Computer Codes and Methods for Simulating Accelerator Driven Systems

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Abstract

A large set of computer codes and associated data libraries have been developed by nuclear research and industry over the past half century. A large number of them are in the public domain and can be obtained under agreed conditions from different Information Centres. The areas covered comprise: basic nuclear data and models, reactor spectra and cell calculations, static and dynamic reactor analysis, criticality, radiation shielding, dosimetry and material damage, fuel behaviour, safety and hazard analysis, heat conduction and fluid flow in reactor systems, spent fuel and waste management (handling, transportation, and storage), economics of fuel cycles, impact on the environment of nuclear activities etc. These codes and models have been developed mostly for critical systems used for research or power generation and other technological applications. Many of them have not been designed for accelerator driven systems (ADS), but with competent use, they can be used for studying such systems or can form the basis for adapting existing methods to the specific needs of ADS's.

The present paper describes the types of methods, codes and associated data available and their role in the applications. It provides Web addresses for facilitating searches for such tools. Some indications are given on the effect of non appropriate or 'blind' use of existing tools to ADS. Reference is made to available experimental data that can be used for validating the methods use. Finally, some international activities linked to the different computational aspects are described briefly.

Contents

Introduction: Can standard codes be used for ADS studies?

Power reactors and research reactors operate at a multiplication factor of $k_{eff} \approx 1$. The behaviour of a reactor in this status has been investigated very extensively, and reactors have been operated for several decades with a cumulative experience of many thousands of 'reactor years'. A large number of experiments were carried out in support of the design and operation of such reactors and were mostly tuned to the analysis of the critical state. Thus the nuclear data derived from experiments, the physics and the mathematical methods developed have focussed to a very large extent to presently operating systems.

Accelerator driven systems (ADS) are operated at a sub-critical state and the most frequent value of k_{eff} considered in this case is 0.95. This choice is linked to criticality safety issues and regulations. It is well known that a sub-critical system, in order to sustain a continuous neutron flux requires an 'external' source as the neutrons released through fission are not sufficient to sustain a chain reaction due to the fact that the neutron loss is higher than its production. The 'external' source becomes thus an essential component of the system. The external sources can be quite different in nature: a neutron source such as AmBe, d-t , neutrons produced by proton (or hadron) accelerators through spallation, the photo-fission neutrons induced by intensive gamma fields from electrons beams hitting heavy targets, etc.

In the ADS proposed or studied today the preferred external neutron source is the spallation source from proton accelerators, because of its high yield in neutrons. The sub-critical facility contains the spallation target made of material having high atomic mass, that has a large number of excess neutrons available when the nucleus is split up in spallation residues. The spallation source is surrounded by a sub-critical configuration with the purpose of multiplying the neutrons produced by the source. The closer to criticality this surrounding system is, the higher the neutron multiplication. When increasing the k_{eff} from say 0.95 to 1.00 the neutron multiplication increases from 20 to 'infinity'. A critical reactor is thus a most powerful neutron multiplier.

As most nuclear data, reactor physics and computational methods were developed for critical reactors, ***how can we apply these tools for ADS systems? Are they suitable? To what extent? What should be done so that we are not fooled by the results from their use?***

Several equations needed for studying the system behaviour in general (i.e. the macroscopic result of many microscopic phenomena) do not need further

development compared to those used for critical reactors as they are general enough; examples are equations describing the mechanical behaviour, the conduction of heat and flow of fluids. Some computer codes may have though 'specific hard-wired' elements or data included used for present systems. These must be adapted or generalised to cover a larger scope (e.g. Pb/Bi instead of Na as coolant). There are other equations and codes that are not directly applicable to ADS. A very important element at this early stage of studies and development of ADS is the proper understanding of the physics equations and the investigation of their properties that describe the neutrons populating the system.

The equations describing the very basic phenomena such as interaction of the neutron, photon, proton, electron, e.g. Schrödinger / Dirac equations, in nuclear model codes need to be extended to the energy ranges covered by the spallation source. As the proton beam is in the 1 GeV range, intra-nuclear cascade models need to be used covering a number of more 'exotic' particles produced in these interactions. The neutron spectrum of a spallation source is much 'harder' than the one of fission and fusion devices. Therefore nuclear models applicable to energies beyond those used for reactor and fusion applications need to be used. Only the lower energy part is covered by some of the existing codes.

