INTERNATIONAL ATOMIC ENERGY AGENCY

INDC(NDS)-469
Distr. AC,AD

I N D C INTERNATIONAL NUCLEAR DATA COMMITTEE

Report on the IAEA

Technical Meeting on

Application Libraries for ADS and Transmutation

IAEA Headquarters, Vienna, Austria
15 – 17 December 2004

Prepared by

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Nuclear Power Technical Development Section

and

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International Atomic Energy Agency
Vienna, Austria

December 2004

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Produced by the IAEA in Austria
December 2004

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Abstract

Highlights of the technical meeting are given with respect to the source of evaluated nuclear data, codes for ADS analysis with associated application libraries, content of these libraries, and the procedure for producing them. Participants debated their requirements and formulated an action plan, with work divided between four sub-groups: review/analysis of ADS benchmarks; selection of evaluated nuclear data files; preparation of the cross-section libraries; and benchmarking. Specific tasks were assigned with deadlines.

December 2004

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INTRODUCTION

The advantages that are put forward for accelerator driven systems (ADS) – apart from their intrinsic low production of long-lived radioactive waste, and transmutation capability – are also enhanced safety characteristics and better long-term resources utilization (e.g., in connection with thorium fuels). Important R&D programmes are being undertaken by various institutions in many Member States to substantiate these claims and advance the basic knowledge in this innovative area of nuclear energy development. In response to expressed Member States' needs, the IAEA initiated [within the frame of the Nuclear Power technology Development Section project on *Technology Advances in Fast Reactors and Accelerator Driven Systems for Actinide and Long-lived Fission Product Transmutation* (http://www.iaea.org/inis/aws/fnss/)], a number of activities on utilization of plutonium and transmutation of long-lived radioactive waste, accelerator driven systems, thorium fuel options, innovative nuclear reactors and fuel cycles, non-conventional nuclear energy systems, and fusion/fission hybrids.

At various occasions (the most recent being the 2004 International Nuclear Data Conference held in Santa Fe, New Mexico), the groups involved in ADS neutronics calculations formulated their nuclear data needs. While there are, in some cases, still needs for additional nuclear data measurements, as well as theoretical data based on nuclear models, it is clearly perceived that the community also needs formatted cross section libraries for both deterministic and Monte Carlo codes.

The IAEA is initiating a collaborative effort between its Nuclear Data (ND) and Nuclear Power Technology Development (NPTD) Sections to contribute towards meeting these needs. Given that the NPTD Section is also starting a Coordinated Research Project (CRP) to benchmark and validate ADS computational tools through both inter-comparisons of the results of calculations, as well as with integral measurements [CRP on *Analytical and Experimental Benchmark Analyses of Accelerator Driven Systems (ADS)*], the production of application libraries for ADS neutronics analyses at this moment appears to be particularly timely, since it would allow, at the same time, to decouple the contribution to differences in computed results due to different methods from the influence of different data, and also to start the validation process for such application libraries.

Thus, the overall objective of the collaborative effort between the ND and NPTD Sections is to generate, in a first stage, limited scope application libraries for a number of code systems used in the analysis of ADS so that selected benchmark cases can be analyzed within the frame of the CRP mentioned above.

The specific objective of the present Technical Meeting was to define the library specifications, e.g., library formats, list of temperatures, list of background cross sections for self-shielding calculations, minimum list of materials necessary for the analysis of selected benchmark cases, etc.

CONCLUSIONS

Source of the evaluated nuclear data

The meeting concluded that it is necessary to prepare a "reference evaluated nuclear data file" that should contain a compilation of nuclide data based on the qualified selection from the various evaluated nuclear data files (ENDF/B-VI.8, JEF-3.1, JENDL-3.3, BROND-2.2, CENDL-2.1). The selection criteria should be clearly defined. The "reference nuclear evaluated data file" should contain also the data at intermediate energy, at least up to 150 MeV. It is preferable that the "reference nuclear evaluated data file" contains also covariance matrices. The data library should be readable by the ENDF processing tools, such as NJOY. The "reference evaluated nuclear data file" should be updated at regular time intervals of three years.

Codes for ADS analysis and corresponding cross section libraries

The participants noted that both Monte Carlo and deterministic codes are necessary for the neutronics analysis of the ADS, and that a diversity of codes exists today. It was concluded that it is important to give due consideration to this diversity, and that there is a need to prepare reference cross section libraries with group structure and continuous energy for Monte Carlo codes (ACE format), as well as group structure cross section libraries for deterministic codes (MATXS format). Ideally, the users would also need ready scripts for processing ENDF files into those libraries. The participants stressed that in addition to cross-section libraries for (sub-critical) core calculations, there is also the need for cross-section libraries for shielding or radiation protection calculations

Content of the cross-section libraries

The participants determined that the following reference cross-section libraries are required:

- Cross-section library for deterministic, broad-scope engineering ADS core design calculations (fast core driven by high energy spallation source)
- Multi-group as well as continuous energy cross-section libraries up to 150 MeV for ADS core design calculations using Monte-Carlo codes
- Cross-section libraries for ADS shielding calculations, both multi-group (for deterministic and for Monte Carlo codes), as well as continuous energy libraries (for Monte Carlo codes).

