https://doi.org/10.61092/iaea.yjj0-2zgy

INDC(NDS)-0822
Distr. Web only

IAEA
International Atomic Energy Agency

INDC International Nuclear Data Committee

Summary report of the IAEA Consultants' Meeting on

Nuclear Data Forms and Observables for the Safe Monitoring, Characterization, Dismantling, Decommissioning and Disposal of Nuclear Fuel and Irradiated Material from Pile, Experiment, Facility and Nuclear Power Plant

(MCDDD)

2-4 November 2020, IAEA Headquarters, Vienna, Austria

Editors

Jean-Christophe Sublet
IAEA, Nuclear Data Section
&
Mark DeHart
Idaho National Laboratory
&
Mark Gilbert
United Kingdom Atomic Energy Authority

November 2020

IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

Selected INDC documents may be downloaded in electronic form from
http://nds.iaea.org/publications
or sent as an e-mail attachment.
Requests for hardcopy or e-mail transmittal should be directed to
NDS.Contact-Point@iaea.org
or to:
Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100
1400 Vienna
Austria

Printed by the IAEA in Austria

November 2020

INDC(NDS)-0822
Distr. Web only

Summary report of the IAEA Consultants' Meeting on

Nuclear Data Forms and Observables for the Safe Monitoring, Characterization, Dismantling, Decommissioning and Disposal of Nuclear Fuel and Irradiated Material from Pile, Experiment, Facility and Nuclear Power Plant

(MCDDD)

2-4 November 2020, IAEA Headquarters, Vienna, Austria

Editors

Jean-Christophe Sublet
IAEA, Nuclear Data Section
&
Mark DeHart
Idaho National Laboratory
&
Mark Gilbert
United Kingdom Atomic Energy Authority

November 2020

Table of Contents

Presentations URL https://nds.iaea.org/index-meeting-crp/CM-McDDD/

Introduction

The purpose of the Consultancy Meeting on nuclear data form and observables for the safe monitoring, characterisation, dismantling, decommissioning and disposal of nuclear fuel and irradiated material from nuclear power plant, pile, experiment and facility is to assess members' needs in terms of research, compilation and assembling of the specific nuclear data forms and observables databases needed for robust nominal and conceptual simulations of time dependant nuclear inventory, radiological characterisation and source terms for fission, fusion, accelerator, life, earth, research sciences applications.

Brief

It is foreseen that during the next few decades a significant number of piles, facilities and nuclear power plants (NPPs) will have reached their operational end of life. From a global inventory of circa 840 piles and research reactors, 226 still operational in 2020, 450 operational nuclear power plants generating electricity (of which 44 having been loaded with MOX fuel since the 1970's), numerous research experiments, and industrial and medical facilities of different types, one notices that quite a few have been closed, become defunct, put in a safe storage condition or are near the end of their active life, while inevitably more will also reach those stages in the next decades.

The purpose of this consultancy meeting is to understand the needs for the data forms and observables, services and capabilities in the processes, research and technological areas that are important for time-dependent radiological source term simulations, in support of the safe monitoring, characterisation, dismantling, decommissioning and disposal (even if only temporary) of irradiated and contaminated materials, structure and fuel in existence, or expected in the future. This should also include preparation for conceptual designs that might become reality by the middle of the 21st century. The simulation protocols involved rely heavily on both a comprehensive set of nuclear reactions and nuclear decays chains in unison. The aim is to research, compile and assemble, deliver and deploy the data forms and observables needed for robust simulations of nuclear inventory and radiological source terms for all applications: from the back end of the fuel cycle to the millennia scale not only for fission but also for accelerator, fusion, non-energy life, material and earth science applications related to radioactive material. One imperative will be to streamline and automate the evaluation, processing and verification of the multistep protocols capable of delivering the practical data forms needed, while also providing uncertainty quantification and propagation methodologies. Such undertakings would also benefit activities related to novel reactor or facility concepts, fuel cycles and materials research, existing protocol optimisation, development and demonstration activities, and completing the nuclear forms landscape beyond and above the traditional and well-understood envelope.

Proceedings

UKAEA; Mark Gilbert; UK

Importance of nuclear data for fusion reactor predictions of material activity and waste

Radioactive waste predictions are an important part of the conceptual and engineering design process of nuclear systems. For the burgeoning fusion industry this is particularly important, to allow reactors to be designed to meet the expectations of low radioactive waste production from nuclear fusion (in comparison to fission). This presentation highlights some of the current computational analyses being performed to quantify the waste arising from conceptual fusion reactor designs, including the detailed material analyses, comparisons and radionuclide contribution assessments required. Via the example of molybdenum, we also discuss where data may be deficient when predicting long-term activity (and hence waste) from some of the novel materials being considered for fusion applications. Decay data libraries are also a vital tool for activity (and hence waste) predictions performed using inventory simulations and UKAEA's recent work to produce an updated library is briefly discussed. There we highlight the need to continuously update to keep pace with modern nuclear cross section libraries, where new radionuclides are constantly being added.

