Development of a CanmetMATERIALS Gen IV Materials Property Database for Materials Selection[1]

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Abstract

The Canadian GIF team has chosen to focus on the development of a Super-critical water-cooledreactor (SCWR), requiring material stability atboth higher temperatures and pressures than theolder CANDU(R) reactor designs. Preliminaryconcept designs peg core operating temperaturesat close to 650 °C and pressures at 25 MPa. Assuch there are a number of materials challengesthat must be considered in the process of de-signing a prototype reactor. The Gen IV SCWRconceptual design requires the identification andtesting of materials used in all components ofthe new reactor design under these conditions.While a large amount of experimental data exists on materials properties in SCW, no databasewas available to consolidate access and assessthis data. A dynamic web-based database forstoring materials corrosion and mechanical datarelevant to the Gen IV SCWR Canadian concept is developed. Data has been collected for, at present, 87 different alloys.

1. Introduction

Canada is one of thirteen members[2] forming the Generation IV International Forum (GIF). The Generation IV International Forum has set a framework for "*international cooperation in research and development for the next generation of nuclear energy systems*" with considerations that such nuclear energy systems "*must be licensed, constructed, and operated in a manner that will provide a competitively priced supply of energy, keeping in consideration an optimum use of natural resources, while addressing nuclear safety, waste, and proliferation resistance, and the public perception concerns of the countries in which those systems are deployed*".[1]

The Canadian team has chosen to focus on the development of a Super-critical water-cooled reactor (SCWR), in line with Canadian expertise and technical capabilities. The choice of a Gen IV SCWR concept running at both higher temperatures and pressures than the older CANDU(R) reactor designs leads to an extremely energy efficient reactor. This new reactor technology is being designed for deployment in the 2020-2030 time-frames and requires a significant effort in both research and development.

This new reactor design will run at higher operating temperatures than the CANDU(R) design, under high pressure in super-critical water conditions. Preliminary concept designs pegs core operating temperatures at about 650°C with pressures up to approximately 25 MPa. As such there are a number of materials challenges that must be considered and overcome in the process of

[2]Argentina, Brazil, Canada, People's Republic of China, Euratom, France, Japan, Republic of Korea, Russian Federation, Republic of South Africa, Switzerland, United Kingdom and Unites States

designing, building a prototype and bringing such a reactor to fruition. In the long term the Gen IV SCWR conceptual design requires the identification and testing of materials used in all components of the new reactor design under these conditions.

The Gen IV SCWR efficiency is tied to its ability to run under extreme conditions. As such materials for key in-core and out-of-core components will have stringent operating conditions so as to increase the overall power efficiency of the reactor. Under these conditions the materials will be subjected to high temperatures, radiation, high pressure and a corrosive environment. The limits to which the reactor can be pushed will be determined by both the materials selected and the configuration of the reactor design. This leads to a multi-component selection problem where each choice made for one component can impact the viable material and configurational choices of the other components in the reactor.

While a large amount of experimental data exists on materials properties in SCW, no database was available to consolidate access and assess this data. The work summarized in this report is on the database development at CanmetMATERIALS and builds on other CanmetMATERIALS, Atomic Energy Canada Limited (AECL) and other Canadian partner data collection projects under the Canadian GIF deliverables. The project brings together the data in one collection allowing for data mining and analysis of the different datasets. Specifically, the database structure expansion and collection efforts will include both corrosion and mechanical properties of materials. This work builds the framework for, and begins population of, a materials property database to help in the selection of candidate materials for the various components of the SCWR reactor. This framework can be used to carry forward into future stages of the SCWR reactor development, increasing the availability of data pertinent to the reactor design.

This document is broken down into 4 sections, the goals of this specific report for the materials property database, an overview of the data currently collected, the organization of the data and a description of the software framework for the database.