It is recognized that a stepwise creation of these cross-section libraries would be the best approach. In a first stage, the libraries should be restricted only to the materials needed for the benchmarking efforts linked to short and mid-term experimental results and design concepts. In a later stage, the inventory of these libraries will be extended to as many materials as requested by the ADS and waste transmutation problems.

Based on the on-going/planned experiments and design concepts YALINA, TRADE, SAD, TEF-P, TEF-T, RACE, and XT-ADS, the participants determined the following short list of nuclides:

- For fuel: $^{234, 235, 236, 238}$U, $^{238, 239, 240, 241, 242}$Pu, ^{237}Np, $^{241, 242m, 243}$Am, $^{242, 243, 244, 245, 246, 247}$Cm, O_2, N_2
- For coolants: Pb, Bi, He, H_2 , H_2O, ZrH, C
- For structural materials: Fe, Cr, Mo, Ti, V, Ni, Mn, B, Al, Zr, W, Ta, Mg

- For target materials: Hg

With regard to the temperature points to be considered, the participants agreed that the reference application libraries should consider the 3 – 4 temperature points in the interval from room temperature up to 1200 °C.

Procedure for producing the cross-section libraries

It was concluded that the most efficient way to produce the reference applications cross-section libraries is through an Expert Group. Specifically, four sub-groups should work in parallel and address the following tasks:

- Sub-Group to **analyse the various ADS benchmarks** that had been performed in the framework of IAEA, OECD/NEA, and EC. The output of this sub-group will be (a) synthetic conclusions on the state-of-the-art of the present discrepancies, and (b) recommendations for the benchmark definition, keeping in mind the objective of being representative of the short-term experimental results and design concepts. The working programme of this sub-group could be structured along the following lines:
  - Review of existing benchmark exercises
  - Selection of simple and well documented benchmarks for testing the first-stage reference cross-section libraries (format wise, or application wise)
  - Selection of the short list of the needed elements in the first-stage reference cross-section libraries
- Sub-group of nuclear data evaluators to **create the reference evaluated nuclear data file** that would serve as the starting point for the reference application cross-section libraries
- Sub-group of **cross-section libraries generators** which will have the task of generating the core physics continuous and multi-group libraries for Monte Carlo codes, the multi-group libraries for deterministic codes, as well as the shielding libraries for Monte Carlo and deterministic codes
- Sub-group for the proposed CRP on *Analytical and Experimental Benchmark Analyses of Accelerator Driven Systems (ADS)* which will have the task of **running the benchmarking effort** and reporting on the shortcomings of the libraries.

It was concluded that this procedure should apply for the first-stage, as well as for the stage in which the final full reference ADS cross-section libraries would be prepared.

Conclusions and recommendations for the work of the expert group

The meeting agreed on the following conclusions and recommendations with regard to the activities of the Expert Group:

- The benchmarking of codes and of the cross-section application libraries should be conducted in terms of energy separation below 20 MeV and full scope energy (up to 150 MeV)
- The benchmarking efforts should include sensitivity studies conducted for particular design concepts.
- It is preferable to involve code developers in the codes benchmarking efforts
- The activities of the Expert Group must be defined and implemented in a complementary and synergetic way with other ongoing IAEA, EC, and OECD/NEA projects

- The outcome of sub-group 1 (charged with analyzing the existing ADS benchmarks) and of sub-group 2 (charged with creating the evaluated nuclear data file) should include recommendations on the need for new nuclear data measurements. Already at this Technical Meeting, the participants noted that improved nuclear data of minor actinides, especially for radioactive targets and in particular for Am and Cm, are needed.

General recommendations

When implementing the IAEA activity under discussion (i.e., the production of reference application libraries for ADS studies), due consideration has to be given to on-going and long-term international R&D efforts and plans in the area of advanced nuclear systems for energy production and actinide utilization and transmutation.

