Reactor Sector



Reactor

José Gonçalves Marques

The Portuguese Research Reactor (RPI), as a unique infrastructure in the Iberian Peninsula, houses as well the *Atmospheric Elemental Dispersion* and *Applied Dynamics* groups. The RPI also supports activities in the Chemistry Sector, the Physics Sector and in the Department for Radiological Protection and Nuclear Safety. The use of the RPI by external users was approximately at the same level as last year and accounted for 25% of the total irradiation time in 2005.

The staff involved in all aspects of the operation and use of the RPI presents its activities under the common headline of *Operation and Exploitation of the Reactor, Dosimetry (RPI) and Reactor Calculations*. New research projects approved in 2004 could finally start this year, covering areas of dosimetry, materials science and neutron tomography.

The *Atmospheric Elemental Dispersion* group uses the k_0 INAA technique in the RPI and was again the main user of the reactor in 2005, accounting for 25% of the total irradiation time. The group is dedicated to study the cycle and impact of trace elements in the atmosphere. It addresses, specifically, the development and application of nuclear techniques,

source apportionment and tracking in the atmosphere, chemical speciation, uptake and release of chemical elements in biomonitoring and monitoring, as well as health linkage through epidemiology and nutrition studies. These objectives are approached through research, included mostly in PhD theses. The activities are essentially financed by the Foundation for Science and Technology.

The research performed by the Applied Dynamics group is mostly concerned by vibration and acoustic problems displayed by components of nuclear and conventional power plants. As such, a significant part of their research results has been motivated and funded by the French Commissariat à l'Energie Atomique (CEA) and the Portuguese Electricidade de Portugal (EDP). However, the techniques developed by this group can and have been used to solve problems, both of industrial and fundamental nature, outside the realm of power generation. In spite of being one of the smallest groups in terms of ITN staff, this fact is compensated by an active collaboration with Universities and Research Laboratories, both in Portugal and abroad. The vitality of this group is well demonstrated by their research contracts and publications.

Reactor Staff

Researchers

J. G. MARQUES, Aux. M. C. FREITAS, Principal A. V. ANTUNES, Principal A. FALCÃO, Principal A. KLING, Aux.(90%) N. P. BARRADAS, Aux. (95%) A. R. RAMOS, Aux. (90%)

Technical Personnel

J. S. SOUSA J. A. M. RIBEIRO J. C. ROXON. SERROTE, V. PÁSCOA R. SANTOS R. POMBO F. B. GOMES A. RODRIGUES A. ANASTÁCIO V. TOMÁS I. DIONÍSIO

Administrative Personnel

T. FERNANDES A. SILVA

Operation and Exploitation of the Reactor, Dosimetry (RPI) and Reactor Calculations

José Gonçalves Marques

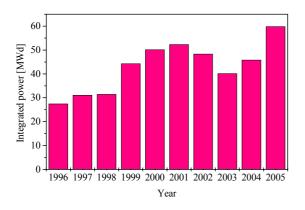
The main objective of the Operation and Exploitation of the Portuguese Research Reactor (RPI) is to be able to satisfy the users' needs while conducting all tasks with the assurance that the reactor is operated in a safe and reliable manner. The year 2005 was a transition year, with some research projects near completion and others just starting.

The laboratory for fabrication of Superheated Droplet Detectors installed in 2004 is now in full use. Three new research projects are using this laboratory.

The Emission Channelling/Blocking Setup is now operational and its optimization is underway, within the scope of a PhD thesis.

The programme for testing of electronic components under fast neutron irradiation for LHC/CERN is near completion. A PhD thesis was presented in the Complutense University of Madrid.

Two projects for installation of setups for neutron tomography and for Perturbed Angular Correlations using short lived isotopes started in late 2005.



The operation of the reactor requires the calculation of parameters such as effective multiplication, control rod worth and safety parameters. An intensive activity in this field has continued, in order to prepare the core conversion to low enriched fuel. A feasibility study for conversion to high density U₃Si₂-Al fuel was done with assistance from the Argonne National Laboratory (USA). No significant loss of performance of the reactor is expected after the core conversion.

The main users of the reactor are described in the Table. The main activity in 2005 was Neutron Activation Analysis (NAA), to users in the Reactor and Chemistry (33%), followed by Isotope Production (30%) and the study of radiation effects in materials and seeds (21%). Isotope production again increased by about 60% from last year and more than doubled relatively to 2004.

User	Area	Time (%)
RPI	NAA	25.0
	Dosimetry and Test of	7.5
	Detectors	
	Other (training, etc)	0.1
Physics	Radiation Effects	18.8
	Neutron Scattering	8.5
Chemistry	NAA	8.0
	Isotope Production	3.8
DPRSN	Isotope Production	3.7
Univ. Lisboa	Isotope Production	20.4
CERN	Radiation Effects	1.8
LIP/Lisbon	Isotope Production	1.5
Univ. Coimbra	Isotope Production	0.8
IVIA	Radiation Effects	0.1

The figure indicates the integrated power produced by the RPI in the last 10 years. A clear increase is seen since 1999, reflecting an increase in its use. The integrated power for 2004 was 60 MWd, about 30% higher than last year and the highest value since 1979. On average, 1.8 irradiations were performed at the same time.

