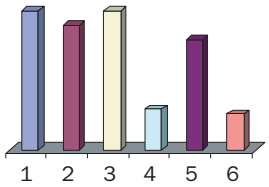
PHYSICAL AND CHEMICAL SCIENCES

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.

Regular budget expenditure: $8 273 873
Extrabudgetary programme expenditure (not included in chart): $13 485



1. Nuclear and Atomic Data for Applications: $1 955 333
2. Nuclear Instrumentation: $1 747 334.
3. Theoretical Physics (contribution): $1 950 000
4. Utilization of Research Reactors and Particle Accelerators: $574 362
5. Radiochemical Applications: $1 543 047
6. Plasma Physics Applications and Controlled Fusion Research: $503 797

OVERVIEW

The Agency continued its global role of providing up to date nuclear and atomic data for use in all facets of nuclear science and technology, through the World Wide Web, CD-ROMs and Telnet retrievals. The setting up of a 'mirror site' in Brazil has been completed and this will greatly benefit scientists in the Latin American and Caribbean region. Injections of charged particle beams is a common mode of plasma heating in fusion devices, and a CRP on the topic resulted in the production of a data set for charge exchange cross sections. Special materials are used on the walls of fusion reactors that face plasma and the results of a CRP on this topic will provide valuable data on plasma-material interaction.

Individuals from Member State in East Asia and Latin America were trained in the operation and maintenance of nuclear electronics; educational kits were developed for this purpose. Two technical documents on the applications of research reactors and on strategic planning for their use will help improve the utilization of research reactors. The results of a CRP provided valuable information on the use of ion beams for optoelectronic and semiconductor materials and devices. Another CRP advanced the field of peptide based radiopharmaceuticals labelled with cyclotron produced radioisotopes. Indigenous capabilities in producing kits for the assay of prostate specific antigen (PSA), and other tumour markers, were built up in Member States through a CRP. A document on good manufacturing practices (GMP) in radiopharmaceutical production was completed and is expected to be included in a WHO manual on this subject. Radioanalytical chemistry and archaeology were combined for the first time in a CRP devoted to archaeological investigations in the Latin America region. The Agency continued to help Member States in introducing quality assurance and quality control measures in their radioanalytical laboratories and encouraged them to obtain ISO accreditation when involved in the commercial endeavours. In the field of plasma physics and controlled fusion research, steady progress is being made towards construction of the International Thermonuclear Experimental Reactor (ITER). The parties involved have requested that activities related to the phase of design adaptation to specific site conditions continue under the Agency's auspices.

NUCLEAR AND ATOMIC DATA FOR APPLICATIONS

The Agency focused its efforts on providing Member States with convenient and cost free access to the numerical nuclear and atomic data needed for the development and maintenance of nuclear technologies and applications. These applications rely on accurate and up to date data to provide a realistic description of the underlying physical processes. After dramatic annual increases in usage in the first years following the introduction of Web based on-line services for the main nuclear databases, the number of user retrievals from the Agency's nuclear data server (*http://www-nds.iaea.org/*) stabilized this year at a constant level. However, retrievals from specialized data libraries and files created in the framework of CRPs and similar projects show a steady increase in user access. There has also been steady growth in off-line requests for data products prepared by the Agency. These trends in the patterns of use of the Agency nuclear data services are summarized in Table I.

An Agency mirror site at the Nuclear and Energy Research Institute of Brazil (IPEN) began operation. Implemented through a technical co-operation project for Latin America and the Caribbean, the site has the same capabilities for nuclear data search and retrieval as the main Agency data server in Vienna and offers much faster access to data for many users in the region, especially in Brazil. With improved connectivity of Latin American and Caribbean regional networks, this site will also benefit other countries of the region. Overall, there is a clear trend in the growth of the number of users from developing countries (see Fig. 1)

Data distributed on CD-ROMs are regularly updated and interface programs have been developed that provide a quality of access to the data similar to on-line services. A test CD-ROM version of the EXFOR database of experimental reaction cross-sections implemented as a relational database, containing extended searching and interactive plotting capabilities, was prepared and distributed to co-operating data centres for evaluation. Other CD-ROMs that were distributed by the Agency include: a new version of CINDA containing a bibliographical index on microscopic neutron data; updated pre-processing codes for evaluated nuclear data files (PREPRO2000); a new release of the ENDF/B-VI library of evaluated cross-sections and the JENDL library of neutron dosimetry reaction cross-sections.

