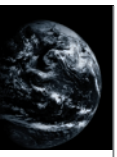
PHYSICAL AND CHEMICAL SCIENCES

PROGRAMME OBJECTIVE

To promote research and development in specific applications of nuclear, physical and chemical sciences for solving practical problems in the fields of energy, environment, nuclear medicine, material sciences and industry; and to enhance the utilization of existing research reactors and accelerators and help national analytical laboratories in acquiring skills in international quality in their analytical measurements.



OVERVIEW

A significant outcome of the Agency's activities in the physical and chemical sciences programme was the preparation of the first international library on photonuclear data, which has important medical and shielding applications. A charged particle reaction data library for medical cyclotrons was also completed. Scientists in Member States continued to make increasing use of the nuclear data centre of the Agency. A new software package was produced for gamma ray spectrometry and distributed to many Member States. Work on nuclear technologies for humanitarian demining was initiated. Training in nuclear instrumentation continued to be provided to developing Member States. The research reactor database was made available on the Internet. New technetium-99m based radiopharmaceuticals for tumour imaging were developed. Emphasis was also placed on good manufacturing practices and quality assurance (QA) methodology in making radiopharmaceuticals. In radioanalytical analysis, there was increasing emphasis on introducing quality control and QA procedures in Member State laboratories. In the area of nuclear fusion, the Agency assisted in the formulation of a revised Memorandum of Understanding between the European Union, the Russian Federation and Japan on work related to the International Thermonuclear Experimental Reactor (ITER) project.

NUCLEAR AND ATOMIC DATA FOR APPLICATIONS

Use of the Agency's nuclear data services by scientists in Member States showed steady growth. As shown in the table below, the number of individual data retrievals via the Internet (*http://www-nds.iaea.or.at*) from the continuously updated main nuclear databases (containing compiled experimental nuclear data and evaluated data libraries from national projects) increased by more than 30% in 1999. Telnet based retrievals, after a decrease in 1998 owing to rising competition from more user friendly Web interface, stabilized at a level of about 2000 retrievals per year, indicating that Telnet based interactive data retrieval tools are still preferred by a number of users, most likely those with low capacity Internet connections.

The Agency has developed the capability to produce and distribute CD-ROM versions of all of its main nuclear data databases. Through the use of this medium, users not connected to the Internet can avail themselves of fast desktop access to the same data available from the nuclear data server at the time that the CD-ROM was produced. In addition, the CD-ROM is the medium preferred by scientists working with large data libraries with relatively static content. A good example is the very large FENDL-2 library. As shown in the table below, the number of CD-ROMs distributed in response to individual data requests doubled in 1999.

The number of off-line retrievals, which include mainly responses to requests for printed material, increased by 15% in 1999. In an attempt to contain costs, about 50% of all reports in the INDC(NDS) series have been made available on the Internet. More than 1200 such reports were downloaded by users in 1999. Informal reports, containing short summary descriptions of the available services, databases and data processing codes, have also been made available on the Internet.

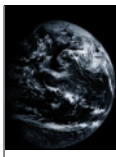
As a result of co-operation with other nuclear data centres, a new reactor dosimetry file, 'RRDF-98', and a library of evaluated cross-sections of nuclear interactions between light charged particles were made available to users. This file can be used to 'unfold' the spectra of neutrons incident on a reactor pressure vessel (RPV) to deduce neutron induced lattice displacements. Such information is important for the assessment of the lifetime of the RPV. The library can also be used in fusion and astrophysical applications.

A new computer package, 'ZVView', designed for interactive graphical display of nuclear reaction cross-sections retrieved from Agency experimental and evaluated nuclear databases, was made available. Also, a new program was developed to facilitate the display of statistical information concerning Internet access to Agency services, broken down, for example, by data topic or geographical region. This provides valuable feedback on the evolving requirements of data users.

A CRP on the compilation and evaluation of photonuclear data for applications was completed, with the final Research Co-ordination meeting held in Tokyo in October. The project produced the first international library of photonuclear data, with information on 164 isotopes of importance for medical,

Dissemination of Nuclear Data

	1995	1996	1997	1998	1999
Retrievals from main Internet nuclear databases	—	—	40	6830	8970
Telnet based nuclear data retrievals	4400	5700	7350	2700	2180
Information on CD-ROMS	—	—	—	205	420
Off-line retrievals	1550	800	1900	1995	2290



shielding and other applications in a format suitable for transport calculations.