UKAEA; Greg Bailey; UK

Towards beta-neutrino spectra from complex nuclear inventories

It is desired that activation and transmutation calculations provide information on the expected decay spectra from a given sample. Currently these spectra are often found for photons, but the equivalent for beta particle spectra are ignored. This is because, due to the three-body nature of the decay system, the beta and associated neutrino energy spectra are continuums and not commonly included in decay data libraries. This presentation covers ongoing work to develop a beta-neutrino continuum spectra library to improve decay data as well as its applications to calculations with the activation and transmutation code FISPACT-II.

Massachusetts Institute of Technology; Benoit Forget; US

Nuclear Data Issues for High Fidelity, High Performance Reactor Modelling and Simulation

This talk introduces the windowed multipole (WMP) cross-section representation and the opportunities it presents for high fidelity reactor simulations. The WMP formalism is very powerful for capturing temperature effects efficiently in multiphysics simulations, but also presents a novel way for embedding nuclear data uncertainty in Monte Carlo simulations. Doing so can provide feedback to evaluators on uncertainties related to specific resonance parameters. The WMP representation of the resolved resonance range of nuclear data has proven quite efficient on modern computing architecture and relies on the benefits of massive data library size reduction and sequential data access.

In the development of this formalism, many issues were encountered in generating the library from current evaluations. The first issue can be summarized as the reliance on ENDF File 3 in the resolved resonance region. File 2 provides resonance parameters while File 3 is a pointwise representation of data that needs to be added to the File 2 values. Modern evaluations rarely use File 3 in the resolved resonance range (e.g., U-238) and rely instead on more faithful resonance models to capture the interference effects. Older libraries, however, rely on File 3 to correct cross-sections in certain energy ranges to better match experiments, which often leads to discontinuities in data. Some evaluations use File 3 to patch two different resonance models, like in the case of Na-23. These discontinuities in data or models make it quite difficult to convert to other resonance formalisms. The second issue highlighted is the use of pointwise values in the evaluations for nuclides that were generated using a resonance formalism. The example of B-11 is used where the provided data lacks sufficient resolution to facilitate conversion to alternative resonance representation.

On the uncertainty quantification side, WMP allows for explicit computation of sensitivities to resonance parameters and, with its much smaller data footprint, enables possibilities for randomly sampling cross-section representations during the random walk to calculate the true impact of nuclear uncertainties on tallied quantities. Covariance data is however quite sparse and when available it is not necessarily a good representation to the uncertainties of the resonance parameters. One example is that codes that generate the covariance matrix do so on variables that are different than the ones reported in the evaluations, which can lead to sampling issues. Additionally, the covariance matrices have sometimes been adjusted to reflect experimental uncertainties using first-order propagation methods, but this can lead to reconstruction issues when sampling parameters from the covariance matrix.

This talk also introduces another area of high relevance for the nuclear engineering community unrelated to WMP. Thermal scattering libraries are essential for the proper modelling of thermal systems and the current proliferation of new designs highlights many gaps in thermal scattering data. From molten salts to metal hydrides (with proper non-stochiometric ratios), many new evaluations are needed. Additionally, greater interaction with the materials community that has developed tools for computing density of states could provide a pathway for new evaluations.

PSI; Dimitri Rochman; CH

Nuclear data needs for spent fuel characterization: a review of PSI experience

Spent fuel characterization is essential for the safe and economical long-term storage of SNF (spent nuclear fuel). A number of quantities need to be precisely known, often from calculations (assembly burnup, isotopic compositions, decay heat, neutron/gamma emission), and also from accounting and irradiation history (e.g., assembly enrichment, cladding, cooling time). In the case of casks and canisters, their criticality values are also needed, as a function of time. Such calculated quantities naturally depend on isotopic compositions and decay data, which can be rephrased by “depend on nuclear data (cross sections and decay data)”. In this presentation, a number of examples are given, where nuclear data uncertainties are affecting the SNF characteristics, significantly enough so that they can impact the design (and cost) of storage facilities. As important as the estimation of uncertainties, the quantification of errors and biases due to nominal cross sections also needs to be performed. As a conclusion, not only better nuclear data can improve simulations, but also more comprehensive nuclear data libraries can help for the assessment of SNF characteristics.

ORNL; Germina Ilas; US

Spent Nuclear Fuel Applications: ORNL Validation Experience

Experiments are essential to validate nuclear data and methods for spent nuclear fuel modelling and simulation (M&S). Validity of safety assessments for spent nuclear fuel transportation, storage, and repository applications is largely based on capabilities to accurately predict the evolution of nuclides during and after irradiation in fuel and structural materials. This presentation highlights experimental data resources for validation and their usage to assess the M&S capabilities and associated nuclear data in the SCALE nuclear analysis code system for spent nuclear fuel applications, with a focus on the ORIGEN nuclear transmutation and decay physics code. The validation examples include nuclide inventory, decay heat, and radiation emissions for light water reactor spent fuel with various characteristics (burnup, cooling time after discharge, assembly design, etc.) and illustrate the use of uncertainty analysis capabilities in SCALE to estimate uncertainties in spent fuel metrics that are due to uncertainties in nuclear data and input parameters.

