Overview of Canada’s National Nuclear Forensics Library Development Programme

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Abstract. The Canadian Nuclear Safety Commission (CNSC) has been charged with the task of leading the development of a national nuclear forensics library (NNFL) cataloguing nuclear and other radioactive material under Canadian regulatory control. Canada’s NNFL will consist of a set of databases and an analytical component that consolidate information about Canada’s material holdings in a manner that allows for the determination of whether or not material that is intercepted or interdicted in the response to a radiological and/or nuclear (RN) threat and/or security event is consistent with nuclear and other radioactive material under Canadian regulatory control. This paper will provide an overview of Canada’s NNFL development programme, including a discussion regarding the instruments that enable it. In addition, the paper will discuss the technology development component of the programme for addressing high-level NNFL requirements related to the generation of analytical data, data management and pattern recognition methods for comparative query and analysis.

1. Introduction

In May 2013, the Government of Canada officially launched the Canadian National Nuclear Forensics Capability Project (CNNFCP) as a whole-of-Government initiative under the Canadian Safety and Security Programme (CSSP) to augment Canada’s national capability to respond to threats associated with nuclear and other radioactive material out of regulatory control[1]. The Government of Canada considers a national nuclear forensics capability as a means to enhance the investigation of radiological and/or nuclear (RN) security threats and/or events; and to assist in the evaluation of RN

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[1] The term *regulatory control* is used in this paper as defined in the IAEA Nuclear Security Series No. 15 – Nuclear Security Recommendations on Nuclear an Other Radioactive Material out of Regulatory Control.

material that is about to be used, or that has been used, in a RN security event. To that end, a national nuclear forensics library (NNFL) was identified as a critical component of Canada's national nuclear forensics capability.

The Canadian Nuclear Safety Commission (CNSC) has been charged with the task of leading the development of a NNFL which includes regulatory and analytical information and data pertaining to nuclear and other radioactive materials produced, used or stored within Canada. The purpose of Canada's NNFL development programme is to provide a tool that can assist in conducting comparative queries and assessments as part of a broader investigation into RN security threats and/or events for the purpose of attributing nuclear and other radioactive materials encountered out of regulatory control. Canada's NNFL development programme leverages existing operational and analytical capabilities within the scope of the CNSC's regulatory oversight and compliance verification activities, as well as subject matter expertise and assets of partner departments and agencies within the Government of Canada for the analysis of nuclear and other radioactive material.

2. Programme scope, objective and success criterion

Canada's NNFL development programme is pursuing an incremental approach in order to assess the viability and long-term sustainability of operating and maintaining a NNFL by first demonstrating a technological and operational proof-of-concept using one material group. As such, under the framework of the CNNFCP, the objective of the programme is to develop, design and deploy a NNFL prototype cataloguing a known population of uranium ore concentrate (UOC) material under Canadian regulatory control. The principal success criterion by which the NNFL prototype will be judged is that it must provide a determination, with a reasonable quantifiable degree of confidence, of whether or not the characterisations of independently analyzed, random and blind UOC samples are consistent with the known UOC population captured in the NNFL prototype.

3. Enabling instruments

3.1. Charter of the CNNFCP

The need for a national nuclear forensics capability and the identification of a NNFL as a critical component of that capability are captured in the Charter of the CNNFCP. The Charter is the principal instrument articulating the directive to establish a national nuclear forensics capability in Canada. As part of the process for establishing the CNNFCP Charter, various departments and agencies within the Government of Canada's RN community of practice were identified to contribute their subject matter expertise and assets to the establishment of a national nuclear forensics capability. Given the CNSC's mandate as the competent authority in Canada for the regulation of the use of nuclear energy and material to protect the health, safety, security and the environment, as well as for the implementation of Canada's international obligations, it was charged with the task of leading the development of Canada's NNFL.

3.2. Nuclear Safety and Control Act

The CNSC was established in May 2000 under the *Nuclear Safety and Control Act* (NSCA) [1] to replace the Atomic Energy Control Board (AECB). Under the NSCA, one of the objects of the CNSC is [1]:

(a) to regulate the development, production and use of nuclear energy and the production, possession and use of nuclear substances, prescribed equipment and prescribed information in order to:

    (i) prevent unreasonable risk, to the environment and to the health and safety of persons, associated with that development, production, possession or use,

(ii) prevent unreasonable risk to national security associated with that development, production, possession or use, and

(iii) achieve conformity with measures of control and international obligations to which Canada has agreed.

The mandated authority of the CNSC under the NSCA allows it to carry out central tasks related to the development of Canada's NNFL by leveraging its operational and analytical regulatory and compliance verification activities related to the accountancy of nuclear and other radioactive material; and combining them with the development of key science & technology (S&T) capabilities through collaborative initiatives with, and the support of, Government of Canada partners within the RN community of practice.

3.3. Domestic and international obligations

The *Nuclear Terrorism Act* [2] amended the Canadian *Criminal Code* [3] to create four new offences related to nuclear terrorism in order to implement the *Amendment to the Convention on the Physical Protection of Nuclear Material* (CPPNM/A) [4] and the *International Convention for the Suppression of Acts of Nuclear Terrorism* (ICSANT) [5]. These four new offences make it illegal to [6]:

(a) possess, use or dispose of nuclear or radioactive material or a nuclear or radioactive device, or commit an act against a nuclear facility or its operations, with the intent to cause death, serious bodily harm or substantial damage to property or the environment;

(b) use or alter nuclear or radioactive material or a nuclear or radioactive device, or commit an act against a nuclear facility or its operation, with the intent to compel a person, government or international organization to do or refrain from doing anything;

(c) commit an indictable offence under federal law for the purpose of obtaining nuclear or radioactive material, a nuclear or radioactive device, or access or control of a nuclear facility; and

(d) threaten to commit these offences.

The *Nuclear Terrorism Act* received Royal Assent on 19 June 2013, paving the way for Canada to ratify the CPPNM/A on 3 December 2013 and the ICSANT on 21 November 2013.

As noted in Section 3.2, the CNSC carries out its mandated function under the NSCA *"…in order to achieve conformity with measures of control and international obligations to which Canada has agreed."* Through the development of a NNFL, and its broader participation in the CNNFCP, the CNSC is undertaking a task consistent with enabling Canada to fulfill its international obligations, as well as its domestic obligations under the NSCA by enhancing its capability to support the investigations and prosecutions of nuclear terrorism offences under the *Criminal Code*.