A new CRP on the development of a database for prompt gamma ray neutron activation analysis was initiated. The database, to be developed in both electronic and printed forms, will include the most recent data on 80 elements, such as capture gamma ray energies, intensities, k_0 factors and neutron cross-sections, and will extend the capabilities of this powerful analytical technique. Because the technique does not rely on the creation of a long lived activation product, it is useful for imaging practically any element, including important light elements such as hydrogen and carbon, in applications such as materials science, food analysis, medicine and the environment.

A charged particle cross-section database for medical radioisotope production was completed. The database includes 26 reactions for the most important diagnostic radioisotopes and 22 beam monitor reactions which are of importance for users of more than 200 medical cyclotrons.

Support was provided to two technical co-operation projects whose goal was to enhance regional use of Agency and local nuclear data services. The first was a regional project to establish a mirror site of the Agency's on-line nuclear data services in São Paulo, Brazil, to serve users in Latin American and Caribbean countries. In addition to providing improved services, the mirror server will be used as a training facility for future technical co-operation workshops and courses. The other project concerned greater utilization of the Ghana research reactor, with the focus on creating a local area network to provide nuclear data services at the reactor facility.

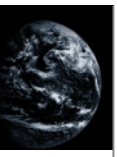
A major numerical database for atomic and molecular data applications was completed for electron impact processes on excited hydrogen molecules and their isotopes. Collision processes in these systems play an important role in the kinetics of low temperature plasmas. In collaboration with the FOM-Institute for Atomic and Molecular Physics in Amsterdam, a new, critically assessed atomic database for the electron impact excitation of helium atoms was completed. These data will be used by fusion plasma modellers and reactor engineers and will also be used for diagnostic studies in low temperature plasmas.

NUCLEAR INSTRUMENTATION

The final Research Co-ordination meeting for a CRP on software utilities for gamma ray spectrometry was held in October. The CRP dealt with the basic applications of nuclear data handling and with new PC computer codes and libraries for gamma ray spectrometry. As a

Reference Input Parameter Library for Nuclear Reaction Modelling

Evaluators of nuclear data in Member States make substantial use of nuclear physics calculations in order to correctly interpolate between available measurements and to ensure that the final recommended values satisfy physics requirements, such as conservation of energy. The main theoretical methods used in evaluating nuclear reaction data below 100 MeV are based on optical and statistical models. Such calculations must be supplied with a large number of input 'parameters', inferred from extensive comparisons of theoretical predictions with data measurements. In an effort to formalize this process of parameter selection, and thereby improve the quality and consistency of nuclear data evaluations, a CRP was conducted to develop a Reference Input Parameter Library (RIPL). The primary output of this CRP is the 'RIPL Starter File', describing nuclear reactions due to incident neutrons, protons and gamma rays, as well as hydrogen–2, –3, and helium–3 and –4 nuclei. RIPL is documented in an Agency technical document (IAEA-TECDOC-1034), which contains a full description of the library and includes the basis of the parameter selection. The topics covered include: atomic masses and deformations; discrete level schemes; average neutron resonance parameters; optical model parameters; level densities; gamma ray strength functions; and continuum angular distributions. ■



result of this CRP, new software packages were developed for: measurements involving low level sodium iodide spectra; gamma ray spectra from high purity germanium detectors; Doppler broadened annihilation peaks; gamma ray libraries; true coincidence corrections; efficiency calculation for large sources; and library driven analysis of gamma ray spectra. These new computer codes will help Member States make more accurate measurements of materials constituents in many fields, such as physics, chemistry, life sciences, industry, archaeology and environmental monitoring.

A new CRP on the application of nuclear techniques to anti-personnel land mines was initiated in 1999. The first Research Co-ordination meeting was held in Zagreb, Croatia. The meeting emphasized the potential of nuclear based methods for the identification of land mines and pointed out the possibility of combining nuclear sensors with other methods for the localization of such buried objects.