Research Team

Researchers

J. G. MARQUES, Aux. A. KLING, Aux. (90%) N. P. BARRADAS, Aux. (95%) A. FALCÃO, Principal A. R. RAMOS, Aux. (90%)

Students

M.A.F. da COSTA, MSc Student, IST, ITN grant

Reactor Operators

J. A. M. RIBEIRO J. C. ROXO N. SERROTE V. PÁSCOA R. SANTOS

Technical Personnel

R. POMBO F. B. GOMES V. TOMÁS A. RODRIGUES J. S. SOUSA

Collaborators

A. FERNANDES, POST-DOC, ITN, FCT GRANT T. GIRARD, CFNUL T. MORLAT, POST DOC, CFNUL F. GIULIANI, POST DOC, CFNUL

Core Conversion of the RPI to LEU Fuel: Feasibility Study

J.G. Marques, N.P.Barradas, A.R. Ramos, J.G. Stevens¹, E.E. Feldman¹, J.A. Stillman¹, J.E. Matos¹

Objectives

The core conversion of the Portuguese Research Reactor (RPI) to Low Enriched Uranium (LEU) fuel will be performed within IAEA's Technical Cooperation project POR/4/016. This project was approved in the end of 2004 and will have financial support of the US and Portuguese governments. As a first step to the core conversion, a joint feasibility study [1] was made by ITN and the RERTR program at Argonne National Laboratory.

Results

LEU uranium silicide (U₃Si₂-Al) dispersion fuel with a uranium density of 4.8 g/cm³ was selected because of its widespread use in research reactors and for the relatively large number of manufacturers.

The study was done for two assembly designs with the same number of plates (18) as the HEU standard assembly. The first design (LEU-1) had the same geometry as the HEU design and a ²³⁵U loading of 320 g for the standard assembly. The second design (LEU-2) is identical to the first one, except that the fuel meat thickness was increased to 0.6 mm from 0.5 mm, increasing the ²³⁵U content to 376 g. Besides establishing the safety margins of the new core, the feasibility study also had a goal of minimizing the number of assemblies required for 10 years of operation of the RPI, or an equivalent 500 MW•d integrated power.

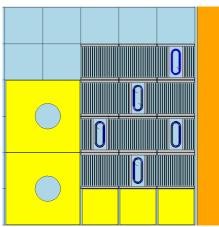


Fig 1. MCNP model of RPI's core configuration P1/2 selected as reference.

The original MCNP Monte Carlo model of the RPI made at ITN for dosimetry studies was modified at ANL to perform the conversion calculations. Relevant experimental data for the HEU cores were reproduced using this model, thus establishing its credibility. While the performance of cores using the LEU-1 design was found to be very similar to the ones of the corresponding HEU cores, the use of LEU-2 assemblies was found to reduce the required number of assemblies from 17 down to 13.

Preliminary values for the thermal-hydraulic safety margins for the HEU fuel design and two LEU fuel designs were determined using the PLTEMP code developed at ANL. Detailed MCNP calculations with the control rods at their critical positions were examined to determine the location of the peak power density in the core. All cores were found to have acceptable safety margins.

The LEU core conversion will not require changes to the control rods, control rod drive mechanisms, the instrumentation and control system, or other reactor components except for the fuel.

The operational and safety analyses for conversion of the core are planned to be completed around March 2006 and the documentation to support the request for licensing the new core will be submitted around June 2006. It is expected that the licensing process will be completed before the end of 2006, when the LEU fuel is anticipated to arrive at the reactor. The HEU fuel, regardless of its irradiation status, will be returned to the US before May 2009.

Published or in press work

1. J.G. Marques, N.P. Barradas, A.R. Ramos, J.G. Stevens, E.E. Feldman, J.A. Stillman, J.E. Matos, Core Conversion of the Portuguese Research Reactor: First Results, *Proc. Int. Meeting on Reduced Enrichment for Research and Test Reactors*, Boston, 2005, Argonne National Laboratory, Paper 16-1.

¹RERTR Program, Argonne National Laboratory Argonne, IL USA 60439

OPERATION AND EXPLOITATION OF THE REACTOR, DOSIMETRY (RPI) AND REACTOR CALCULATIONS

Fast Neutron Irradiation of Electronic Circuits for the LHC/CERN

J.G. Marques, A.C. Fernandes, J.A. Agapito¹, F.J. Franco¹, Y. Zong¹, J. Casas-Cubillos²

Temperature measurement is a key issue in the LHC facility at CERN, as it will be used to regulate the cooling of the superconductor magnets. The signal conditioners for cryogenic thermometry are expected to receive a fast neutron fluence of the order of $2x10^{13}$ n/cm² during a 10 year period, as well as a gamma dose of 500 Gy, and this can affect the operation of the commercial circuits used in their construction. The operating conditions of these circuits are simulated using a fast neutron irradiation facility built in the RPI in 2000. On-line measurements of properties of the circuits and components are performed before, during and after irradiation and stand-by periods, to evaluate the irradiation damages as well as possible annealing effects. A PhD thesis (F.J. Franco) was presented in the Universidad Complutense de Madrid with work done in the previous years. The irradiations will continue in 2006 with the test of more components in statistically significant amounts, as well as prototypes of the final circuit boards, as they become available.

