TOWARDS A DIRECT COMPARISON OF PRACTICAL CSE WITH BUC APPROACHES: BENCHMARK FOR A PSEUDO-APPLICATION CASE WITH USER-DEFINED NCS CRITERIA

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ABSTRACT

This paper aims to introduce the recently initiated OECD/NEA/WPNCS subgroup (SG13) calculation benchmark exercise. The SG13 objective is to provide a comparison of existing Nuclear Criticality Safety (NCS) approaches in application to final disposal canisters loaded with used nuclear fuel (UNF). An output of such a study would inform/support practical applications for UNF safe transportation and final disposal, by enabling a better understanding of important aspects of the loading curve determination methodology, such as the Upper Safety Limit (USL) definition, and providing further insight into the expected methodological uncertainties. Furthermore, this study would provide very valuable information for nuclear waste management organizations to facilitate and optimize the designing process of the UNF disposal canisters and geological repositories. The scope of the envisioned required computations will be limited to criticality calculations, optionally complemented with the nuclear data (ND) uncertainty propagation, in accordance with the participants' implementation. The requested result is the loading curve (LC) in the form of the required burnup (BU) vs. the initial U-235 enrichment. The participants' task is to determine the BU values at which the model k_{eff} meets the NCS criteria for each initial enrichment by performing their own criticality calculations (i.e. following their own methodologies). Based on this determination, the participants will obtain the loading curves, which represent the final result of the task. The NCS criteria are to be defined by the participants individually, whereby a common administrative margin for subcriticality equal to 5% (Δk_{eff}) will be used.

KEYWORDS

OECD/NEA/WPNCS, Nuclear Criticality Safety, Burnup Credit, Calculation benchmark

1. INTRODUCTION

Criticality Safety Evaluation (CSE) methodologies, including their validation bases, may have different levels of conservatism and comprehensiveness, depending on the application type, as in general described in [1]. Some methodologies can be based on generic NCS criteria, while for others case-specific criteria can be defined, for instance, involving adjusted ND or an adjusted calculation bias and the related uncertainty for an application system k_{eff}, based on either Bayesian [2] or frequentist statistics [3] (or even their combination). An optimal level of complexity of CSE methodologies can be an open question, in particular in the context of potential industrial applications such as NCS for UNF final disposal canisters. For example, the use of a single generic USL would simplify the derivation of the LC for UNF noticeably. On the other hand, case-specific (e.g. burnup (BU)-dependent USL) approaches could be more cost-efficient by reducing the number of required disposal canisters (or through cost savings on the canister design). The effects of such potential methodological differences on the LC, in terms of required minimal BU vs. initial fuel assemblies' enrichment, are not obvious. The objective of the proposed benchmark is to examine such effects by a direct comparison of participants' results for a well-defined and simplified pseudo-application case.

The verification and validation of k_{eff} calculations together with the comparison of criticality calculations using different codes and ND libraries as well as burnup credit (BUC) related studies have been in the focus of WPNCS activities since its creation. The EG UACSA Phases I and V exercises were focused on the k_{eff} bias and its uncertainty for test applications. The SG11 [4] goal was to perform a clean comparison of the bias-corrected k_{eff} values and their uncertainties for the specified test cases, between different methodologies and validation approaches (Bayes, Maximum Likelihood, Trending Analysis, etc.). The studies listed above required the use of appropriate tools and methodologies which, however, did not necessarily represent methodologies applied or being developed for realistic practical applications.

The comparison of existing NCS criteria was never a specific subject for analysis at the WPNCS. Such a study would be very useful, in particular to assess the level of maturity and reliability of the CSE+BUC methodologies for applications related to such important and complex tasks as NCS for final disposal canisters loaded with UNF. Making this study as an international exercise under the auspices of OECD/NEA/WPNCS will provide an opportunity to collect solutions from the NEA member countries and different organizations, including industrial, research and Technical Safety Organisations (TSO).

2. CALCULATION MODELS

2.1. Benchmark model for analysis by participants

As a pseudo-application case, it is proposed to use a model roughly approximating a disposal canister filled with four similar PWR 17x17 UO_2 fuel assemblies, but without the canister walls at this stage. For the given exercise, it is proposed to use only water reflector in order to be as representative as possible for general CSE application cases with PWR fuel (i.e., including the spent nuclear fuel pools). Because the goal of this exercise is to compare different methodologies and validation approaches, the calculation model does not need to be fully realistic. It will be sufficient to use a simplified model, in general representative enough for the task of the LC derivation. The proposed fuel assembly specifications are similar to those used in the WPNCS/ BUC-VII benchmark [5]. The horizontal cross-section of the 3D model is illustrated in Fig. 1. Uniform fuel compositions are to be used for every pin, also axially. The model temperature is 20°C.

