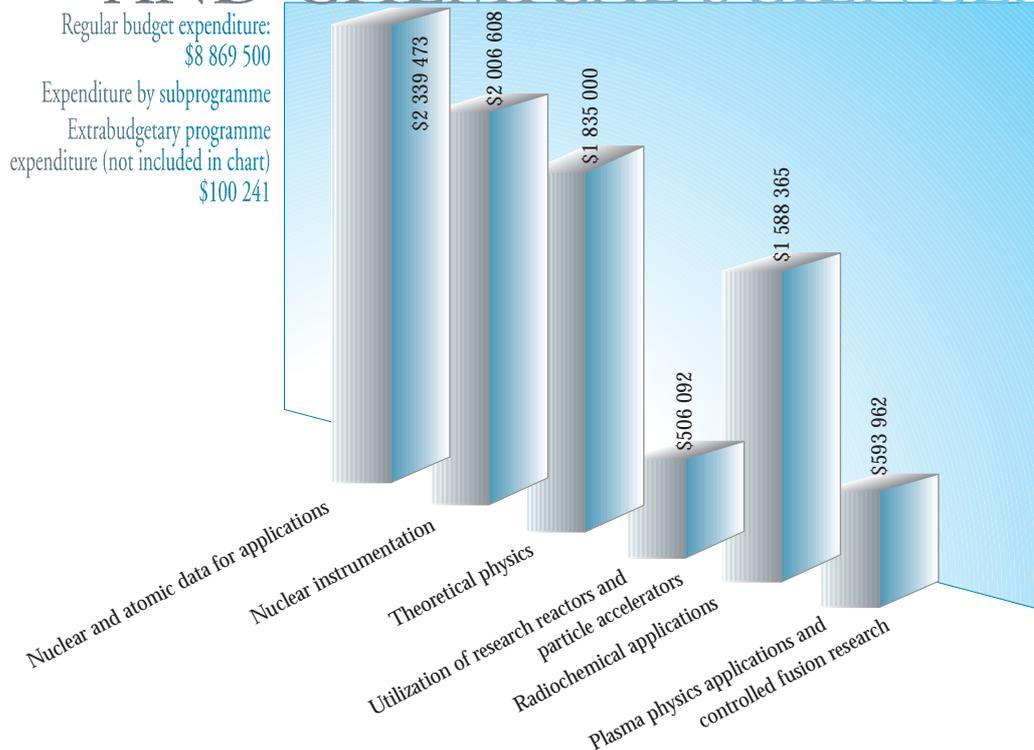


# PHYSICAL AND CHEMICAL SCIENCES



In the physical and chemical sciences programme, nuclear and atomic data services on the Internet registered a substantial increase in retrievals, while four major new nuclear databases and an improved data library for fusion applications were added. An intercomparison of widely available particle spectral analysis software was carried out to provide information on the performance, capabilities and limitations of these software packages. This is a follow-up of an earlier similar effort to compare gamma spectroscopy software. An Advisory Group meeting recommended that the neutron interrogation technique, in conjunction with other non-nuclear techniques, could provide a means to detect buried land mines in fields, a problem of considerable humanitarian interest worldwide. Experts studied ways to implement quality assurance procedures for analytical services in laboratories using

nuclear and nuclear related techniques in developing Member States. An assessment was made of the suitability of emerging new technologies for molybdenum-99 and technitium-99m generators, which are extensively used in nuclear medicine. A global directory on radioisotope production using cyclotrons and usage statistics was compiled.

## Nuclear and atomic data for applications

On-line nuclear data services to Member States were improved by incorporating direct links to three major

### NUCLEAR AND ATOMIC DATA RETRIEVALS

Year	1993	1994	1995	1996	1997
Nuclear data on-line retrievals	600	3200	4400	5700	7350
Atomic data on-line retrievals	—	—	450	900	1050
Off-line retrievals	1200	1950	1550	800	1900

databases (EXFOR, CINDA and NUDAT) and one large, special purpose library (NGATLAS) into the Agency's nuclear data services Internet home page. Accesses to this page rose sharply over the previous year. A new page was created to facilitate user access to Agency atomic and molecular databases. Data retrievals through the Internet increased by 27% over 1996, continuing the strong upward trend in the use of on-line services in recent years. In addition, there remains a steady demand for conventional, postal-based, off-line services.

To better serve data users who have limited access to the Internet, especially those in developing countries, development began of CD-ROM versions of major nuclear databases, together with user friendly retrieval software. The first searchable CD-ROM, of the EXFOR database of experimental nuclear data, has already been produced.

Co-ordination of the International Data Network of Nuclear Data Centres resulted in the testing of four major databases, release of the MENDL-2P database (which is of interest for the accelerator transmutation of nuclear waste) and processing and testing of the Chinese CENDL-2.1 general purpose library. The Atomic and Molecular Data Center Network was expanded with the inclusion of data centres in Israel and the Republic of Korea.