The neutron transport equation as applied to fissionable systems also requires further analysis. The homogeneous radiation transport or Boltzmann equation, having $1/k_{eff}$ as the eigenvalue, is the one most widely known and used, but if used in connection with an external source requires a closer look to understand its meaning. This equation has as 'eigenvector' the fundamental mode observed in critical reactors. k_{eff} is a convenient scale for criticality safety **calculations** as it is often the parameter used to determine safety margins. In a sub-critical system however the 'eigenvector' calculated represents a distribution in which the neutron production is artificially increased by the $1/k_{eff}$ factor, thus biasing the neutron distribution of the actual system. In a sub-critical system k_{eff} is kind of an artifice, for computing a reactivity scale. The homogeneous transport equation is still widely used, because of its convenience when using with existing computer codes and because of the familiarity many researches have with it. The actual neutron distribution in an external source driven system can be very different from the fundamental mode of the homogeneous balance equation. The shape of the external source is the more influential, the more the system is sub-critical. Neutron populations in strongly sub-critical systems remember where they come from and as we approach criticality due to the large multiplication and the increasing number of subsequent neutron generations the shape of the source is forgotten. Neutron populations in a critical system have no recall of the source (they have gone through a large number of generations), they populate the system

with a distribution determined by the fundamental mode of the homogeneous critical equation.

The neutrons of an external source driven sub-critical system follow distributions made of super-positions of the fundamental and many higher modes, not of the homogeneous equation, but of the inhomogeneous equation containing the external source term. The eigenvalues of the inhomogeneous equations are very different from the $1/k_{eff}$ of the homogeneous equation. The fundamental eigenvalue of the prompt neutrons is known as the α-Rossi, that is negative for systems below prompt critical. The fundamental eigenvalues of the delayed neutrons are close but not identical to the delayed neutron precursor decay constant. The fundamental eigenvectors of prompt and delayed neutrons are not identical and differ from the one of the homogeneous equation with $1/k_{eff}$. A closer look at the Boltzmann equation including the delayed neutrons shows that there are large numbers of higher mode eigenvalues for both prompt and delayed neutron populations. The eigenvalues of the lower modes are all real, but for higher modes we find a continuum of eigenvalues in the complex domain. Studies on the properties of these equations have been published extensively in the late Sixties / early Seventies in Nuclear Science and Engineering.

A new form of multiplication factor (source multiplication factor k_S) has been introduced for assessing the integral behaviour of ADS. This factor is different from k_{eff} in that it contains the higher modes excited by the source and converges to 1 when approaching criticality as does k_{eff}. It represents a different criticality scale considered more appropriate for ADS. k_S does not represent an eigenvalue of an equation. It represents the factor by which the neutron loss must be reduced to balance the insufficient number of neutrons produced by fission. Formulations of couplings between k_{eff} and k_S have been made. Such couplings can only be calculated, not measured. In fact functions of the homogeneous and inhomogeneous equations are used concurrently in such formulations; both cannot represent the actual neutronic behaviour, but are convenient for analyses of such systems.

The models we use in computer codes and the associated data libraries contain somehow the cumulative knowledge acquired during several decades of research. These do a good job if used by qualified staff in the parameter range for which they were validated and qualified. This was done by comparing the computed predictions with the results of ‘integral’ experiments, i.e. data describing some macroscopic quantities of the system. In essence our ‘prediction’ with computer code models is valid as long as it consists in ‘interpolating’ between sound knowledge we have accumulated. Calculations

outside that range are ‘extrapolations’ into the unknown. The results may be reasonable with some luck but we are moving in this case into ‘forecasting’ that may well be of the quality of the weather forecasting we see daily in the media. In essence, with ADS systems we move to some unknown ground, an area very interesting and challenging for research. But all new models developed for describing its ‘neutronic’ / ‘photonic’ behaviour must be validated against experiments that cover the parameter space of ADS. A sound mistrust should animate users of standard codes when they look at results from calculations and investigate to what extent their calculation represents the system in reality. Another source of caution concerns the following: computer codes provide in most cases only the result of the ‘expected’ value without any confidence bounds. For engineering and safety applications, confidence bounds and margins need to be quantified. Therefore sensitivity and uncertainty analysis should be integral part of design studies that go beyond just scoping with some parameter variations. Codes for carrying out such work exist, but again some extension of scope may well be required.

Role of Modelling Tools

When studying applications in nuclear technology we need to understand and be able to predict the behaviour of systems manufactured by human enterprise. First, the underlying basic physical and chemical phenomena need to be understood. We have then to predict the results from the interplay of the large number of the different basic events: i.e. the macroscopic effects. In order to be able to build confidence in our modelling capability, we need then to compare these results against measurements carried out on such systems. The different levels of modelling require the solution of different types of equations using different type of parameters. The tools required for carrying out a complete validated analysis are:

- The basic nuclear or chemical data
- The computer codes, and
- The integral experiments.

