#### CORROSION DATABASE FOR SCWR DEVELOPMENT

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#### Abstract

The development of the Gen IV CANDU-Supercritical Water Reactor (SCWR) requires the identification and evaluation of candidate materials that can be used for in-core and out-of-core components. One initial goal of the Materials Database project under the Canadian National Gen IV program is to identify a short-list of candidate materials for longer-term testing. A large amount of data is now available on materials properties (e.g., corrosion, creep) under SCWR conditions (for temperature between 374 and 732°C, P = 35 MPa). To facilitate the collection and assessment of these data, a materials database has been developed by AECL and MTL. This paper describes the development of this database, outlining basic data requirements and design. Illustrations include the functional view of the database, guery tables and user interface plots. Examples of corrosion rate assessments of some 3XX stainless steels and of Alloy 800H under various test conditions will be presented. The project is still in an early stage and development is underway, including data collection and Visual Basic programming. Even at this preliminary stage, the database is proving to be a valuable tool for the corrosion evaluation of alloys.

Keywords: Corrosion Database, SCWR, Materials Corrosion and Analysis etc.

## **1.0 INTRODUCTION**

Of the six reactor systems in the Generation IV International Forum, Canada has chosen to focus on the development of the Supercritical-Water-Cooled Reactor (SCWR) system, the system that best fits its national expertise, technical capabilities and interests [1]. The Generation IV CANDU SCWR is a conceptual design for a novel, extremely energy-efficient advanced reactor that would come on line in about 2025.

The Gen IV SCWR concept would produce supercritical water at temperatures as high as 625°C to generate electricity, hydrogen and district heating. The use of supercritical water to carry heat from the reactor core to the turbine will generate much more extreme water chemistry conditions than those found in the current CANDU-PHW design, which operates from 250 to 320°C [2]. The long-term viability of the Gen IV CANDU-SCWR concept requires the identification and testing of classes of candidate materials that can be used for in-core and out-of-

core components, including a fuel channel design for fuel cladding material (up to 850°C during normal operation and higher temperatures during short upset conditions). Coating or surface alloying and modification may be required for some key in-core (e.g., fuel cladding) and out-of-core (e.g., outlet feeders) components to minimize degradation. Material performance will need to be demonstrated in the key areas of corrosion and stress corrosion cracking, strength, embrittlement and creep resistance and dimensional and microstructural stability [3-7]. Measuring irradiation deformation and mechanical properties after irradiation are essential for in-core materials.

One initial goal of the Canadian Materials and Chemistry SCWR R&D program is to identify and evaluate classes of commercial materials that can be used in an SCWR for in-core and out-core components, and assemble these data into a database. In recent years, a significant international effort has produced a large amount of test data for corrosion in SCW. The establishment of a materials database will consolidate these data and provide a tool that can be used for identification of suitable materials for use for all out-of-core components, as well as for in-core components such as the fuel cladding and liner. These candidate materials will require longer term, more detailed corrosion testing. Existing reactor designs will also benefit from improved understanding of the mechanisms of corrosion in high temperature water, as well as from the availability of the improved facilities and enhanced knowledge acquired in this effort. Advanced supercritical fossil plants operate under conditions similar to propose SCWR regimes for components in the heat-transfer and electricity generation portions of the plant, and this database could also find applications in this area.

# 2.0 DATABASE SYSTEM DEVELOPMENT

The goal of the current project is to develop a corrosion database for storing, querying and analyzing corrosion data under proposed SCWR conditions. Corrosion data will be obtained from the open literature and from international partners. In the initial phase of this project, the work has focused on building the structure of the database; its construction process includes the following development stages:

- Requirements Development User needs are explored and both users and the development team acquire a detailed understanding of what software should be created.
- Architecture Senior developers design the project's organizational structure, its communication rules, and system wide design and implementation guidelines.
- Design During this phase the requirements are translated into an operational program.

- Construction The detailed design, coding, unit testing and debugging phase.
- QA & Testing Planned and systematic pattern of activities designed to ensure that a system has the desired characteristics.
- Release Software is delivered to users who are outside the group responsible for the development of the software.