A starter file of input parameters for calculations of nuclear data was assembled and is being prepared for release in response to nuclear data evaluation needs for emerging nuclear applications. An improved nuclear data library for fusion applications (FENDL-2) was released, including an extensive library of activation data for the production of radioactive isotopes. This is of particular importance for the design activities of the International Thermonuclear Experimental Reactor (ITER).

A personal computer version of the Agency's nuclear database for safeguards was upgraded. A comprehensive atlas of neutron capture cross-sections, of interest in a wide range of applications, including reactor calculations, was completed and published. In response to the needs of the medical research community, a technical document on nuclear data for neutron therapy was prepared. Finally, a new CRP was established on X and gamma ray decay data for detector calibration for improved quality in spectroscopy measurements for safeguards, dosimetry and in industry.

A CRP on atomic and plasma-wall interaction data for fusion reactor divertor modelling generated a significant amount of data which were urgently needed for fusion divertor design, particularly ITER. A handbook containing data on the chemical erosion of carbon based plasma facing materials under particle impact was completed. These data are of interest to the fusion community and the semiconductor industry. Responding to the needs of plasma fusion researchers, particularly ITER, two CRPs, on charged exchange cross-section data and on the erosion and hydrogen retention properties of mixed plasma facing fusion materials, were initiated.

## Nuclear instrumentation

A low cost, modular counting system (based on the Agency's 'Eurocard' standard and driven by a personal computer) and a field applicable pulser were developed. An Advisory Group meeting on nuclear instrument maintenance and repair was held in June in Vienna to assist Member States in using instruments based on microprocessors, large scale integrated circuits, programmable array logic and surface mounted technology (SMT). New training kits and laboratory manuals were developed to train technical staff in the skills required to repair modern nuclear instruments, such as those based on SMT.

A new CRP was initiated on specialized software utilities for gamma ray spectrometry. The goal is to help Member States improve their ability to analyse trace quantities of materials using computer assisted nuclide identification, quality assurance techniques, calculation of true coincidence corrections, detector response from extended sources and analysis of positron annihilation gamma ray peaks.

An intercomparison of widely available software packages for alpha particle spectral analysis was carried out in Vienna in November using prepared test spectra. The results will provide Member States with information on the performance, capabilities and limitations of software packages for alpha spectrometry.

Bulk hydrogen analysis using neutrons is the subject of a new CRP that was initiated in 1997. The aim is to explore improved methods of quantifying hydrogen content for a variety of applications, such as moisture in industrial and agricultural products, hydrogen

corrosion in metal aircraft components (metal fatigue) and the microscopic behaviour of hydrogen in reactor fuel rods.

The Agency's Laboratories at Seibersdorf developed educational kits (including manuals) for nuclear instrument repair and maintenance, such as a timing single channel analyser, a pulsed optical feedback preamplifier, power supplies, and sensor acquisition and interface modules. The provision of spare parts, technical advice and documentation was expanded to cover all African countries with active technical co-operation projects in nuclear instrumentation.

Two technical documents were published on sampling and sample preparation procedures for environmental materials. The purpose is to improve the accuracy and extend the applicability range of the X ray fluorescence (XRF) method, including total reflection XRF and X ray microfluorescence. The documents provide information on optimized sample preparation techniques readily applicable by XRF laboratories in developing Member States. In related work, two quantitative methods for laboratory and portable XRF units were developed at the Agency's Laboratories at Seibersdorf. One method can be applied without extensive calibration of the portable XRF set-up, while the second is based on a concept that is particularly suitable for the quantitative determination of selected elements in environmental materials with complex and variable matrices. Finally, a new procedure for the homogeneity test of candidate reference materials (including those for microanalytical techniques) was developed, and a feasibility study of individual particle analysis by X-ray microfluorescence was also completed.

## Utilization of research reactors and particle accelerators

A scientific session on turning military nuclear technology to peaceful uses was held during the General Conference. It covered the experience with space, submarine, and laser nuclear technology for civil applications in the Russian Federation, technology for the utilization of military plutonium for peaceful purposes, International Science and Technology Centre

activities related to redirecting the work of former Soviet military scientists to peaceful research and conversion of defence equipment into commercial high power electron beam equipment.

A Technical Committee meeting on neutron beam research, held in Portugal in September, provided a comprehensive review of the applications of neutron scattering in many fields, such as magnetism, superconductivity, stress analysis, superalloys, quantum physics, polymers and neutron radiography.

A new CRP was established on the application of mega-electron-volt ion beams for the development and characterization of semiconductor materials. This research will help developing Member States acquire skills in ion beam analysis and in the modification of semiconductor materials, including impurity transport, real-time monitoring, passivation, gettering, lattice location and microfabrication using ion beams.

At an Advisory Group meeting on regional accelerator centres and user networks, held in Vienna in November, it was concluded that ion beam analysis and related accelerator technology should be the focal points in establishing regional ion accelerator centres, networks and training programmes for developing countries. Such centres would enhance access to accelerator facilities and ion beam applications.

