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The forward-problem approach in Safeguards verification: directly comparing simulated and measured observables

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Abstract:

Physical verification by NDA in nuclear safeguards implies typically the adoption of an inverse-problem approach. This is, indeed, the definition of a problem, in which we use physical observables to deduct other physical quantities, which in our case are contained in the operator's declaration. A typical example is the Plutonium mass, measured using Pu isotopics and neutron coincidence doubles counts, linked to the Pu 240 effective mass by a calibration.

An alternative approach has been recently proposed and is now close to the in-field deployment by the Euratom Safeguards Directorate of European Commission's DG ENER. In fact, the detailed knowledge of the physical processes that are taking place in the sample and within the detector allows computing the amount of the measured observable, by modelling the physical system as it results from the operator's declaration, in a forward-problem approach.

The present paper describes the first two examples of the forward-problem approach's application to actual real-life safeguards verification. The first example deals with a Monte-Carlo-based modelling tool that has been developed to enable the inspectors to perform an improved verification of fresh fuel assemblies by neutron coincidence collar (NCC), taking into account the growing complexity of the fuel's design. The second example shows how the verification of spent fuel is improved regarding the false alarm rate and the partial defect detection capability, by the integration of the automated review package iRAP and the modelling by the Oak Ridge transmutation code (ORIGEN).

The potential applications of the new approach are not limited to the two described in this article, which, however, represent relevant proofs of concept of the potential that a change of perspective in verification by NDA may generate.

Keywords: NDA, Forward problem, Spent Fuel, Fresh Fuel, ORIGEN, Neutron Coincidence Collar

1. Introduction

In 2017, Euratom Safeguards celebrates its 60th anniversary – the legal being the Euratom Treaty, signed in Rome on March 25, 1957. During this long history, a number of field practices, approaches and methods have been developed, consolidating Euratom inspectorate position as one of the reference institutions in the international Safeguards community.

An essential component of the conformity controls, which allow the inspectors to draw independent conclusions, is the Credibility Control, linking the declarations by the nuclear operators to the physical reality, as observed by the inspectors. The physical verifications, that the inspectors carry out in order to perform a credibility control, often consist in the measurement of physical quantities, related to the declared nuclear material properties, by Non-Destructive Assay (NDA).

The advantage of NDA measurements is the possibility to perform the necessary verification, without excessive interference with the operator's industrial process and without alteration of the nuclear material under assay, its physical form or its container. However, one drawback of NDA methods is the not always obvious interpretation of discrepancies, because of an imperfect estimate of measurement uncertainty, especially caused by the difficult quantification of uncertainty in the instrument calibration. Moreover, for the measurement methods used in NDA verification, an appropriate metrological traceability is made impossible by the non-existence of reference materials of the same type, quantity range and physical form of the samples to be measured.

The growing availability of technologies allowing high performance calculations, since the late 1990s, has allowed tackling these limitations of the NDA methods, by using physical-model-based simulation to define the instruments' calibration, starting from a detailed knowledge of the physical system defined by the instrument, the sample and by their mutual interactions. In this perspective, although modeling was used to overcome some of its limitations, simulation did not change the traditional calibration approach, relating an observable physical quantity (for instance, a neutron or gamma count rate) to the values of the quantity of interest (for instance, the quantity of nuclear material).

More recently, a further step has been taken, by using real-time simulation to predict directly the observable physical quantities (corresponding to declarations from the operator), which are then compared with the measurement results [1][2]. This different forward-problem approach, has allowed overcoming some limitations of the traditional calibration approach in particularly complex cases. The

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following paragraphs will describe its consequent practical and conceptual implications.

2. Inverse and Direct problems: definition and application to Nuclear Safeguards Measurements

During verification, as in every measurement operation, we establish a relation between two different abstract spaces. One, which we define as Model Space ($\mathcal{M}$), contains all the knowledge we have from the physical system, defined by a set of parameters including the information contained in the operator declaration. The other abstract space, which we define as Data Space ($\mathcal{D}$), consists of the data from the observable quantities.

The general measurement problem is defined by the following relationship:

$$d = \boldsymbol{G}(m)$$

where $d \in \mathcal{D}$, $m \in \mathcal{M}$ and $\boldsymbol{G}$ is a generic operator linking explicitly the observed data and the model parameter.