2. Goals

The focus of the database collection is centredaround materials selection for components under high pressures and high temperatures. The data collection will focus on properties in the temperature range of 300°C- 850°Cand at pressures up to 60MPa. Data in the mechanical properties will focus on basic mechanical properties, yield strength, elongation and UTS, and also rupture time data and creep rate data. Data in the corrosion properties database focuses on weight gain rate data in super-critical water conditions but will also collect data in super-heated steam. Additionally database structures are to be built for irradiation effects on the material properties.

The database is structured so as to allow users to retain ownership of their data, maintain a level of moderation over the data and to potentially expand to restrict data queries based on a certain level of security, i.e. confidential data restricted to particular users. At present the confidential data feature has not been implemented, though access to the data requires a registered account. The two major user features are as a contributor of data and as a user of data. With this organization the following features are required before expanding the tool-base:

- Organize data in a common format

- Begin the population of the database with existing data extracted from literature sources
- Allow users to contribute to the data collection efforts of the database
- Allow users to query the data for specific searches

Once a sufficient dataset is acquired tools for interpolation using models and datamining can be explored and implemented.

3. Organization Overview

The organization of the database is built around the concept of future modular expansions, allowing cross-property queries while maintaining an organized and secure database structure. This organization is broken down into 5 categories:

- Access and Moderation
- User Management
- Material Properties
- Material Characteristics
- Book keeping and Referencing

The strategy of the database is to make the specific material property the top of the search criteria, where common items are fed into sub-tables. This modular dependence is illustrated in Fig.1.

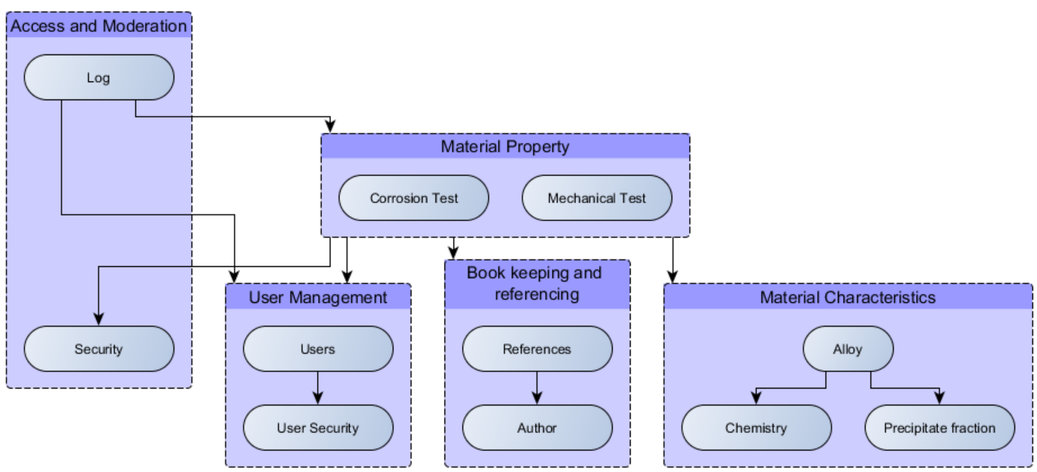

Figure 1Modular organization design of the database and dependency flow

The access and moderation module logs all changes to the database and contains information as to who has access to specific data. The user management module controls the users access level to the database. The material properties module contains the specific measurables from an experiment about the material properties. The Material Characteristics contains the information about what defines the material such as the chemistry and structure. The book keeping and referencing module contains information about the sources of the data. These 5 modules are described below in more detail.

3.1 Access and Moderation

The access and moderation module is responsible for keeping track of the security levels for each of the data entries and for tracking any changes made to the datasets. This kind of moderation is important in a dynamic, community driven, data collection effort, maintaining the quality of the data queries. At present there are two sources of information stored in the access and moderation module.

The first is a log of changes that are made to database. This log contains a list of each data point that was entered, deleted or altered, by whom and when the alteration was made. This will allow a moderator to reverse changes made to data sets in the database if they were altered in error.

