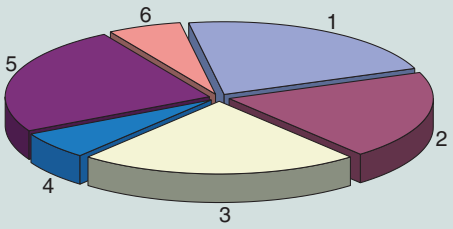
APPLICATIONS OF PHYSICAL AND CHEMICAL SCIENCES

PROGRAMME OBJECTIVE

To enhance the contribution of a wide spectrum of nuclear technologies in meeting the needs of Member States by: providing up to date nuclear and atomic data; supporting programmes based on research reactors and particle accelerators; improving capabilities in the development and use of radioisotope and radiation technology, radioanalytical measurements and nuclear instrumentation; encouraging environmentally friendly technologies based on the use of radiation; and providing a forum for the co-ordination of fusion research worldwide.

Regular budget expenditure: $8 822 587
Extrabudgetary programme expenditure (not included in chart): $20 412



1. Nuclear and Atomic Data for Applications: $1 942 099
2. Nuclear Instrumentation: $1 722 187
3. Theoretical Physics (contribution): $1 983 000
4. Utilization of Research Reactors and Particle Accelerators: $520 573
5. Radioisotopes and Radiation Technology: $2 139 348
6. Nuclear Fusion Research and Plasma Physics Applications: $515 380

KEY ISSUES AND HIGHLIGHTS

- The layout and content of the Agency's nuclear data web site was improved to provide easier access to users for their nuclear data needs. As a consequence, there was a 30% increase in retrievals from the site.
- Research carried out through a CRP resulted in the development of a nuclear data library (WIMS-IAEA) for research reactor calculations.
- An Agency symposium in São Paulo, Brazil, highlighted the role of accelerators for analytical, materials and medical applications.
- Educational kits were provided by the Agency for training in the use and maintenance of nuclear instrumentation employing microcontrollers and microprocessors.
- Techniques were developed through a recently concluded CRP for the labelling of small peptides with rhenium-188 for radiopharmaceutical applications.
- The Agency and WHO, in a joint effort, defined good manufacturing practices (GMP) in radiopharmaceuticals; they will be published as a special section of a WHO manual on GMP for pharmaceuticals.
- The International Thermonuclear Experimental Reactor (ITER) Council declared the successful completion of Engineering Design Activities in July 2001. The next phase is under way, and involves co-ordinated technical activities among ITER parties under Agency auspices.

NUCLEAR AND ATOMIC DATA FOR APPLICATIONS

The results of a CRP that ended in 2001 were published in a technical document, *Charged Particle Cross-Section Database for Medical Radioisotope Production: Diagnostic Radioisotopes and Monitor Reactions* (IAEA-TECDOC-1211). Fully complementing the information available on the Agency's web site *(http://www-nds.iaea.org/medical)*, the document presents recommended cross-sections for 22 beam monitor reactions and 26 production reactions of radioisotopes used in nuclear medicine for diagnostic purposes. These recommended data are sufficiently accurate to meet the demands of the production criteria for high purity diagnostic applications in single photon emission computed tomography and positron emission tomography for biofunctional studies.

The ENDF Verification Support Package (ENDVER) was completed to display the contents of Evaluated Nuclear Data Files (ENDFs) and compare them with experimental data from the Experimental Exchange Format (EXFOR) database. Special features include the capability to display and compare angular distributions, energy spectra and double differential cross-sections. This software package has aided considerably in data verification.

The Atomic and Molecular Data Information System (AMDIS) has been enhanced by the addition of comprehensive data for physical sputtering with both angular and energy dependence. These new data include fusion relevant projectiles impacting on beryllium, carbon, tungsten and related compounds. Furthermore, a comprehensive database for the radiation enhanced sublimation (RES) of carbon and carbon related compounds was developed and added to AMDIS. The results of this work, summarized in the Agency publication *Atomic and Plasma-Material Interaction Data for Fusion*, show the dependency of physical sputtering and RES yields on the temperature of the material, incident projectile energy and incident flux. Version 1.2 of the International Database on Irradiated Nuclear Graphites, developed and maintained through extrabudgetary funding, was also distributed. These databases are of great importance in the design of fusion energy research machines where the interaction of plasmas with the reactor wall is critical to the success of the machine.