4. Overall structure of the NNFL prototype

The NNFL prototype for UOC material will consist of a separate database and analysis utility. The function of the database is to store and manage administrative (licensing, accountancy, facility, transport, etc.) and analytical characterization information and data pertaining to each constituent of the known UOC material population captured in the NNFL prototype. The function of the analysis utility is to interrogate, query and analyze the analytical data in order to provide a comparative assessment regarding the consistency of a UOC sample against the known UOC population.

4.1. Separation of the database and analysis utility

The separation of the database and the analysis utility into two separate entities is driven by three key factors:

(a) the preservation of data and information integrity,

(b) the requirement to protect sensitive data and information, and

(c) considerations related to technology development and implementation.

The strength of any comparative assessment carried out through the use of a NNFL depends heavily on the quality and validity of the information and data contained in the database. As part of its interrogative function, the analysis utility will manipulate data in order to identify key variables in order to resolve patterns of interest. In order to ensure that this function cannot alter the data in the database, a decision was taken to fully separate the two entities, with the only connection being a "read-only" capability from the analysis utility to the database. In this configuration, the analysis utility will perform a targeted query in order to identify and select the data it needs, before undertaking the necessary steps to manipulate the selected data outside of the database.

The CNSC currently operates multiple databases tracking the quantities, movements and associated regulatory information of nuclear and other radioactive materials under Canadian regulatory control. Given the purpose of the NNFL prototype and potential long-term implementation thereof, Canada's NNFL will be held, operated and maintained by the CNSC. The information contained in the NNFL prototype will be of a requisite sensitive nature such that steps will be taken to secure it through the implementation of protective measures and strict access control regimes. Access to the database and analysis utility of the NNFL prototype will be restricted to specific CNSC personnel, and will be graded subject to the operational needs and roles of the personnel involved in sustaining the capability. By separating the database from the analysis utility, the effectiveness of protective measures and access control regimes can be maximized.

The separation of the database from the analysis utility provides the added advantage of decoupling technology development and maintenance requirements of each component. Furthermore, the underlying subject matter expertise for database design and that of the analysis utility are very different, and separating them allows for a more focused development strategy for each. In addition, it is anticipated that each component will evolve independently, and thus their separation will provide the added benefit of flexibility in implementing potential design changes, software upgrade and maintenance activities, as well as allowing for their development to occur in parallel.

4.2. S&T development

Canada's NNFL development programme is divided into three core S&T development activities, including:

(a) analysis of UOC material for the generation of analytical characterization data,

(b) development, design and deployment of a database, and

(c) development, design and deployment of a multivariate analysis (MVA) chemometrics analytical tool.

4.2.1. UOC material analysis

UOC material was identified as the preferred material group for development purposes of the NNFL prototype; and was/is not related to any specific security concern associated to that material group. UOC material is a signature-rich material group with established methods for its analysis and characterization [7-12]. In addition, the use of this material group allows for the leveraging of current CNSC capabilities, as well as those of Government of Canada partner departments and agencies, in the characterization of UOC. For the initial phase of the NNFL prototype development, the primary method for UOC material characterization and data generation will be through the use of inductively coupled plasma mass spectroscopy (ICP-MS), relying on a method that has been developed, optimized and validated by the CNSC Laboratory for the quantitative analysis of 57 elements in UOC.

4.2.2. Database development, design and deployment

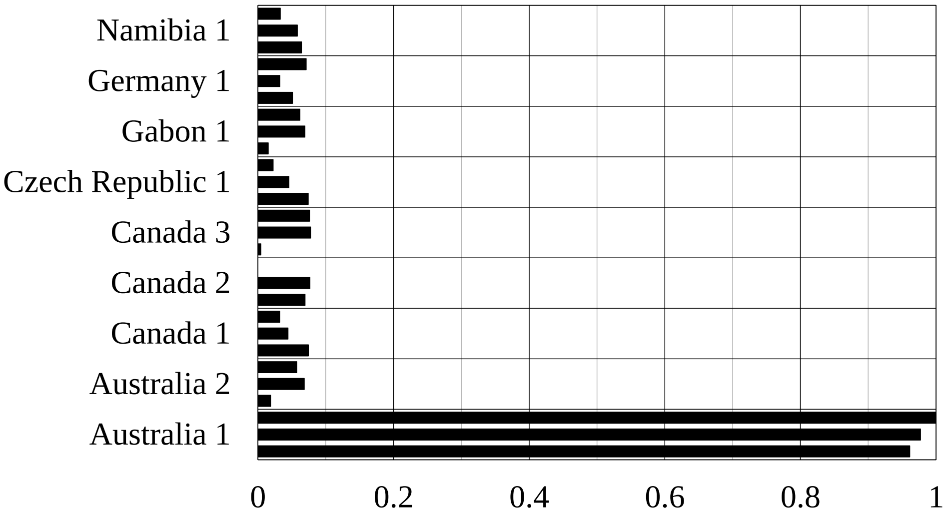
The development, design and deployment of the database for the NNFL prototype will rely on the internal capabilities of the CNSC Information Management Technology Directorate (IMTD). The CNSC, with the support of its IMTD, has extensive experience in the development and operation of databases for the purposes of tracking the quantities, movements and associated regulatory information of nuclear and other radioactive materials under Canadian regulatory control.

Notwithstanding the nuclear forensic value of geolocating an intercepted or interdicted UOC sample to a point of origin, geolocation in and of itself provides insufficient information regarding the broader investigative question as to how a UOC sample was lost from regulatory control. As such, steps will be taken to design the database in a manner so as to link the analytical UOC material characterization data for each constituent of the known UOC population with the regulatory information associated with it. This link is intended to provide a summary of the regulatory information and data regarding facilities, material accountancy, transport and import/export transactions, which will provide valuable insights into any potential diversion path(s) out of regulatory control.