This article describes the role each component plays in a computational scheme designed for modelling purposes. It describes also which tools have been developed and are internationally available.

Tools Required for Modelling

The three basic components required for modelling in nuclear energy applications are:

1. **basic nuclear data, material properties data, chemical-thermodynamics data and derived application data libraries, group constants, continuous energy data.** The basic particle interaction data is described in numerical form in ***evaluated nuclear data*** libraries such as ENDF/B-VI, JEF-2, JENDL-3 and others. These libraries are very general and describe within the energy range considered (10^{-5} - $2 \cdot 10^{7}$ eV with some extensions to $1.5 \cdot 10^{8}$ eV) all basic phenomena (neutron interaction cross-section, photon production, photon interaction cross-section, fission yields and radioactive decay data). These contain information in great detail and in a form not directly usable by computer codes. There is consequently a need to filter out relevant information and to condense it to a form appropriate for applications (e.g. multi-group cross-section libraries, continuous energy cross-section libraries, etc.). The computer code system most widely used for that purpose is NJOY.

   Detailed information on these data can be found for example by visiting the following Web sites:

   USA: http://www.nndc.bnl.gov/ (National Nuclear Data Center-Brookhaven - NNDC)
   http://epicws.epm.ornl.gov/rsic.html (RSICC)
   http://t2.lanl.gov/data/data.html (LANL)

   Europe: http://www.nea.fr/html/dbdata/ (OECD/NEA Data Bank)
   http://www-nds.iaea.or.at/ (Nuclear Data Centre IAEA)
   http://csnwww.in2p3.fr/amdc/ (Atomic Mass Data Centre)

   Japan: http://cracker.tokai.jaeri.go.jp/index.html (JAERI Nuclear Data Center)

   Other basic data such as TDB (***chemical thermodynamics*** data needed for speciation studies - http://www.nea.fr/html/dbtdb/) and MATPRO (http://www.nrc.gov/RES/SCDAP/nrc.html) for ***material properties*** are available. Many other basic data are distributed together with the computer codes using them.

2. **computer codes carrying out different modelling aspects such as:**

   - nuclear models (URL: http://www.nea.fr/html/dbprog/nucmod.htm)
   - experimental data processing (http://www.nea.fr/html/dbprog/cpsabs_o.html)

- basic and evaluated data processing,(http://www.nea.fr/html/dbprog/categ-a.html)
- spectral calculations, reactor cells and lattices (http://www.nea.fr/html/dbprog/cpsabs_b.html)
- multi-dimensional radiation transport, criticality , power distributions (http://www.nea.fr/html/dbprog/cpsabs_c.html)
- radiation shielding, heating and damage (http://www.nea.fr/html/dbprog/cpsabs_j.html)
- isotopic inventories, burn-up and build-up (http://www.nea.fr/html/dbprog/cpsabs_d.html)
- in-core fuel management, economic aspects of the fuel cycle, optimisation (ditto)
- reactor dynamics, coupling of neutronics and thermal-hydraulics (http://www.nea.fr/html/dbprog/cpsabs_f.html)
- heat transfer and fluid flow, (http://www.nea.fr/html/dbprog/cpsabs_h.html)
- fuel behaviour , (http://www.nea.fr/html/dbprog/cpsabs_i.html)
- deformations, stress and structural analysis, (http://www.nea.fr/html/dbprog/cpsabs_i.html)
- radiological safety, hazard and accident analysis (http://www.nea.fr/html/dbprog/cpsabs_g.html)
- environmental impact, confinement and dispersion in geosphere, biosphere and atmosphere (http://www.nea.fr/html/dbprog/categ-r.html)

The computer codes used in most nuclear applications have the role of bridging the gap between the underlying microscopic phenomena and the macroscopic effects. They also accumulate, in a readily usable way using a mathematical and algorithmic language, the wealth of physics knowledge that science and technology have acquired during the last half century. In many cases these computer codes can have a relatively complex structure: in addition to several modular codes they also contain associated data libraries (for generic applications or project oriented), application dependent code/data sequences, test problems, etc.

Many computer codes for nuclear applications are in the public domain, but there is also proprietary software that is widely used. The best sources for computer codes in the nuclear energy fields are as follows:

USA: ESTSC (Energy Science and Technology Software Center – DOE-OSTI Oak Ridge)
http://www.osti.gov/estsc/
RSICC (Radiation Safety Information Computational Center – ORNL Oak Ridge)
http://www-rsicc.ornl.gov/rsic.html

International: OECD/NEA Data Bank – France
(http://www.nea.fr/html/dbprog/)
A computerised and searchable program abstracts database is available free of charge on CD-ROM.