Efforts to produce an Internet based search engine for atomic data led to the development of a prototype version that has undergone extensive testing. The initial version of the search engine, released in December 2001, operates on servers at the Agency, the Weizmann Institute of Science (Rehevot, Israel) and at the GAPHYOR Data Center of the Centre National de la Recherche Scientifique (Orsay, France). This project was initiated in response to the difficulties faced by users of atomic and molecular data in easily formulating the correct query for a number of different databases. The search engine permits the user to formulate and pass along one query in the correct form to many databases and to have all search results gathered for display simultaneously, an approach that will allow plasma modellers to access many more data.

The adoption by the Agency of alternative relational database management systems has substantially improved the quality of its computerized data services. These new methods of data storage and distribution also comply with the information technology policy of the Agency. In addition, these systems are expected to have a major impact on the nature, flexibility and cost of all nuclear data services, including the formulation of nuclear reaction databases in multisystem or multimedia environments that will provide a common solution to the handling of different software and hardware platforms and result in more user friendly access.

Access to the Agency's nuclear data server for the Internet (*http://www-nds.iaea.org*) has stabilized over 2000–2001 at a level of 15 000 queries per year (see Table I and Fig. 1). Nevertheless, the total number of data retrievals has increased by 30%, due mainly to customer requirements for data from the general purpose and special applications libraries. The latter are being successfully formulated and introduced through CRPs. Another noteworthy point is that the number of queries from developing countries has continued to grow in 2001. In addition, the layout and design of the web page has been significantly

improved to ease user access to the data. New data libraries have also been added to the site, as well as program packages to verify the evaluated data files and for nuclear model calculations

NUCLEAR INSTRUMENTATION

In supporting the utilization and maintenance of instruments used for nuclear applications in Member States, the Agency develops and disseminates spectrometry software and educational kits for instrument maintenance. Knowledge and competence are imparted through training courses. For example, the Agency's software packages for spectrometry and the related reference spectra are now available on its web site and can be downloaded by users. In this connection, an exercise to compare commercially available software packages for analysing particle induced X ray emission spectra revealed that there is room for improvement in quantifying results from low intensity peaks.

Various distance learning tools for the maintenance of instruments were developed through Agency technical co-operation projects. For example, a CRP was started to develop modules for the troubleshooting of such commonly used instruments as radioimmunoassay and liquid scintillator counters, and electrometers. The aim of the CRP is to develop information

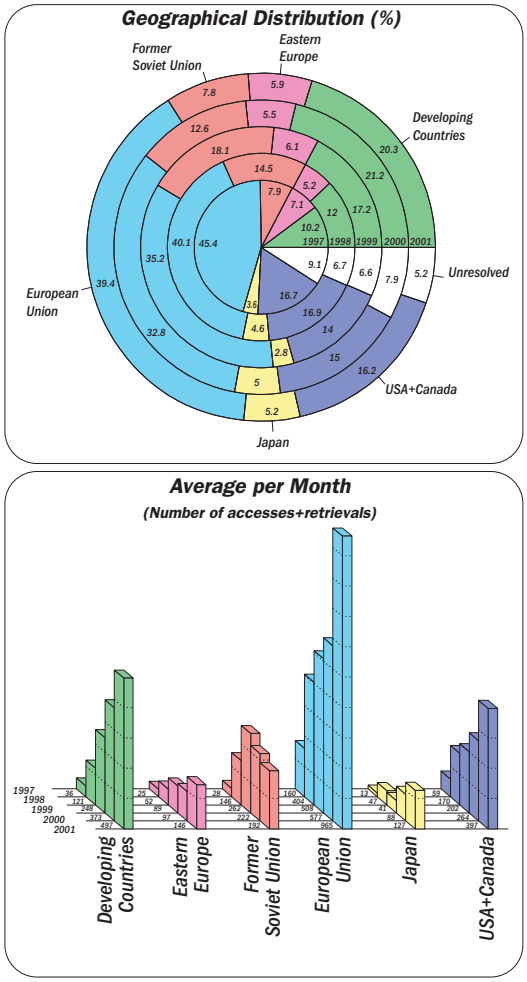


FIG. 1. Number of data accesses and retrievals from the Agency's nuclear data web site and from the mirror server at the Nuclear and Energy Research Institute (IPEN) in Brazil.