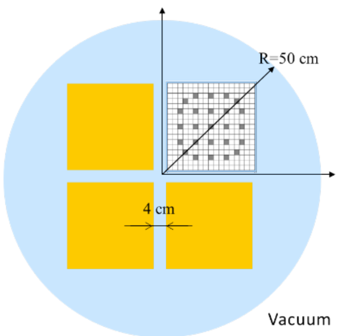

Figure 1. SG13 calculation model of a canister filled with four identical UNF assemblies (schematic)

The water gap between the fuel assemblies is arbitrary defined to be 4 cm (the fuel assemblies pitch is 25.505 cm). The outer model radius is 50 cm.

The UNF isotopic densities [at/cm^3] for the same set of nuclides as used in the WPNCS/BUC-VII benchmark will be provided in the detailed specifications as a function of the initial enrichment and discharged burnup. It is proposed to use the following sets of the initial U-235 wt% enrichment and burnups: 2.0, 3.0, 4.0, 5.0 wt% (arbitrarily chosen round numbers) and 0, 0.1, 10, 20, 30, 40, 50, 60, 70 MWd/kg respectively.

As concerns the USL definition, it is only proposed to use the same administrative margin for subcriticality, being equal to 5% (Δk_{eff}) for all participants. Other USL components are to be defined by the participants on their choice, according to their practical CSE(+BUC) methodologies.

2.1. Pin cell model for preparation of the UNF compositions by the coordinators

The fuel depletion calculations are not to be performed by the participants, as calculations have already been done by the benchmark coordinating team. For that, calculations with the CASMO5 code and the ENDF/B-VII.1 library were realised at PSI. Thus, UNF compositions will be provided in the benchmark specifications. For the depletion calculations, the pin cell model from the WPNCS/BUC-2D benchmark [6] was used. The parameters for depletion calculations were taken also from [6]: Fuel temperature = 873 K, Moderator temperature = 573 K, Power density = 38 W/gU, Boron concentration = 456 ppm.

The simulations were done with the CASMO5 "PIC" card. Note that at this stage a simple pin cell model was used and not an equivalent model to represent the entire fuel assembly moderating conditions. Actually, a full fuel assembly depletion or also a pin cell depletion with an equivalent pitch size could be used instead of the regular fuel pin cell model, illustrated on the left side of Fig. 2 [6]. Fig. 2 also shows k_{inf} for the three versions of the depletion calculations: for the simple pin cell, for the pin cell with the equivalent pitch size and for the entire fuel assembly (FA) simulated explicitly. One can see that the equivalent pin cell k_{inf} results are very close to the full FA results, while the regular pin cell results are noticeably different.

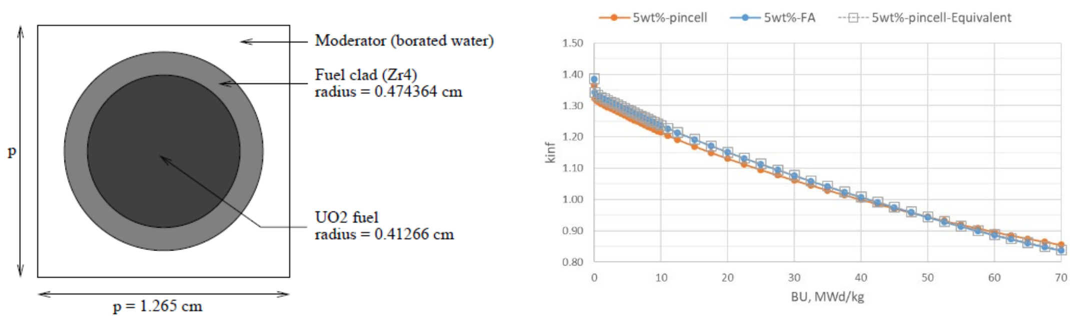

Figure 2. On the depletion model choice; left: the simple pin cell model [6]**; right: k_{inf} results**

In general, a more realistic irradiation history can be simulated as well, including cooling times between reactor cycles, etc… However, all such (in principle important) details are not the focus of the given exercise objectives. Furthermore, as long as the same FA-average compositions are to be used for all pins in the criticality calculations, the use of the simple pin cell depletion instead of a FA depletion model looks reasonable.