1 Universidad Complutense de Madrid. 2 CERN, LHC/ACR Division.

Monitoring of Airborne Effluents in the RPI Stack Exhaust and Assessment of their Radiological Impact A. Kling

The monitoring of airborne radioactive effluents is of high importance for the safe operation of a research reactor and the determination of its radiological impact. In the existing monitoring system (AIRMON-91) all aerosols are stopped by a paper filter before entering the iodine detection channel allowing only to detect elemental ¹³¹I in the effluents. Since ¹³¹I bound to aerosols could represent a significant contribution to the dose received by members of the public an additional monitoring system (Merlin-Gerin IM201S) capable of the detection of the total ¹³¹I release has been installed is now fully operational.

A further important issue was to estimate the annual doses delivered to the public due to the release of airborne radioactive effluents from the RPI stack. The source term was based on measured airborne radioactivity release data for 2003 (⁴¹Ar, ¹³¹I and aerosols). In addition, the ³H and ¹⁴C releases were calculated based on information on their concentration in the reactor pool water and evaporation rates. For the calculation of the radiological impact the code PC-CREAM was used. In order to obtain a conservative estimate of the dose rates unfavourable meteorological conditions were assumed. The results show that for children and adults the radiation dose is vastly dominated by the effect of ⁴¹Ar while for infants the contributions due to ⁴¹Ar and ¹³¹I are about equally important. The dose rates for all three age groups (infants, children and adults) are, even at the shortest calculable distance (300 m), more than two orders of magnitude below the limit of 1 mSv/a established by law.

Development of Superheated Droplet Detectors for Neutron Dosimetry and Spectrometry Applications A. R. Ramos, M. Felizardo, T. Morlat¹, J. G. Marques, F. Giuliani¹, A. Fernandes, T. A. Girard¹

This project proposes to study the fabrication and use of SDDs based on ecologically sound, easily manipulated halocarbons such as Octofluoropropane (C3F8), Octofluorocyclobutane (C4F8) and Hexafluoropropylene (C3F6). The chemistry of these particular halocarbons will be investigated. Particular emphasis will be put on strategies for increased detector shelf life: a) chemical: increased gel matrix stability (by adding reagents to increase the gel fracture energy, e.g. agarose) and droplet stability (by adding surfactants); b) physical (repressurization of detectors). The manufactured SDDs will be tested and calibrated using the neutron beam facilities of the Portuguese Research Reactor (RPI). After calibration, the SDDs developed will be tested for use as neutron spectrometers. Finally the detector dosimetric performance will be experimentally evaluated in comparison with thermoluminescent dosimeters based on lithium fluoride, calcium sulphate and alumina. This project is funded by FCT under contract POCTI/FIS/55930/2004. Development of new quasi-monochromatic beams for installation in the E4 tube began in 2005 and the geometries for the main filters (Si+Ti and Si+S filter) have been studied.

1 Centro de Física Nuclear da Universidade de Lisboa.

Installation and Testing of the Emission Channeling Experiment

P. Marques, A. Kling, J. G. Marques

Emission channeling is a powerful tool for the investigation of structural properties of crystalline materials. In contrast to the classical method using radioactive probe atoms incorporated in the lattice, the set-up at RPI uses charged particles arising from thermal neutron induced nuclear reactions, e.g. $^6\text{Li}(n,\tau)\alpha$. Channeled particles leaving the crystal are detected by a two-dimensional position sensitive detector located about 60 cm from the target. In the course of the set-up installation one of the main tasks during 2005 was the thorough testing and optimization of the various parameters available in the data acquisition and read-out system. For this purpose sources with different α -emitters were used in order to determine the optimum operational conditions for the detector and the data acquisition system as well as to perform the energy calibration. First two-dimensional patterns were obtained by putting collimators in front of the sources. A further task was to adapt the beam-line D1 in order to host the reaction chamber of the emission channeling set-up. It has been assured that all features of the radiological protection of the beam line stayed intact. Additional lead and lithium carbonate shielding placed at the set-up itself improved the protection of sensitive components located inside the reaction chamber (detector, preamplifier electronics).