In other terms, the general measurement problem is about establishing a relationship linking the causes (the physical theory leading to the model parameters) and the effect (the observed data). As shown in Figure 1, the direction we choose interpreting this link determines whether we are dealing with a direct (forward) or with an inverse problem.

The inverse problem approach will be, then, the one starting from the measured data (e.g. correlated neutron flux) to determine one or more *unknown* parameters (e.g. fissile material mass and/or isotopic composition) defining the physical system under observation. Those parameters subject to verification are thus not measured directly, but they are rather the result of inversion algorithms solving complex equations, deriving the unknowns from the measured observables.

Figure 2 schematically represents the inverse problem in the specific case of nuclear safeguards verification: the measured data go through a model, in order to deduct the unknowns, which are eventually compared to the declared values in the verification phase. One of the implications of this process is that measurement uncertainties on the initial observables need to be propagated throughout the inversion model, which is not trivial from the mathematical point of view.

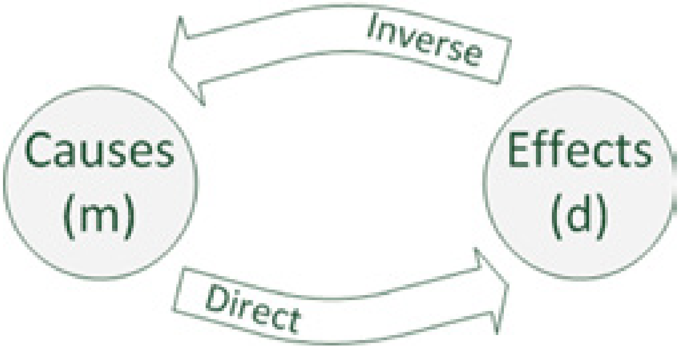

Figure 1: Schematic representation of direct and inverse problems

Sometimes, to simplify the model, assumptions like "infinite thickness" of the samples need to be taken or the model is replaced by empirical calibration curves. These latter suffer from a critical drawback: the Certified Reference Materials of the same type (i.e. in size, weight, matrix, fissile mass, package form) do not exist; therefore, selected samples from the operator's facility are used for calibration. In this way, a measurement's metrological traceability not directly possible; sometimes, indirect traceability can be established, e.g. by help of destructive assay of samples. Interpreting discrepancies in the verification results is then only possible with the intervention of experts in the specific measurement technique, who are able to assess uncertainties including knowledge from additional information sources.

Moreover, the inverse problem can represent a case of *ill-posed* problem in the sense of Hadamard [3], where the *well-posedness* conditions are that

a. A solution exists;

b. The solution is unique;

c. The solution's behavior changes continuously with the initial conditions.

In particular, we can immediately understand why the condition b. is not met in a simple practical case: two fuel assemblies with different ^{235}U masses, but different location of burnable poison rods, may give the same (i.e. statistically comparable) double neutrons count rate, if measured in a thermal-mode neutron collar. In this case, thus, the solution of the observed data inversion is not unique.

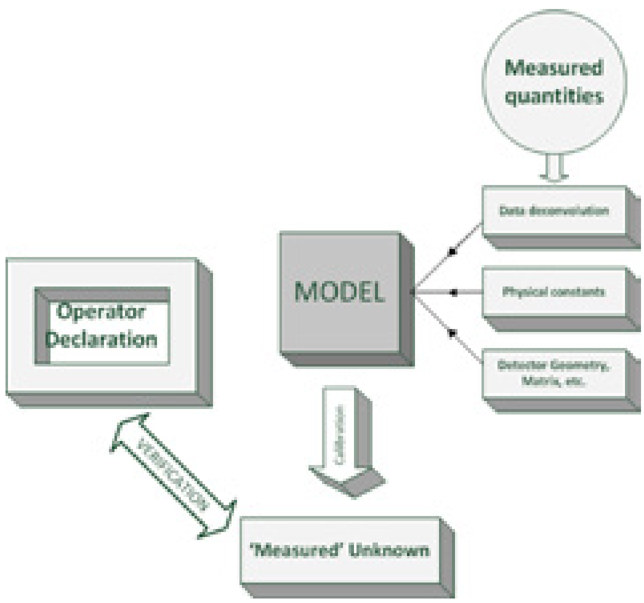

Figure 2: Schematic representation of the inverse problem as applied to nuclear safeguards verification.