Uncertainties related to the depletion calculations are also not considered for the SG13 exercises (though this can be one of the major parts of the computations of a realistic loading curve). Note that such uncertainties are going to be analyzed within the follow up of the WPNCS/SG10 activities[1]. It should be stressed that the SG13 exercise is not about an accurate fuel assembly depletion, but about the LC derivation with the provided (approximately realistic) fuel compositions.

[1] Very relevant benchmarks were also defined for quantifying the fuel reactivity depletion uncertainty in [7].

3. PREPARATORY WORK FOR THE BENCHMARK DEFINITION

3.1. CASMO5 pin cell depletion

The pin cell depletion calculation results obtained with CASMO5 are illustrated on Fig. 3 as a function of k_{inf} vs. burnup and the initial fuel enrichment.

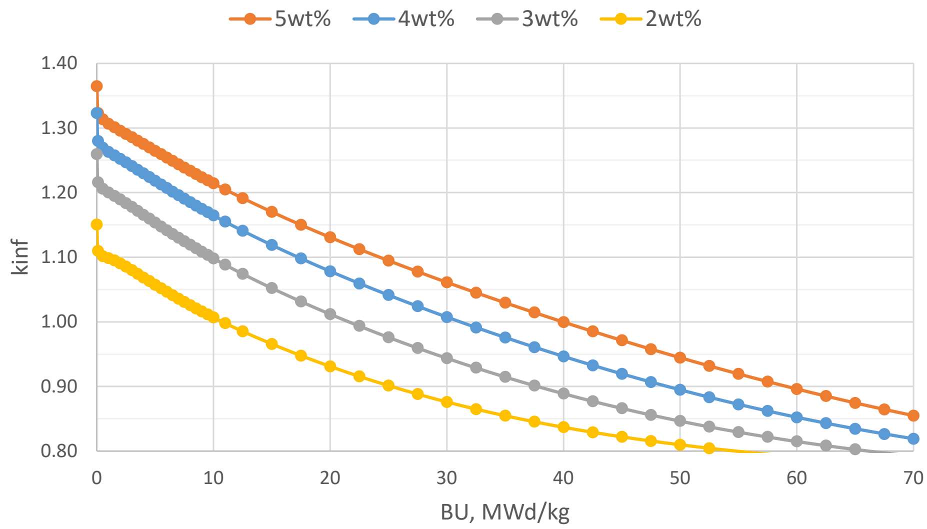

Figure 3. CASMO5 depletion illustration: k_{inf} results

As an illustration, the isotopic compositions as functions of burnup for the case of 5wt% initial enrichment are shown on Fig. 4 (each isotope is indicated by a number equal to Z*1000+A, with Z and A denoting the nuclear charge and mass, respectively). The detailed benchmark specifications will provide such data in the text format for all considered enrichments.