The second source of information is a list of data security information. This emerges in two forms. The first is the restriction levels of specific data entries, if the data entered is not for general dissemination then the data, when entered into the database can be restricted to particular user groups as defined by the security groups. The second form of security information is the list of the security groups. At present there are 3 security groups; a moderator which has complete access to the database, including the moderation logs, a contributor which has access to push data into the database and to edit the data that they pushed and a viewer which has the ability to perform queries on the data sets but cannot edit or push data onto the system.

The access and moderation module is controlled and viewed by the moderator only.

3.2 User Management

The user management module contains the information necessary to allow users access to the database, restricting the different users' access according to their specific group level. In this particular module the user’s username, contact information and security levels will be stored. Passwords are stored in a separate database, are encrypted and cannot be viewed even by the moderator but can be reset.

The user management module is controlled and viewed by the moderator only.

3.3 Material Properties

The material properties module contains the information about the specific measureables from the experiments and/or simulations. The present database has two submodules for the materials properties, corrosion data containing average weight gain rate information of materials under super-critical water conditions and super-heated steam conditions and mechanical property data containing rupture time due to creep. These datasets are described in more detail below in sections 4.1 and 4.2.

The materials property module is viewable by a viewer level of security and editable and viewed by both contributor and moderator.

3.4 Material characteristics

The materials characteristics module contains the information about the materials in the database. At present the database stores information about the alloy class, the alloys chemistry, and if relevant, the precipitate fractional amounts.

The materials characteristics module is viewable by a viewer level of security and editable and viewed by both contributor and moderator.

3.5 Book keeping and referencing

This module is responsible for keeping track of the sources from which the data in the data sets are collected. This module will store and track the lists of publications, reports or experiments from which any particular data entry into the data sets is taken.

The Referencing module is viewable by a viewer level of security and editable and viewed by both contributor and moderator.

4. Data collection overview

Data has been extracted from the literature by a number of partners and has been loaded into the database software designed in this project. This sectionoverviews the data, as it currently stands, in the data base. The data collection efforts have focused on corrosion properties and mechanical properties of many potential candidates. This data was used to narrow the selection for the fuel cladding to a number of potential candidate alloys.

4.1 Corrosion data

Corrosion at the higher operating temperatures of the super-critical water reactors (SCWR) was an important concern for the selection of materials for the in and out of core components. The data collected in the database was selected over a range of pressures, temperatures and exposure times under both super-critical water(SCW) and super-heated steam(SHS) conditions. The control variable ranges for the data are outlined in Tbl.1.

Table 1 Parameter range for corrosion properties in database collection

Parameter	Min	Max
Pressure	24 MPa	60 MPa
Temperature	50°C	732°C
Time	4 hours	22000 hours

Corrosion data has been collected for, at present, 87 different alloys, a sampling of the alloys are shown in Tbl.2.

Table 2 Sample of some alloys stored in the data collection. The corrosion component of the database has, at present, data for 87 different alloys

Category	Type
F/M Steel	Grade 91 Grade 92 Grade 122
Austenitic Stainless Steels	304 309 310/310S 316 347
Iron-Nickel Base Superalloy	800 800H
Nickel Base Superalloy	600 625 718

The corrosion data collected consists of samples under particular test conditions and a measurement, which as used to characterize the corrosion properties of the sample. A corrosion data entry contains information on the experimental conditions (SCW, SHS or in water), the total time the test was run in hours and the temperature and pressure of the water. The measurable quantities presently used are the average weight gain rate in $\mu m/dm^2$and/or the metal loss after the sample had been descaled if available. This dependency in the database structure is outlined in Fig.2.

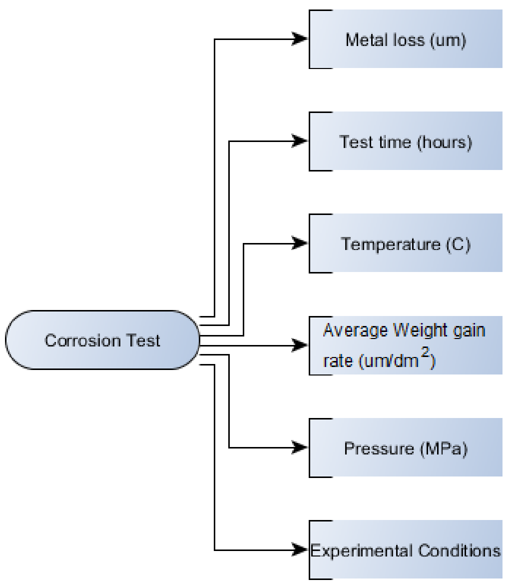

Figure 2Corrosion test specific values required

Candidate alloys for the fuel cladding were identified as 310S, 800H, 625 and 3033. Once identified, the data collection efforts were focused on these alloys.