The approach is to develop a generic database system that serves as a base for corrosion data analysis and assessment. The system is intended to be a user-friendly data storage and management tool. The system is designed to be scaleable and generic in terms of data manipulation and sharing. An interface will allow integration with various existing databases for data interpreting, analyzing, processing and reporting. Simulation and predictive modeling that enhance the analytical ability of the database will be incorporated at a later time. This system will provide controlled remote access for the user or the system administrator via a standard telecommunication protocol. This feature is particularly useful for a national program that involves many participants across the country.

## 3.0 SYSTEM REQUIREMENTS OF THE DATABASE

The high level functionality or feature requirements of the database are listed below:

<u>Scope:</u> It should easily be able to handle the large quantities of data that are involved. It should handle the scenarios of (i) modifying or editing data, (ii) adding new data, (iii) updating data that needs to be shared between users, and (iv) security of the data.

<u>User Interface:</u> It should provide a generic, user interface for user operations. It should have a user-friendly data display interface to allow the authorized user to manipulate the database, including query, edit, add, delete and other data process operations.

<u>Data Import/Export:</u> It should allow data transfer between existing databases. In particular, it should support data transfer among different file formats.

#### Data Processing

A database may be simply a repository of data to be entered and retrieved. However, many databases also process or analyze the data. Microsoft Access is particularly strong in this area, with its excellent object-oriented Visual Basic programming environment. <u>Report and Display:</u> Database reports are often one of the last things to be considered when writing the requirements specification, probably because they are standalone objects which simply extract data from the database and therefore cannot upset its overall architecture. However, this is a very important function.

#### Database Administration:

An operational Access database usually requires less administration than a client-server system. However, it will still require attention from time to time. Someone in-house may be assigned to perform these tasks. It is useful to define up-front how the following will be handled: security features and restricted editing by general users; database backups; user training and support; compact and repair procedures should the database be corrupted; installation of the application on new client machines; addition and deletion of logins; password reset; installation of database upgrades on client machines; and feedback of error logs and problems via email or phone.

# 4.0 DATABASE DEVELOPMENT: DESIGN

A database is a collection of information organized in such a way that a computer program can quickly select desired pieces of data. Traditional databases are organized by fields, records, and files. A field is a single piece of information, a record is one complete set of fields, and a file is a collection of records. Modern databases are not only information organizers, but also perform data processing, analysis and display to make it easier for the user to extract the desired information. Our corrosion database contains four important modules:

- 1. Data Storage Module
- 2. Data Query Module
- 3. Data Display and User Interface Module
- 4. Existing Database and Scientific Model Integration

The Data Storage Module stores the raw data in table format with unique IDs. The columns are specified fields with pre-defined data types and the rows are data entries or specific data records. There will be a number of tables. The Data Query Module is the most complicated module; it contains intelligent data queries and displays that require sophisticated data processes and analyses. It is very difficult to handle dynamic data queries in which the user decides what to query. The Data Display and User Interface Module is also important since it provides the interface for the user to access the database and to review query results, either in table or figure format. The last module will be developed later in the project; it is useful to leave a "plug" for further integration of scientific models to enhance the analytical capabilities of the database. In this project, Microsoft Access is being used to implement module (1) and Visual Basic to implement

modules (2) and (3). In the following sections, brief design descriptions of modules (1) to (3) are given, along with simple implementation examples.

As noted above, the data storage module stores the raw data in table form. It contains data on test conditions, alloys, corrosion and mechanical performance, and microstructure characterization. The data query module consists of query tables that can be accessed by the user via the user interface using query objects (programmed in Visual Basic). The query tables hide the raw data from the users; only the database administrator has the right to access the raw data for database maintenance.

Figure 1 lays out the basic structural relationship among the tables. For instance, the material table contains identifiers and alloy names and it has one to one relationships with most tables including the microstructure and composition tables. However, the relationship between the reference table and the material table is 1 to n because one paper or reference may contain information about a number of alloys. As database development and data collection continues, the relationships may change and new relationships may be added.