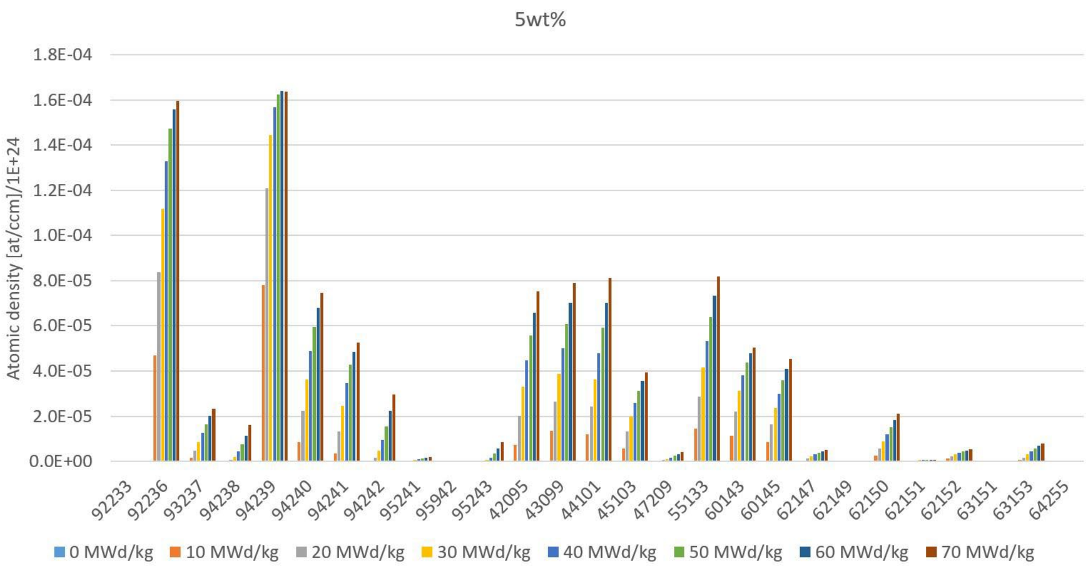

Figure 4. CASMO5 depletion illustration: Isotopic compositions as functions of BU

3.2. Monte Carlo criticality calculations

The isotopic compositions from the CASMO5 calculations were transferred to a 3D MCNP6® model (see https://mcnp.lanl.gov for details on the MCNP® software trademark) illustrated in Fig. 1. The model height was selected as 370 cm with vacuum boundary conditions at the top and bottom surfaces. The MCNP6 k_{eff} results are shown in Fig. 4.

Taking into account the proposed administrative margin for subcriticality of 5% (Δk_{eff}) and based on the previous experience for similar tasks [8-10], it is assumed that the expected relevant range of the k_{eff} safety limits will be somewhere in the range between 0.90 and 0.95, as indicated in Fig. 4.

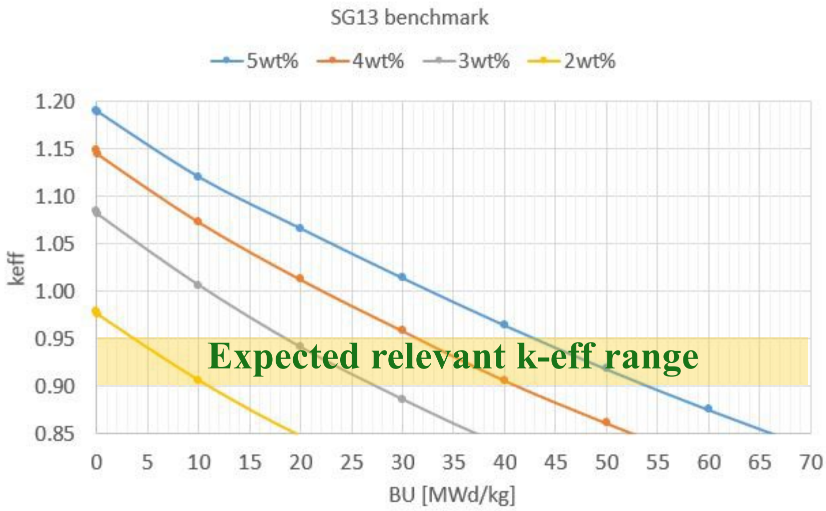

Figure 4. k_{eff} results as functions of burnup, obtained with the provided UNF compositions

Based on this data, it is possible to derive very approximate estimations of the BU ranges which should be relevant for the considered initial enrichments, in order to comply with the assumed k_{eff} safety limits between 0.9 and 0.95 (the minimum and maximum relevant burnups can be determined at the intersections of the k_{eff} curves with the k_{eff}=0.95 and k_{eff} =0.90 lines). As a result, an approximate range of the anticipated loading curves can be predicted, as given in Fig. 5.