At the Technical Meeting, the status of these R&D efforts was briefly summarized:

- Belarus

  YALINA ADS experimental programme

- China

  Program of basic research for ADS physics and related technology within the frame of the national energy "Basic Research Programme 973" sponsored by the China Ministry of Science and Technology

- EU

  IP EUROTRANS FP6 aiming at the demonstration of the feasibility of transmutation of high level waste through the ADS route
  IP NURESIM aiming at the creation of an integrated nuclear reactor simulation platform of deterministic and statistical codes covering a wide spread spectrum of topics from data treatment up to fuel cycle analysis
  RED-IMPACT assessing the impact of transmutation and reduction of nuclear waste on geological waste repositories
  MYRRHA experimental ADS design concept at SCK·CEN Mol

- India

  ADS-related projects and planning within the framework of thorium utilization schemes of India's nuclear power programme, involving three main R&D institutions (Bhabha Atomic Research Centre (BARC) at Mumbai, Variable Energy Cyclotron Centre (VECC) at Kolkata, and the Centre for Advanced Technology (CAT) at Indore)

- Japan

  ADS related programs within the J-PARC project (TEP and TEF facilities)
  Japanese consortium initiative for ADS technology

- Republic of Korea

  HYPER Project, aiming at the design of a large ADS transmuter
  DUPIC fuel development for waste management

- Russia

  Various ISTC projects related to nuclear data generation for ADS and innovative fuel cycles
  National programme related to new generation reactors (BREST, Pb-Bi modular reactor…)
  ADS experimental projects such as SAD (Sub-critical Assembly Dubna)

- USA

  AFCI, Advanced Fuel Cycle Initiative concentrating on innovative fuel development and present generation reactors fuel reprocessing,
  GEN IV
  Initiative for global reactor and fuel cycle simulation
  RACE initiative among five US universities aiming at the basic knowledge development and education in the ADS field
  SNS project

- International initiatives

  GEN IV International Forum
  INPRO

The participants formulated general recommendations that are summarized as follows:

- The IAEA should play a more active role in developing and supporting an ENDF processing code for preparing ACE format files
- Reference application cross-sections libraries with group structures and continuous energy for Monte Carlo codes (ACE format), as well as reference application cross-sections libraries with group structure for deterministic codes (MATXS format) should be prepared under IAEA aegis. Ideally, the Agency should also prepare ready scripts for processing ENDF files into those libraries. Specific cross-section libraries for core calculation and for shielding or radiation protection purposes should be prepared. Specifically, the following cross-section libraries should be prepared: (a) cross-section library for broad-scope engineering deterministic ADS core design calculations, (b) multi-group as well as continuous energy cross-section libraries up to 150 MeV for ADS core design calculations using Monte-Carlo codes, and (c) cross-section libraries for ADS shielding calculations, both multi-group (for deterministic and for Monte Carlo codes), as well as continuous energy libraries (for Monte Carlo codes)
- The libraries should be created for both thermal and fast spectrum systems

ACTION PLAN

Sub-Group Members

1. Review/analysis of ADS benchmarks

E. Gonzalez, CIEMAT
H. Aït Abderrahim, SCK·CEN
A. Ignatyuk, IPPE
Y. Kadi, CERN
W. Gudowski, KTH
S. Chigrinov, SOSNY
Japanese representative (to be proposed by T. Fukahori)
F. Mellier, CEA (to be confirmed)
US representative (proposed names E. Pitcher (LANL) or G. Palmiotti (ANL)
Y. Titarenko, ITEP
A. Stanculescu, IAEA

2. Review/preparation of an evaluated nuclear data file

A. Ignatyuk, IPPE
T. Fukahori, JAERI
A. Mengoni, CERN
A. Trkov, IAEA
Y. Shubin, IPPE
A. Koning, NRG
Y.O. Lee, KAERI
M. Chadwick, LANL

3. Preparation of the cross-section libraries

A. Trkov, IAEA
T. Fukahori, JAERI
Y. Kadi, CERN
S. Ganesan, BARC (to be confirmed)

4. Benchmarking

W. Gudowski, KTH
A. Lebrat, CEA (to be confirmed)
Y. Kadi, CERN
Th. Aoust, SCK·CEN
JAERI Representative (to be defined)
M. Carta, ENEA (to be confirmed)
E. Gonzalez, CIEMAT (C. Vicente to be confirmed)
Y. Batyaev, ITEP

Task assignments (by date)

Task	Responsible person	Deadline	Status
The sub-group on review/analysis of ADS benchmarks: to provide the short list of elements needed to treat the TARC, FEAT, and YALINA-2 benchmarks.	E. Gonzalez	31 January 2005	
Preparation of the TARC and FEAT benchmarks definition.	Y. Kadi	28 February 2005	
Preparation of the YALINA-2 benchmarks definition.	S. Chigrinov	28 February 2005	
The sub-group on review/preparation of an evaluated nuclear data file*:* to make the selection of the evaluated nuclear data to be used for the first stage cross-section libraries.	A. Ignatyuk	1 March 2005	
Review of the data of the two benchmarks defined above and proposal of the list of other benchmarks to be considered by the sub-group on review/analysis of ADS benchmarks.	E. Gonzalez This action is on the whole sub-group.	31 March 2005	
The sub-group on review/analysis of ADS benchmarks to submit a report to IAEA including: - Results of the review of existing benchmarks; - Conclusion on the TARC, FEAT, and YALINA-2 Benchmarks; - Definition of the next bench-marking activity and time schedule. - Recommendations for benchmarks to be performed within the frame of the IAEA CRP on *Analytical and Experimental Benchmark Analyses of Accelerator Driven Systems (ADS.)*	E. Gonzalez	31 March 2005	
The sub-group on review/analysis of ADS benchmarks, and the sub-group on review/preparation of an evaluated nuclear data file: to identify a first list of new nuclear data measurement needed for ADS and transmutation studies.	E. Gonzalez and A. Ignatyuk	31 March 2005	
The sub-group on the preparation of the cross-section libraries: to prepare the first stage cross-section libraries.	A. Trkov	30 April 2005	
The sub-group on benchmarking: to initiate the first benchmarks.	W. Gudowski	31 August 2005	