Development of a CF3I SDD for Spin-Independent Dark Matter Searches

T. Morlat¹, M. Felizardo, A. R. Ramos, J.G. Marques, F. Giuliani, T. A. Girard¹

This project proposes the R&D of a superheated droplet detector (SDD) based on trifluoroiodomethane (CF3I) for implementation by the SIMPLE project in searches for spin-independent dark matter, complementing the project's current search activity for spin-dependent dark matter with pentafluorochloroethane (C₂ClF₅). The reason for the refrigerant change is the necessity of a heavy target component, since the spin-independent WIMP-nucleon cross section varies with A². The R&D involves the investigation of methods for density-matching the device gel matrix with the refrigerant, the development of an experimental protocol within the P-T phase diagram of both refrigerant and gel which will result in a homogeneous dispersion of small refrigerant droplets within the colloid, and the fabrication of a device prototype for characterizations and response testing with alpha's and neutrons. The project is supported by FCT under contract POCI/FP/63407/2005.

1 Centro de Física Nuclear da Universidade de Lisboa.

Dosimetry of Mixed Radiation Fields with Paired Dosemeters

A. C. Fernandes, J. P. Santos, C. Oliveira, J. G. Marques, L. Santos, V. Cardoso, E. Novák¹, M. Osvav²

Mixed-field dosimetry is frequently performed using paired detectors, with one of them practically insensitive to neutrons and the other one with similar sensitivities to photons and neutrons. In the frame of EURATOM project no. FIR-CT2003-40157, twin chambers (Mg(Ar) and TE(TE)) and thermoluminescent (TL) dosemeters (TLD700 and TLD100) were used for dose measurements at a zero-power WWER model at the NRI (Nuclear Research Institute Řež plc., Czech Republic). The results obtained by the two methods were consistent, both among themselves and in comparison with reference data provided by NRI.

New TL materials were investigated for the purpose of mixed-field dosimetry. The neutron response of undoped and Cu-doped LTB (Lithium Tetraborate) crystals produced at NASU (Institute of Electron Physics, Uzhgorod, Ukraine) was studied via radiations at the thermal column of the Portuguese Research Reactor and compared with standard commercial phosphors. The undoped LTB has a low photon sensitivity (10 times lower than TLD100), but the doping increases its sensitivity by a factor of 44. In spite of the fact that undoped LTB has a low photon sensitivity, it is more sensitive to thermal neutrons than the doped material by a factor of 5. Although a significant sensitivity loss was observed for the undoped LTB after neutron irradiations (50% sensitivity decrease after $2x10^{12}$ cm⁻² neutron fluence), the application of undoped/doped LTB pairs is promising for mixed-field dosimetry at lower neutron doses, using doped and undoped LTB as photon and neutron dosemeters, respectively.

¹ Nuclear Power and Safety Division, Nuclear Research Institute Řež plc., Czech Republic

² Radiation Safety Department, Institute of Isotopes, Budapest

Applied Dynamics

José Antunes

The activities at Applied Dynamics Laboratory (ADL) are devoted to research in nuclear engineering, with an emphasis in the vibratory and acoustic behaviour of mechanical components. Our group started in 1986, with the following objectives: (1) Develop theoretical methods, computer tools and experimental techniques, to solve structural problems in nuclear power station components; (2) Use this state-of-the-art know-how, in order to solve structural problems arising in Portuguese power plants and other industrial facilities.

The first objective has been pursued through extensive international collaboration with our main scientific partner - the French Commissariat à l'Energie Atomique (CEA) / Département de Mécanique et Technologie (DMT). More than one decade of fruitful collaboration is attested by a significant number of published results. Important problems have been solved, such as nonlinear vibrations in steamgenerators, flow-induced vibrations of nuclear fuel and stability problems in rotating machinery. Furthermore, new identification techniques have been developed and applied with success to nonlinear dynamical systems.

The second objective has been pursued by starting in 1990 a series of projects with (and for) the Portuguese power supplier Electricidade de Portugal / Companhia Produção de Electricidade Portuguesa de (EDP/CPPE), stemming from actual structural problems in power plants (Sines, Setúbal): These projects enabled us to model and solve vibratory problems arising in rotating machinery, vibroacoustical problems in boilers and heat-exchangers, as well as structural identification problems. Several computer codes have been developed in connection with these projects.

In recent years we also developed research projects of more fundamental nature, mainly funded through the Praxis XXI and POCTI research programmes. These projects have been developed in partnership with several Portuguese institutions (Faculdade de Ciências de Lisboa, Instituto Politécnico do Porto, Instituto Politécnico de Setúbal, Instituto Superior Técnico, Universidade Nova de Lisboa), as well as the Université de Paris and Southampton University. This work, developed in the context of fundamental physics – in particular addressing problems in music acoustics, optimization and structural geology – is centred in modelling nonlinear dynamics and flow-structure phenomena. The methods developed transcend the context of these projects and may be adapted to solve several aspects of industrial problems.