4.2 Mechanical data

Mechanical property data for a number of alloys was collected to identify candidate alloys for the fuel cladding and other in-core and out-of-core components [2,3]. This data collection effort focused around the ultimate tensile strength, yield strength and elongation of the alloy and on creep rupture time data. A sampling of the alloys for which data has been collected is shown in Tbl.3.

Table 3 Example alloys that mechanical data has been collected for and stored in the CanmetMATERIALS database.

Category	Type
F/M Steel	Grade 91 Grade 122
Austenitic Stainless Steels	310/310S 321 347
Super-austenitic Stainless Steel	AL-6XN NF709R Nitronic50
Iron-Nickel Base Superalloy	800 800H
Nickel Base Superalloy	600 625
ODS Alloys	MA 956 PM 2000

The creep failure data consists of samples under particular temperatures(°C) and stresses (MPa) while measuring the time to failure (hrs) and the elongation percent. The creep rate (/s) from these cases are averaged from the total failure time and elongation.

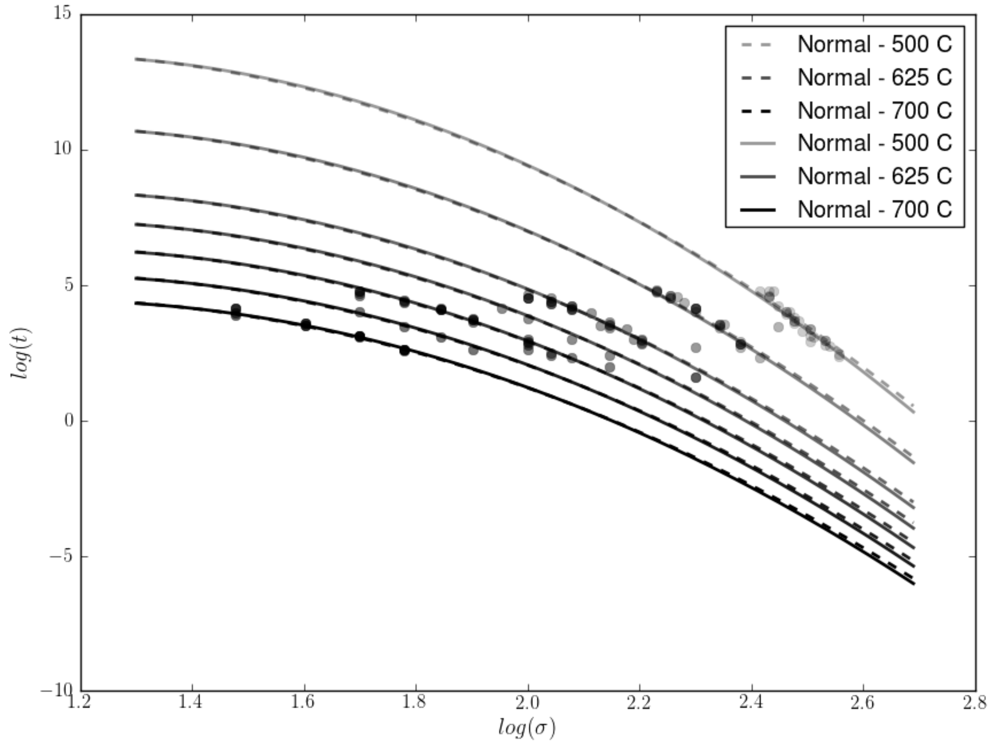

Figure 3Creep rupture times of grade 91 steel at temperatures varies from 500 °C to $700°C fit using the Larson-Miller model assuming a Gaussian and Weibull distribution for the data.