Key points on nuclear data and experimental validation data needs for the end-user are summarized in the presentation. While nuances may slightly differ for different users (industry, government regulator, code developer, nuclear data evaluator, etc.), there are common themes, emphasizing the importance and value of high-quality, low uncertainty experimental data for validation; publicly-available validation data resources with adequate documentation and information visualization capabilities; evaluated benchmarks with comprehensive uncertainty analysis; application-specific guidance and recommendation on data's usage, value, and applicability.

ORNL; Robert Grove; US

Nuclear M&S Tools and Applications at ORNL and Related Nuclear Data Perspectives

Nuclear modelling and simulation (M&S) is becoming much more complex and changing rapidly. Modern engineering design capabilities are influencing nuclear applications in many ways including more complex and higher fidelity geometric descriptions, complex arrangements of materials and the use of novel materials, rapid iterative design cycles, mixed high and low fidelity requirements, coupled multiphysics, and increasing computational requirements, capabilities and platforms. There is a broadening of nuclear applications areas requiring high fidelity solutions well outside the boundaries of traditional reactor physics regimes. These points are illustrated in this presentation through the Virtual Environment for

Reactor Applications (VERA), the Transformational Challenge Reactor (TCR), the Exascale Computing Project (ECP) and the ExaSMR project within ECP, and through large scale facility dose mapping in the fusion neutronics field.

This rapidly increasing complexity in nuclear M&S is driving the needs for advanced nuclear data. The complexity makes it more challenging to assess and assure the efficacy of the underlying nuclear data; stresses the tools and techniques for assessing very large nuclear data sets and the impact of changes in these data; requires robust analyses of uncertainties, covariances, sensitivities, and propagation of uncertainties through multi-step multi-physics M&S; and requires high performance computing (HPC) Monte Carlo capabilities which, in turn require new ways of accessing the huge amounts of nuclear data needed for huge numbers of unique materials. The advancing needs for nuclear data across many applications areas include: increased importance of materials that are being used in environments well outside traditional LWR regimes; increased importance of activation, damage, heating and other nuclear data for facility analyses and for advanced fission, fusion and security applications; increased fidelity in activation, transmutation, production, and decay data; and advanced and robust uncertainty quantification, covariance, and sensitivity data and tools. Finally, the increasing use of Monte Carlo methods for nuclear analysis on HPC systems is driving the need for close collaboration between experts in emerging HPC algorithms and nuclear data forms. We should expect that these trends will continue driving the needs for advanced nuclear data across many nuclear applications areas.

Jean-Christophe Sublet; International Atomic Energy Authority; AT

The nuclear data forms and observables of the lesser Gods

Although general purpose transport libraries are available from every major project and are still now a day receiving the bulk of the attention of the nuclear data community other specialised libraries have had to be assembled over the years to answer the lesser (than neutron transport) needs: high energy, activation-transmutation, fusion, dosimetry, earth and medical sciences, etc., they all contain similar nuclear data forms but are not consistent with one another. Enhanced, all-embracing data forms are needed to supplement the existent and fill the many gaps that exist. Not only total but partial open channels, including the description of all (not only neutron) outgoing emitted particles, transitioning and residual states yield, spectral and angular information, channel variance and covariance, are needed across a much broader nuclei landscape and wider incident particle energy range. The enhanced reaction library needs to be supported by an all-embracing decay data library covering the defined targets, all daughters and emitted particles to support high-fidelity simulation efforts.

O. Cabellos; Universidad Politécnica de Madrid (UPM); ES

Nuclear Data Needs for characterization of nuclear fuel and irradiated materials

Nuclear data is the link between the nuclear physics (and differential experiments) and applications calculations. For application simulations the transport Boltzmann equation and Bateman equation are used to predict neutron flux and isotopic inventory, respectively. This system of equations is solved jointly to predict as accurately as possible the evolution of the isotopic content in nuclear applications. Nuclear data are the parameters characterizing these equations: total cross sections, scattering and reaction cross sections, double differential cautions, etc., multiplicities, emission spectra, production yields (neutron, photons, fission products), decay data (half-life, branching ratios, emission probabilities, emission spectra), thermal scattering laws, etc.

In addition, different conversion factors are used to predict response functions for characterization of nuclear fuel and irradiated installations: radioactivity, photon production, decay heat, contact dose, neutron emission (spontaneous fission, delayed neutron emission, and nuclear reactions, such as (α,n)), primary damage in materials (dpa and gas production), committed effective dose, offsite doses and consequences, waste management (specific activity limits for waste disposal, hands-on and remote recycling, shallow land burial), etc.

An extensive collection of benchmarks and experiments have been identified in different public handbooks for nuclear data validation: SFCOMPO-2.0 for depletion benchmarks, decay heat benchmarks, dose rate benchmarks, etc. This compilation of integral benchmarks allows to easily test nuclear data evaluations.

