges from (++) , meaning high performance, to (--) meaning low performance. As one can see the advantages and disadvantages in this case are fairly balanced. In general the GRS uses both methods redundant or picks out the favourable method for specific problems.

As we can see in Table 1 both methods have difficulties for the items 7, 8 and 9. The problems <Labyrinthe> and <Skyshine> in 8 and 9 concern scenarios, in which starting at a TSC the radiation in the surrounding area, e.g. an interim storage facility, shall be calculated taking into account only completely and multiple scattered radiation. <Skyshine> means the backscattering of radiation - after passing through the concrete of the roof - in wide-ranging air layers. In DORT a precalculation with GRTUNCL [3] is needed to get a "first collision source". <Slots> in point 7 concerns the problem of radiation transport through small slots, which is difficult to describe as well. In particular for the items 7 and 8 no physically satisfying solution exists so far, which can handle the problems in only one step.

Table 1 Comparison of deterministic and statistical systems applied to dose calculations

Item	Monte-Carlo method MCNP and GRS experiences in dose calculations	Deterministic method DORT/TORT and GRS experiences in dose calculations
1. Flux-convergence properties	(-) Flux and dose values only at certain positions. Limited capabilities for further analysis. Statistics vary in different areas.	(+ +) Equally converged solution for flux in all cells. Variety of further analysis possible.
2. CPU time	(-) relatively time expensive due to statistics (in case of TC)	(+) relatively short (in case of TC)
3. Source specifications	(-) proper scanning of spread source areas leads to statistical problems	(+) spread source areas handled well
4. Determination of cell allocations	(+) no problems	(-) done by hand. Influences the quality and convergence of the system. Auxiliary calculations necessary
5. Energy spectrum in source area	(-) proper scanning of energetically wide-ranged sources leads to statistical problems	(+/-) arbitrary energy ranges of source terms can be handled well. Eventually problems in condensation to „broad group“ libraries
6. Radiation transport in vacuum	(+) no problems for vacuum as well as air	(-) problems due to ray-effect for discrete meshes and solid angles already in air. Auxiliary calculations necessary
7. Radiation transport through slots	(-) problems due to statistics. Auxiliary calculations necessary	(-) problems due to discrete meshes and discrete solid angles. Auxiliary calculations necessary.
8. Radiation transport through labyrinths	(-) problems due to statistics. Auxiliary calculations necessary for cascade calculations.	(-) problems due to ray-effect for discrete meshes and solid. Auxiliary calculations necessary for cascade calculations
9. Radiation transport <skyshine>	(-) problems due to statistics	(-) problems due to ray-effekt for discrete meshes and solid angles. Auxiliary calculations necessary.
10. Radiation transport <deep penetration>	(-) problems due to statistics / <Importance>-problem must be solved	(+ +) no problems for proper determination of meshes
11. Describing 3d geometries	(++) 3d geometries easy to handle. High flexibility and mixture of different geometries (e.g. R-Z, X-Y-Z) possible	(-) 3d geometries difficult to handle. Auxiliary calculations necessary for 3d effects for DORT
12. cross-section libraries	(+) neutron-pointdata does not need resonance treatment for induced fission and remaining reactivity	(-) neutron “broad group” data need external resonance treatment for induced fission and remaining reactivity. Remarkable influence of varying group structures

4 CALCULATION OF DOSE RATE FOR A TRANSPORT AND STORAGE CASK CONTAINING SPENT FUEL ELEMENTS

In the following we discuss the problems and their solutions for the dose rate calculation of a transport and storage container typ CASTOR V/19 by using the deterministic code DORT. Afterwards the results will be compared to an additional calculation employing the Monte Carlo code MCNP.