The Applied Dynamics team is mainly concerned with the following scientific fields: structural dynamics, flow-induced vibrations, nonlinear dynamics, vibroacoustics, experimental methods, signal processing, system identification, structural and acoustical optimization. As a spin-off from our research activities, teaching has been actively pursued on structural dynamics and acoustics - ranging from university level courses in Portugal (Coimbra, Lisbon) to several post¬graduation short courses abroad (Paris, Dublin). Also, student training and several university thesis (MSc and PhD) have been successfully supervised, for both Portuguese and foreign students. An extensive book on fluid-structure dynamics and acoustics, co-authored by two CEA and ADL researchers will be published early 2006.

Among the above-mentioned scientific fields one should stress those features which give our small group a distinct profile from others working in structural dynamics in Portugal. Those features are: (1) a proven expertise and output in flow-excited systems and nonlinear vibrations; (2) a complementary theoretical/experimental approach for every problem.

Most of the research projects pursued at ADL have been based on research contracts.

Research Team

Researchers

J. ANTUNES, Princ.

Students

O. INÁCIO (25%) PhD Student, Inv. Professor (1)

Technical Personnel

A. ANASTÁCIO

Collaborators

L. HENRIQUE (15%), PhD, Adj. Professor (1) M. MOREIRA (30%), PhD, Adj. Professor (2) M. PAULINO (20%), MSc, Inv. Professor (3) R. SAMPAIO (10%), PhD, Adj. Professor (4)

- (1) IPP, Porto
- (2) IPS, Setúbal
- (3) IPL. Lisboa
- (4) ENIDH, Lisboa

Dynamical modelling and optimization of nonlinear vibratory and acoustical systems

J. Antunes, O. Inácio¹, L. Henrique¹, M. Wright²

Objectives

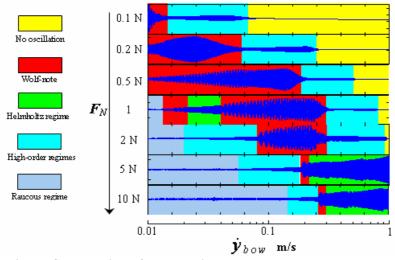
This research started a few years ago as a POCTI funded project, an international cooperative effort to develop theoretical methods and numerical techniques for dealing with strongly non-linear dynamical problems, such as involving impacts and friction phenomena. The main objective was the development of modeling techniques for nonlinear multi-modal structures. These techniques have been applied to a paradigmatic problem in nonlinear physics – bowed instruments – but can be easily adapted to industrial problems of the same nature. In recent years, coupling of vibratory and acoustical systems has also been addressed, namely through the point of view of dynamical optimization.

Results

Last year we extended our modal computational approach in order to address the dynamics of several complex vibratory sub-systems coupled by frictional phenomena. During 2005 these two computational interaction models have been explored in order to assert the merits and disadvantages of each approach. At the same time, the prototypical computed system has been explored, in order to highlight interesting features. Concerning dynamical dynamical optimization, we started to exploit a recently built experimental set-up, in order to obtain test data to substantiate a theoretical model for the vibroacoustics and radiation of vibrating bars or plates coupled to acoustical resonators. Both have been designed using optimisation techniques, which enabled us to tune their resonances at will. A significant number of papers emerged from this research, a PhD thesis anchored on the optimization results was concluded with success, and another PhD related to the nonlinear aspects of this project will be concluded early next year.

Published work or in press

- 1. O. Inácio, L. Henrique, J. Antunes, "The dynamics of tibetan singing bowls", Acta Acústica united with Acustica (in press).
- 2. O. Inácio, J. Antunes, "Simulation methods for the nonlinear string/body coupled dynamics of bowed musical instruments: A comparative analysis", *Proceedings of the Forum Acusticum*, Budapest, August 29-September 2, 2005.
- 3. O. Inácio, J. Antunes, "Dynamical regimes of bowed-string instruments with body-coupling", *Proceedings of the Twelfth International Congress on Sound and Vibration*, Lisboa, July 11-14, 2005.
- 4. L. Henrique, O. Inácio, J. Paulino, J. Antunes, "Optimization of vibratory and acoustical components of percussion instruments: Theoretical and experimental results" (Invited Paper), *Proceedings of the Forum Acusticum*, Budapest, August 29-September 2, 2005.
- 5. O. Inácio, L. Henrique, J. Antunes, "Optimized bass-trapping resonators for control rooms: A preliminary study", *Proceedings of the Internoise*, Rio de Janeiro, Brasil, August 7-10, 2005.
- L. Henrique, J. Antunes, O. Inácio, J. Paulino, "Application of optimization techniques for acoustical resonators", Proceedings of the Twelfth International Congress on Sound and Vibration, Lisboa, July 11-14, 2005.