Work at the Agency's Laboratories at Seibersdorf included:

- Establishment of training facilities for the design and repair of electronic modules based on surface mounted technology (SMT);
- Development of educational kits for training in nuclear electronics, including SMT and photovoltaic kits (based on solar energy) for instruments with switch mode power supplies;
- Development and testing of an original scanning system (including hardware and software) for large volume cadium–zinc–telluride detectors applied to portable gamma spectrometry;
- Construction of miniature power supplies for in-field gamma spectrometry applications and improvements to hardware and software for a new generation of hand held radiation monitors;
- Development and implementation of a Windows 95/NT software package for a total reflection X ray fluorescence (XRF) module;
- Adaptation for practical application of optimum XRF sample preparation procedures, and training provided in parts per billion concentration measurements of iodide and arsenic in water samples.

UTILIZATION OF RESEARCH REACTORS AND LOW ENERGY ACCELERATORS

With 60% of all research reactors in the world being 30 years or older, the issue of ageing is of increasing concern. To address this and other related subjects, the Agency held an international symposium on research reactor utilization, safety and management near Lisbon in September. Age induced problems such as corrosion, irradiation damage effects and reduced component reliability were identified as key areas requiring active in-service inspection programmes. In addition, the importance of proper documentation and advance planning for decommissioning was stressed for ageing reactors. The symposium also highlighted the fact that more new research reactors are now being planned, designed and built than at any time in the recent past, with most being of higher power (i.e. approximately 20 MW). In a changing environment, many of these facilities need to develop a strategic plan, with input from all concerned, in order to remain viable. Another issue of concern in the research reactor community is the handling of spent fuel, particularly in light of the planned cessation by the USA of its fuel repatriation programme by mid-2006. In practice, this may force many otherwise productive research reactors to close down because of the lack of any suitable alternative fuel disposal options. It was emphasized that for many research reactors, only the eventual implementation of regional or international facilities for the interim storage and eventual disposal of spent fuel would permit their continued operation.

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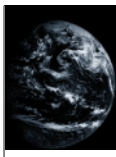


At a Technical Committee meeting in Debrecen, Hungary, in October, on the applications of accelerator based neutron sources, the recent development of small portable 'sealed tube' electrostatic neutron generators was reviewed. The potential of these types of sources in fields such as humanitarian demining, elemental analysis and industry was emphasized. In many cases a neutron source of a sealed tube or inertial electrostatic confinement type could replace an isotopic neutron source, thereby minimizing the risk of radioactive contamination of the environment.

A Technical Committee meeting was held in June in Vienna on current issues in neutron capture therapy (NCT). This was a timely meeting since some operators of research reactors are considering involvement in this area. The meeting highlighted the fact that this is still an unproven therapy, and that there is little need for more facilities to spend the large amounts of money necessary to set up NCT clinical trials.

Work in support of technical co-operation activities included monitoring of projects dealing with the utilization of research reactors and accelerators, and assistance to neutron beam utilization projects and to projects related to new reactors. A significant outcome from one research reactor project was the development of a neutron diffraction beam in Greece, which will be used in research work sponsored by the European Union.

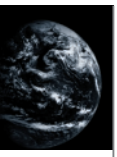
RADIOCHEMICAL APPLICATIONS

At an international seminar on therapeutic applications of radiopharmaceuticals, organized in Hyderabad, India, in January, current developments and future trends of this promising nuclear medicine modality were reviewed. In particular, the use of beta and alpha particle radionuclide emitters tagged to biomolecule carriers, such as monoclonal antibodies and peptides, was emphasized.

The current status of and future trends in target and processing technologies for cyclotron production of medically important radionuclides were reviewed using the services of consultants. Recognizing the needs of developing countries which have established cyclotron centres for radionuclide production, it was concluded that further development and research were required to improve solid target preparation techniques. This in turn would contribute to better utilization of cyclotron facilities and greater availability of important radionuclides such as palladium-103, which has become an extremely important radionuclide for the treatment of prostate cancer when incorporated into sealed sources.

Technetium-99m Labelled Peptides for Tumour Imaging

The introduction of indium-111–octreotide for imaging neuro-endocrine tumours marked a new turn in radiopharmaceutical development, opening up the vast potential of peptide based agents for diagnosis and therapy. However, indium-111–octreotide is not ideal for imaging studies and is also expensive and not available in countries that do not have cyclotrons. The availability of technetium-99m–octreotide will make this technique available in almost all countries at an affordable cost. Developing such an agent based on the octreotide analogue was the aim of a CRP which was concluded in 1999. The results of work carried out in laboratories in Europe, Asia and Latin America resulted in the development of a promising technetium-99m complex, which exhibits similar properties to indium-111–octreotide in laboratory studies. This compound has shown comparable if not better images in preliminary studies in patients. The work carried out in this CRP has paved the way for the use of technetium-99m–octreotide analogues and extended the benefits of the imaging procedure to all parts of the world. The CRP also helped many participants from developing countries acquire expertise in current interdisciplinary areas of radiopharmaceutical R&D, including peptide conjugation and purification, technetium-99m labelling of the conjugate, HPLC techniques for purification and radiochemical analysis, in vitro receptor binding and ligand displacement assays and animal biodistribution studies. ■