Sensitivity/Uncertainty analysis and uncertainty quantification are needed to assess the impact of nuclear data uncertainties in response functions. This analysis will help to identify the most important nuclear data contributing to bias and uncertainties.

Finally, target accuracies for response functions should aim "*to point out and to quantify priority nuclear data needs or uncertainties reduction to meet design*".

Osamu Iwamoto; Japan Atomic Energy Agency; JP

Recent development of nuclear data libraries for nuclear decommissioning and transmutation in the JENDL project

After the release of JENDL-4.0, the JENDL project released several special purpose files especially focusing on nuclear back ends such as decommissioning of facilities (JENDL/AD-2017) and transmutation of high-level radioactive wastes (JENDL/ImPACT-2018) as well as accelerator applications including activation data (JENDL/PD-2016, JENDL/PD-2016.1, JENDL-4.0/HE). The JENDL/AD-2017 was developed for evaluation of neutron activation of nuclear power plants, including 311 target nuclides which have enough neutron reaction data for light water reactors. The JENDL/ImPACT-2018 aimed at facilitating research works of nuclear transmutation of long-lived fission products (LLFP) of ^{79}Se, ^{93}Zr, ^{107}Pd and ^{135}Cs within the R&D program for Reduction and Resource Recycling of High-level Radioactive Wastes through

Nuclear Transmutation funded by the ImPACT Program (Cabinet Office, Government of Japan), whose data covers proton and neutron induced reactions up to 200 MeV on long lived fission products and their secondary products during nuclear transmutations. The photonuclear reaction data library JENDL/PD-2016 increased the stored number of nuclei to 2,681 from 68 of previous version JENDL/PD-2004 to satisfy the materials of various application fields. In connection with the collaboration of the IAEA photonuclear data library, JENDL/PD-2016.1 was developed with revising data of more than 1,000 nuclides and adding new evaluation for 4 nuclides with extending the upper energy range from 140 MeV to 200 MeV.

Mark DeHart; Idaho National Laboratory, US

Simulation Needs for Advanced Reactor Technologies

At present, a number of advanced reactor concepts are being evaluated by industry with government support. These include both prismatic and pebble bed high temperature gas reactors (HTGR), fluoride-salt cooled high-temperature reactors (FHR), molten salt reactors (MSR), micro-reactor (µR), fast reactor (FR) and nuclear thermal propulsion (NTP) engines. The driving physics vary for different reactor types. Many designs are based on TRISO fuel; MSR, FR and FHR utilize a liquid coolant (Na, Pb, and salts), where as the salt contains the fuel in the MSR. HTGR, some µR and NTP designs are gas cooled; HTGR, FHR and NTP designs will operate at high temperatures. Each of these designs introduces geometric complexities of various levels, new materials and will be a challenge in terms of cross section processing and the level of coupled physics relative to methods developed over decades for light water reactors.

Challenges in these designs include chemistry, thermomechanical behaviour, fuel performance, thermo-fluids and ipso facto neutronics. Each of these physics have multiple multiphysics methods, deterministic by their very nature, require advanced techniques to couple physics that have strong non-linear relationships as a result of material properties, geometry changes and temperature and density feedback effects. Advanced non-linear solvers are only as good as underlying data, both thermomechanical and neutronic. Needs for multiphysics simulations of advanced reactors include (a) needs for cross sections and scattering data for reactor-grade graphite and a better understanding of TRISO fuel physics, (b) thermal scattering data for FLiBe and other salt concepts, including molecular subcomponents of the salt, (c) higher temperature evaluations for high temperature systems, i.e., for NTP and for accident scenarios for high temperature reactors, (d) beryllium is expected to play a significant role in micro-reactor designs, the current ATR and potentially for a replacement ATR design, (e) changes in cross sections for Na, iron, specifically Fe-56, have had an effect on sodium FR designs; similarly changes in carbon data have had a significant effect on graphite systems; a convergence on data improvements in these materials is important, (f) data is not well qualified for fission product yield data, decay constants, and branching fractions to support spectra outside typical LWR spectra; (g) as simulations make possible detailed time-dependent simulations, there is a corresponding need for improvements in time-dependent parameters, specifically kinetics data. Improvements along these lines will improve the accuracy of simulations that will ultimately be used to design experiments, develop prototypes and perhaps by applied in the safety analysis of advanced reactor systems.

Young-Ouk LEE, Korean Atomic Energy Institute, KR

Analysis and Validation of SNF Characterization via Ultra-Fine Grid Core Tracking with Improved Nuclear Data

The issues of Spent Nuclear Fuel is long-standing culprit in Korea. Recently Korean government set forth a long-term nuclear R&D program, in which spent nuclear fuel characterization become one of important key words. Strongest need of reliable Spent Nuclear Fuel Characterization comes from the regulation and management fields. Reliable Spent Nuclear Fuel Characterization is also needed in the Fuel cycle R&D. Currently, SCALE-based code package is under study in rod-wise grid for a whole reactor core burnup, which requires a huge computing resource.