TABLE I. **STATISTICAL ANALYSIS OF DATA SERVICES**

	1997	1998	1999	2000	2001
Internet retrievals from the main Agency nuclear databases	23	4276	9581	9642	12 894
Accesses through the Internet to other Agency files and information	4400	7443	7757	11 472	16 153
Telnet based nuclear data retrievals	7350	2700	2180	1387	550
Information on CD-ROMs	—	205	420	648	883
Off-line retrievals	1900	1995	2290	2557	2231

communication technology (ICT) based training modules, including animation and other multimedia techniques, as educational tools to increase the number of trained technical staff in Member States.

Laboratories participating in the second Research Co-ordination Meeting of a CRP on the application of nuclear techniques for the identification of anti-personnel land mines reported advances in the development of portable detection devices. A hand held sensor based on backscattered, thermalized neutrons was identified as a promising tool. The Agency's work in this area was also presented at a European Commission meeting in Brussels.

A new CRP on in situ application of the X ray fluorescence (XRF) technique has the objectives of: developing optimum sampling methodologies; improving performance for field portable XRF spectrometers; and validating quantitative procedures for in situ XRF analysis. The results will benefit applications in environmental monitoring, mineral exploration, cultural heritage preservation and industrial process control.

The Agency's Laboratories at Seibersdorf provided basic technical support for activities related to the use and maintenance of nuclear instrumentation in Member States. Key efforts included the following:

— Assembling and providing educational kits for training on microcontroller and microprocessor based equipment.
— Selecting, testing and implementing ICT based training materials for basic nuclear electronics and for the maintenance and repair of nuclear instruments.
— Establishing a new training station for the repair of printed circuit boards.
— Assessing new radiation detectors for X ray and gamma ray spectrometry.
— Developing instruments for environmental pollution monitoring, dosimetry and agricultural studies.
— Developing a power supply for silicon drift detectors.
— Assisting in the establishment of regional centres for the maintenance and repair of nuclear instruments.
— Providing technical guidelines to Member States on the development and maintenance of instruments for nuclear spectroscopy.
— Assessing the total uncertainty of secondary target/X ray tube based energy dispersive XRF spectrometry, following the ISO standard.

UTILIZATION OF RESEARCH REACTORS AND PARTICLE ACCELERATORS

The main result of a recently concluded CRP to update the Winfrith Improved Multigroup Scheme (WIMS) has been to make available on request an updated, multi-group, neutron cross-section library, WIMS-IAEA, along with calculations for more than 200 benchmark problems. This library will improve the core physics modelling capability at many research reactors.

In addressing the issue of under-utilized research reactors, the Agency has assisted Member States in preparing utilization programmes tailored to the specific capabilities of the reactors. This assistance has taken the form of the publication of three technical documents to guide reactor operators. In addition, a utilization plan for a new research reactor in Nigeria was developed through a technical co-operation project.

Promoting education and training in nuclear technology in Member States is a major aspect of the Agency's technical assistance programme. A report prepared by a Technical Committee presents an overview of educational opportunities in accelerator technology and its applications. In particular, the report focuses on enhancing information exchange and establishing technology transfer mechanisms among different countries, and identifying training opportunities and needs in developing countries. In related work, Agency technical co-operation projects provided assistance in the procurement of an ion beam accelerator for materials development and analysis in the Syrian Arab Republic, and Thailand received helped in the operation and use of accelerators for ion implantation and materials analysis.

At a symposium held in São Paulo, Brazil, on the utilization of accelerators, the different uses of accelerators around the world and the new applications that lie ahead were reviewed. Target areas for Agency supported collaborative R&D programmes in the field of accelerator applications were also defined. Furthermore, the role of accelerators in nano-technology, environmental remediation and the sanitation of mail were considered.

