Development of a NIST Database of Nuclear Analytical Measurements

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*646.05 Chemical Process and Nuclear Methods Group **646.04 Chemical Informatics Group Nuclear methods have been used to provide measurements at NIST/NBS for more than 50 years.

- A huge amount of data generated from measurements performed for:
- Certification of Standard Reference Materials
- Stakeholders (including users of the NIST Center for Neutron Research (NCNR) cold neutron research facility)
- Interlaboratory comparisons (e.g., CCQM, IAEA)
- Basic research.
- Data can be found in:
- Reports of Analysis and NCNR reports
- Publications
- Memos and personal communications
- Spreadsheets and lab notebooks

Goal:

- Create a searchable database of data generated by Nuclear Analytical Methods at NIST
- Why?
- Transparency
- Conveyance of NAM capabilities to potential stakeholders and NIST scientists and management
- Historical interest

Creation of the Database

- Data compiled from:
- 442 Reports of Analysis 382 on Docushare, 60 found in offices
- >80 Publications
- 100 Memos and personal communications to users
- **35 Spreadsheets**
- Includes data from:
- >200 SRMs and RMs certifications and 30 intercomparisons
- >150 Measurements for stakeholders

Data compiled into spreadsheets and organized by:

- Material
 - SRMs and Intercomparisons
 - non-SRMs (users)

• Element

Data uploaded online at:

http://callisto.nist.gov/nuclearmethods/

Nuclear Methods Database Demonstration

- Start with Landing Page (Periodic Table)
 - Demonstrate how search fields can be displayed and undisplayed by clicking check boxes
 - Analysis method and subcategory
 - Go to next slide for definitions
 - Go through different fields. Hit +/- icon to show information for an individual measurement.
 - Point different units.
 - Most mass fractions (SRM) shown in mg/kg (values originally in % or ug/kg converted for convention)
 - mole ratios for many user measurements
 - Comments field information which is not easily displayed elsewhere
- Go to "View all Elements" to show data for all elements measured.
 - Demonstrate filters for displaying range of values: measured quant, % unc, sample mass.
- Demonstrate graphing capabilities all data that can be converted to mg/kg are displayed. Analysis methods indicated by symbol.
 - By element
 - By material
 - Zoom in and pan capabilities, hover to display information.

Analysis Method	Description	Subcategory	Description
Instrumental Neutron Activation Analysis (INAA)	Decay gamma rays measured after neutron irradiation.	Shorts	Half lives< 12 h
		Intermediates and Longs	Half lives > 12 h
		In Beam	Irradiated in beam.
Radiochemical Neutron Activation Analysis (RNAA)	Post-irradiation chemistry before counting	gamma	Count emitted gamma rays
		beta	Count betas (e.g. P-14, S-35, C-14)
Prompt Gamma-ray Activation Analysis (PGAA)	Simultaneous irradiation and counting of sample – prompt gamma rays measured.	Thermal Neutron PGAA (TNPGAA)	Reactor neutrons moderated at room temperature
		Cold Neutron PGAA (CNPGAA)	Reactor neutrons moderated at 20K by liquid hydrogen
Preconcentration Neutron Activation Analysis (PNAA)	Pre-irradiation chemistry before irradiation and counting.		
Delay Neutron Activation Analysis (DNAA)	Delayed neutrons counted from uranium/thorium fission.		
Neutron Depth Profiling (NDP)	Measure charged particles emitted upon neutron capture. B, Li in silicon wafers		
Neutron Incoherent Scattering (NES)	Hydrogen measured by detecting neutrons scattered from sample.		

Ongoing work:

- Debug database. Correct errors. Fix significant figures.
- Improve graphical interface make icons clickable to view data summary
- Add definitions for acronyms, especially for methods and submethods.
- Add embedded figures
- Make NIST users aware of the existence of the database, get feedback from NIST, and eventually to make it available to users outside NIST.

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Continue to add data.

H (mg/kg vs. position) in Ti alloy failed Turbine Blade