The goal of this proposal is to achieve highly reliable spent nuclear fuel characterization and validation through ultra-fine core tracking technique, with improved nuclear data. A model & simulation code will be developed for tracking core burnup based on highly reliable nuclear data and analyzing pellet-wise nuclear characteristics according to the burnup history of nuclear fuel. Target accuracies of number density for major actinides is set less than 1 %, for minor actinides less than 5 %, for major fission products less than 5 %, and, for minor fission products less than 10%. Internal collaboration on nuclear data improvement is inevitable to meet those targets.

In the first three years of the project, nuclear data, code, and M&S system will be improved, and developed. In the 4th year, the system will be updated with open benchmarks. In the final year, the system will be validated by measurement, utilizing existing post irradiation data. Direct validation will be the next step, which includes destructive analyses of the nuclear characteristics in some sampled Spent Nuclear Fuel assemblies.

Mark DeHart, Idaho National Laboratory, US

Multiphysics Simulations of Advanced Reactors

Multiphysics modelling is an expanding field for analysis and design of nuclear systems. Internationally a number of simulation packages have been developed for multiphysics analysis of both LWRs and/or advanced reactor designs. These packages include (but certainly are not limited to) MOOSE based tools (MAMMOTH, Rattlesnake, Griffin, BISON, RELAP-7, Sockeye, etc.), GeN-Foam, VERA and NURESAFE, along with commercial products such as ANSYS and COMSOL. International interest led OECD/NEA to form an Expert Group on Multi-physics Experimental Data, Benchmarks and Validation (EGMPEBV). The US DOE is also sponsoring university research to develop multiphysics benchmarks from existing datasets or at research reactors; however, this data, while valuable, is generally limited to LWR-type environments. For advanced reactors new experimental measurements relative to the nature of designs are needed. Leading candidates for advanced reactor deployment are prismatic and pebble bed high temperature gas reactors (HTGR), fluoride-salt cooled high-temperature reactors (FHR), molten salt reactors (MSR), micro-reactor (µR), fast reactor (FR) and the nuclear thermal propulsion (NTP) engine. Experimental facilities have been disappearing for quite some time, and often potentially relevant experiments designed to measure X fail to adequately document the states of Y and Z, or data are incomplete. The primary physics of concern for advanced reactors are (1) fuel integrity (release of fission products, relocation, structural integrity), (2) thermal-fluids (coolant, heat pipes, MSR fuel), (3) chemistry (corrosion, molecular disassociation), (4) mechanics (stress/strain, thermal expansion) and neutronics (reaction rates, leakage, activation, depletion). The importance of the various physics varies by reactor type: fuel integrity is primary in pebble systems, very minor in MSRs; thermal fluids in heat pipe µRs is limited to heat pipe performance and ex-core Stirling engine; neutronic depletion is minor in µRs and NTP due to low burnup; thermal expansion is important in FRs, NTP and HTGRs; chemistry is perhaps most important in MSRs but may also be of concern for NTP systems. Appropriate data are relatively sparse. However, new and planned experiments and facilities within the next 6-8 years may alleviate this situation: the Microreactor Agile Non-nuclear Experimental Testbed (MAGNET), the Microreactor Applications Research, Validation and Evaluation (MARVEL), the US Department of Defence Strategic Capabilities Office microreactor design down-select and prototype, DOE Advanced Reactor Design Program (ARDP) awards, NASA hydrogen flow loop fuel sample test and sodium test loop in TREAT, the Versatile Test Reactor, MYRRHA, Jules Horowitz, the prototype Gen IV sodium cooled fast reactor (PGSFR), ASTRID and others. Test data will become available and hopefully shared internationally from many programs, although industrial testing data and data from certain countries may have limited availability. However, it is clear that there is a need for data to properly validate multiphysics analysis tools.

Discussions and motivations

Nuclear observables and data forms are at the foundation of most nuclear programs. IAEA’s member countries’ traditional efforts in research, development and technologies have been in support of each member’s dominance and need. However, the scenarios are shifting in support of more cross-country, cross-continent collaborations on new technologies and standards (to raise acceptability) while regulations and licensing protocols also need to account for export markets (to reach critical mass, benefit from series effects, drive the cost down) and neighbourhood considerations.

