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ITINERIS

D4.8.1: Implementation plan for the operation of the 3 MV Tandetron accelerator at LABEC with the upgraded computer control systems (software and hardware) [B6]

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1. INTRODUCTION

This deliverable is prepared in the context of the ITINERIS project, within the Work Package 4, Atmosphere, that deals with the integration of Research infrastructures working in the atmospheric domain through synergistic approaches and cross boundaries developments.

The aim of this document is to describe the implementation plan for the specific task of the WP 4 Atmosphere about the upgrade of the computer control systems, including hardware and software, for the 3.0 MV Tandetron accelerator at LABEC to increase accuracy and reliability of datasets of the elemental composition of particulate matter samples as obtained by PIXE and other IBA measurements performed at LABEC. This in the context of 100% digital outcome of the ITINERIS project.

The document is structured in five (5) different sections. After this introduction, an overview of the LABEC laboratory at INFN Firenze and its role in ACTRIS ERIC, the European Aerosol, Clouds, and Trace Gases Research Infrastructure Consortium, is reported in section 2. Section 3 reports the gaps and the needs for the implementation of upgrading the accelerator computer control system. Finally, section 4 and 5 report the procedures for recruiting personnel and procuring equipment, respectively, for the achievement of the upgrade of the Tandetron accelerator system controls. Annexes and references are reported at the end of the document.

2. INFN FIRENZE LABEC LABORATORY AND ITS ROLE IN ATMOSPHERIC RIS

The INFN Firenze LABEC laboratory ("Laboratorio di Tecniche Nucleari per l'Ambiente e i Beni Culturali", Laboratory of nuclear techniques for the Environment and the Cultural Heritage) is located in the scientific campus of the University of Florence (Italy). LABEC is a high-qualified centre for the development of new technologies based on particle accelerators and ionizing radiations, and for their applications in environmental contexts and in heritage science [1]. The LABEC laboratory was born in 2003 with the installation of a "small" particle accelerator, namely a 3.0 MV Tandetron produced by High Voltage Engineering Europe, HVEE, and stems from more than thirty years of experience of the research group members with accelerator-related analytical techniques. Accelerated particles are used to characterize the elemental composition of aerosol samples collected on filters by Ion Beam Analysis (IBA) techniques. IBA are a suite of analytical techniques that exploit the detection (and analysis) of radiation such as X-rays and gamma-rays, or charged particles, as emitted in the interactions obtained by the bombardment of the sample with an accelerated particle (usually proton) beam. Among IBA, the particle-induced X-ray emission (PIXE) technique has been widely used for the study of the aerosol composition [2], since up to 20 key elements (from Na to Pb) including important anthropogenic elements (S, V, Ni, Cu, Zn, As and Pb) and all the crustal elements (Al, Si, K, Ca, Ti, Mn and Fe) can be detected in only few minutes of measurement. Moreover, PIXE is sensitive to concentrations down to μg/g, it is highly quantitative (few %) and traceable, and it is a non-destructive technique, so further measurements with other complementary techniques can be carried out on the same samples. The analysis of the elemental composition of aerosol samples gives important information on several markers that may help in disentangling the contributions of different atmospheric aerosol sources.

LABEC hosts the ECAC-CAIS unit Elemental Mass Calibration Centre (EMC2) of the CAIS-ECAC (Center for Aerosol In-Situ - European Center for Aerosol Calibration and Characterization) of ACTRIS ERIC [3]. The main goal of EMC2 in ACTRIS ERIC is to provide proficiency tests of individual laboratory analysis through the organization of inter-comparison and round-robin exercises, operation support for quality assurance and quality control for the measurement of mass concentration of particulate heavy metals and inorganic elements, and hands-on training of operators and scientists from ACTRIS user community. EMC2 will work with the aim of harmonizing the analyses of the elemental composition of atmospheric aerosol samples, in order to make data from different atmospheric observatories fully comparable.

The list of current available instruments (including status, repository where data are stored, link to data and metadata example) is included in the ANNEX 1.

3. IDENTIFIED GAPS AND NEEDS FOR INTEGRATION

The activity of INFN Firenze will be focused to increase the availability of digital datasets concerning elemental composition of particulate matter samples with enhanced propensity for reuse according to the FAIR principles. This aim will be reached through an upgrade of the analytical performances of the LABEC accelerator laboratory for elemental in-situ analysis of atmospheric aerosol sample for ITINERIS and, in general, for the atmospheric aerosol community. This will be accomplished by improving both the offline, laboratory-based measurements (PIXE, XRF, EC/OC) and the online, near-real time measurements.

For laboratory-based measurements, the main activity will involve the upgrade of the computer control systems including hardware and software for the existing 3.0 MV Tandetron accelerator at LABEC to increase accuracy and reliability of PIXE and other IBA measurements performed at LABEC for automatic high-throughput analysis of particulate matter samples to meet user requests.