Appendix 1

International Atomic Energy Agency
Technical Meeting on
"Application Libraries for ADS and Transmutation"
IAEA Headquarters, Vienna, Austria
15 – 17 December 2004
Meeting Room A2774

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Appendix 2

International Atomic Energy Agency
Technical Meeting on
"Application Libraries for ADS and Transmutation"
IAEA Headquarters, Vienna, Austria
Meeting Room A 2774
15 – 17 December 2004

AGENDA

Objectives of the Technical Meeting (TM)

The overall objective of the TM is to provide guidelines to the Agency on the specifications and definitions needed to produce cross section libraries for ADS neutronics calculations. The libraries will constitute a package suitable to perform neutronics ADS simulations based on different codes (i.e., using different formats). All the libraries will be based on the same evaluated nuclear data files, thus allowing to identify the impact of different calculational methods on the integral parameters of an ADS through benchmark exercises, as planned, e.g., within the frame of the IAEA Coordinated Research Project CRP on "Analytical and Experimental Benchmark Analyses of Accelerator Driven Systems (ADS)" (to start in 2005).
The participants in the TM are asked to provide guidance to the Agency with regard to the following topics:

- Recommended source evaluated nuclear data library for generating the libraries
- Transport code(s) to be used for neutronics analysis: name, reference, availability from the NEA Data Bank, or from RSICC
- Format of the data library for each of the proposed neutronics analysis codes
- Can the data library be generated by data processing systems available from the NEA Data Bank or RSICC, e.g., NJOY?
- Minimum list of materials contained in the library (note: this is a pilot project for selected benchmarks; a full reference library can be generated later, based on the experience from the pilot project)
- Data processing specifications:
  - Temperature
  - Group structure
  - Background cross-section list for self-shielding

Wednesday, 15 December

08:30	**Registration** (IAEA registration desk, Gate 1)	
09:30	**Opening of the Meeting**	IAEA
	Introduction of participants	All
	Appointment of chairperson	IAEA
	Discussion and approval of the agenda	All
10:00	**Coffee break and Administrative Matters**	
11:00	**Presentation** of the scope of the IAEA initiative to produce cross section libraries for ADS neutronics calculations A. Trkov	
11:20	**Presentation** of the IAEA CRP on "Analytical and Experimental Benchmark Analyses of Accelerator Driven Systems (ADS)" A. Stanculescu	
11:40	**Discussion** on the scope and objectives of the Meeting	All
12:30	**Lunch break**	
	Technical presentations	
	Participants	
14:00 – 14:30	A. Stanculescu	
14:30 – 15:00	A. Ignatyuk	
15:00 – 15:45	Y. Kadi	
15:45 – 16:00	**Coffee Break**	
16:00 – 16:30	T. Fukahori, Nuclear Data	
16:30 – 17:00	A. Mengoni	
17:30	**Reception A23**	

Thursday, 16 December

	Technical presentations cont'd	
09:00 – 09:30	Y. Shubin, Intermediate Library	
09:30 – 10:00	V. Batyaev	
10:00 – 10:45	V. Shvetsov	
10:45 – 11:15	**Coffee Break**	
11:15 – 12:00	H. Ait Abderrahim	
12:00 – 13:30	**Lunch break**	
13:30 – 14:00	T. Fukahori	
14:00 – 14:30	E.M. Gonzalez-Romero (to be presented by A. Stanculescu)	
14:30 – 15:00	R. Klein Meulekamp	
15:00 – 17:00	**Discussions**, consolidation, summary of the specifications and definitions for the cross section libraries (Coffee break as appropriate)	All

Friday, 17 December

09:00 – 09:30	**Technical Presentations** cont'd S. Monti	
09:30 – 12:00	**Finalisation of Action Plan**	
	Drafting of the meeting report (Coffee break as appropriate)	All
~13:00	**Closing of the Meeting**	

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NDSONL for FTP access to files saved in "NDIS" Telnet session.