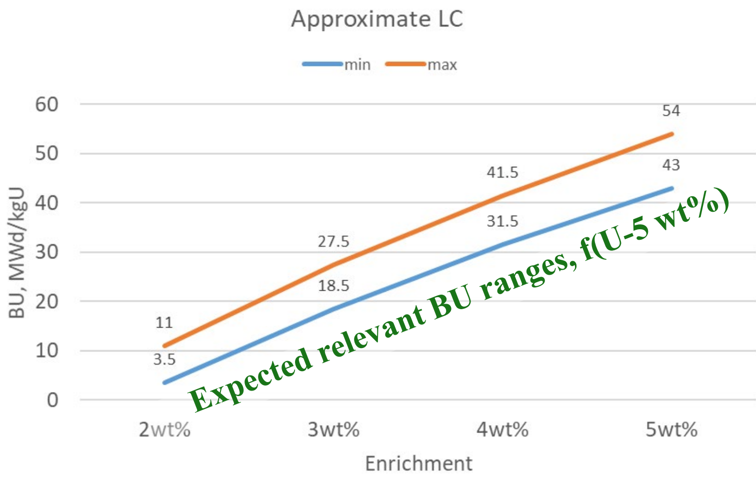

Figure 5. Anticipated BU diapason for the LC to be generated

3.1. On the choice of the validation benchmarks

The following illustration is related to the choice of the critical benchmark experiments from the ICSBEP database, which should be appropriate for the validation of the participants' calculation methodologies for the pseudo-application case. It is postulated that all participants will use, at least at the first stage of this study, the same set of validation benchmarks. It is also desirable to have only a limited number of benchmarks in the validation suite, to minimize the participants' efforts.

Fig. 6 shows the weight percent of U-235 and fissile Plutonium isotopes as function of burnup for the considered initial fuel enrichments. The vertical yellow rectangles indicate the burnup ranges identified in Fig. 5 as relevant for the given enrichments. The numbers in the rectangles show the fraction of U-235 isotopes weight vs. the fissile Plutonium isotopes weight. Obviously, a more accurate assessment could be done with the fractions of fission reaction rates instead of the weight fractions, however for the sake of the given rough assessment the latter should be sufficient.

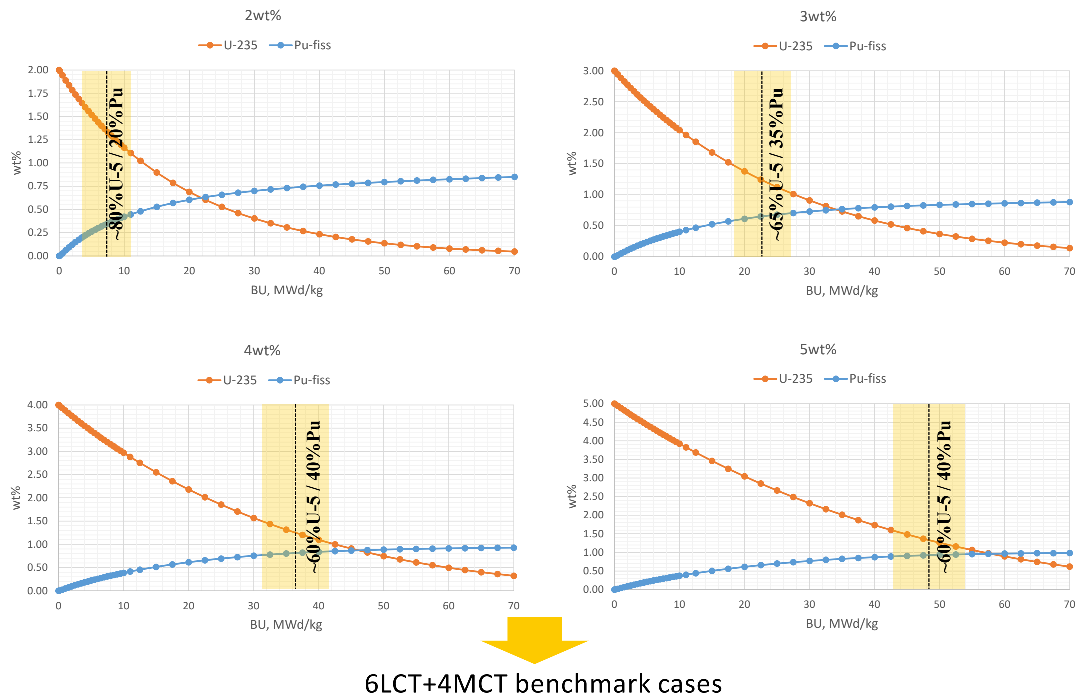

Figure 6. Weight percent of U-235 and fissile Plutonium as function of burnup

It can be seen that the relevant fractions of isotopes change with the increase of enrichment. However, for the sake of simplicity, it is proposed to assume that on average the relevant fraction of U-235 vs. fissile Plutonium isotopes for the whole range of enrichments and burnups is about 60% to 40%. On such a simplified basis, it can be concluded that, for instance, having six Low-enriched uranium Compound Thermal systems (LCT) and four Mixed plutonium–uranium Compound Thermal (MCT) ICSBEP benchmark cases could be a reasonable choice.