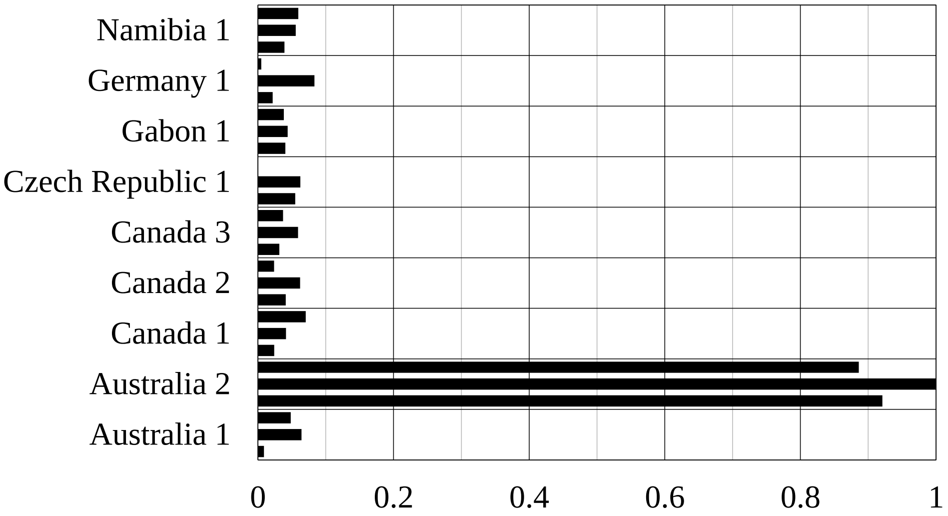
4.2.3. MVA/chemometrics analysis utility

Previous development work carried out by the CNSC and the National Research Council Energy, Mining and Environment (NRC-EME) portfolio in the area of laser-induced breakdown spectroscopy (LIBS) for UOC material characterization and origin assessment [13-17] provides the basis for the development of the MVA/chemometrics analysis utility for the NNFL prototype. Chemometrics is the application of data-analytic disciplines for the interrogation and identification of patterns in chemical systems. The analytical methodology of the MVA/chemometrics analysis utility will be built using a combination of principal component analysis (PCA), partial least squares discriminant analysis (PLS-DA) and soft independent modelling of class analogy (SIMCA) procedures in a complex multistage pattern recognition algorithm in a hierarchical multi-class arrangement.

(a) LIBS test sample for Australia 1



(b) LIBS test sample for Australia 2



(c) LIBS test sample for Canada 1

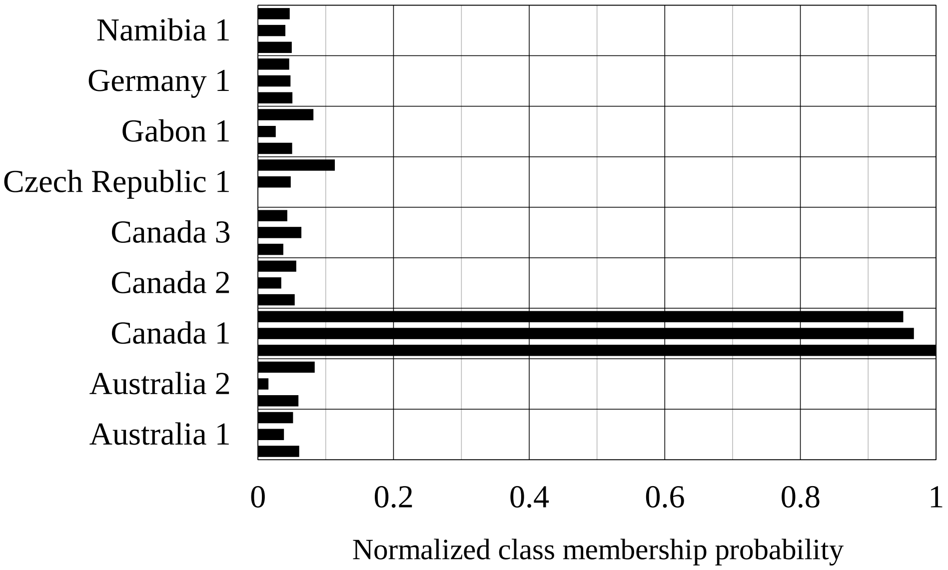
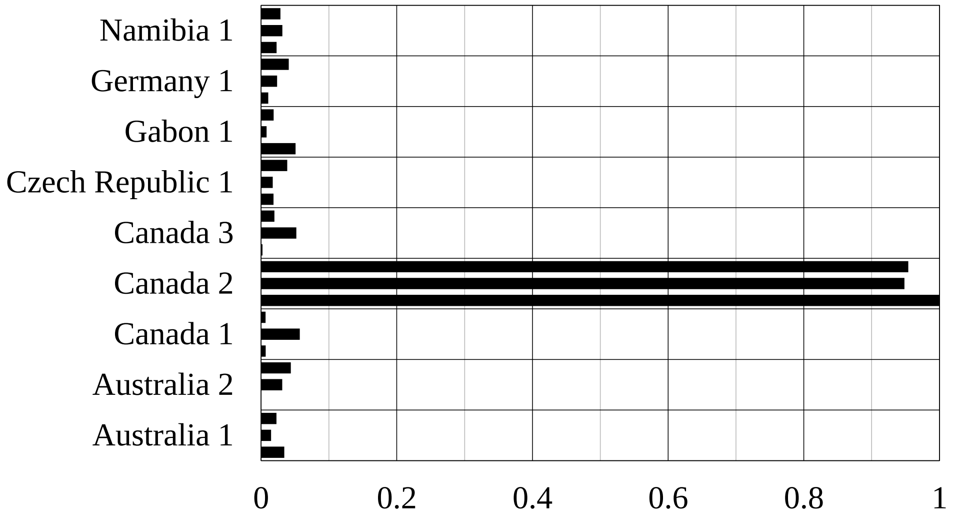
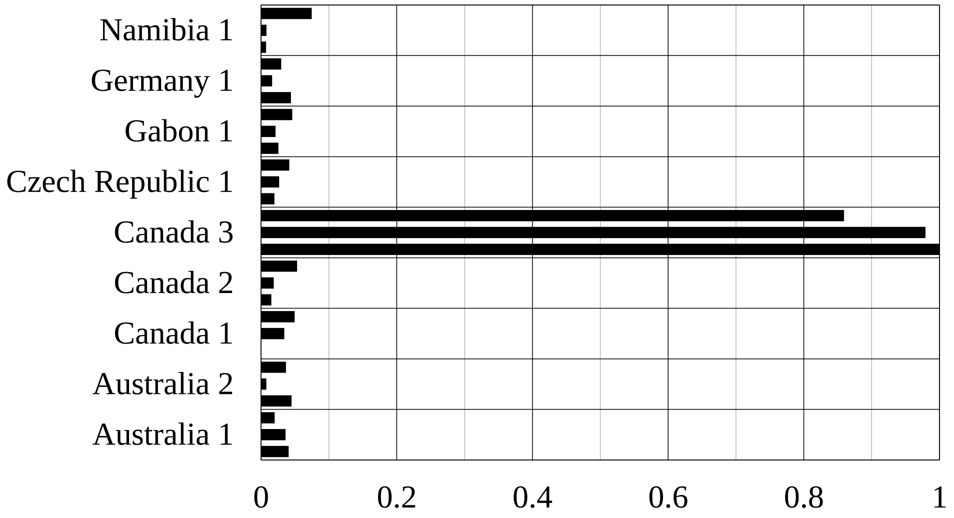


Figure 1 – UOC LIBS test sample normalized class membership probability against three reference characterizations for each location of UOC origin.