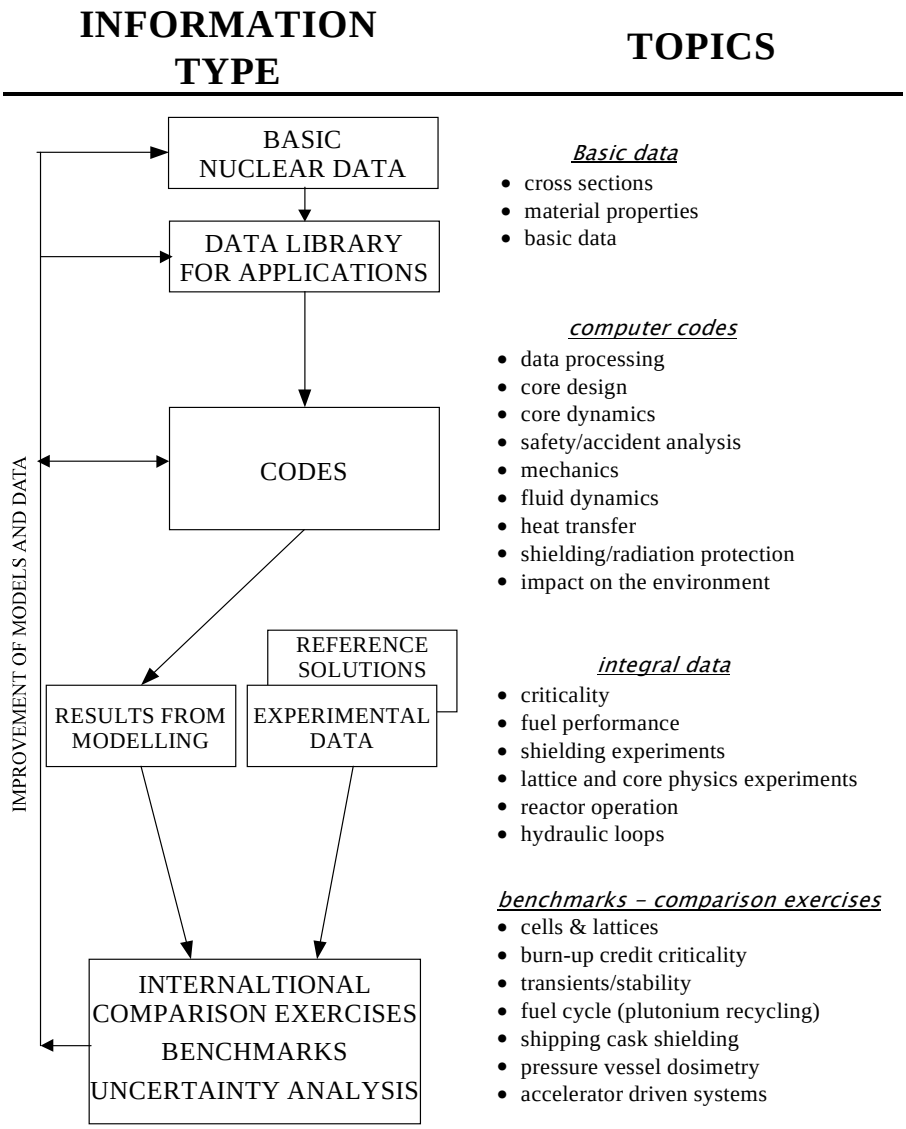
These codes, before they are released, are subject to a series of tests, model validation and benchmarking. Their scope includes practically all the important aspects of modelling in nuclear technology applications.

3. integral experiments data bases

- radiation shielding experiments
- criticality experiments
- reactor core and lattice experiments
- thin and thick target yields
- data from reactor operation
- fuel behaviour experiments
- thermal hydraulic loops experiments
- seismic and material strength data bases

Integral experiments are the references needed for model development, verification, and validation.

Fig. 1: Procedures, Data and Computer Codes for Model Validation and Improvement



International Benchmark Studies

What is a benchmark?