On the other hand, the choice of a forward problem approach would start from the modeling of the physical system involved in the measurement, where the quantities of interest (e.g. fissile material mass/isotopic composition) become parameters of the model. As shown in Figure 3, the operator's declaration will then identify specific values of the mentioned parameters, while the model will predict the observable's quantities under these specific conditions. The verification phase will then consist in the direct comparison of the measured versus the predicted observables. The whole verification task becomes, in this way, a typical *hypothesis testing* exercise, in which a predicted quantity undergoes a direct comparison with its experimental value, under the hypothesis defined by the operator declaration.

We can then observe that a forward problem approach avoids the most difficult aspects of the mathematical inversion (deconvolution algorithms, non-unique solution, experimental error propagation), which are no longer needed in the verification task. At the same time, using the same set of information available and the same set of data, the credibility of the verification conclusion is not affected. Even in a forward-problem approach, though, one can still postulate other operator declarations that could result in the same or similar predicted quantities (within measurements and model uncertainties). However, we have to keep in mind that the primary task of the inspectorate is to verify the declarations provided by operator and not necessarily to develop the declared parameters independently.

It is also worth pointing out that measurement uncertainties are not eliminated by modelling: rather, a clear distinction is made between the uncertainty components arising from the calculation and those originating from the measurement itself (e.g. sample positioning, homogeneity, counting statistics).

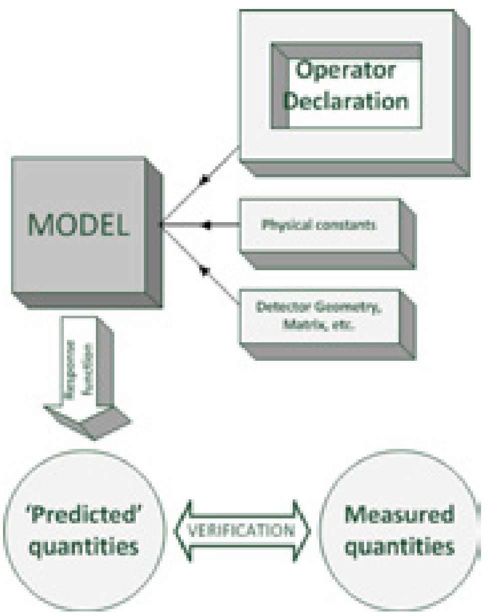

Figure 3: Schematic representation of the forward problem as applied to nuclear safeguards verification.

3. Euratom field-ready inspection tools using a forward-problem approach

Euratom Safeguards directorate makes use of Monte Carlo modeling in several deployed instruments, thus overcoming the issues with lack of reference materials and metrologically traceable calibration standards [4][5]. The improved computing capabilities and some specific verification issues have recently suggested that a forward problem approach with real-time simulation can improve the current verification practices. Clearly, every model needs to be appropriately benchmarked against well-characterised reference materials.

3.1 XFuelBuilder tool for Fresh LWR Fuel verification

Fresh fuel verification by Neutron Coincidence Collar (NCC) poses difficulties, in particular due to the increasing optimization of fuel performance, resulting in greater complexity of fuel design. In particular, fuel producers optimize the fuel assemblies by the use of strategically located burnable poison-enriched rods and by pins that have a variation in ^{235}U enrichment both axially and radially in the assembly.

In order to allow the inspectors to cope with this complexity, European Commission's Joint Research Centre and iScience have developed for Euratom Safeguards inspectorate *XFuelbuilder*, a tool based on the Monte Carlo simulation of NCC measurements. *XFuelbuilder* is in fact a software package, with a user friendly graphical interface, that allows the inspector to prepare a MCNP input file in a simple visual way and then run the simulation of the fuel + collar physical system. The modelling has been done using the MCNP-PTA code, developed at the Joint Research Centre of the European Commission in Ispra, in order to simulate the electronics pulse train analysis (PTA), including a shift register logic for coincidence counting. A benchmark of the modelling has been done at the PERLA laboratory at the Joint Research Centre in Ispra and is reported in past articles [4][5][6].