Below are listed some of the discussed motivations:

- Enhanced characterisation of radiological streams: solid, liquid and gas
- Providing the nuclear data forms to support the follow up, characterisation and monitoring of legacy, spent fuel and other component nuclear wastes

- Robust nuclide inventory, radiological assessment for monitoring, re-cycling, decommissioning, storage, disposal activities
- Adequately manage decommissioning and/or support the arguments for deferral
- Optimise/ascertain fast-track robust radiological simulation studies
- Providing uncertainty quantification metrics on radiological quantities
- Empower optimisation, innovative simulation activation-transmutation studies
- Enhanced, heightened simulation for novel build and experimental facilities
- Complement the nuclear landscape where no or few experimental information exists
- Answer the accidental, damaged-facility, non-traditional pile, plant scenario simulation needs
- Improved fissile decay chains, major (with proper branching, larger coverage) and minor actinides (more robust, verified in need of validation)
- Improved structural materials decay, transmutation and activation mixed reaction-decay chains under irradiation
- Improved build-up and burnup simulations: poison transmutation/activation chains
- Providing the nuclear data forms to support high-fidelity simulation efforts
- Scrutinising the low-level and intermediate-level waste frontier simulation
- Empowering the processing, radiochemical plant clean-up
- Inspiring down-blending activities, depleted uranium valorisation

- Driving the costs down and the acceptability up, for monitoring, safe storage, decommissioning and dismantling
- Fortifying, encouraging and fostering cross-country, cross-continent collaboration
- Conveying to all nuclear sciences as opposed to the one only: fission, fusion, accelerator, medical, space, earth-life sciences

Overview and recommendations

UKAEA: there is an ongoing effort to identify the nuclear data needs for fusion, highlighting deficiencies in cross sections and decay data for critical materials being considered for fusion applications. There are ongoing efforts to develop validation and verification benchmarks and cases to test nuclear data libraries as applied to waste and decommissioning interests of structural and function materials for fusion (and other advanced nuclear systems such as next generation fission). Included in this will be assessment of where the nuclear data uncertainties are generating unacceptable safety/handling margins in waste and decommissioning assessments and thus where nuclear data evaluation efforts (to reduce uncertainty) need to be directed. This could potentially include assessment of experimental data sets (e.g., EXFOR) to determine where historical data is potentially misleading the evaluation community.

Rolls-Royce: It is important to be able to provide support for molecular modelling in nuclear engineering simulations. Molten salt mixtures and metal hydrides comprehensive nuclear data forms are needed for compact reactor designs.

KAERI: Concrete has a complex molecular structure and crowded storage ponds would benefit from improved simulations protocol that rely on all-inclusive nuclear data. Time dependant nuclides number density prediction requires all-embracing, reaction and decay, nuclear data forms. Prediction validation should be done through time dependant sampling measurement of SNF and irradiated structure.

UPM: This community should explore new data science techniques, such as Machine Learning, to identify problems in nuclear data via integral experiments. It will help to explore and assess future nuclear data needs

LLNL: provide the nuclear data forms to support high-fidelity simulation efforts. Fundamental sciences and applications are a partnership

MIT: The nuclear data community should continue focusing their efforts on better measurements and improved evaluations, as these are essentials for improving the predictive capabilities of our tools, but in doing so they should also consider these issues:

- Continue the development and support of open-source well-documented data processing codes
- Review evaluations of older nuclides so that they do not prevent the development of novel nuclear data models (e.g., remove unnecessary discontinuities in models and/or data, reduce reliance on File 3 in resolved resonance range, etc.)
- Provide unaltered covariance data (i.e., on the parameters on which the data was fitted and not adjusted to match certain experiments) and also provide nuclide-to-nuclide covariance data.
- Include resonance parameters for all nuclides even if they were generated in a non-standard format, in addition to the pointwise data
- Create a repository of files and data such that evaluations can easily be replicated and accessed (e.g., SAMMY input files, DFT/MD input files for TSL libraries, etc.)

The nuclear data community and the nuclear code developers need to work in closer collaboration. Providing data without context or how it was generated should be avoided. High-fidelity simulations and high-performance computing open doors for better integration of nuclear data processing in the simulations, and could enable better, faster feedback to the nuclear data community for further improvements.

ORNL: Ideas/plans on how to synergize existing validation resources and efforts (databases, expert groups, organizations) world-wide are essential for addressing nuclear data and validation data needs of the end-user community. Ideas/plans on how to create a mothership database, mega-resource of validation data to direct/inform/advise an interested user on available resources/websites/guidance, based on their application of interest, may be a valuable starting point. Development of benchmarks based on experimental data, to assess the impact on spent fuel metrics of nuclear data and nuclear data uncertainties, are always valuable in identifying data gaps and needs and in informing efforts on how to augment/extrapolate/interpolate the existing validation space via data science approaches.

The rapidly increasing complexity in advanced nuclear modelling and simulation across all applications areas is driving a need for a closer collaboration between nuclear data and nuclear analysis experts. A salient example brought forward by both MIT and ORNL in this consultancy is the need for novel ways of efficiently accessing huge amounts of nuclear data driven by the application of advanced Monte Carlo methods on high performance computing systems. This is driving development of "on-the-fly" evaluations rather than traditional table lookup techniques.

INL: it is clear that there is a need for enhanced data forms to properly validate multiphysics analysis tools and provide high fidelity simulation results. In addition, the wealth of nuclear data available has been measured and vetted primarily in light-water and some heavy-water spectra. Such data may not be appropriate or may be deficient for application to advanced reactor design concepts. Rapid cross-section evaluation capabilities will also be needed to be able to simulate spatially varying properties resultant from multiphysics coupling.