(d) LIBS test sample for Canada 2



(e) LIBS test sample for Canada 3



(f) LIBS test sample for Czech Republic 1

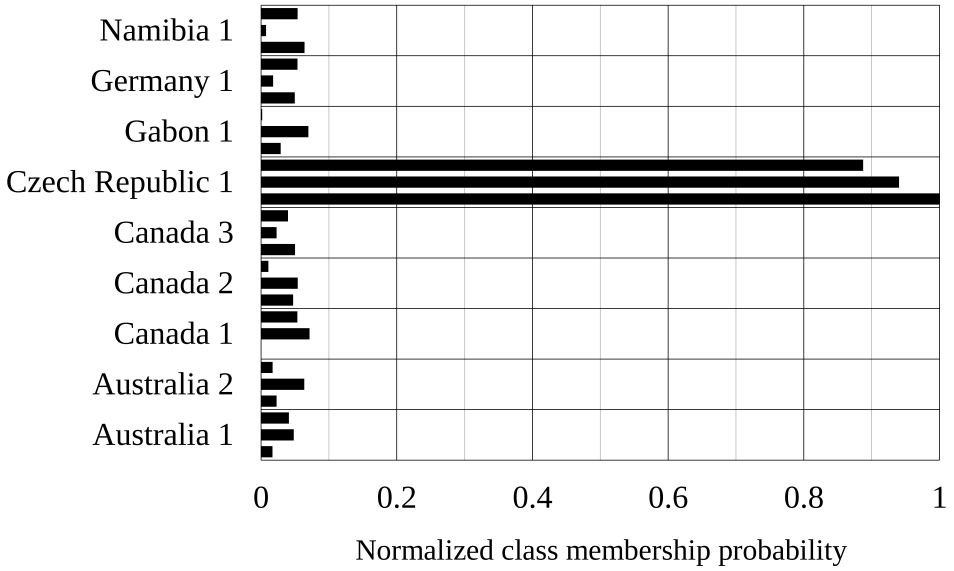
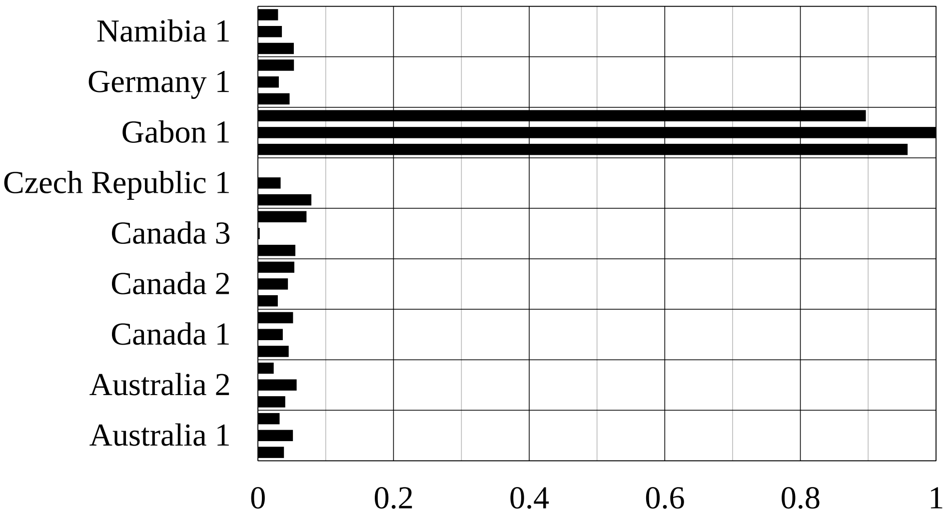
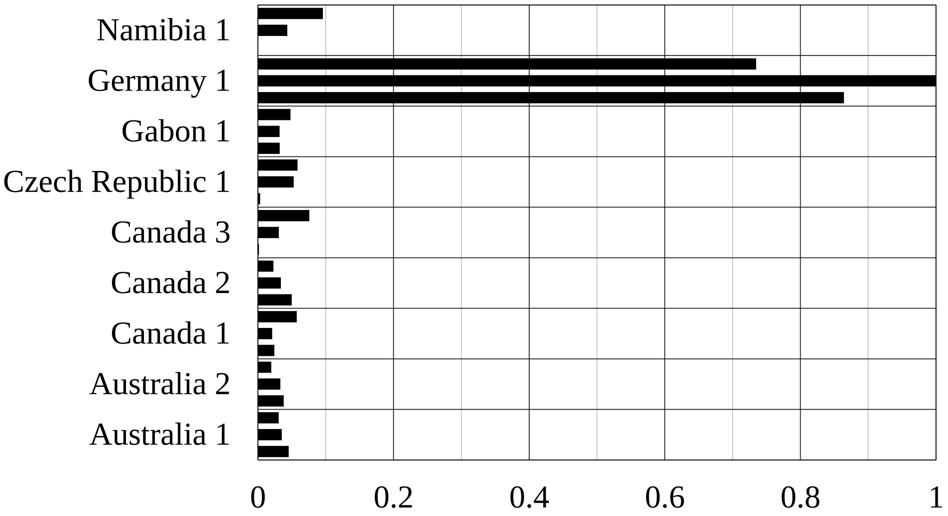


Figure 1 (continued) – UOC LIBS test sample normalized class membership probability against three reference characterizations for each location of UOC origin.