XFuelbuilder includes already the built-in models of the NCCs used by Safeguards inspectorates, both in thermal and fast mode configuration. The inspector can retrieve a stored assembly model or add a new pin or assembly design. Once chosen the collar type, the fuel design and the collar position along the fuel's active length, the inspector can run the simulation, thus obtaining the Reals, the Accidentals and the Totals as he or she would do in any neutron measurement. These values are then easily compared with the measured data, acquired by NCC assay of the assembly. Figure 4 describes the data flow of the whole verification task.

XFuelbuilder, choosing a forward-problem approach, is not affected by the already mentioned ill-posedness of the NCC verification problem, being at the same time a user friendly tool for the inspector. Moreover, it is capable to integrate many of the declared fuel details in the verification itself. This approach is also going to improve practical aspects of NCC verification, usually needing a passive measurement before the active one, in order to take into account for the correlated neutrons from ^{238}U spontaneous fission. While this two-phase process obliges the inspector to deploy and remove the source and is a practical limit to the possibility to make such measurements as unattended, in *XFuelbuilder* both induced and spontaneous fission are taken into account. Then, in principle, only the active measurement needs to be done, thus giving the inspectorate the possibility of unattended measurements. After a refinement phase, aimed at maching the inspectors' needs, Euratom Safeguards is starting to deploy *XFuelbuilder* as of 2018, starting from facilities where unattended NCC verification is needed.

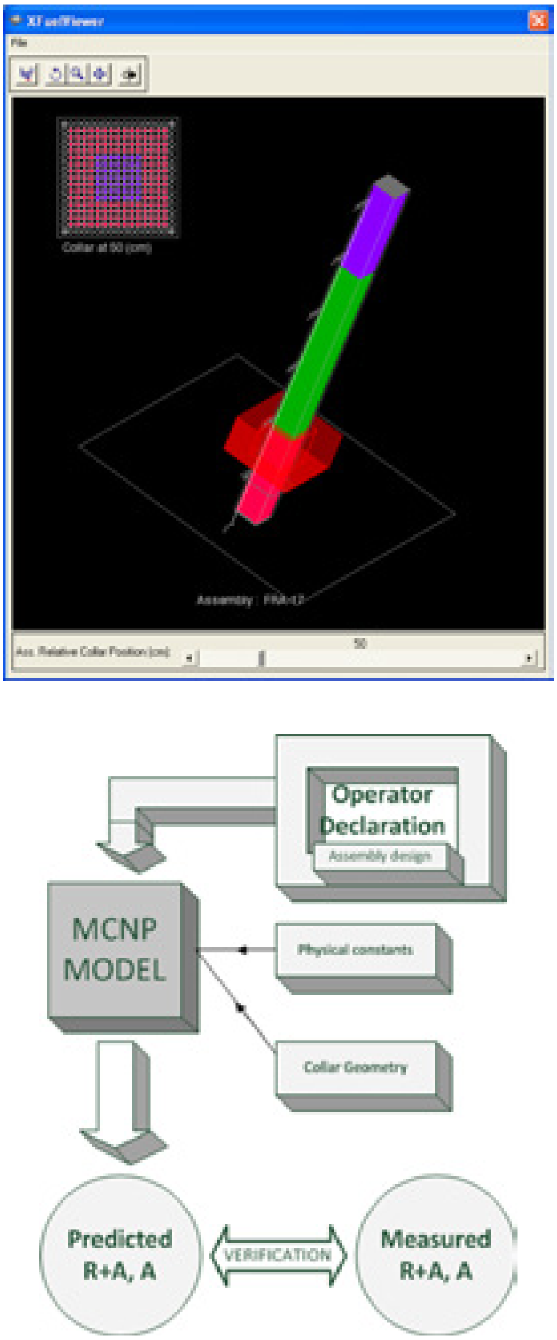

Figure 4: Screenshot and data flow of XFuel Builder

3.2 iRAP-ORIGEN method for improved Fork detector measurement results evaluation

Spent-fuel is one of the big challenges for NDA. In fact the high neutron and gamma activity from irradiated assemblies make it extremely difficult to measure and quantify fissile material in a simple and direct way. Although some promising methods may address this issue in the future [8], the Fork detector is at present the workhorse for the verification of fuel in preparation of intermediate/long term or final, geological storage, where recovery (and re-measurement) is practically not possible. In Fork detector verifications, safeguards inspectors measure the neutron and total gamma fluxes from an irradiated fuel assembly to check its consistency with the declared burn up, initial enrichment and cooling time of the assembly itself.