The term means a fixed 'point of reference' used in comparisons. For our purpose it can take two different forms:

1. ***theoretical benchmark***, an 'exact' reference to a specified precision, obtained by solving mathematical equations describing a physical phenomenon or process. While a theoretical benchmark is an exact solution to a mathematical problem, it does not make statements about the precision in predicting the physical phenomenon itself. It simply asserts what the measure of the physical phenomenon would be if the equations represented exactly the physical world. Theoretical benchmarks are used essentially to validate approximations inherent to algorithms used in large computer codes and their correct coding,
2. ***experimental benchmark***, a well designed and instrumented measurement, addressing a well-defined physical phenomenon or aspect thereof. Some of them are called 'clean' because the experimental set-up used contains few and relatively simple components, which facilitates meeting the objective of unfolding the requested data. It consists of a precise description of the apparatus, geometrical set-up and data analysis tools. The experimental benchmark data have associated uncertainties, the derivation of which is precisely documented. Experimental benchmarks are needed to validate the physics models used in the computer codes together with the associated basic data used to describe for instance the microscopic phenomena underlying the macroscopic behaviour. They are normally used to check the correct ***integral*** behaviour of algorithms and the basic data working together.

Both types of benchmarks are widely used. They have a complementary function. Theoretical benchmarks often cover also aspects, which would otherwise be difficult or too expensive to measure. The community concerned with establishing well qualified computing tools for the design and operation of nuclear technology facilities has established international co-operations to facilitate the comparison of their methodologies. International comparison exercises (called also standard problems) have been designed covering the diverse needs of methods validation. The purpose of such comparison exercises is twofold:

- familiarisation with working methods and assumptions made by experts from different teams

· assessing the own skills in modelling, gaining experience and building confidence in the methods used

Role of code comparison and benchmarks

Essentially three elements are required to ensure modelling tools meet the requirements of nuclear industry and licensing needs:

- state of the art computer code design and programming according to quality assurance principles
- quality assurance in maintenance of the code
- model assessment and validation of codes through benchmarking and code comparison exercises.

There is a further element of different nature. Even though a code has undergone the best development and validation praxis, the quality of the results depend in the end from the user. Therefore user qualification through training courses is essential. One of the best training methodologies is benchmarking and comparison with others. In such a procedure much is learned about how a well-defined problem can be translated into input to a code. The sensitivity and uncertainty analysis that normally goes with benchmarks give much insight into the role basic data used, the implication of their uncertainty onto the results, in other words a wealth of understanding is achieved.

Over the years the OECD/NEA NSC has organised a large number and comprehensive set of international comparison exercises. A list is provided as Annex I. They have been instrumental for achieving model improvements and ensure a common understanding of modelling issues. More recently, two theoretical benchmarks relevant for ADS have been organised by the OECD/NEA.

The first benchmark exercise, initiated in 1994, was based on a transmutation strategy involving light water reactors, fast reactors and an accelerator-driven system (ADS). For the ADS, a sodium-cooled system with a tungsten target and MA-Pu nitride fuel, was analysed by JAERI (Japan), PSI (Switzerland) and IPPE (Russian Federation). The basic nuclear data used were JENDL-3.2 by JAERI, JEF-2.2 by PSI, and FOND-2 based ABBN-93 by IPPE. In the analysis of the spallation neutron in the energy range from 1 GeV to 15-20 MeV, the NMTC/JAERI, HETC-PSI, and HETC codes were used, respectively. For the nuclear data processing, NJOY, MILER, and BONAMI-S were applied by JAERI, NJOY, MICROR, and MICROX-2 by PSI, and CONSYST2 by IPPE. All the three institutions used the two-dimensional S_N code TWODANT for simulating the sub-critical core. However, they used different energy group

structures (73 groups for JAERI, 33 for PSI, and 28 for IPPE). Burn-up calculations were made by using the BURNER (JAERI), 2DTB (PSI) and CARE (IPPE) codes. Considerable differences in calculated initial k_{eff} values and burn-up reactivity swings indicated a need for refining the benchmark specification and continuing the exercise with a wider participation. The full results of the benchmark can be found in the OECD/NEA report [NEA/NSC/DOC(2000)6].

The benchmark was therefore launched in July 1999 to resolve the discrepancies observed in the previous exercise and to check the performances of reactor codes and nuclear data for ADS with unconventional fuel and coolant. A model of a lead-bismuth cooled sub-critical system driven by a beam of 1 GeV protons was chosen for the exercise. The choice of lead-bismuth as a coolant and target material reflects the increased interest in this technology. Since emphasis was on code and data validation in the energy region below 20 MeV, a standard spallation neutron source spectrum and distribution was prescribed and distributed to participants. The spallation neutron source was produced with the PSI version of HETC assuming a proton energy of 1 GeV and a beam radius of 10 cm. Seven solutions from ANL (USA), CIEMAT (Spain), KAERI (Korea), JAERI (Japan), PSI/CEA (Switzerland and France), RIT (Sweden) and SCK-CEN (Belgium) were contributed. The list of basic libraries, codes and methods used are summarised in the Table below.