RADIOISOTOPES AND RADIATION TECHNOLOGY

Receptor imaging of the central nervous system (CNS) has been shown to be very valuable in the management of neurological disorders using radiopharmaceuticals labelled with cyclotron produced isotopes, namely, carbon-11, fluorine-18 and iodine-123. However these isotopes are expensive and not readily available. A CNS receptor imaging agent based on technetium-99m will make such techniques widely available at an affordable cost. A CRP that ended in 2001 studied several approaches to synthesize, characterize and evaluate technetium-99m labelled molecules with potential for CNS receptor imaging. Technetium-99m mixed ligand complexes were prepared and in vitro receptor binding methods were developed to determine the receptor affinity and specificity of the compounds, followed by in vivo studies in animals. The CRP succeeded in establishing the radiochemical approaches for the preparation and evaluation of technetium-99m CNS receptor agents, which could pave the way for developing a suitable radiopharmaceutical.

Radioimmunoassays (RIAs) are widely used in clinical chemistry, but also have applications in non-clinical fields, including veterinary medicine, animal reproduction, food processing and the drug industry. A new CRP was started in 2001 to extend the capabilities of national laboratories in developing RIA kits for non-clinical applications. The goal of the CRP is to focus on RIA kit development for aflotoxin B1 — an important contaminant in food, atrazine — an environmental contaminant, and progesterone — for veterinary applications.

Good manufacturing practices, which have long been applied to pharmaceuticals, are also being increasingly used for the manufacture of radiopharmaceuticals. However, there has been a need for international guidelines, particularly for the benefit of developing Member States. The Agency and WHO have jointly prepared such guidelines, which were then approved by the WHO Expert Committee on Specifications for Pharmaceutical Preparations in October 2001. They will be published as a special section of WHO's *GMP Manual for Pharmaceuticals*.

In a recently concluded CRP, several techniques to label small peptides with therapeutic radionuclides were investigated. In particular, the peptide lanreotide was labelled with rhenium-188. This labelling technique can also be extended to several other peptides and biomolecules.

The scientific community became aware of the varying toxicological properties of different chemical forms of trace elements more than thirty years ago, when accidental releases of certain organometallic compounds caused severe health problems in populations eating crops from affected areas. However, the appropriate tools for method validation of speciation analysis, such as natural matrix reference materials, are not easily available. Nuclear analytical techniques are particularly well suited for method development and validation because of their non-destructive nature and their ability to use radioisotopes to determine the fate of compounds and elements. Labelled compounds can be introduced into biological tissues and act as a probe in the same way as natural analogues. A CRP was therefore started in 2001 to validate speciation analysis using nuclear techniques. The objective is to disseminate improved speciation techniques to Member States affected by impaired element concentrations in drinking water, soil or nutrition to monitor the toxic potential to their population.

Another CRP that started in 2001 had as its goal the upgrading of the most popular Agency reference materials to achieve full traceability to the International System of Units for radionuclide concentrations. Five laboratories

and the Agency's Laboratories at Seibersdorf developed traceable measurement techniques for the most important natural radionuclides, fission products and transuranium isotopes in natural matrix materials. Prior to the certification of the radionuclide concentrations, the homogeneity of the different batches of reference materials was verified. The measurement results for evaluation and certification of the materials are expected in 2002.

One of the tasks of the Agency's Laboratories at Seibersdorf was to organize intercomparisons and proficiency tests for CRPs and technical cooperation projects. Two such tests were organized for a project that included samples spiked with anthropogenic, alpha, beta and gamma emitting radionuclides. In addition, a very specialized proficiency test was organized for eight laboratories involving the preparation of 48 different samples representing four matrices (milk, vegetation, soil and water) with varying concentrations and mixtures of both anthropogenic and primordial radionuclides. The Seibersdorf Laboratories provided technical support to Member State counterpart staff in evaluating, interpreting and preparing the individual and summary reports as well as certificates for this proficiency test.

In 2001, orders for products from the Agency's Analytical Quality Control Services (AQCS) were received from approximately 200 customers (Table II).

The training and certification of non-destructive testing (NDT) personnel has significance in any country's industrialization programme. To this end, a revised version of an Agency technical document was prepared (*Training Guidelines in Non-destructive Testing Techniques, 2002 Edition*, IAEA-TECDOC-628/Rev.1). The new version is expected to help end users in Member Sates update their materials and programmes. It will also play an important role in international harmonization efforts in the field of NDT.