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TABLE I. **DISSEMINATION OF NUCLEAR DATA BY THE AGENCY**

	1996	1997	1998	1999	2000
Retrievals through the Web from main nuclear databases	—	23	4276	9581	9642
Telnet based nuclear data retrievals	5700	7350	2700	2180	1387
Information on CD-ROMs	—	—	205	420	648
Off-line retrievals	800	1900	1995	2290	2557
Accesses through the Web to other files and information materials	—	4400	7413	7757	11472

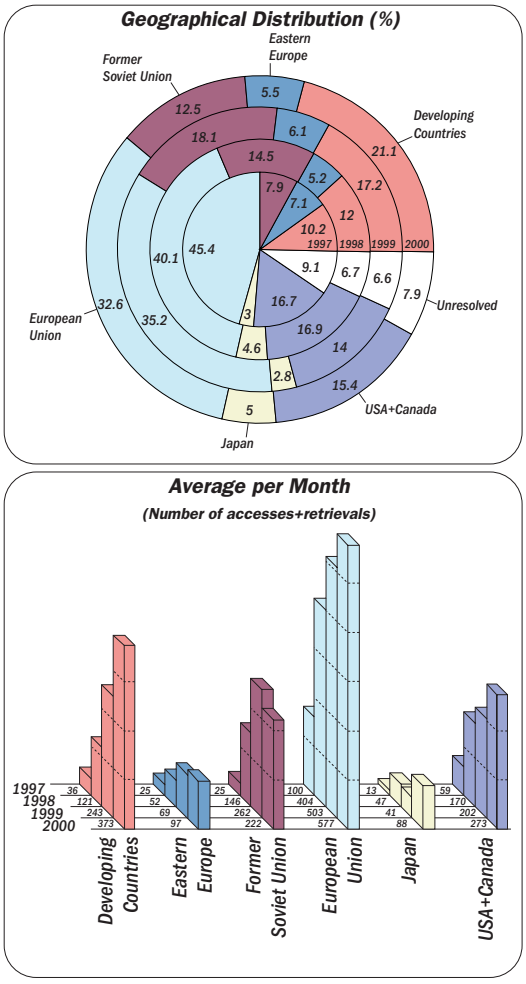

FIG. 1. Developing countries represent the second largest group of users (after the countries of the European Union) of the Agency's nuclear data server, accounting for more than 20% of all data retrievals and accesses. The figure shows Internet statistics for the Agency's nuclear data services, including the mirror server at IPEN.

A new project on the development of platform independent solutions for network shared nuclear databases began in co-operation with other data centres. The objective of this effort in database programming and data access is to broaden the participation of co-operating data centres working on different platforms (including PCs). The technology will also permit access to nuclear data services over local networks, which is important for isolated laboratories in developing countries with inadequate access to the Internet.

A large amount of data on the chemical erosion of wall materials of fusion devices was added to the on-line Atomic and Molecular (A+M) Data Information System, AMDIS. These data, the output of a recently completed CRP, are highly important in the modelling of nuclear fusion reactor experiments around the world. The results represent a major step forward in the amount and accuracy of such data. And two databases for physical sputtering and radiation enhanced sublimation for beryllium, carbon and tungsten and related compounds were completed in 2000.

A CRP on charge-exchange cross-section data for fusion plasma studies that ended in 2000 produced particularly important data in the modelling of beams injected into plasmas generated in nuclear fusion experimental devices. The data include results of experimental measurements and theoretical calculations that are especially important in validating theoretical models. A notable feature of this CRP was the use of some of the best experimental techniques available in the field.

NUCLEAR INSTRUMENTATION

The objective of a CRP that started in 2000 is to develop and foster the application of alpha particle spectrometry. Benefits will include better instrumental systems, Frisch-grid ionization chambers for large area samples, software for alpha spectrum analysis and the development of natural reference materials for alpha spectrometry.

An Advisory Group report concluded that nuclear techniques are well suited to determine whether a buried object contains an explosive. Nuclear sensors, because of their specificity to explosives, can therefore be used on a multi-sensor platform to provide confirmation of the presence of explosives. In this connection, the Agency described the possibilities and advantages of using nuclear techniques for humanitarian demining at two meetings of the Standing Committee of Experts on Technologies for Mine Action, a working group within the Ottawa Treaty.