Organisation	Basic library	Codes used	Method
ANL (USA)	ENDF/B-VI ENDF/B-V for lumped FP	MC^2-2, TWODANT, REBUS-3	Deterministic
CIEMAT (Spain)	JENDL-3.2 ENDF/B-VI for fission yields	EVOLCODE system (NJOY, MCNP-4B, ORIGEN-2.1)	Monte Carlo
KAERI (Korea)	JEF-2.2 JENDL-3.2 for Pb and ^{242m}Am	TRANSX-2.15, TWODANT, DIF3D-7.0, REBUS-3	Deterministic
JAERI (Japan)	JENDL-3.2	ATRAS (SCALE, TWODANT, BURNER, ORIGEN-2)	Deterministic
PSI/CEA (CH/France)	ERALIB I (JEF-2.2 based)	ERANOS, ORIHET	Deterministic
RIT (Sweden)	JEF-2.2	NJOY, MCNP-4B, MCB, ORIGEN-2	Monte Carlo
SCK-CEN (Belgium)	JEF-2.2 ENDF/B-VI for Pb and ^{233}U	NJOY97.95, MCNP-4B, ORIGEN-2 and BATEMAN2	Monte Carlo

The analysis of the results showed significant discrepancies in important neutronic parameters such as one-group microscopic cross-sections, k_{inf}, initial k_{eff}, burn-up reactivity swing, flux distribution and safety parameters. Strong discrepancies appear also in the estimation of the external neutron source, an

important parameter for an ADS because it determines the requested accelerator power.

The discrepancies were mainly due to deficiencies in the nuclear data of actinides which are abundant in minor actinide dominated cores but do not significantly influence the reaction rate balance of conventional MOX cores. However, the impact of the different nuclear data could not fully explain the discrepancies observed in the results. In future benchmark exercises, attention should therefore be given to both the data processing route and the neutron transport approximations. Concerning the burn-up calculations, attention should be given to the treatment of the fission products and to the actinide decay chains, taking into account that minor actinide burner cores feature unusual fuel compositions.

The causes for many of these discrepancies still require clarification, and efforts in this direction should continue if the calculation tools are to be applied to detailed design calculations for minor actinide dominated ADS cores. A benchmark based on experimental results would be necessary to better understand the origin of discrepancies observed. A complete analysis of the results can be found in an OECD/NEA report [NEA/NSC/DOC(2001)13].

As a follow-up to the two theoretical benchmarks mentioned above, the OECD/NEA developed a benchmark based on the MUSE-4 experiments in co-operation with CIEMAT (Spain) and CEA (France). This “Benchmark on Computer Simulation of MASURCA Critical and Sub-critical Experiments (MUSE-4 Benchmark)” will be performed during 2002. The benchmark is divided in three steps. The first step will allow understanding the simulation methods of the different groups and tuning of the simulations programs with the experimental data of one already measured configuration (COSMO). In the second step, the MUSE-4 reference configuration will be modelled investigating different reactor parameters (criticality constant, flux distribution, etc.) in a nearly critical configuration. The third step is oriented to the simulation of reactor response to the external source in the sub-critical reference configuration. Static parameters are also considered in this sub-critical reference configuration. A wide participation is expected for this first experiment-based ADS benchmark and the latest version of deterministic and Monte Carlo codes will be used together with the state-of-the-art nuclear data sets.

Integral Experiments Data Bases

The assessment of calculation tools and the validation of nuclear data performance have been crucial issues of Reactor Physics, Shielding, Criticality Safety etc. for Reactor and Fuel Cycle installation design. In most countries with significant nuclear power activities, research and development institutes, often with the support of the nuclear industry, have been developing an approach of global method and data validation, using integral experiments. These experiments have been designed according to two main "philosophies": a) to muck-up the reference configuration (core, shielding, storage lattice etc.) b) to analytically investigate separated basic phenomena. In both approaches, highly sophisticated experimental techniques have been developed and used in order to reduce uncertainties and to allow the definition of resulting bias factors, design margin or cross-section adjustments, which could have a clear impact on cost reductions and safety improvement.

A very large number of these integral experiments have been performed in the last forty years and they have contributed in an essential way to the present state-of-the-art in designing existing reactors or fuel cycle installations. Results from these experiments remain of great value today, as they provide the record on which development and validation of present data and methods are based.