(g) LIBS test sample for Gabon 1



(h) LIBS test sample for Germany 1



(i) LIBS test sample for Namibia 1

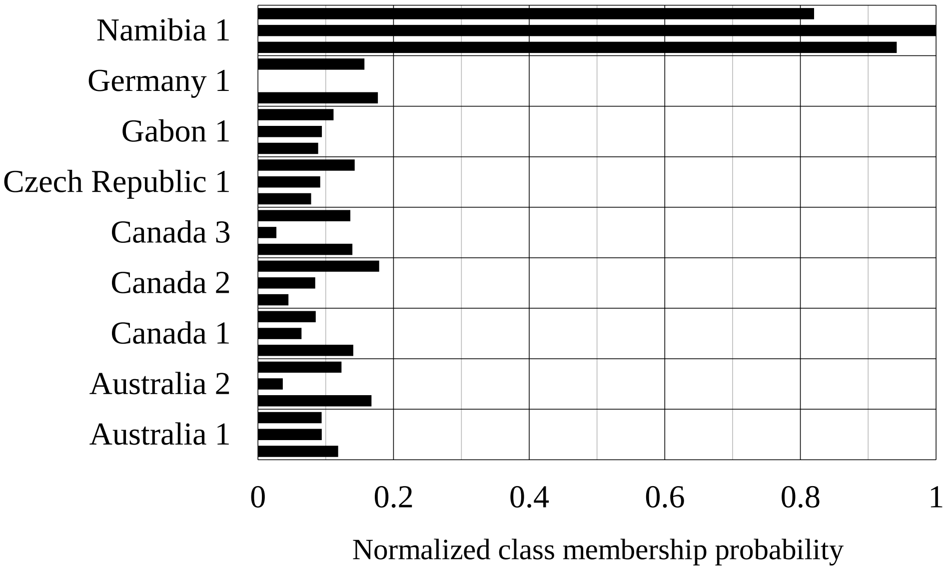


Figure 1 (continued) – UOC LIBS test sample normalized class membership probability against three reference characterizations for each location of UOC origin.

The application of PCA, PLS-DA and SIMCA procedures in a multistage pattern recognition algorithm for the analysis of UOC data for the purposes of geolocation has been tested through the development of LIBS technology [13-17]. Figure 1 shows preliminary results for the origin assessment of UOC material based on the chemometric analysis of LIBS spectrochemical data. Here, three UOC samples from each location (or class) were characterized with the average of 100 LIBS characterization spectra each to create a LIBS UOC signature library for the nine locations: Australia 1, Australia 2, Canada 1, Canada 2, Canada 3, Czech Republic 1, Gabon 1, Germany 1 and Namibia 1. A blind UOC sample from each location was then characterized using LIBS to produce a spectrochemical signature, which was then compared against the library of LIBS UOC spectra using a multistage pattern recognition model in order to determine a class membership probability (i.e., origin attribution).

The preliminary results shown in Figure 1, which have been normalized to show the proportional membership probability for each sample against the LIBS UOC spectrochemical library, demonstrate that the chemometric analysis of LIBS spectrochemical data of UOC material can provide a highly-discriminant class membership probability between origins of UOC material. In addition, Figure 1 demonstrates the robustness of the underlying multistage pattern recognition algorithm of the chemometric analysis given that LIBS provides a relatively crude characterization compared to higher-sensitivity and higher-selectivity methods such as ICP-MS. As such, it is anticipated that the chemometric interrogation of the ICP-MS generated UOC data for the NNFL prototype will yield higher-fidelity discrimination between UOC material signatures.

It is important to note that the application of a multistage pattern recognition modelling approach in the MVA/chemometrics analysis utility allows for the ability to provide a probabilistic output at a certain (pre-defined) confidence interval. This is crucial given that the degree of confidence of a NNFL comparative query and assessment result must be quantified and well-understood.

5. Conclusion

The Government of Canada has engaged in a whole-of-Government initiative to establish a national nuclear forensics capability. A NNFL has been identified as a critical component of this capability, the development of which is being led by the CNSC. Canada’s NNFL development programme has established a plan that will simultaneously leverage existing operational activities and capabilities, as well as key S&T for the development, design and deployment of a NNFL prototype cataloguing a known population of UOC material under Canadian regulatory control. The NNFL prototype will constitute a technological and operational proof-of-concept used to assess the viability and long-term sustainability of operating and maintaining a full-scale NNFL.

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The Uranium Sourcing Database Project: Practical Insights into the Establishment and Application of a Nuclear Forensics Library

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Abstract. The Uranium Sourcing Database is a working nuclear forensics database containing data on thousands of samples of uranium ore concentrate (UOC) and related products. The database is part of a broader effort to characterize and document distinguishing properties of UOC for use in assessing the probable source of sample of material absent any packaging or identifying marks. While this project has focused on UOC, the lessons learned are equally relevant to a wide range of nuclear and radiological materials. We will present a number of practical insights, including nuclear forensics database development and population, user interface requirements, analytical laboratory to database interface, and database utilization.

1. Introduction

The Uranium Sourcing Database is a working nuclear forensics database containing data on thousands of samples of uranium ore concentrate (UOC) and related products. The database is part of a broader effort to characterize and document distinguishing properties of UOC for use in assessing the probable source of sample of material absent any packaging or identifying marks [1]. While this project has focused on UOC, the lessons learned are equally relevant to a wide range of nuclear and radiological materials. We will present a number of practical insights, including nuclear forensics database development and population, user interface requirements, analytical laboratory to database interface, and database utilization.

Nuclear forensic methods can be broadly divided into two categories: predictive and comparative. Predictive forensics requires detailed, accurate, and validated models of physical processes governing the production and alteration of nuclear materials. For some types of materials, such as spent reactor fuel, such models do exist at a level of refinement that makes them useful for nuclear forensic analysis [2]. However, for many types of material, including uranium ore concentrates, no validated models exist that capture the complexity and variability of the associated signatures. For this reason, the best tools available for forensic analysis are comparative. Conclusions are drawn after considering the similarities and differences between the unknown and a reference set of known materials. The principal purpose of a nuclear forensics (NF) database is to serve as a data repository from which to draw these reference sets for comparative nuclear forensics. However, the NF database has utility beyond simply storing data for use in a comparative forensic investigation. A collection of data and metadata from a number of samples representing a variety of sources can also serve as an empirical foundation upon which to begin the development of predictive insights and models to complement comparative models in the forensic process.

In this paper, we describe our insights acquired from years of practical experience with a database of uranium ore concentrate sourced from around the world. The Uranium Sourcing Database was established as a tool to research the application of comparative signatures to the problem of safeguards verification. The goal of this work is to verify that the characteristics a collected sample are consistent with the declared source of the material. For nuclear forensics, the process is very similar, and hence the database requirements are also very similar. In fact, we have utilized the Uranium Sourcing Database for nuclear forensic investigations [3]. Hence, for the purposes of this paper, we will be referring to the Uranium Sourcing Database as a nuclear forensics database.

2. Database design, administration, and personnel considerations

The first task involved with the establishment of a nuclear forensic (NF) database, following the decision to implement such an effort, is to identify an individual or team to design, administer, and manage the database.