A significant milestone was the inauguration in November of a cyclotron–PET centre in Prague, the first of its kind in Eastern Europe. Developed as part of an Agency technical co-operation project, this centre features dedicated radiochemical facilities for the production of a metabolic tracer widely used in cardiology and oncology. It is planned to produce and distribute this tracer to hospitals in the Czech Republic.

Analytical data for the certification of two algae reference materials (IAEA-392 and IAEA-413) were reviewed. The results indicate that the certification exercise was a success and that both materials can be certified for approximately 20 elements.

Work in the field of chemistry at the Agency's Laboratories at Seibersdorf included: a quality system following the guidelines of ISO-17025; assistance to laboratories in Member States in Eastern Europe to establish and/or improve their level of quality assurance through the establishment of a quality system; participation in a workshop for auditors and preparation of proficiency test material to evaluate the performance of these laboratories.

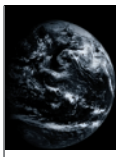
PLASMA PHYSICS APPLICATIONS AND CONTROLLED FUSION RESEARCH

Controlled fusion research activities are carried out in around 50 Agency Member States to develop a new energy source using the nuclear fusion reactions that power the sun and the stars. To promote international collaboration that will be of benefit to a significant number of Member States in selected areas of plasma physics and controlled fusion research and development, the Agency provides assistance through a variety of activities such as the convening of conferences, technical meetings and CRPs. These activities: facilitate the exchange of technical information; foster co-operation between major laboratories and developing Member States; promote spin-off applications; help developing Member States strengthen their research programmes; and provide support for the ITER Engineering Design Activities.

A Technical Committee meeting on first principle based transport theory, held in Kloster Seeon, Germany, in June, provided a forum for discussion of a wide range of plasma physics theories that aim to predict the rate of heat loss ('transport') from a magnetically confined thermonuclear plasma. Three dimensional computer simulations of plasma particle motion using millions of grid points show the occurrence of plasma 'streamers' or 'zonal flows' that cross the magnetic field, causing rapid local heat flows. The plasma theory is now able to predict the conditions under which 'internal transport barriers' reduce the plasma heat loss rate, resulting in better operation. A summary of the meeting is being published in the Agency's *Nuclear Fusion* journal.

Another Technical Committee meeting on electron cyclotron resonance heating (ECRH) physics and technology for fusion devices was held in Oarai, Japan, in October. ECRH may be used in the future to reduce tearing modes, to suppress sawtooth oscillations, and to help sustain internal transport barriers in tokamaks. After microwave heat pulses are injected into a plasma, the thermal diffusivity can be calculated from the rate at which the heat pulse spreads. Several laboratories are working to develop gyrotrons that can generate about 1 MW steady state with good efficiency (i.e. >30%). Diamond windows are being developed because their low microwave absorption and high thermal conductivity permit them to transmit much higher power than ordinary windows without cracking.

Control, data acquisition and remote participation for fusion research formed the subject of a Technical Committee meeting held in Lisbon in June. A large variety of plasma and machine control systems as well as remote handling systems were presented from many experiments. In addition, reports were presented on new Internet based user interfaces providing complete read/write access to entry tables for authorized users via common browsers. There was consensus that unification of the different systems was needed to facilitate remote collaboration in



fusion research, because all major experiments in operation and those currently under construction support multiple groups interactively participating in ongoing experiments from off-site locations.

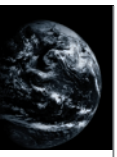
H-mode (high confinement) physics/transport barriers in magnetically confined fusion plasmas were studied in a Technical Committee meeting held in Oxford, United Kingdom, in September. Results indicated improved confinement and stability performance with internal and edge transport barriers in various devices in long pulse discharges with reversed magnetic shear through a large number of control schemes. The transport barrier which exists at the plasma edge in high confinement regimes is now recognized to be as important as the global energy confinement. The goal for the near future is to reproduce favourable 'small' edge localized mode regimes in several experimental devices with different plasma sizes and parameters before the extrapolation to ITER is implemented. High density *H*-mode operation with high field side pellet refuelling allows both good *H*-mode confinement and high plasma density near the empirical Greenwald density limit. Such operation could provide significant advantages for a fusion reactor.