Moreover these data represent a cultural and scientific heritage of high relevance. In fact this information will certainly be extremely useful in the future in assessing promising new concepts, whenever the further development of nuclear energy takes off again. The gap between the old and new generations of experimenters is growing and special attention should be given to the transfer of this heritage of the old generation to the new ones.

The OECD/NEA Nuclear Science Committee (NSC) has identified the need to establish international databases containing all the important experiments that are available for sharing among the specialists. The NSC has set up or sponsored specific activities to achieve this. The aim is to preserve them in an agreed standard format in computer accessible form, to use them for international activities involving validation of current and new calculational schemes including computer codes and nuclear data libraries, for assessing uncertainties, confidence bounds and safety margins, and to record measurement methods and techniques.

Integral experiments concern measurements on a system consisting of different components. The measured values are the macroscopic behaviour of the system

(e.g. attenuation of dose through a complex shield, level of reactivity of a reactor or a spent fuel transportation cask, decay heat, level of burnup, etc.). They allow to gauge the combined use of computational methods and basic data used to the real world values. At the beginning of nuclear reactor development, computational methods were still in their infancy, the models used did not include sufficient knowledge to make reliable predictions. Integral experiments were then 'the reference' to be used for any design.

Integral experiments come with clearly stated and documented uncertainties in the form of confidence bounds of the measured values and a correlation matrix describing the relative independence of the measurements carried out. An integral experiment is complete if it includes a final phase of interpretation of the results. The interpretation is the part that gives insight into the phenomena and into the way they are appropriately modelled.

Computer codes and basic nuclear data have been thoroughly checked on a number of cases, be it known reference solutions or experiments. However, the number of possible combinations of their use is so big that a large and possibly comprehensive database of well-characterised experiments is needed. With such databases sufficient confidence can be built that methods and procedures used for design, operation and safety analysis are adequate.

Nuclear industries and licensing authorities need to be able to rely on the good performance of computer programs and nuclear data in all important nuclear energy calculations. It is important that the methods and data issued should be internationally accepted. This is best achieved by validation and benchmarking on an international scale, with all countries concerned participating in the testing.

List of different integral databases

In the following a few integral databases are described that have been established through the OECD/NEA:

FUEL BEHAVIOUR

A Public Domain Database on Nuclear Fuel Performance or the Purpose of Code Development and Validation (IFPE)

Visit → http://www.nea.fr/html/science/fuel/ifpelst.html

CRITICALITY SAFETY

International Criticality Safety Benchmark Evaluation Project (ICSBEP)

Visit → http://icsbep.inel.gov/icsbep/

THERMAL HYDRAULICS IN NUCLEAR POWER PLANT

CSNI Code Validation Matrix of Thermal-Hydraulic Codes for LWR LOCA and Transients (CCVM)

Visit → http://www.nea.fr/html/dbprog/ccvm/

REACTOR PHYSICS

Reactor lattice and core experiments (IRPhE)

Visit → http://www.inel.gov/energy/nuclear/irphep/

RADIATION SHIELDING EXPERIMENTS (SINBAD)

Visit → http://www.nea.fr/html/science/shielding/

COMPUTER CODES SPECIFICALLY ADDRESSING HIGH ENERGY PARTICLES PHENOMENA or USEFUL IN ADS STUDIES

(Distributed by RSICC, OECD/NEA Data Bank or ESTSC)

Nuclear Models :

- **ALICE91 (PSR-0146)** precompound/compound nuclear decay model
- **CEM95 (IAEA1247)** MC calculation of nuclear reactions (Cascade Exciton Model)
- **DWBA98 (NEA-1209)**, The distorted wave Born approximation (DWBA) is used.
- **EMPIRE-II (IAEA1169),** calculates nuclear reactions in the frame of combined optical, Multistep Direct (TUL), Multistep Compound (NVWY) and statistical (Hauser-Feshbach) models.
- **GNASH-FKK (PSR-0125)** multi-step direct and compound and Hauser-Feshbach models
- **HETC NMTC (CCC-0178)** MC high energy nucleon meson cascade transport
- **HETC-KFA (CCC-0496)** MC high energy nucleon-meson cascades
- **ISABEL (NEA 1413)** intra-nuclear cascade model allowing hydrogen and helium ions and antiprotons as projectiles
- **MECC-7 (CCC-0156)** medium energy intra-nuclear cascade model

- **NMTC/JAERI97** (**NEA-0974)** high-energy p, n, π reaction M-C simulation
- **PICA (CCC-0160)** MC nuclear cascade reactions by the collision of photons (30 < E < 400 MeV) with nuclei