One approach to designing a nuclear forensics database, is to work with an experienced database developer to design and implement the new database. This approach has many advantages, including efficiency of implementation, potential cost savings over training internal staff, and avoiding overtaxing staff with additional duties. However, the lack of familiarity of the database developer with the particular needs of a nuclear forensics database may be a liability. Additionally, the involvement of a dedicated database administrator will usually be required beyond the initial implementation period, and it will likely be essential to have a database administrator available on an ongoing basis to maintain the database and make periodic improvements to the system.

It is also possible to develop the necessary database development skills for database design and implementation within an already established nuclear forensics work group. This is a good approach if resources are limited, but places an increased workload on staff. This approach requires at least one staff member to possess or develop specialized skills in database design and implementation. One significant advantage to database design without the aid of an external database developer is that the in-house developer is likely to possess greater familiarity with nuclear forensic data. Cultivating database skills internally to the nuclear forensics working group will also likely facilitate greater interaction with, and collaboration between, the database administrator/designer and the analytical staff.

2.1. Designing a database for nuclear forensic data

The term database is used in many different ways; in this work we define a database as a collection of data stored in some organized fashion. Data is stored within a database in one or more tables; a table is a structured list of data of a specific type. The way the tables are designed and relate to each other is referred to as the database structure. The simplest structure is a flat database, in which all of the data is stored in the rows and columns of a single table. An example of such a flat structure is an Excel worksheet, or a single table in Microsoft Access. Flat databases are quite straightforward to set up and implement, and require a minimum of specialized database knowledge. For a very small database that will be accessed by only one person at a time, it is possible that an Excel spreadsheet might be sufficient. For anything beyond the most basic and limited database, however, a more robust model that allows for multiple users across many computers is far preferable.

2.2. A data model for nuclear forensic data

The data model describes the underlying entities and relationships that a database is designed to represent and capture. The entity relationship diagram is used to develop and document the data model. There are many ways to organize a given dataset, which includes both data (e.g., measured values) and metadata (e.g., the type of instrument used to make the measurements). The data model for the Uranium Sourcing Database was developed through an iterative design process. The primary design goals for the Uranium Sourcing Database are ease of use for nuclear forensic queries; ease of use by subject matter experts; and maximizing utility for end users. The structure that we developed emphasizes the importance of samples and measurements, since these are the starting point for a nuclear forensic investigation.

2.3. Database Structure

In the Uranium Sourcing Database, data are grouped into two primary logical units (*tables*), 15 secondary derivative tables, and relationships are defined to link the tables. This structure provides efficient storage of information, and provides for built-in data validation. For example, all entries (*records*) in the result table must have corresponding sample and parameter information. The presence of lookup tables supports consistency in the data sets by limiting valid values to, for example, correct spellings and consistent abbreviations. The relational database structure is useful for efficient retrieval of subsets of data to meet user requirements.

The two principal tables in the database are the **Sample** and **Result** tables (**Figure 1**).

The **Sample** table contains information about each of the samples in the database. This includes sample composition, provider, and date received by the lab, among other things. Each analyzed sample has a unique Sample ID, and also sometimes additional ID numbers that were provided by the sample provider. *Sample* is the key field that links the sample to its chemical, physical, and image data found in the **Result** and **Image** tables. *Sample* also links the sample to data found in the **Class**, **Source**, and **Location** derivative tables. The date of sample receipt and mass of the sample are noted in the **Sample** table as well. The Sample table is linked to the **Class** table, which contains information about the "*class*" of the sample (usually the location of collection or production), the *source* of the sample, and the *country* of origin of the sample. The **Source** table contains information about the geologic provenance of the sample (*geologic_province*) and the type of deposit from which the sample was derived (*deposit_type*). The **Sample** table is linked to a number of lookup tables including **Material** (i.e. specific type of UOC compound), **Provider**, and **Location**. Image files associated with specific samples are included in the **Image** table. It is important to note that a given sample may have more than one associated image, i.e. several photographs, SEM images, or other graphic data. The **Image** table is therefore linked to the sample table with a many-to-one relationship.

The **Result** table contains quantitative laboratory measurements, expressed as numeric values, and qualitative results (i.e. XRD interpretations) expressed as text. The **Result** table is linked to the **Sample** table by the *Sample* ID field. The **Result** table is also linked to the **Parameter**, **Analysis**, **Units**, **Instrument**, and **Lab** tables. Another important link is between the **Result** table and the **Document** table, which links directly to the original source data for a given measurement. Typically documents in the **Document** table are either Excel files, or pdf files from which the data was extracted for uploading to the database. It has proven useful to have an easily accessible archive (i.e., a data repository) of the source documents that have been used to populate the database. Relationships between the **Sample** table, **Result** table and other tables in the database are shown in **Figure 1**.

2.4. Analytical laboratory to database interface

The Uranium Sourcing Database effort includes a substantial sample characterization component. In addition to data from outside sources, much data is generated in our labs specifically for the purpose of populating the database. Once an analyst finishes a set of measurements (e.g., strontium isotopic ratios), they send a file containing the data to the analytical lead for the database, who then vets, formats, and uploads the data to the database. When external reports are required for a sample analysis, the data can be easily downloaded from the database into a reporting template.

Incorporating some LIMS functionality into a NF database

Rather than stand up a separate laboratory information management system (LIMS), we have opted to utilize the Uranium Sourcing Database to track the status of sample analyses. This can be seen in the sample table in **Figure 1**; most of the fields are for tracking.