4.1 Geometrical setup

Figure 4 shows the geometrical setup of the storage container used in the MCNP-simulation and more simplified used in the DORT-calculation. One can clearly see the axially varying material-structure of the basket. The fuel elements are modelled separately, but assuming homogenized material mixtures. This means we do not model the fuel element rod by rod, which is not necessary for this problem. In both models the cooling fins of the outer cask surface are modelled by smear density taking into account mass and volume conservation. The DORT geometry model coinciding basically with the MCNP calculation model, but deviates in the following three points:

- Also the fuel elements including the basket structure are homogenized taking into account mass and volume conservation.
- The moderator rods in the cast iron wall are modelled by two effective cylinder rings taking into account volume but not mass conservation. The density is determined by an auxiliary calculation using either DORT with a 90 degree rotated geometry or directly with MCNP. A factor of 0.8 has been determined, which coincides with the previously determined value by CASYST in earlier studies (1985).
- The local wall attenuation in the outer cast iron wall at the trunnion positions can only be considered by using a cylinder ring surrounding the whole cask. In the following calculations we considered this effect for the lower trunnion and neglected the effect of the upper one.

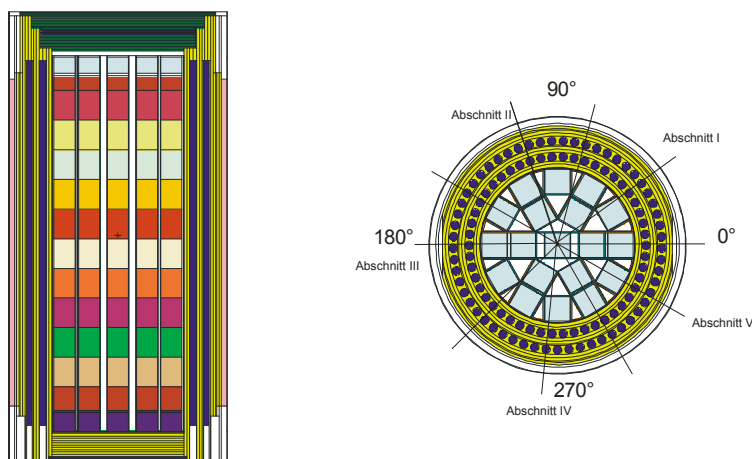


Figure 4: Geometry setup of the CASTOR V/19 in MCNP

We assumed the TSC to be loaded with 19 fuel elements of the PWR-convoy type with an initial enrichment of 3.6 % ^{235}U , an average burn-up of 40 GWd/tHM and a storage/decay time of 10 years. An axial burnup profile shown in Figure 5 was used, which represents the average of numerous measured profiles of PWR fuel elements. The variety of data points have been condensed to a burn-up profile with 10 axial zones as it is shown in Figure 6.

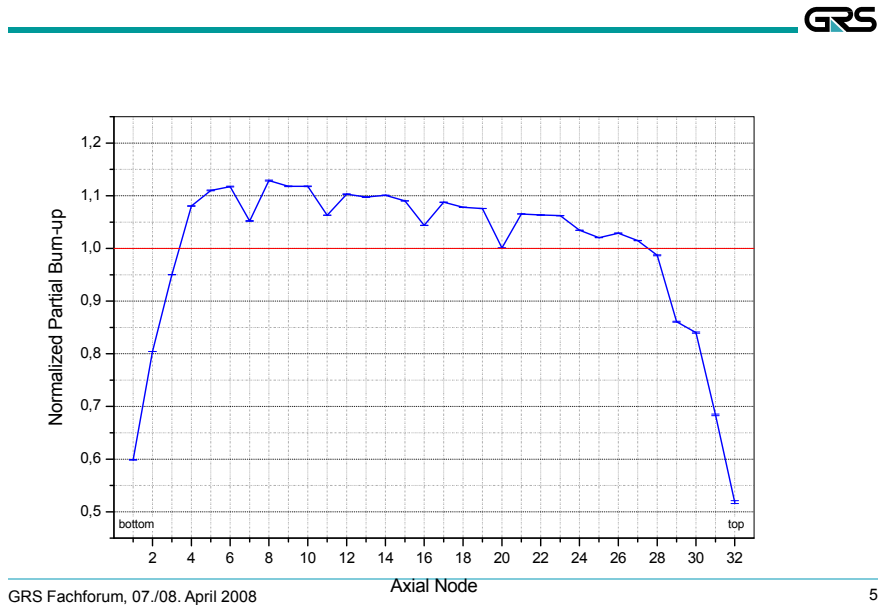


Figure 5 Axial burnup profile of a generic PWR fuel element.