Evaluated Nuclear Data processing

- **NJOY99 (PSR-0480),**: a comprehensive nuclear data processing computer code system for producing continuous-energy and multi-group neutron, photon, and charged particle cross sections from ENDF format evaluated nuclear data
- **TRANSX (PSR-0317)** code to produce neutron, photon transport tables for discrete ordinates and diffusion codes

Radiation Transport / Evaluation (Stochastic)

- **CALOR95 (CCC-0610),** High-Energy Calorimeter Design & Data Evaluation By M-C
- **CASIM (NESC0742)** MC high energy cascades in complex shields
- **LAHET 2.8 (CCC-0696)** Code System for High Energy Particle Transport Calculations.
- **MCNPX (CCC-0705),** Monte Carlo Code System for Multiparticle & High Energy Applications

Radiation Transport / Evaluation (Deterministic)

- **DANTSYS (CCC-0547)** 1-D, 2-D, 3-D Sn neutron, photon transport
- **DIF3D 8.0/VARIANT8.0 (CCC-0649),** 2-D 3-D multigroup diffusion/transport theory nodal & finite difference solver, variational method
- **DOORS3.2 (CCC-0650)** discrete ordinates system for deep penetration neutron and gamma transport
- **MOSRA-LIGHT (NEA-1633),** High Speed 3-D x-y-z Nodal Diffusion Code for Vector Computers
- **TORT (CCC-0543)** 3-D S_N n, photon transport with deep penetration

Sensitivity / Uncertainty Analysis

- **SUSD-3D (NEA-1628),** 1-, 2-, 3-Dimensional Cross Section Sensitivity and Uncertainty Code

Burnup codes

- **MONTEBURNS 1.0 (PSR-0455):** An Automated, Multi-Step Monte Carlo Burnup Code System.
- **REBUS3/VARIANT8.0 (CCC-0653),** Code System for Analysis of Fast Reactor Fuel Cycles.

Radiation damage:

- **MARLOWE15 (PSR-0137),** The MARLOWE program simulates atomic collisions in crystalline targets using the binary collision approximation
- **SRIM2000 (NEA-0919),** stopping power & range of ions in matter
- **SPECTER-ANL (PSR-0263)** damage for material irradiation
- **RECOIL/B (DLC-0055)** heavy charged particle recoil spectra lib. for radiation damage

Sources from decay

- **SOURCES4A (CCC-0661),** Calculating (α, n), spontaneous fission, (β,n), delayed neutron sources & spectra

Charged particle interaction / ranges

- **ASTROS (CCC-0073)** primary/secondary proton dose in sphere/slab tissue
- **LPPC (CCC-0051)** proton penetration, slab
- **LRSPC(CCC-0050)** range and stopping power calculator
- **PTRAN (CCC-0618)** MC proton transport for 50 to 250 MeV
- **STARCODES (PSR-0330),** stopping-power and range tables for electrons, protons, and α
- **LPSC (CCC-0064)** p, n flux, spectra behind slab shield from p irradiation

Medium-High-Energy data

- **EPDL-VI/MOD (USCD1187)** photon interaction x-sections library (10 eV to 100 GeV)
- **HILO86R (DLC-0187)** 66 N, 22 γ-group cross-sections, up to 400 MeV (neutron) and 20 MeV (γ)
- **LA100 (DLC-0168)** evaluated data library for n, p up to 100 MeV, ENDF-6 format
- **LAHIMACK (DLC-0128)** multi-group neutron and γ cross-sections up to 800 MeV
- **LEP (DLC-0001)** results from intra-nuclear cascade and evaporation
- **MCNPXDATA (DLC-0205),** Neutron, Photon, and Electron Data Libraries for MCNPX.
- **MENDL-2P (IAEA1376),** Proton Medium Energy Nuclear Data Library
- **MENSLIB (DLC-0084)** neutron 60 group cross-sections, E<60MeV
- **PNESD (IAEA1235)** elastic cross-sections of 3 MeV to 1000 MeV protons on natural isotopes
- **XCOM (DLC-0174)** photon cross-sections from 1 keV to 100 GeV

NOTE: This list does not address codes for safety and hazard analysis as this can be carried out to a large extent with methods used for reactor applications. Codes coupling neutronics and thermal / hydraulics have been omitted. In sub-critical systems such couplings are weak or negligible. However these should be used for ADS approaching criticality (k_{eff} ~0.98-0.99).

For the studying the behaviour of ADS in the spectral range of reactors or fusion systems, a wealth of other codes exist and can be found by searching the Internet sites e.g. of RSICC and the OECD/NEA Data Bank.

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