PSI: more comprehensive, all-inclusive nuclear data libraries can help for the assessment of SNF characteristics

JAEA: In the JENDL project, many evaluated nuclear data libraries have been released. The targets of MCDDD would be widespread over various application fields of nuclear data. It is important to validate the evaluated nuclear data depending on target accuracy for each purpose. Collaboration may give a good framework for collecting the data for the validations and making comparison between evaluated data.

The expert's panel recommend the IAEA to nurture a dedicated Coordinated Research Project capable of answering some of the needs and motivations expressed above. A major aspect of it should be to endeavour to unify the research and development fields across the continents while bridging the gaps between the different sciences and physics at play.

The end-product will be to fully integrate the data forms and observables needed beyond the normal and safe operational NPPs, pile or experimental needs, for in-depth activation, transmutation, characterisation, burnup, build-up, decay heat and dose, hazard indices, radiological simulations to support the existing fleet but also novel concepts, including innovative multiphysics aspects covering the high to low energy incident particle ranges and the timescale from milli-second to millennia.

Appendix 1 Virtual meeting agenda

Consultancy Meeting on

Nuclear Data Forms and Observables for the Safe Monitoring, Characterization, Dismantling, Decommissioning and Disposal of Nuclear Fuel and Irradiated Material from Pile, Experiment, Facility and Nuclear Power Plant

(MCDDD)

November 2nd – 4th, 2020, IAEA Headquarters, Vienna, Austria

Virtual Event - MCDDD

The purpose of the Consultancy Meeting on Nuclear Data Form and Observable for the Safe Monitoring, Characterisation, Dismantling, Decommissioning and Disposal of Nuclear Fuel and Irradiated Material from Nuclear Power Plant, Pile, Experiment and Facility is to assess members' needs in terms of research, compilation and assembling of the specific nuclear data forms and observables databases needed for robust nominal and conceptual simulations of time dependant nuclear inventory, radiological characterisation and source terms for the fission, fusion, accelerator, life, earth, research sciences applications.

Agenda

14:00 – 18:00 CET
Monday November 2nd, Virtual Room

14:00 Welcoming address – Arjan Koning, SH-NDS

Election of chairman and rapporteur Adoption of agenda, administrative matters

Introduction, Scope of the CM - J.-Ch. Sublet, UH-NDSU

14:10 J.-Ch. Sublet (IAEA) "McDDD white paper"

14:30 Dimitri Rochman (PSI - Switzerland) "Nuclear data needs for Spent Fuel

Characterization: a PSI outlook"

15:00 Young-Ouk LEE (KAERI - Korea) "Analysis and Validation of SNF Characterization via Ultra-Fine Grid Core Tracking with Improved Nuclear Data"

15:30 Mark D. DeHart (INL - USA) "Simulation needs for advanced reactor"

16:00 Oscar L. Cabellos de Francisco (UPM - Spain) "Nuclear Data Needs for characterization of nuclear fuel and irradiated materials

16:30 Benoit Forget (MIT – USA) "Nuclear Data Issues for High Fidelity, High Performance Reactor Modelling and Simulation"

17:00 Luiz Leal (IRSN - France) "IRSN methods and tools for data needs identification"

17:30

18:00 End of Day One

Tuesday November 3rd, Virtual Room

14:00 Osamu Iwamoto (JAEA - Japan) "Recent development of nuclear data libraries for nuclear decommissioning and transmutation in the JENDL project"

14:30 Anders Sjöland (SKB - Sweden) "Perspectives and needs for nuclear data activities with a focus on spent nuclear fuel characterization"

15:00 J.-Ch. Sublet (IAEA) "The nuclear data forms and observables of the lesser Gods"

15:30 Mark R. Gilbert (UKAEA – United Kingdom) "Importance of nuclear data for fusion reactor predictions of material activity and waste"

16:00 Mark D. DeHart (INL - USA) "Validation Challenges in Multiphysics Simulations of Advanced Reactors"

16:30 Germina Ilas (ORNL - USA) "Spent Nuclear Fuel Applications: ORNL Validation Experience"

17:00 Caleb Mattoon (LLNL - USA) "LLNL Nuclear Data Needs and GNDS"

18:00 End of Day two

Wednesday November 4th, Virtual Room

14:00 Kenichi Tanaka (NUPEC – Japan) "Needs for Nuclear data - Aiming to improve radiological characterization reliability for decommissioning, and disposal of radioactive waste from nuclear power plants"

14:30 Greg Bailey (UKAEA – United Kingdom) "Towards beta-neutrino spectra from complex nuclear inventories".