Euratom Safeguards is presently field testing a data evaluation tool [9][10], based on the integration of the review code iRAP (joint development of Euratom and IAEA) and the ORIGEN code (Oak Ridge Isotope GENeration), which is part of the package SCALE developed by Oak Ridge National Laboratory [11]. The iRAP-ORIGEN integration has been developed and improved under various Action Sheets on the EC-US DOE agreement in the field of nuclear material safeguards R&D. This cooperation has submitted a paper (now under review) summarising the work performed and including a more detailed uncertainty analysis of the calculations that are the basis of the method and of the assumptions made in the modelling of the fuel assemblies that are calculated [12].

The iRAP-ORIGEN tool allows, on the one hand, to process unattended Fork measurements, and extract the assembly neutron and gamma signature. On the other hand, a simulation combining an ORIGEN irradiation and depletion calculation, using the operator's declarations as input data, and a Monte Carlo computed detector response function compute the expected values of the same signature. The data flow of the complete process is explained in Figure 5.

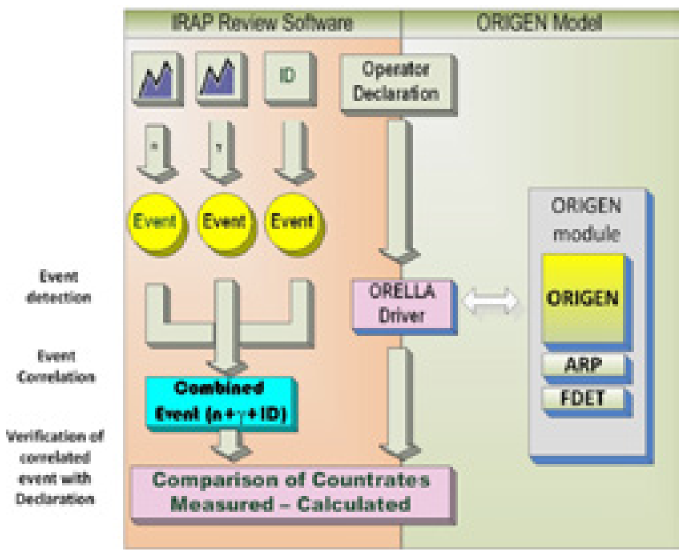

Figure 5: Data flow of an iRAP-ORIGEN Verification

This tool has already proven to be accurate in in taking into account the factors, which may influence the neutron and gamma signatures of spent fuel (e.g. cooling between irradiation cycles, within-assembly neutron multiplication). iRAP-ORIGEN is also ready for unattended measurements evaluation and is proving particularly inspector-friendly in installations where remote data transmission is available. The tool assists both the Inspectors and the Facility Operators: by providing a convenient mechanism for rapidly comparing operator declarations with measurement results. Alarms that are due to simple clerical or transcription errors may be resolved quickly, without need for further reverification activities at a later date.

Finally, still remaining a rather simple and limited technique, this improved version of Fork measurements is complementary to other techniques, aimed at the assembly integrity verification, like tomography [13], or aimed at other types of fuel characterization, like Passive Neutron Albedo Reactivity (PNAR) [8].

4. Conclusions

A forward-problem approach, consisting in real-time simulations using declaration data as parameters in a model that predicts directly measured observables, may be helpful in nuclear safeguards NDA verification, especially in cases where calibration can hardly take into account the complexities of the specific sample.

Euratom Safeguards Directorate, in partnership with research institutions such as the European Commission's Joint Research Centre and the Oak Ridge National Laboratory, has already developed tools, which are ready to bring this *hypothesis testing* approach into every day's inspection activities. The first two application fields are the verification of fresh LWR fuel by Neutron Coincidence Collar and the verification of irradiated fuel assemblies by Fork detector.

The forward-problem approach is also an opportunity for resource optimization, as it can be very well integrated in a remote data infrastructure, which allows performing the computational part of the verification at the headquarters.

Finally, it is worth mentioning that the use of a forward-problem approach is going to require a corresponding reflection of such physical verifications in the safeguards approaches, especially regarding the meaning of anomalies in terms of diversion scenarios and Material Balance Evaluation.

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