A CRP on the use of radiation processing for the sterilization or decontamination of pharmaceuticals and pharmaceutical raw materials was completed. The results of various physico-chemical and pharmacological studies and tests indicated the possibility of radiation treatment of drugs such as cefotaxime, amoxycillin, spyramicine, tetracyclines, cyclophosphamide and sulphonamides. In the case of trifluorothymidine, fluorometholone, deferroxamine and a new peptide, radiation sterilization was found to be better than or equivalent to heat sterilization. The usefulness of radiation processing for the decontamination of various herbal medicines and plant extracts was also shown.

Fumes and other gaseous emissions from industrial activities often contain toxic volatile organic compounds (VOCs). These include by definition all organic compounds that are detrimental to the ozone layer and are considered to contribute to global warming because of their extremely long atmospheric lifetimes. They also include organic compounds that are hazardous materials, causing headaches, dizziness or sore throats, and those that are carcinogenic. Using the services of consultants, the Agency prepared a report that demonstrated that electron beam technology is the most energy efficient treatment technology for all VOCs with the exception of hydrofluorocarbons. Its key advantage over other technologies is in treating low concentrations of VOCs (<1000 ppm), since it does not merely transfer the waste from one medium to another (unlike activated carbon adsorption or scrubbing). It was also shown to have great promise for the remediation of contaminated sites and exhaust gases from various industrial applications.

TABLE II. **NUMBER OF AQCS UNITS SOLD IN 2001**

Analyte group	Number of units sold
Radionuclides	629
Trace elements	257
Methylmercury	17
Organic contaminants	18
Total	**921**

The technical, economic and environmental advantages of the radiation processing of cellulose and wood by-products were assessed in a study. For example, electron beam processing of cellulose pulps provides a technically and commercially viable method that can replace the energy intensive ageing step in conventional viscose processes. Significant reductions in chemical use and toxic emissions benefit the industry in terms of reducing manufacturing costs as well as the pollution associated with the process.

A new CRP entitled 'Integration of Residence Time Distribution (RTD) Tracing with Computational Fluid Dynamics (CFD) Simulation for Industrial Process Visualization and Optimization' began in 2001. The main objective is to develop and validate a method for analysing and diagnosing industrial engineering processes using radiotracer experiment and CFD modelling. Experimental protocols and software codes of a combined experimental and computational method will be elaborated to obtain reliable quantitative results on process performance in industrial vessels and process units to improve and optimize their design and efficiency.

NUCLEAR FUSION RESEARCH AND PLASMA PHYSICS APPLICATIONS

In July 2001, the ITER Council held its final meeting at Agency Headquarters to mark the successful completion of the Engineering Design Activities carried out by the ITER Joint Central Team and the ITER Parties' National Teams between 1992 and 2001. In preparation for the construction of ITER, the current ITER Parties (Canada, the European Union, Japan and the Russian Federation) have agreed to conduct, under Agency auspices, Co-ordinated Technical Activities (CTA) until the end of 2002. One goal is to adapt the final ITER design to site specific conditions. Thereafter, the Joint Implementation (Construction, Operation and Decommissioning) of the ITER Project is expected to start.

A CRP was started to investigate dense magnetized plasma applications for harnessing nuclear fusion, both as a power source and as an intense radiation source. Dense magnetized plasmas can be generated by various types of devices, including pinches, focuses, plasma accelerators, open switches, sparks and hollow

TABLE III. **AGENCY TECHNICAL COMMITTEE MEETINGS ON NUCLEAR FUSION**

Title	Location
Control, data acquisition and remote participation for fusion research	Padova, Italy
Research using small fusion devices	São Paulo, Brazil
Spherical tori	São Jose dos Campos, Brazil
Divertor concepts	Aix-en-Provence, France
H-mode physics and transport barriers	Tokai, Japan
High average power drivers for inertial fusion energy	Kyoto, Japan
Energetic particles in magnetic confinement systems	Gothenburg, Sweden

cathode discharges. Magnetized plasmas may provide a more efficient route to achieving fusion ignition.

The Agency continued to be a catalyst in fusion research and information exchange, with a range of Technical Committee meetings conducted under its auspices (Table III). At the meeting on H mode physics and transport barriers, it was reported that after new divertors were installed, the Wendelstein 7-AS Stellarator in Garching, Germany, achieved the highest densities ever in a magnetic confinement experiment (up to $n_e \sim 4 \times 10^{20}$ m^{-3}).