An Advisory Group meeting on the detection of explosives (in particular land mines) by low cost methods was held in Vienna in December. This was the first Agency meeting on this subject which is of great humanitarian interest, especially to developing Member States. Nuclear and non-nuclear methods were compared and recommendations were made to increase the reliability of detection and to reduce costs.

In order to check the accuracy of analytical data, an interlaboratory comparison of PIXE analyses of fly ash embedded in paper filters was carried out. The results were evaluated according to recognized international protocols for proficiency testing which ensured both comparability and the proper classification of the participating laboratories. Approximately half of the laboratories involved were classified as being satisfactory.

On the basis of responses received to a questionnaire, a directory of cyclotrons for isotope production with 206 entries covering 34 Member States was compiled.

# Radiochemical applications

In a CRP on the development of technitium-99m labelled peptides for imaging peripheral receptors, a comparative evaluation was carried out on iodine-125 and technitium-99m labelling of the somatostatin analogue vapreotide (RC160). Technitium-99m octreotide analogues are potentially useful for imaging neuroendocrine tumours.

A CRP on labelled biomolecules for targeted radiotherapy was initiated. This CRP will build on experience in producing therapeutic radionuclides and chemical modifications of monoclonal antibodies and peptides for achieving specific targeting of radionuclides in vivo for radiotherapy of different cancers.

Radioimmunometric assays of tumour markers can play a very useful role in early cancer detection and management. Accordingly, a new CRP was started on the development of affordable kits using local resources for such assays. The research programme focuses on: the prostate specific antigen (PSA) and free PSA, used in prostate cancer screening; the tissue polypeptide antigen (TPA), for breast cancer screening; and solid phase immunoradiometric assay systems for PSA and free PSA with the objective of developing them into user friendly kits.

Several developing Member States operate research reactors and cyclotrons and have developed programmes for radioisotope production. The services of consultants were used to survey the emerging new technologies for molybdenum-99 and technitium-99m generator production, which will have a significant impact on nuclear medicine practice. The proposed methods for producing these radioisotopes using accelerators were reviewed.

As part of efforts to publish an updated edition of *Radioisotope Production and Quality Control* (Technical Reports Series No. 128), questionnaires were sent to several research reactor operators requesting details of the radioisotopes they regularly produce, the quantities produced, reactions and the radiochemical process used.

The Agency's Laboratories at Seibersdorf provided analytical support for a number of CRPs through

intercomparisons and preparation and distribution of a number of reference materials. Four new reference materials were under evaluation: a lichen and two new algae materials for toxic element content, including one certified for platinum, and an Asian soil for caesium-137 content. A statistical evaluation and draft report on two of the intercomparisons (ALMERA-I and IAEA-326/327) was completed.

Progress was made in the certification of IAEA-392 and IAEA-393 according to the guidelines of the International Organization for Standardization (ISO). In addition to the analyses performed by the Agency's Laboratories at Seibersdorf, four other laboratories were contracted to perform certification analyses for elemental concentrations in these two algae materials. This is the first time this approach has been taken under the Analytical Quality Control Services (AQCS) programme.

To provide better support and feedback to laboratories in Member States concerning their performance in intercomparisons, detailed questionnaires on their analytical methodologies were prepared for distribution and evaluation during the next intercomparison. A new version of the intercomparison data evaluation software was also introduced.

Trace element analysis of objects, especially ceramic materials, recovered in archaeological excavations are very useful in establishing archaeological chronologies. Of the various techniques available with sufficient sensitivity and precision, instrumental neutron activation analysis (INAA) is one of the most effective. A new CRP that applies INAA for archaeological investigations was initiated with the collaboration of the Smithsonian Institution in the USA. The CRP will focus on promoting interdisciplinary research, using nuclear analytical techniques in archaeological investigations and developing facilities for such research at nuclear installations in Latin America.

Nuclear analytical techniques (NATs) are useful in the mineral industry for: determining the contents of major, minor and trace elements; optimizing the yield of separation processes; quality control programmes; and waste and pollution minimization. A CRP on developing nuclear techniques for the analysis of precious and rare metals in mineral concentrates was initiated. It is expected to help realize the enormous potential of NATs in improving raw material utilization in ore processing and effecting savings in the energy and materials used in these processes.

## Plasma physics applications and controlled fusion research

A final Research Co-ordination meeting was held in Vienna in December on the development of plasma heating and diagnostic systems in institutes in developing countries using middle and small scale plasma devices. This CRP used the scientific potential of these countries to develop methods of plasma heating and diagnostics and to resolve specific problems using tokamaks, alternative magnetic traps and other plasma discharge devices.

The ITER Council approved the ITER Detailed Design Report, Cost Review and Safety Analysis (DDR) and the Report on the Technical Basis for the DDR. The work reported was a collaborative effort relying on the ITER Joint Central Team and the home teams of the ITER parties. Both reports were published by the Agency.