Coupled String/Body Computations for Increasing Normal Bow Force and Tangential Velocity

ITN Annual Report - 2005

¹ Instituto Politécnico do Porto, ESMAE, Laboratory of Music Acoustics

² University of Southampton, Institute of Sound and Vibration Reserarch, UK

Dynamical Modelling of Geological Inclusions

F. Ornelas¹, R. Taborda¹, J. Antunes

This has been a fruitful project, funded by a FCT/POCTI grant, developed in collaboration with the group of structural geology of FCL. The expertise of our colleagues in geologic experiments and field interpretation has been enriched by our experience in flow modelling, leading to a growing corpus of published theoretical and experimental results. Recently, 2-D finite element modelling was used to investigate the influence of a permanent low-viscosity layer between matrix and inclusion on matrix flow and inclusion rotation under viscous simple shear flow. Rigid inclusions of different shape (circle, square, ellipse, lozenge, rectangle and skewed rectangles) and aspect ratio (R) were used. The calculated matrix flow pattern is neither bow tie nor eye-shaped, the two classically accepted flow configurations. New results and interpretations on the inclusion rotations have also been obtained, showing that a low-viscosity layer (LVL) makes inclusions with R = 1 rotate synthetically, but the rotation rate depends upon shape (circle or square) and orientation. Therefore, shape matters in the slipping mode. The present numerical results closely agree with previous results of analogue experiments with a permanent low viscosity interface. On the other hand, analogue and numerical modelling was used to show that the flow of a Newtonian viscous fluid around a rigid body, in simple shear, depends strongly on the degree of confinement, i.e. the ratio between the shear zone width (H) and the rigid inclusion's least axis (e2) (S=H/e2). It also depends on how closely we look at the inclusion, which leads to the definition of an effective channel length and an effective flow pattern, compatible with micro-tectonics observations. If we consider a long channel, the flow pattern is bow tie-shaped, but tends to become eye-shaped as S approaches infinity. Therefore, special care must be taken when trying to infer rock rheology (e.g. viscous Newtonian or non-Newtonian) from geometrical patterns (e.g. geometry of a mantle and tails of recrystallized material around a rigid body), which are assumed to reflect the flow type. Finally, incompressible Navier-Stokes in 2D finite element modelling was used to investigate rigid inclusion rotation under confined bulk simple shear flow.

1 Faculdade de Ciências de Lisboa, Structural Geology.

Noise Reduction Optimization in Tubular Heat Exchangers

M. Moreira¹, J. Antunes, H. Pina², J. Paulino³

The interaction between a gaseous flow and the tube banks of heat exchangers can lead to the self-excitation of acoustic resonances, originating the formation of stationary acoustic waves in the fluid. These lead to highamplitude pressure fluctuations inside the equipment, with the consequent vibratory excitation of structural elements. When the frequencies of the excited acoustic modes near-coincide with the modal frequencies of tubes, high vibratory levels can seriously affect the system integrity. It is worthwhile to point out that this problem only arises in gaseous heat exchangers, since the typical sound speed in liquids lead to acoustical frequencies typically beyond those of the structural component vibrations. To the present date, in spite of the industry concern by this problem, the physical mechanisms of sound excitation of by cross-flows within tubular banks are not yet fully understood, therefore the available criteria for predicting such flow-acoustic instabilities are not trustfully. Typically, this problem is solved by inserting plates inside the tubular banks (so-called acoustic baffles), in order to inhibit the acoustical instabilities by modifying the acoustic field. However the physical mechanism that renders a given baffle configuration effective or not is still insufficiently known and controversial. In this three years project, funded by a FCT/POCTI grant, we started by developing techniques for optimizing the acoustic baffle configurations. In particular, an efficient method for achieving fast acoustical computations of realistic baffled enclosures, based on a constrained approach of acoustical modal synthesis, has been developed. We expect this will enable us, in the next stage, to achieve baffle configuration optimization with computational savings of one to two orders of magnitude. Then, optimization algorithms will be coupled to suitable flowacoustical interaction models, to be developed and experimentally validated by wind-tunnel experiments.

¹ Instituto Politécnico de Setúbal, Escola Superior de Tecnologia, Department of Mathematics

² Instituto Superior Técnico de Lisboa, Department of Mechanical Engineering

³ Instituto Superior de Engenharia de Lisboa, Department of Mechanical Engineering

Atmospheric Elemental Dispersion

Maria do Carmo Freitas

The research is focused on studies of atmospheric environment, nutrition and health. The investigation appeared as a natural application of the potentialities of k_0 -INAA (instrumental neutron activation analysis using the k_0 -method). The unit activities include six main lines:

Monitoring, Biomonitoring, Quality Control, and Data Handling aiming at characterising areas of Portugal using lichen transplants, air particulate matter collection, and (wet+dry) deposition. The data are analysed for factors aiming at identifying emission sources and the spread of elements through the atmosphere, both locally and by long-range transport. Data analysis methods and their development are very important due to the multielement nature of the analytical technique used. To assure the quality of the data, accuracy and precision studies are being performed, both in biomonitoring and monitoring fields, aiming at better understanding differences found in the results for the same element and sample. Air particulate matter obtained by different air samplers is compared. So-called conventional analytical techniques are applied to complement the research unit's results. Within this activity line, the following are being done: services to industry (monitoring), FCT funded project research (both biomonitoring and aerosol monitoring) and training (one post-doctorate on monitoring and two current PhD theses on biomonitoring).