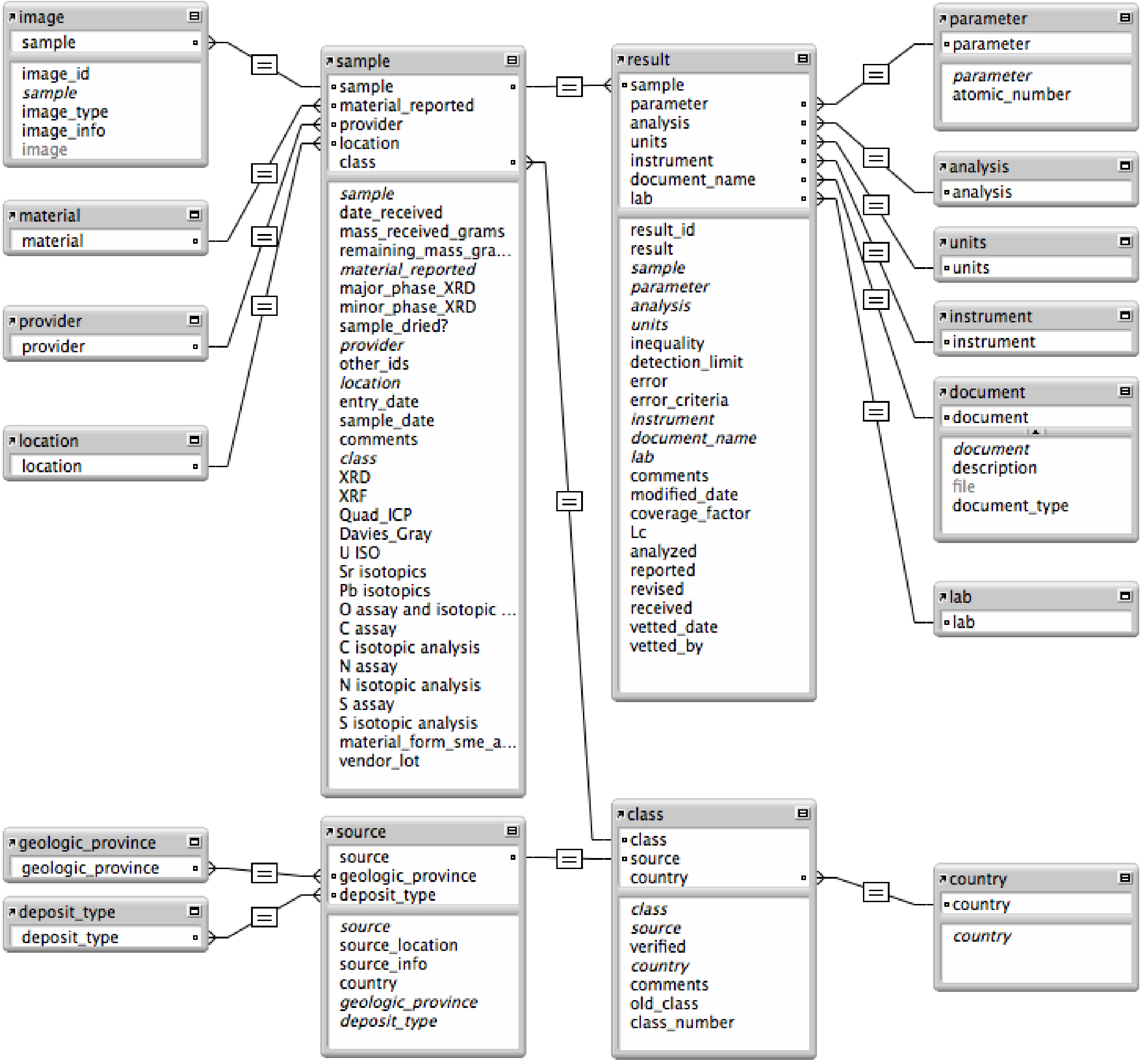

Figure 1. Uranium Sourcing Database core database diagram.

2.5. Choosing a platform for the database

There are a wide variety of database management software platforms that provide the necessary functionality for a nuclear forensic database. We have experimented with a few different platforms for the Uranium Sourcing Database; each has its own advantages and drawbacks.

Most nuclear forensic databases will likely be of a size and scale that will require a relational structure and a robust, multi-user interface. A general-purpose database management system is a software package designed to allow the creation, querying, updating, and administration of databases. A number of widely used platforms meet these requirements, including Oracle, MySQL, Microsoft SQL Server, Microsoft Access, and FileMaker Pro, to name a few. Some primary considerations in selecting a particular platform are the ability to allow and control user access, institutional support, and familiarity with the software.

While desktop systems like Microsoft Access are relatively user-friendly, they are not designed for multiple simultaneous users. FileMaker Pro is unusual in that it is both relatively user-friendly and also designed for multiple users on a network. One limitation to the FileMaker platform is that it does not use structured query language (SQL) and is therefore a non-standard database platform. Despite this limitation, we have used FileMaker Pro for the Uranium Sourcing Database because it was already part of the standard software package at LLNL. The institutional support for FileMaker Pro made implementation over the LLNL network straightforward. Our preferred approach is to employ a database with institutional support, at least for the initial database implementation.

As goals or priorities change, it may be necessary or desirable to migrate the NF database to a new platform. Choosing a relatively simple structure and avoiding the use of business logic (e.g., in the form of *stored procedures*) in the database makes migration easier. If business logic is kept at the application layer level (i.e., not part of the database), it may be reused with the new platform with relatively minor changes.

The cost of database software varies substantially, depending on the scale and level of support. For databases on the scale of nuclear forensics data, there are many no-cost options, including both open source, unlimited platforms like MySQL as well as free, size-limited versions of proprietary platforms like Oracle and SQL Server. No-cost versions typically lack customer support, but online user forums are a rich source of information as well as voluntary “crowd-source” support.

2.6. Data types

Data can be stored in database tables in a number of numeric and non-numeric formats. Selecting the appropriate format for data storage within the database has been an important component of designing and maintaining the Uranium Sourcing Database. In this context ‘data type’ refers to a storage format that constrains the type of information stored by a computer in a variable. For example, the ‘tiny int’ data type used by Transact-SQL only allows storage of integers from 0 – 255 in a variable that uses 1 byte of memory [4]. There are many different data types used by database programs and many of them have cryptic names like ‘varchar(50).’ This situation is further complicated by the fact that there are many deprecated data types. Since data types are not standardized across all databases, we will not go into further detail on these specifics. There are a few broad categories of data type that are needed for a NF database. These include text, integer, decimal, and time.

One important lesson learned from the Uranium Sourcing Database effort is that database data types don’t necessarily easily accommodate the range of data types represented in geochemical datasets. For example, the decimal data types specify the number of digits allocated before and after the decimal. This poses a problem when attempting to store data with variability in the number of significant digits (e.g. storing isotopic data good to six significant figures cannot be stored in the same format as trace element data good only to two significant figures, unless they are stored as text).

Another common problem occurs when the database administrator receives measurement data on spreadsheets with the display setting adjusted to show the correct significant digits. Uploading these data into a numeric data type field will result in numbers with far more digits reported than intended or appropriate. It is therefore preferable to have analysts submit data to the database administrator in text format, such that the correct significant figures are preserved. It is also essential to perform quality assurance/quality control on the data, ensuring that analytical results are truncated to the appropriate number of significant figures prior to uploading data to the database. One imperfect and counter-intuitive solution to *preserving* significant figures in the database is to use a text data type for the measurement data. Unfortunately, this creates other problems: database software typically cannot sort numbers-stored-as-text properly. This will require another workaround. One could, for example, have a duplicate column with the same data stored as numbers (with the incorrect significant digits), simply to use as a field for sorting or other mathematical operations. There are probably many other solutions that will work as well. Our aim is not to declare a universal solution to this problem, but rather to call attention to it.