In order to select ten cases from the ICSBEP Handbook, it is proposed to restrict the (postulated) selection criteria as follows: 1) Pitch < 2 cm; enrichment < 5%; Benchmark k_{eff} uncertainty < 0.5%; square lattices; no neutron absorbers; water reflector. Preferences should be given to most simple and easy for modelling benchmarks. The actual list of the benchmarks to be used is under finalization. It can be noted that, in general, a more sophisticated selection of the ICSBEP benchmarks could be done [1]. However, advanced approaches would be more resource consuming, although not principally necessary for the comparison of different methodologies.

4. OUTLOOK ON THE EXPECTED RESULTS

The following results are provided just as an illustration of how a solution of the proposed benchmark could look like, based on the previous experience gained at PSI and Nagra [10]. In the given illustration it is assumed that the USL, taking into account the nuclear data uncertainties, is about ~0.9335 (to be verified). In general, the USL can be BU-dependent. However, for the sake of simplicity, in the given illustration it is assumed that the USL is constant over burnup. Thus, combining the USL limit with the data from Fig. 4, one can produce Fig. 7, where the intersections of the USL and k_{eff} lines give the burnup values required for the loading curve.

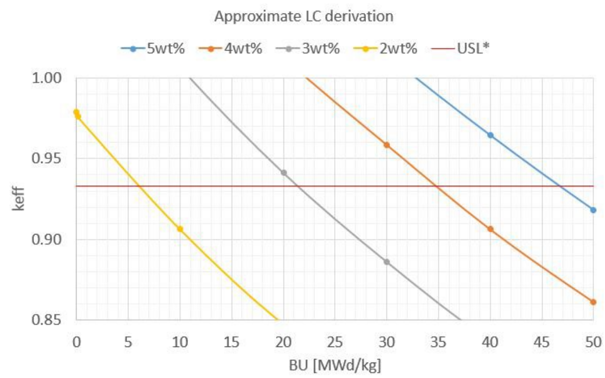

Figure 7. On the determination of the burnup to meet the USL for the considered enrichments

Using the above results, one can produce the loading curve like the example shown in Fig. 8.

Figure 8. An illustrative loading curve

5. CONCLUSIONS

The given paper presents the concept of the OECD/NEA/WPNCS SG13 benchmark. The main benchmark objective is to assess the influence of differences in the existing CSE+BUC methodologies and their validation approaches on the evaluation of the UNF LC. The LC is to be produced by the participants as a function of required minimum burnup vs. initial fuel enrichment. In the present phase, only UO_2 fuel is considered with some representative but fictitious enrichment values. Participants are free to use their own criticality safety criteria to solve the task. It is also up to the participants' choice to use any ND or calculation bias and its uncertainties adjustments based on the validation studies. To minimise the sources of disagreements, it is proposed that all participants should use (if possible) the same ND library, i.e. ENDF/B-VII.1 and its covariances (in the nomenclature of the ENDF-6 formatted files: MF-31, -32, -33, -35).

On the basis of the given exercise, more advanced and comprehensive numerical tests may be developed in the future to address other potential sources of discrepancies and uncertainties. This may include:

- Independent choice of validation benchmarks, including proprietary databases, especially for BUC applications,
- Depletion and decay calculations and associated k_{eff} uncertainties,
- 3D modelling effects, including the axial burnup distribution or the “end effect”,
- Models with metal reflectors,
- Models with solid absorbers,
- Refining the depletion steps and enrichment values,
- Adding other fuel designs / MOX fuel,
- Usage of other ND libraries, etc.

However, it is proposed for the given first exercise to minimise participants’ efforts and the number of parameters that can lead to the results variability, to make the exercise as clean as possible for evaluation of the methodological differences only. In this sense, SG13 specifications follow the concept of WPNCS SG11 benchmark, which in fact served as the valuable basis for proposing the current SG13 activity.

ACKNOWLEDGMENTS

This benchmark proposal is prepared under the auspice of the OECD/NEA/WPNCS. The preparatory work was realized partly in relation to the PSI-Nagra research project BUCSS-R. The authors are grateful to their colleagues from WPNCS. Special thanks go to OECD/NEA staff, Dr. J.-F. Martin and Dr. O. Buss for the assistance with the WPNCS/SG13 organisational matters.

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