Epidemiological studies include health related problems. The objective is to link biomonitoring and monitoring to epidemiological studies, at local, regional and European scale. Currently, one PhD and one post-doctorate are dedicated to this subject.

Element Uptake Processes. The group also enters the plant physiology looking for effects on plants due to atmospheric chemical components. The underlying questions are related to the extent in which lichens may reflect the element contents of particulate matter, which may possibly be dominated by its soluble element concentration fractions. This is the subject of one PhD thesis.

Nutrition. The group is increasing the investigation in nutrition studies through a PhD thesis aiming at a better knowledge of selenium in the Portuguese diets. Selenium is a nutrient, which should be included in the human organism within a very narrow mass a ount range, otherwise severe diseases should be expected. Also nutrition contents in spices and rice originated from Sri Lanka are still being studied, following a IAEA fellowship. Honey analysis is being surveyed for Azores islands and Portugal mainland, a more complete study is now taken in Algarve region.

Training. The research unit has a strong component in post graduation training.

Services. Analytical services are also provided under request (private companies).

Research Team

Researchers

M. CARMO FREITAS, Princ., Group Leader

Students

A. P. MARQUES, PhD student, FCT grant M.G. VENTURA, PhD student, FCT grant R. GODINHO, PhD student, FCT grant S. SARMENTO, PhD student, FCT grant

Technical Personnel

I. DIONISIO

Collaborators

A.M.G. PACHECO, Aux. Professor, CVRM/IST, Portugal H. TH. WOLTERBEEK, Senior Researcher, Netherlands B. VIEIRA, Horta Airport, Portugal S. M. ALMEIDA, FCT post-doctorate grant M.M. FARINHA, ISQ, Portugal (on-going PhD)

Calibration of *in situ* Biomonitors for Quantification of the Atmospheric Dispersion of Heavy Metals

M.C. Freitas, A.M.G. Pacheco, S. Sarmento, I. Dionísio, M.S. Baptista, M.T.S.D. Vasconcelos, J.P. Cabral

Objectives

Within BioCAL project (POCTI/CTA/38411/2001, co-funded by EU through FEDER), a full study was conducted in three different locations in Portugal (Lisbon, Viana do Castelo and Sines) in order to compare responses of biological (lichen *Parmelia caperata* and tree bark of *Platanus hybrida*) and non-biological (cellulose acetate) monitors. Alternate forms of lichen exposure were also tested (with substrate and in roughly square pieces).

Results

Two-month exposures, performed during Winter, Spring and Summer, at three Portuguese coastal cities, revealed that airborne accumulations of copper, lead, nickel and strontium were partially dependent of meteorological conditions but essentially dependent of nature of exposed material. No reduction in variability of standardized synthetic materials or homogenized biomasses was shown when compared to lichen. The synthetic materials only accumulated Cu and Ni, being therefore considered an alternative to traditional transplants when these are the elements of interest. The biological materials accumulation of studied elements was comparable to lichen transplant accumulation. The tested biomasses did not present higher ability to accumulate metals, thus their replacement of the traditional transplants was not considered advantageous since their attainment is a time-consuming process. Lichen exposure in detached form was suitable in biomonitoring studies instead of traditional transplants and accurate measurement of area/volume is useful to relate atmospheric deposition rates with lichen metal content.

For lichens, low-methylated arsenic species were found in long-term exposure experiments, whereas in short-term exposure experiments no increase in total arsenic concentration was observed although some degree of biomethylation occurred. Tree bark experiments were not conclusive; no arsenic species could be determined due to too low initial total arsenic concentrations. It was concluded that transplanted lichens can only be used for long-term exposure studies. Looking at the extent of methylation seems probable that lichens do not act as simple passive biomonitors but are actively involved in uptake, accumulation and/or biotransformation of arsenic, possibly other elements as well.

The exposed samples were analysed by INAA, ICP-MS, AAS. It could be concluded that analytical precision was similar for all elements but Br, Cu, Na by INAA, which also did not agree with their certified values in first place. A nonparametric assessment of

correlation between field replicates by paired techniques showed that Spearman coefficients could be asserted at any significance level (asymptotic p=0.000), in all cases and elements. Identical results – based on Wilcoxon's T statistic at p<0.05 – were only found for Na by INAA, Mg, Mn, Ti by INAA and ICP-MS, and Cu by ICP-MS and AAS. In a few cases, biological-matrix effects appeared to underlie the results of the techniques' intercomparison, such as for Ca and Sr (unbiased results for lichen set alone, when separated from bark set) and Pb (unbiased results for bark set alone, when separated from the lichen set).