Using an AIRBAGS loop over 10 axial zones we start an OREST burn-up calculation assuming varying power and coolant properties and store the calculated inventories. The following points should be mentioned:

- The n-γ-source material of the spent fuel with about 1000 important isotopes and the inventory (providing scattering, absorption and multiplication to the emitted radiation) in the axial zones for the radiation transport in principal should be identical. But due to computational constraints, an approximation has to be applied, for ensuring maximum consistency, with respect to radiation source and radiation transport properties of the inventory. The limited capability of the transport libraries, does not admit a one-to-one transfer. We solve this consistency problem as follows: all 1000 isotopes from ORIGEN are considered in the source term determination by NGSRC at the desired decay time. This means that also material dependent calculations of α-n neutrons and Bremsstrahlung are consistent. In the axial material lists of DORT the 50 OREST nuclear number densities are basically used the same way by MCNP and DORT, except that DORT updates the densities according to the resonance-corrected cross sections from OREST. This step corresponds exactly to the procedure taking care of the reactivity balance in OREST and also KENOEST. Thus, the consistent calculation of the induced fission and the influence on the absorption in the burned fuel is given. Only a small uncertainty remains concerning the time difference between the end of the burn-up and the chosen decay time in the source term determination. In the present case the axial material lists also have to be mixed with

structure material of the fuel elements zircaloy and steel from the basket. Head and foot piece are treated separately.

- The subcritical neutron multiplication in the partially burned fuel element inventory, which leads to an increase of neutron emission from spontaneous fission and α -n-processes by about 30 %, as well as the subcritical multiplication factor is determined directly during the calculation in DORT and of course also in MCNP. While in [5] the transport calculation DOT3.5 had to be cancelled after a single outer iteration, DORT determines by about 10 or more iteration the neutron-flux-dependent induced fission source up to the desired accuracy of 0.01%.
- The additional production of secondary gammas from neutron capture and their contribution to the dose rate is in principle possible in one n- γ -run, but now this contribution to the dose rate can not be extracted separately in numbers. Thus, in DORTABLE as well as in MCNP we perform two separate calculations. The first one includes a neutron source term only and thus all gammas are secondary gammas. The second calculation then includes the gamma source term only. The gamma dose from both calculations is then added up to get the entire dose rate.

The DORT calculation of the TSC includes 420 spatial zones and 29 different structure materials. The zones are split altogether in about 18000 cells, for which convergence with a relative error of 0.01 % could be achieved.

4.2 Results of MCNP and DORT

Both models MCNP and DORT start with identical materials, dose conversion factors and n- γ source terms, as well as with basically the same geometrical model, as has been discussed above.

In Figure 6 the neutron dose rates calculated by MCNP at the surface of the cask is shown. The TSC in this figure is in horizontal orientation with the bottom to the left and the top to the right. The dose has been determined at different angles and been averaged yielding the mean value (red circles). The curve (ABP) shows the burn-up profile of the fuel. One can see that in the mid of the container the dose rate basically follows the burnup profile and a maximum of 40 μ Sv/h is determined. Local dose rate maxima occur at the top and the bottom of the cask with values up to 50 μ Sv/h. This maxima appear at the material attenuation at the positions of the trunnions.

In Figure 7 the DORT results are shown. In the mid of the cask the neutron dose rate also follows the burn-up profile and the maximum reaches again a value of 40 μ Sv/h. The local maxima in the dose rate at the bottom and top are also clearly visible. However, as described above we take into account the trunnion only at the bottom of the cask and not at the top. Therefore, the maximum reaches the value of 50 μ Sv/h only at the bottom and is much less significant at the top. This difference shows nicely the influence of the material attenuation in these positions. The shape of the calculated γ dose basically follows the shape of the neutron dose, but the maximum only reaches a value of about 25 μ Sv/h. The local γ -peaks at the bottom and the top are, however, visibly moved from the n-peaks, which can be attributed to the different scattering, absorption and escape properties for neutrons and γ s in the head piece and the bottom.