Through its laboratories at Seibersdorf, the Agency provides essential support and transfers technology to Member States. Significant activities in 2000 included:

- New educational kits for training in nuclear electronics, including power supplies, micro-controllers and protection instruments.
- Developing power supply and control systems for portable X ray fluorescence (XRF) spectrometers.
- Developing and testing of a portable XRF spectrometer based on a low power X ray tube and thermoelectrically cooled semiconductor detector. The spectrometer can be used to study art objects.
- Developing a database to store the results of experiments obtained by using an automatic scanning system for large area detectors.
- Adapting selected commercially available information and communication technology based training tools for nuclear electronics and the maintenance/repair of surface mounted technology based instruments.
- Installing and assessing an energy dispersive XRF system based on a high voltage X ray tube.
- Assessing a backscatter fundamental parameter method for quantitative in situ XRF analysis.
- Establishing a worldwide information network for XRF laboratories

UTILIZATION OF RESEARCH REACTORS AND PARTICLE ACCELERATORS

The focus of activities in 2000 was on developing a set of documents and information services to enable the reactor manager to effectively deal with the current environment. In this regard, the Research Reactor Database included, for the first time, quantitative research reactor utilization information in order to track the effectiveness of Agency activities in this area.

The goal of an innovative new CRP is to pair mentor research reactor facilities with recipient institutions to expand the use of small angle neutron scattering (SANS). The paired facilities will work together on developing aspects of SANS to make it applicable to a broader range of facilities, such as those with lower power, or in harsher environments where support services for high technology equipment are not available.

Another new CRP will examine the use of ion beam techniques for the analysis of light elements in thin films, including depth profiling. The first Research Co-ordination meeting emphasized the importance of ion beam techniques in providing unique information in important materials research areas such as corrosion degradation, and the role of light elements like hydrogen, carbon, nitrogen and oxygen on the electrical and structural properties of advanced materials.

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Finally, a CRP on the application of MeV ion beams for the development and characterization of semiconductor materials helped the participating laboratories to significantly improve their analytical capability for materials characterization. Another benefit was greater collaboration between participating research groups, resulting in many scientific journal publications in the fields of optoelectronic characterization of semiconductor materials and devices, elemental characterization of thin semiconductor films, and defect transformations in semiconductors. In addition, several participating laboratories significantly improved their analytical capability for materials characterization.

At the Agency's Laboratories at Seibersdorf, an electronic version of the Accelerator Database was developed and is available on the

Agency's Web site (*http://www.iaea.org/worldatom/*). In addition, archaeological samples were analysed under an agreement with the Ruder Boskovic Institute in Zagreb.

RADIOCHEMICAL APPLICATIONS

Diagnostic and therapeutic radionuclides produced in cyclotrons are finding increasing use in nuclear medicine. Improved and more economical production procedures and efficient methods of target recovery will increase their availability and reduce costs. In order to realize this objective, a new CRP was started to develop improved targets for the production of iodine-123, iodine-124, palladium-103 and thallium-201.

"Assay of serum PSA (prostate specific antigen) levels is a valuable adjunct to the diagnosis and management of patients with prostate cancer ..."

A CRP on the optimization of synthesis and quality control procedures for the preparation of fluorine-18 and iodine-123 labelled peptides ended in 2000. The participants investigated improved synthetic routes for the production of prosthetic groups, including procedures for their purification and quality control. Three new peptides were identified, synthesized, radiolabelled and evaluated in vitro and in vivo. Among the radiopharmaceuticals tested, one holds significant promise and can lead to a new generation of somatostatin receptor specific agents.

Infectious diseases remain a major health problem and cause of death worldwide, particularly in developing countries. Nuclear medicine imaging, because of its sensitivity, offers an attractive option for the diagnosis of focal infections. A new CRP on the development of kits for technetium-99m radiopharmaceuticals for infection imaging has the goal of developing technetium-99m labelled compounds with better specificity and faster blood clearance, needed for clinical use

Assay of serum PSA (prostate specific antigen) levels is a valuable adjunct to the diagnosis and management of patients with prostate cancer, the second most prevalent cancer in males. Doctors recommend annual PSA tests in conjunction with digital rectal examinations in males over the age of 50. The local capability to produce PSA assay kits in sufficient quantities and at a reasonable cost is crucial for undertaking such screening programmes in developing countries. A CRP that ended in 2000 built on earlier expertise acquired in developing radioimmunometric assays for hormones generated in national laboratories. Among the main achievements: (i) a methodology was developed for the purification of PSA from seminal plasma, (ii) anti-PSA secreting hybridomas were produced; (iii) matched pair monoclonal antibodies (MoAbs) for use in the assays were obtained; and (iv) other key assay reagents including PSA standards, iodine-125 labelled MoAb tracer and MoAb coated tubes, were produced. In addition, the CRP participants developed PSA–immunoradiometric assay (IRMA) kits using reagents and validated them against imported kits. With this expertise, the participants will be able to produce IRMA kits for total and free PSA at an affordable cost to meet national and even regional demands, in addition to developing such kits for other tumour markers.