Presently data can be queried and extracted for analysis, for example in Fig.3. In this query the rupture time data for grade 91 steel was extracted from the database and analysed using Python to examine the effects of choice of statistical distribution on the data. The rupture time data was fit using a method of maximum likelihood for the two distribution choices after querying the database for the relevant data. In this example, data for temperatures at 500 °C, 550 °C, 600°C, 625 °C, 650 °C, 675 °C and 700 °C was extracted and simultaneously fit to the model for each distribution choice. Plotted is the fit for the 50^{th} percentile of failure.

5. Software overview

To achieve the goal of dynamic access and collaborative collection and use of data, a web access database was developed using a combination of HTML[3], PHP[4] and Javascript which accesses a central database using MySQL for storage and queries. The software and algorithms will be detailed in another report, an overview of the strategies and organization of the software is provided below.

The database structure is broken down into security and access algorithms, data moderation algorithms, SQL[5] Table organization, and queried access of data. The software around the security and access is overviewed in section 5.1, Data moderation algorithms are overviewed in section 5.2, the SQL Table

[3]Hyper Text Markup Language
[4]PHP: Hypertext Preprocessor
[5]Structured Query Language

structure is overviewed in section 5.3 and the data queries functionality is overviewed in section 5.4. The details of the software are documented in the software documentation.

5.1 Security and access algorithms

Access to the database is secured by a separate encrypted irreversible hashing algorithm written in javascript. The user passwords are stored in their encrypted state. This encrypted password is passed to the php server and compared to the stored, encrypted, password. Each page access requires a comparison on server side to retrieve the correct page, otherwise the user is redirected to the log in screen.

Additionally, when logged in, the server (php) will identify the user sub-group and build the webpage according to their particular access. Presently there are three user sub-groups, as described in section 3.

5.2 Data moderation algorithms

The moderation algorithms are written in php and are controlled by the server to avoid possible client tampering. When a request to alter the data in the database is made, in addition to the requested change the server will create a log in the moderation SQL table of which table entry was added, altered or deleted, by whom and when. The moderation is a combination of SQL and php calls.

5.3 SQL Tables

The user login security is stored in a separate database consisting of two tables, a members table which contains an id, username, email, encrypted password and password salt, and a table of login attempts which records failed and successful log in attempts to the database. The remaining database information is stored in the materials database and is broken down into the modular design in section 3. Algorithms have been written in php to allow for dynamic queries of the relevant data in the data base.

5.4 Data Queries

There are presently two primary queries for the database, the ability to push data into the database by batch loading data and references to the database and to pull data from the database.

To push data to the database a user uploads a file containing the relevant data in a predefined format along with a corresponding bibtex file. Javascript algorithms extract the information from these two files and organize it into two tables (data and references) for the user to confirm. Once confirmation has been made, the user may submit the data to the database. Javascript will then organize each data entry in turn and submit to a messaging system in the background to pass each entry to a php function for entry into the database. The php function will hash out the corresponding entry deciding which table is to be altered and build the corresponding SQL command to load the data by preparing an SQL statement. Once prepared the SQL statement is sent to the database and the data is pushed into the database and corresponding moderation logs are built.

To pull data from the database the user performs a dynamic query which allows the user to narrow the results of their search by continually adding more query restrictions. As additional restrictions are added to the form, and the query is submitted by the user, the query is posted to a php function and a corresponding prepared SQL statement is dynamically built and queried to the database. Once the data is retrieved, the information is passed back to Javascript where the functions build a table of the relevant data that can be saved and analyzed as needed.

6. References

[1] Charter of the generation IV international forum

[2] S Xu, S.M. Jun and P.Le.Dreff-KerwinPresented paper at AMR pressure vessels and piping conference, Paris, France, July 2013

[3] S Xu, W. Zheng and L. Yang, CMAT Open technical report, 2014-2480-RT, 2015