15:00 Oliver Köberl (AXPO – Switzerland) "A utility perspective Beznau NPP"

15:30 A. Ferrari (HZDR - Germany) "Challenges in shielding design at accelerator systems in special environments"

16:00 Bob Grove (ORNL – USA) "Nuclear M&S Tools and Applications at ORNL and related Nuclear Data Perspectives"

16:30 Discussions, Resume

17:00

17:30 Conclusions

18:00 Close of meeting

Presentations URL https://nds.iaea.org/index-meeting-crp/CM-McDDD/

Appendix 2 Virtual meeting list of participants

F4-CS-2004968
(Virtual Meeting) Consultancy Meeting on Nuclear Data Form and Observable for the Safe Monitoring, Characterisation, Dismantling, Decommissioning and Disposal of Irradiated Materials and Nuclear Fuels from Nuclear Power Plant, Pile and Experiment
Vienna, Austria
2 to 4 November 2020

List of Participants

Mr Greg BAILEY Culham Science Centre Abingdon OXFORDSHIRE UNITED KINGDOM
Mr Jeremy BEZ Institut de Radioprotection et de Sûreté Nucléaire 31 avenue de la division Leclerc Fontenay aux roses, CEDEX FRANCE
Mr Oscar Luis CABELLOS DE FRANCISCO Universidad Politecnica de Madrid Energy Engineering Department ETS de Ingenieros Industriales de Madrid 28006 MADRID SPAIN
Mr Mark DEHART Idaho National Laboratory 2525 Fremont St. IDAHO FALLS, ID UNITED STATES OF AMERICA
Ms Anna FERRARI Helmholtz Zentrum Dresden Rossendorf Bautzner Landstrasse 400 01328 DRESDEN GERMANY
Mr Benoit FORGET Massachusetts Institute of Technology 77 Massachusetts Ave. CAMBRIDGE, MA UNITED STATES OF AMERICA
Mr Zhigang GE China Nuclear Data Center China Institute of Atomic Energy P.O. Box 275 (41) BEIJING CHINA

Mr Mark GILBERT United Kingdom Atomic Energy Agency ABINGDON OXFORDSHIRE UNITED KINGDOM
Mr Enrique Miguel GONZALEZ-ROMERO Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas (CIEMAT) Avenida Complutense 40 28040 MADRID SPAIN
Mr Bob GROVE Oak Ridge National Laboratory 1 Bethel Valley Road OAK RIDGE, TN UNITED STATES OF AMERICA
Ms Germina ILAS Oak Ridge National Laboratory (ORNL) 1 Bethel Valley Road OAK RIDGE, TN UNITED STATES OF AMERICA
Mr Osamu IWAMOTO Japan Atomic Energy Agency (JAEA) Shirakata 2-4 Naka-gun 319-1195 TOKAI-MURA, IBARAKI JAPAN
Mr Arnd JUNGHANS Helmholtz-Zentrum Dresden-Rossendorf (HZDR) Institute of Radiation Physics Bautzner Landstr. 400 01328 DRESDEN GERMANY
Mr Oliver KOEBERL AXPO Power AG Beznau DÖTTINGEN SWITZERLAND
Mr Luiz LEAL Institut de Radioprotection et de Surete Nucleaire (IRSN) PSN-EXP/SNC/LNR - batiment 25 31 avenue de la Division Leclerc, BP17 92262 FONTENAY-AUX-ROSES CEDEX FRANCE
Mr Young-Ouk LEE Laboratory of Nuclear Data Evaluation; Korea Atomic Energy Research Institute (KAERI) P.O. Box 105 DAEJEON KOREA, REPUBLIC OF

Mr Caleb MATTOON Lawrence Livermore National Laboratory 7000 East Avenue, L-414 CA 94550 LIVERMORE UNITED STATES OF AMERICA
Mr Gareth MORGAN Rolls-Royce Analytical Engineering Raynesway, DERBY UNITED KINGDOM
Mr Joseph REES Rolls-Royce plc PO Box 2000, Raynesway, DERBY ENGLAND UNITED KINGDOM
Mr Dimitri ROCHMAN Paul Scherrer Institut (PSI) 5232 VILLIGEN SWITZERLAND
Mr Anders SJÖLAND Swedish Nuclear Fuel and Waste Management Co (SKB) Evenemangsgatan 13, PO Box 3091 169 03 SOLNA SWEDEN
Mr Kenichi TANAKA Nuclear Power Engineering Center (NUPEC) 14-2, Nishi-Shinbashi, Minato-ku 105-0003 TOKYO JAPAN

IAEA Vienna International Centre P.O. Box 100 Wagramer Strasse 5 1400 VIENNA **AUSTRIA**	**Mr Jean-Christophe Sublet – Scientific Secretary** Head - Nuclear Data Services Unit Nuclear Data Section Email: j.c.sublet@iaea.org
	Ms Shin Okumura Nuclear Data Services Unit Nuclear Data Section Email: s.okumura@iaea.org
	Mr Koning Adrianus Johannes Section Head - Nuclear Data Section Email: A.Koning@iaea.org

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre, P.O. Box 100
A-1400 Vienna, Austria

E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Telephone: (43-1) 2600 21725
Web: http://nds.iaea.org