Significantly higher contents were determined by ICP-MS for As, Ba, Cr, Cs, La, Sc, Ta whereas a few others resulted higher by INAA (Ce, Hf, Se, Zn). Statistically convincing evidence of difference in techniques' output could not be found for Ca, Co, Fe, K, Na, Rb, Sb, Sm, Tb, Th, U, at stringent significance levels. Residual variability may reach 37 % (*P. caperata* thalli) or even 57 % (*P. hybrida* bark), not to mention the biological variability in accumulation during the period(s) of exposure (or assessment, in native lichens). For some elements, experimental issues may arise from digestion procedures (ICP-MS) and/or sample heterogeneity (INAA).

Published or in press work

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- 3. M.C. Freitas, A.M.G. Pacheco, I. Dionísio, S. Sarmento, M.S. Baptista, M.T. Vasconcelos, J.P. Cabral, Instrumental neutron activation analysis and inductively coupled plasma mass spectrometry on atmospheric biomonitors, *J. Radioanalytical and Nuclear Chemistry* (in press).
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Atmospheric Aerosol Impacts on Human Health

S.M. Almeida, M.C. Freitas, S. Sarmento, C.A. Pio¹

This work is supported by the project POCI/AMB/55878/2004. The main objective is to assess the relationship between long term exposure to Air Particulate Matter (APM) and the incidence of Asthma, Chronic Obstructive Pulmonary Disease (COPD) and mortality, for both total APM mass concentration and particle toxic chemical constituents' levels (as Pb, Ni, Cd, As, Hg, Cr). Health risk will be followed relating different concentrations of total APM and some of their constituents. The study of the chemical particles species allowed determining the main sources of particles to atmosphere, using receptor models. The direct relationship between pollutant sources and health impacts will be assessed. From this information, it will be possible to suggest abatement strategies perfectly adapted to the studied area, in order to improve the air quality and, consequently, to decrease the impacts on human health. Time series related to APM concentrations are correlated with asthma and COPD hospital admissions. In 2005, Hospital admission for the respiratory diseases was obtained by analysing the hospital check-out lists from Instituto for Informatic and Financial Management for Health. The health data are analyzed by time series methods in order to exclude potential confounders as seasonal and long term patterns, daily temperature, humidity, precipitation, other pollutants (SO₂, O₃, NO_x) concentration and influenza epidemics. Meteorological and air quality data are obtained in Meteorological and Environment Institutes.

1 Departamento de Ambiente e Ordenamento. Aveiro University, Portugal.

Studies for the Evaluation of Selenium (and Other) Levels in Typical Constituents of Portuguese Diets M.G. Ventura, M.C. Freitas, A.M.G. Pacheco¹, H.T. Wolterbeek²

The aim is to determine the selenium content in a few selected food items commonly consumed and produced in Portugal. Selenium is an essential trace element of fundamental importance to human health. Despite its biological importance, data on selenium in foods are still limited for Portugal. Selenium levels in foods are affected by both content and availability of the element in soil or feed which vary geographically between and within countries. This study provided basic information on selenium content in various foods which can contribute to build a national database. The latter combined with national consumption data can be used to estimate the selenium intake by Portuguese population. Rich protein food, i.e., meat, fish, eggs contribute mostly to the daily dietary Se intake. Vegetables, fruits, cereals, with lower contents on selenium can be an important source on the Mediterranean type diet, where its consumption is considered high. Total selenium content in selected food items have been determined using nuclear activation analysis (NAA) in both versions instrumental (INAA) and replicate sample (RSINAA) through the short-lived nuclide ^{77m}Se, respectively at Interfaculty Reactor Institute/Delft and developed at ITN. Selenium daily intake for two geographically distinct population groups and on selenium species determination in fish samples with high consumption in Portugal, are followed.

1 CVRM-IST, Lisbon Technical University.

2 Interfaculty Reactor Institute - Delft, The Netherlands

Biomonitoring of trace element air pollution

A.P. Marques, R.M. Godinho, M.C. Freitas, H.Th. Wolterbeek¹

This study is about the use of lichens in air pollution studies. Lichens are used in all experiments and elemental analyses are performed by nuclear multi-elemental techniques. One project aimed this year to understand the differences in the results obtained by two elemental techniques in two replicates of the same sample – it was concluded that statistically they do not differ, and to focus on elemental accumulation differentiation in the possible set-ups in transplant monitoring. The other project focus on the (bio)assessment of the elemental burden from selected APM's size classes. The issue is to relate lichen elemental occurrences to elemental occurrences in selected atmospheric size PM, thereby discriminating towards solubility and extractability. Results should make out the usability of lichens in fast and easy estimates of integrative atmospheric. The attention is focused on the multi-element solubility and extractability in both lichens and selected PM size classes, obtained from the same exposure sites. The issue is that lichens may reflect soluble and /or extractable fractions of atmospheric PM's in various or specific size classes. Positive results may lead to an extensive use of lichens in easy, cheap, geographically large scaled and first-line screening of elemental burden from atmospheric particles.

1 Radiochemistry Department, Interfaculty Reactor Institute - University of Delft (IRI - TU Delft), Delft, The Netherlands

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