The control system of the Tandetron accelerator at LABEC laboratory consists of software that controls the components of the accelerator, and corresponding hardware, that enables the communication between the operator and the hardware components. After 20 years from the installation, the present control system is now facing obsolescence in both the software and the hardware: for instance, the industrial PC of the computer control system runs on Windows NT operating system, the control cards are based on ISA bus protocol and the telemetry cards, although custom-built by HVEE, are often not available anymore in case of malfunctioning or failure.

The upgraded control system of LABEC Tandetron accelerator must adequately replace all the existing hardware controls present in the existing old control system of the LABEC Tandetron accelerator, delivered during its installation in 2003, and it must grant sustainability and reliability in performing PIXE and other IBA measurements at LABEC on particulate matter samples for elemental analysis at least for the next 20 years.

The **hardware** that needs to be controlled/read by the new control system, includes:

- focusing elements such as quadrupole doublets and Einzel lens, electrostatic steerers;

- pumping systems and vacuum gauges, valves;
- ion sources (sputtering-type and Duoplasmatron);
- low-energy drift part;
- 3.0 MV Tandetron charge system;
- high energy beamline;
- switching magnet:
- beam diagnostic systems (beam profile monitors and Faraday cups).

The controlling **software** should contain set of panels/routines/features, that enables:

the tuning of the individual hardware components, their operation and diagnostics using mouse and/or keyboard;

the display of all the parameters and readouts for system tuning, monitoring and diagnostics, including e.g. beam profiles, beam cross sections and beam scan area on the computer monitors without the need of any additional hardware;

the display of the status of vacuum pumps and vacuum levels and manipulation of vacuum valves, beam profile monitors and Faraday cups on panels specially configured in line with the overall system layout;

automatic routines for system start-up and shut-down, including start-up and shut-down of ion source(s) and charge-exchange canal, conditioning of the accelerator terminal voltage;

recording and storing all the parameters of the operation with the timing resolution (better than ten seconds), and recalling them and implementing anytime later, using a file saving format compatible with the present system in order to keep historical record of the accelerator system;

scanning and mapping for automated system tuning of e.g. magnetic and electrostatic analyzers, magnetic and electrostatic lenses, steerers and scanners, etc;

scanning of ion beam energy within a user defined range and steps, where the terminal voltage, electrostatic quadrupole lens, and high energy magnet are simultaneously tuned at each energy step.

The control software should run on a new industrial grade computer, equipped with Microsoft Windows 10 or more recent operating system. The control computer contains standard, commercially available communication cards for connection with other hardware components of the control system, and is electrically separated from the control hardware components positioned at the accelerator side: all the hardware control units at the accelerator side are connected with the control computer via optical fibres.

List of instruments/goods to be acquired within ITINERIS:

- Complete set of new interfaces for computer control of the hardware systems along the accelerator (focusing elements such as quadrupole doublets and Einzel lens, electrostatic steerers, pumping systems and vacuum gauges, valves), from the low energy side to the high energy side, including ion sources (sputtering-type and Duoplasmatron), low-energy drift part, 3 MV Tandetron charge system, high energy

beamline, switching magnet, beam diagnostic systems (beam profile monitors and Faraday cups), including spares and links. All these interfaces have to be compatible with existing hardware components, which were specifically designed for the 3 MV accelerator.

- New computer control system, including:
  - interfaces for field bus control system;
  - computer hardware (industrial grade computers);
  - Microsoft Windows based overall system control software – the software is requested to allow for logging hardware controls and indicators and for saving working parameters in file formats which are compatible with the present system (in order to keep historical record of the facility);
  - UPS for control computer.

4. PROCEDURES FOR THE PERSONNEL

No personnel is planned to be hired specifically for this activity of upgrading the HVEE 3.0 MV Tandetron accelerator computer control systems, including software and hardware, since all the work will be done by the accelerator supplier company.

5. EQUIPMENT PROCEDURES

Purchase of Upgrade of HVEE 3.0 MV Tandetron accelerator computer control systems, including software and hardware:

- Single supplier (*Fornitore Unico*), above-threshold procedure (*procedura sopra soglia*)
- Classification by main CPV: 31643000-5 Particle accelerators (*Acceleratori di particelle*)
- Order yet to be issued, but contract vetting (*Determina a contrarre*) already signed.

The purchase of these pieces of equipment is in line with ITINERIS timeline; the purchase of the upgrade of HVEE 3.0 MV Tandetron accelerator computer control systems (software and hardware) has been delayed due to change of the Italian Procurement Code in July 2023 requiring a thorough rewriting of templates and documents, but it is foreseen that the adjudication vetting (*Determina di aggiudicazione*) will be signed within December 2023 and the equipment supplied in 12-15 months. As such it will comply with ITINERIS timeline.

