Elemental Characterization and Speciation
CEEFI

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The Elemental Characterization and Speciation Group of the LFI (CEEFI), was born as such in 2003 in the sequence of a small reorganization of activities using the 2.5 MV Van de Graaff accelerator of ITN. It carries out work of research, development and application of ion beam based nuclear analytical techniques for the characterization of elemental composition of samples, aiming also at speciation methodologies. So far, the main focus has been on particle induced X-ray emission (PIXE) and airborne material. Atmospheric environment related samples like airborne particulate matter and/or biomonitoring samples being different faces of this focus. A tuning of this working line is presently being undertaken in order to cover a broader but more concise focus on small mass samples such as particulate matter (airborne or not), nanoparticles, macromolecules or thin film samples.

Strategically, the group assumes that it is important not to depend exclusively on collaborations neither for sampling nor for data handling processes. Therefore, a strong R&D effort is put on airborne particle sampling and data handling methods. Data handling R&D includes both spectral analysis, as well as environmental data analysis (e.g. inverse methods for source apportionment).

Taking into account that PIXE is already a matured analytical technique, services are provided to the community in general, and to the scientific community in particular. In this cases, analysis of samples other than small mass ones is carried out, and it is not rare that important spin-offs associated to details or specific developments of the PIXE technique, do emerge in this framework.

Within the organics of the Ion Beam Laboratory (LFI), CEEFI is responsible for the maintenance and improvement of PIXE facilities, and assures that, at least, no losses on the installed capacity occur.

In 2006, the groups' activity was focused on launching a large re-equipment project the: Laboratory for Characterization and Speciation of Aerosols (LCEA). Equipment selection, acquisition and installation was therefore one of the main tasks. This project contributed to the acquisition of a refurbished tandem accelerator where the new setup for High Energy-High Resolution PIXE is under installation. The first high energy spectra are scheduled to be obtained during the first two weeks of 2007.

Apart from this the following results were attained: (1) high resolution PIXE (spectra made in IJS, Lubljana) confirmed uncertain results from past low statistics experiments, these results being studied now in the framework of a Ph.D. thesis in ion beam analysis speciation; (2) improvements on the existing data handling software were made and a few papers were published on the subject; (3) the problem of chemical mass balance equations with unknown source signatures was addressed and has been solved for the case of two sources, the general case solution being underway; and (4) the database on airborne element content measurements in Portugal dating back to January 1995 was completed and is now being formatted for publication in the beginning of 2007.

Researchers

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Students

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Technical Personnel

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Characterization and Speciation of Aerosols

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Objectives

The characterization and speciation of aerosols, is the basis and central issue of the CEEFI group work, since it is based on this data that uptake and/or impact models are tentatively established. Each of the specific activities of the group therefore converges towards this aim, or emerges from it. During 2006, the main activity undertaken was the operation of an airborne particle sampling unit at ITN campus, and the launching of the Laboratory for the Characterization and Speciation of Aerosols (LCEA). So far most of the equipment was acquired and the installation procedures are underway. LCEA will be a major demonstration unit infrastructure intended to characterize as best as possible the aerosol present at the ITN Campus, as well as airborne particulate matter sampled in a few locations that will configure a small network spread across the country.

Results

During 2006 the monitoring protocol used was identical to that used during 2005, namely an intermittent (6 minutes on, 18 minutes off) all day sampling with filters being replaced every week. In this way an almost continuous monitoring is achieved while preserving the number of samples within reasonable limits. In parallel to this, a database structure, which includes a historic record of samples, was created. During 2006 this database was under thorough debugging of both structure and data. In the sequence of this work, it was decided to recover data from old work and a large set of samples was analysed. In this way the whole database could be made to contain data starting in January 1995, therefore holding 12 years of airborne elemental contents in airborne particles sampled in Portugal. Data from late November and December 2006 is being analysed in January 2007 prior to publication of the database.

In Fig.1 the time series of annual averages and maxima of chlorine in airborne fine particles (PM2.5) determined in the Lisbon area since 1995 (near Setubal up to 1998 and at ITN since then) is presented. This shows that events of very high Cl concentrations in fine particles identified in 2004 and 2005 were already observed in smaller scale in 1995 in Faralhão and every year since 2000, becoming worse in the last three years. Further data gathered from 2004 and 2005 samples leads to a hypothesis of a problematic situation originated from a combination of anthropogenic emissions (pollution) clear sky and strong marine influence. Still no information is available yet on the chemical species holding this chlorine although the NaCl possibility can be practically excluded based on results from XRD. Further investigation will be necessary to trace this PM2.5 chlorine origin. Studies on possible consequences of these events may now be searched for since there is already a meaningful annual time series to start with.

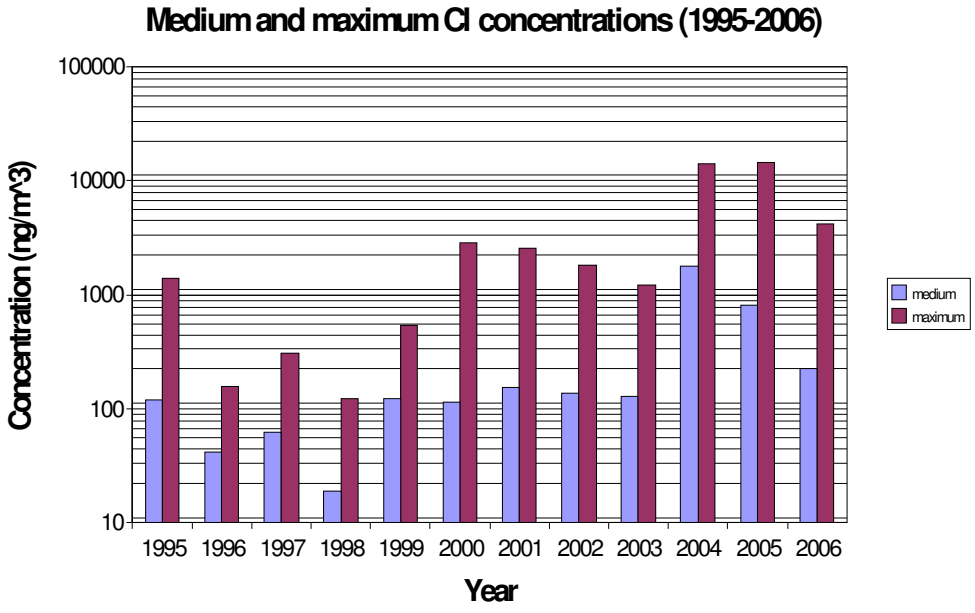

Fig. 1: Variation of airborne chlorine average and maximum concentration in PM2.5 determine at Faralhão (1995 to 1998) and ITN during (1999 to 2006). The growth of the maximum value to unreasonable numbers is clear.