In regional technical co-operation projects in Europe and Latin America on quality assurance/quality control for nuclear analytical laboratories, counterparts were requested to submit regular progress reports, participate in proficiency tests and accept external audit inspections. The goal of these projects — to assist Member State laboratories establish a complete quality system in compliance with the ISO/IEC 17025 — was largely achieved

A recently completed CRP, carried out with the participation of the Smithsonian Institution in the USA, combined for the first time trace element analysis with archaeological investigations. A well established technique involving pattern recognition and 'fingerprint-

ing' through instrumental nuclear activation analysis was introduced to a number of laboratories in various Latin American countries to determine the provenance of ancient pottery. The CRP opened up new fields of application of nuclear sciences. Specifically, partnerships between users of the analytical data (the archaeologist) and the analyst were established. National teams were formed comprising analytical scientists and archaeologists to formulate the working hypothesis, collect and prepare samples, analyse the materials and evaluate the data sets.

In order to meet the need for reliable analytical tools in speciation analysis, isotopic and nuclear techniques must be used for validation and method development. Accordingly, a new CRP was started on the development and validation of speciation analysis using nuclear techniques for the method validation of arsenic, selenium and chromium species in aqueous media. The goal of this CRP is to establish recommended and validated speciation tools for use the laboratories of developing Member States.

PLASMA PHYSICS APPLICATIONS AND CONTROLLED FUSION RESEARCH

Through its work in plasma physics and fusion research, the Agency continued to: facilitate technical information exchange; 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 (EDA). Work related to the ITER EDA facilitates execution of the ITER project and the dissemination of technical information on EDA results, which also benefits developing Member States.

Participants at the 18th Agency Fusion Energy Conference in Sorrento, Italy, reported that several tokamak experiments (DIII-D, JET, JT-60U, ASDEX-U, TEXTOR and HT-7) had exceeded the theoretical plasma density limit (the "Greenwald limit"). Such experiments also demonstrated the creation of a plasma region with reduced heat loss rate (an "internal transport barrier"), which improves the plasma energy balance. Pellets of solid hydrogen have been injected to sustain plasma density. The injection of powerful atomic beams, radio waves or microwaves has been shown to help sustain the plasma current and enhance plasma stability. Impressive results were also achieved in stellarator experiments, especially the superconducting Large Helical Device (LHD).

In inertial fusion energy (IFE) power plants, powerful laser beams or ion beams compress pea sized fuel pellets to a point where intense nuclear fusion reactions occur, resulting in small explosions. If these explosions are confined in a blast chamber and repeated

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several times per second, heat and electricity are generated. On the basis of recent experimental success, IFE is now at the stage where significant benefits can be obtained from international co-operation. A new CRP on the elements of power plant design for IFE will help resolve such key interface issues as the:

- Driver/target interface (focusing and beam uniformity required by the target);
- Driver/chamber interface (final optics, magnet protection, shielding);
- Target/chamber interface (target survival during injection, target positioning and tracking).

This CRP will also assess the systems integration and environmental, safety and economic aspects of IFE power plants.

At a Technical Committee meeting in Chengdu, China, on the applications of fusion energy research to science and technology, various industrial and societal benefits, or

spin-offs, of fusion research were highlighted. For example:

- Hybrid diesel-electric engines first used in the Joint European Torus power supplies are now operating in the "Altrobus" in Italy;
- Patented microcalorimeters developed for fusion research are now being used in industrial plasmas;
- Electronic equipment developed for Langmuir probe diagnostics in fusion research are now being applied to space plasma research;
- Theoretical models (e.g. solution of Fokker–Planck equations) developed for plasma investigations are now being applied in financial modelling.

A Technical Committee meeting in Madrid provided a forum for the discussion of IFE target and chamber investigations worldwide. The key technical issues for successful pellet compression are the uniform illumination of the pellets by smoothed laser beams and the uniformity and sphericity of the fuel pellets. Among the topics discussed were: blast chamber technologies; chamber/laser interfaces; target injection; system integration; and safety and environmental issues. The meeting also helped to develop collaborations between small and large laboratories.