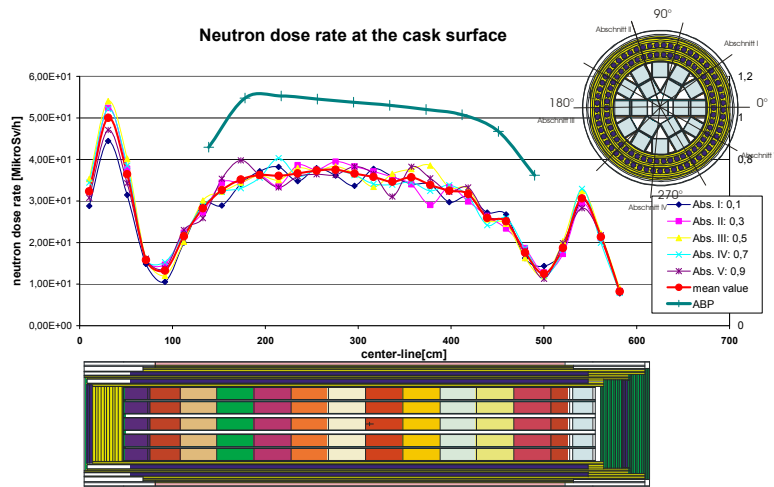


Figure 6: Neutron dose results with MCNP for the CASTOR V/19

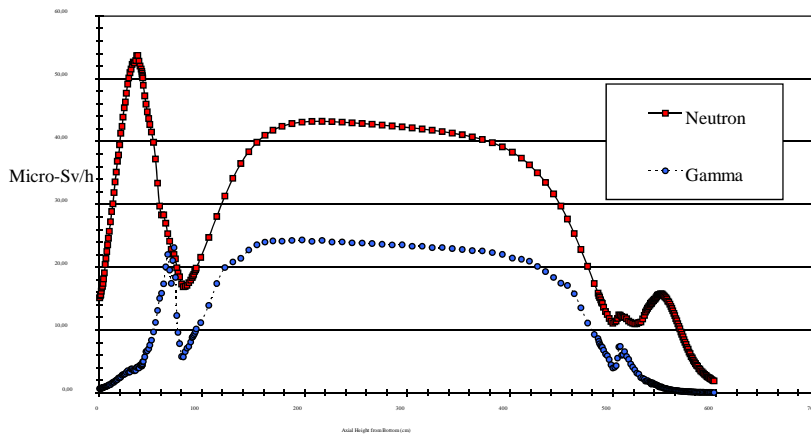


Figure 7: DORTABLE neutron and gamma dose results for the CASTOR V/19

5 SUMMARY AND OUTLOOK

We discussed neutron and γ dose rate rate calculations for transport and TSCs loaded with spent fuel elements with axial-dependent burn-up profiles using the codes MCNP and DORT. We introduced the coupled GRS system DORTABLE, which is based on DORT and is suitable for dose rate calculations at TSCs. The deterministic calculation based on DORT

and the statistical calculation based on MCNP yield similar results for the local dose rate and the remaining reactivity, despite the rather large shielding through the cask. The many necessary computational steps have been implemented physically satisfying and employed in both methods: the axial-dependent inventories of the burn-up calculation with about 1000 isotopes are transformed to axial-dependent n- γ source terms and simultaneously to axial dependent cross section material lists employing conservation of reactivity. Future developments will regard the additional inclusion of the deterministic 3d SN-Code TORT in R-Z- Φ -geometry. Using TORT instead of DORT, the minor geometrical simplifications in the deterministic model are no longer necessary. Currently the inclusion of activated structure material together with burned fuel is in work. In the system CASYST this was already realised in a simplified form for the ^{60}Co radiation of the activated bottom and top zones. Now we intend to include the activation code GRS-ORIGENX [2] in addition to the burn-up module OREST in order to perform the activation of the structure materials of the fuel elements simultaneously. Due to the long computation time a consideration of axial-dependent burnup profiles in shielding calculations has not yet been common approach. In the near future, however, this can become state-of-the-art. The IAEA Draft Safety Guide, Storage of Spent Fuel DS371 [6], p.24 recommends that the source term determination for the shielding calculation also includes axial burn-up effects as well as activation of structure materials besides other boundary conditions as enrichment, burn-up and decay time. These demands can now be met.

ACKNOWLEDGEMENT

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