The ITINERIS scientific team working on this instrument is composed by Massimo Chiari, Giulia Calzolai, Cosimo Fratticioli, Fabio Giardi, Franco Lucarelli and Silvia Nava.

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ANNEX 1 –AVAILABLE INSTRUMENTS AT INFN FIRENZE LABEC LABORATORY

- Tandem accelerator (3.0 MV terminal voltage HVEE Tandetron) with 5 IBA beamlines and 5 measuring end stations. The accelerator is equipped with three independent ion sources, two of which (a single-sample Cs-sputtering and a Duoplasmatron) are used to produce all kind of beams (from protons to heavy ions), mainly for applications of Ion Beam Analysis.
- External proton milli-beam set-up high-current/high-throughput PIXE and PIGE analysis of atmospheric aerosol samples (PMx samples, size-segregated samples, high time-resolution samples) collected on any type of substrate (Teflon, Nuclepore, Quartz fibre...) and by a large variety of commercial samplers.
- External scanning proton microprobe set-up with detectors for PIXE, PIGE and RBS/EBS analysis; the focusing system is an Oxford Microbeam quadrupole doublet and the scanning is achieved by magnetic and mechanical scanning.
- Pulsed beam facility for irradiation of devices in-vacuum or in-air with bunches of ions (ranging from proton to oxygen), counting from 1 ion to a few thousand ions per bunch, at a repetition rate of the bunches from single shot to a few kHz.
- Multi-purpose in-vacuum scattering chamber equipped for PIXE, PIGE and RBS/EBS analysis.
- External proton sub-milli-beam set-up for low-current PIXE, PIGE and RBS/EBS analysis of thick and bulk samples, such as cultural heritage objects.
- Analytical grade micro-balance with automated filter weighing (Sartorius) installed in a controlled environment laboratory for gravimetric analysis of atmospheric aerosols.
- Laboratory ECOC thermo-optical analyser (Sunset Lab Inc.) for filter-based measurements of the Elemental and Organic carbonaceous fractions in atmospheric aerosol samples;
- Field ECOC thermo-optical analyser (Sunset Lab Inc.) for near-real time measurements of the Elemental and Organic carbonaceous fractions in atmospheric aerosol samples with a time resolution down to 1 hour.
- Commercial “Epsilon 5” ED-XRF spectrometer (Panalytical) in polarizing geometry for elemental analysis of aerosol (the spectrometer is currently not operational and needs refurbishing, and software and hardware upgrades).
- Two (2) double channels sequential samplers for PM10, PM2.5 or PM1 (Dado Lab Gemini).
- Two (2) single channels sequential samplers for PM10, PM2.5 or PM1 (TCR Tecora Skypost).
- Three (3) Streaker high-time resolution aerosol samplers (PIXE International) for collection of the fine and coarse aerosol fractions with hourly resolution (instrument out of production).

- Two (2) STRAS (Size and Time Resolved Aerosol Sampler) high-time resolution aerosol samplers (designed by INFN) for collection of the fine and coarse aerosol fractions with hourly resolution.
- Multi-stage cascade impactor (Dekati SDI, Small Deposit Impactor) for the collection of aerosols in 12 dimensional classes from 40 to 8 μm (from nanoparticles to PM10).

The following new instruments are currently under acquisition within ITINERIS:

- XACT 625i Ambient Metal Monitor (SaliBri Cooper, formerly Cooper Environmental) for automatic in-situ sampling and XRF analysis of particulate elemental matter, such as metals and dust.
- Second Laboratory ECOC thermo-optical analyser (Sunset Lab Inc.) with dual mode optics, NDIR CO_2 detector and autosampler for high-throughput filter-based measurements of the Elemental and Organic carbonaceous fractions in atmospheric aerosol samples.

Datasets produced by analysis of aerosol particle samples by PIXE and other IBA techniques, as well by other complementary techniques at LABEC (Thermo-Optical, XRF…) are stored in the INFN Open Access Repository (INFN OAR):

- https://www.openaccessrepository.it/

under the Creative Commons Attribution 4.0 license. The datasets are accessible and reusable.

Stored datasets include, at least:

- Experiment title
- Contributing authors (external and local)
- Description of the experiment
- Funding institution (grant)
- Scientific community of reference
- Raw data file (measured samples and reference standards)
- Scanned copy of the logbook (pdf)
- Spectra files converted for the dedicated IBA analysis codes
- Photos of the measured samples (if any)
- Plot of the temperature in the accelerator hall during the measurements

An example can be found, amongst others, at the repository link https://www.openaccessrepository.it/record/77163 (DOI 10.15161/oar.it/77163)

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