"Key results achieved in environmental applications of plasma assisted discharges included the development and field testing of a prototype plasma pyrolysis system for the treatment of medical wastes."

Energetic particles in magnetic confinement systems were discussed at a Technical Committee meeting in Naka, Japan, in October. The status of runaway electrons produced during disruptions in tokamak plasmas has changed from being an innocuous phenomenon, mainly used to probe magnetic turbulence, to a serious threat to the first wall of future large tokamaks. Reliable avoidance schemes need to be validated for application to ITER. Present theoretical investigations will contribute to the development of the neoclassical theory of fast ions; a non-linear kinetic fluid model was developed that includes kinetic effects of all particle species in high beta plasmas. Several questions still have to be resolved experimentally and theoretically. One concerns runaway electrons: how many electrons will be accelerated, how are they confined, and what can be expected for the electron impact to the first wall of tokamaks. The second question is on fast ions. Many aspects of fast ion behaviour in tokamaks are well understood, but their confinement properties in stellarators need further clarification, as does the role of kinetic and non-linear Alfvén instabilities in magnetic confinement systems.

A finding at a Technical Committee meeting on research using small fusion devices, held in October in Chengdu, China, was that improved machine and diagnostic performance of the HL-1M tokamak resulted in improved confinement and reproducibility of the plasma discharges; the diagnostic systems were also improved. Another finding was that supersonic and helium molecular beam injection experiments showed promising results, and gas doping for impurity transport studies seemed to play an important role for the understanding of the control mechanisms of fusion plasmas. Magnetohydrodynamic studies using Mirnov coils and heavy ion beam probes of the plasma edge were also reported. Measurements with Mirnov coils showed that magnetic turbulences are composed of two components: broadband fluctuations caused by microinstabilities and coherent modes, the latter associated with the rotation of an $m = 2$ magnetic island within the plasma column. A new phenomenon was observed in the single trajectory of an injected heavy ion beam: the sample volume — the area of secondary ionization allowing plasma potential measurements — was split up into two volumes.

A Technical Committee meeting on steady state operation of magnetic fusion devices was held in Fukuoka, Japan, in October. The topics included: long pulse tokamak and stellarator discharges andadvanced configurations;



required technologies for long pulse operation of magnetic fusion devices; plasma facing components; heating and current drive scenarios; control systems, diagnostics for long pulse operation; theory; and modelling. Reports were presented on several new devices currently under construction that will have pulse lengths from 300 to 1000 seconds and plasma currents of 1 to 2 MA, similar to the planned pulse length of the ITER tokamak. Results from the TRIAM-1M tokamak show a regime of enhanced confinement and current drive efficiency by careful tuning of the heating power. The results achieved at the Large Helical Device show steadily increasing performance, with pulse lengths of up to 35 seconds at high power. There were also reports on a comprehensive model developed for transport and electron current drive that is able to describe low confinement modes and reduced transport for low/reversed shear and high poloidal beta required for internal transport control, a key issue for plasma control in ITER. A summary of the meeting and selected papers will be published in the *Nuclear Fusion* journal.

The final Research Co-ordination meeting for a CRP on engineering, industrial and environmental applications of plasma physics and fusion technologies was held in November in Vienna. Among the topics addressed were: plasma assisted surface engineering for enhanced surface properties in laboratory and industry; application of plasma technologies for the processing of hazardous wastes in gaseous, liquid and solid forms; interaction between low temperature plasma and fusion technology; and basic physics studies on these topics. One result of the CRP was greater inter-laboratory collaboration and opportunities for the training of students from developing countries. Key results achieved in environmental applications of plasma assisted discharges included: the development and field testing of a prototype plasma pyrolysis system for the treatment of medical wastes; and the construction of a silent dielectric barrier discharge device as a cheap ozone gas generator. The latter system has been tested in treating sewage water from biological organisms, cleaning coal from sulphur compounds and removing water vapour from the natural gas that accompanies oil.