3. Populating a nuclear forensic database

3.1. Units and conventions

Data for a NF database is likely to come from multiple sources, with differing requirements and standards of reporting. Some data may be generated from laboratory analysis of samples of interest specifically for NF purposes. But there are also numerous potential sources of external data, which was originally collected for other purposes. Data collected for quality control, for example, might be reported in different units with different conventions for dealing with detection limits. There are two ways of dealing with inconsistencies in the data designated for the NF database. One option is to import the data to the database as received, and perform the necessary operations (e.g., converting reported units from ppm to µg/g U) after exporting the data for a specific query. The advantages of this approach are 1) reducing the potential for data corruption through errors in conversion, and 2) reducing the up-front work load by saving these operations until such time as they are needed. The second option is to perform all conversions prior to upload, so that the data in the database is as consistent as possible. This increases the up-front work load, but it makes the database far more useful. Furthermore, if a file repository is used, there is a record of the original data in its original form. This will minimize potential problems from corrupt conversions of data prior to uploading to the database. Regardless of which approach is used, all of the data should be vetted by a technical expert familiar with the measurements that produced the data prior to using it for forensic investigations.

3.2. The file repository

Typically, the database administrator receives data in files that have been vetted by subject matter experts. In addition to uploading these data to the database, it is highly recommended that a link to the original file be facilitated by the database structure. In this way each measurement for every sample in the database can be traced back to the source document. In the Uranium Sourcing Database, this is achieved by the use of a document field in the result table, which links to a document table, which links to a file, as illustrated in **Figure 1**. Some off-the-shelf analytical database solutions do not allow this linking of measurements with documents. We feel this is a critical requirement for a nuclear forensics database.

3.3. Data entry

Databases can either be populated manually, by typing in one entry at a time, or in bulk or batch operations in which data is uploaded as a group of entries. In most cases, a batch/bulk import operation is the most efficient and consistent approach. Batch and bulk imports are accomplished either with a SQL script or through a graphical user interface, or a choice of either method, depending on the database software. In many cases, the format of the data provided to the administrator for input to the database is not in the format required for bulk importing. For repetitive data formatting operations, some kind of automation is highly recommended. This automation can be programmed using a variety of languages; for the Uranium Sourcing Database, Microsoft Visual Basic for Applications (VBA) in Excel is used.

3.4. Queries

The process of interrogating the database for information is referred to as querying. The word ‘query’ can mean a request for information, but it can also refer to a block of SQL code that is not limited to requesting information (it can be used to perform other operations, including deleting data). Queries can be performed by executing SQL commands (for most systems) or though a graphical interface. Since the NF database administrator and end user(s) will not necessarily be SQL coding experts, development of at least two graphical interfaces are suggested: one for the administrator and one for other technical users, such as scientific staff.

4. Utilizing a NF database

In general, there are three categories of users of the NF database, and each has different interface requirements. These are the database administrator/developer, the scientist/investigator, and the 'customer.' The administrator/developer needs full control of the database, including both the structure and the content. We have found that a variety of off-the-shelf applications meet the administrator interface requirements. But these same applications tend to be overwhelming to the scientist/investigator who is typically not a database expert. A custom application layer can be designed to facilitate the functionality desired for this user group. However this requires a significant software development effort. Some platforms provide graphical user interface development environments to aid in this effort. Alternatively, a web programmer can be employed to develop a web browser interface.

The third user category, the customer, probably should not be interacting with the database through any direct interface. Instead, customer queries should probably be directed through a database point of contact, who will likely be a manager or a database administrator. The customer may be asking only for database statistics or they may be requesting utilization of the data for a nuclear forensics investigation.

There are two categories of graphical user interface for databases: off-the-shelf software (e.g., SQL Server Management Studio Express) and custom applications. The off the shelf solution requires less development work, but it requires a higher skill level to utilize (though not as high as the command line SQL interface).

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The third user category, the customer, probably should not be interacting with the database through any direct interface. Instead, customer queries should probably be directed through a database point of contact, who will likely be a manager or a database administrator. The customer may be asking only for database statistics or they may be requesting utilization of the data in for a nuclear forensics investigation.

For utilization in a nuclear forensic investigation, querying the database is only the beginning; a subject matter expert will need to review the data in the context of the query and call upon outside knowledge not necessarily captured in the database. For this reason, customer queries to the NF database for drawing nuclear forensic conclusions should probably only be handled by a small group of technical experts, who will use the data and metadata to develop reports to the originator of the request for comparative NF analysis.

For complex signatures, additional data processing may be called for. In these cases, the data from the query are typically exported to Excel and/or an analysis environment like MATLAB for further processing and analysis. The Uranium Sourcing Database is populated primarily with uranium ore concentrate (UOC) data. Since samples of UOC of forensic interest don't have physical dimensions (like a fuel pellet) or serial numbers (like a sealed source), we must rely on other measurable properties for the process of comparative nuclear forensics. The relatively high abundance of elemental impurities in UOC, comprises a multivariate signature. These, along with isotope ratios are exported from the database and utilized as inputs to a multivariate analysis, such as principal components analysis (PCA) for characterization or partial least squares discriminant analysis (PLS-DA) for discrimination/classification/attribution [5].

Database summary reports involve a special kind of query, and include two types of information: that which can be derived by a direct query of the data and that which requires synthesis and interpretation and/or some kind of calculation. An example of the first type is a report documenting the number of samples in the database from a particular location. An example of the second type is a report documenting how many new sources were added to the database in the past year. Both examples are typical of the kind of information that management requires for metrics. The first example should be easily fulfilled by the most rudimentary database. The latter example requires a date-added field in the sample table, something that may not occur to the developer when deciding what kinds of information needs to be captured. It is recommended that these types of requests be given particular attention when developing the database fields to ensure that all likely requests can be addressed by a database query.

5. Conclusions

The Uranium Sourcing Database effort has yielded many practical insights into nuclear forensic database development and utilization. Lessons learned from this database of uranium ore concentrates should be broadly applicable to a wide variety of nuclear material types. There are a number of factors to evaluate when establishing a nuclear forensic database, from initial design to utilization in a nuclear forensic investigation. In addition to the obvious (database design, population, and management), special consideration should be given to important issues such as analytical laboratory interface; handling significant figures in the database; the linking of data to documents and source files; the unique requirements of each type of database user; and utilization of data in multivariate analysis.

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