Figure 1: Design structure of table relationships.

# 4.1 Data Storage Module

Figure 2 shows a small fraction of the raw corrosion data table. The data were mainly collected by Atomic Energy of Canada Limited over several years from the available literature and from their in-house experiments. On the left side, all the data and query tables are listed. At this stage, there is only one raw data

table, named CorrosionDataBase. The table contains columns (fields) for ID, alloy, pressure, temperature, time, average weight (gain/loss), etc. Fields can be added, deleted or edited. The raw data entries are in the table rows. There are over 470 entries, for 85 different alloys in the current CorrosionDataBase table. Additional tables for other data will be added as the project progresses.

CorrosionDataBase	Corrosion	DataBase Materia	Corrosion	Performance	Jest Condition	Mechanical P	roperty
CorrosionDataBase : Table	ID +	Alloy 🚽	P (Mpa) 🔹	Time (hr) 🔸	Temp •	Avg Weight 👻	Fe
Characterization	1	Ducrolloy SS	40	160	420	0.23	44
Composition	2	Ducrolloy SS	40	400	420	1.079	44
Composition	3	Ducrolloy SS	40	400	420	0.3418	44
Corrosion Performance	4	Sanicro28	25	168	420	0.0595	
🗇 Material	5	Haynes 188	24.1	1000	538	0.004	3
Mechanical Property	6	Haynes 188	24.1	5000	538	0.003	3
Test Condition	7	Haynes 188	24.1	8000	538	0.006	3
	8	Haynes 188	24.1	10000	538	0.0035	3
The second	9	Haynes 188	24.1	11000	538	0.0027	3
	10	Hayes 25	24.1	1000	538	0.005	3
	11	Hayes 25	24.1	5000	538	0.0066	3
	12	Hayes 25	24.1	8000	538	0.0078	3
	13	Hayes 25	24.1	9000	538	0.0056	3
	14	Hayes 25	24.1	11000	538	0.0045	3
	15	12CR-1MO-1WVN	25	500	290	0.02	Bal
	16	12CR-1MO-1WVN	25	500	375	0.04	Bal
	17	12CR-1MO-1WVN	25	500	550	0.9	Bal
	18	403 SS	29	312	455		
	19	406 SS	24.1	11000	538	0.0312	Bal

Figure 2: A portion of the corrosion table (raw data).

CorrosionDataBase 📀 «	Composition	CorrosionDat	taBase 📑 Mate	rial 🗗 Corrosio	on Performance	Test Condition	Mechanica
CorrosionDataBase : Table	Alloy 👻	Fe +	Ni -	Cr 🔸	Co 🔹	C +	N -
Characterization	1.1Cr	Bal	0.25	1.1	<0.05		
- Composition	1.9Cr	Bal	0.2	1.9			
	12Cr	Bal	0.035	11.97		0.02	0.01
Corrosion Performance	12CR-1MO-1WVN	t Bal		11.97		0.11	
Material	13Cr-4Al			13.64		0.04	0
Mechanical Property	14Cr-4Al			13.64		0.04	0
Test Condition	16Cr-4Al			16		0.08	0
	19Cr			18.37		0.05	0.01
	19Cr-4Al			16		0.08	0
	19Cr-4Al			16		0.08	0
	2 1/4Cr-1Mo	Bal	0.16	2.2		0.09	
	2.0Cr	Bal	0.32	2			
	201 SS	Bal	3.5-6.0	16.0-19.0		0.15	0.25
	22Cr-4Al			22.05		0.1	0
	302 SS	Bal	8	18		0.08	
	304 SS	Bal	8.3	18.17		0.04	
	304 SS	Bal	8-0-12.0	18.0-20.0		0.08	
	304L SS	Bal	8.5	18.3		0.035	0.06

Figure 3a: A portion of a composition query table.

## 4.2 Data Query Module

When working with a database, most users only need a specific group of records at any one time (data for a given test temperature or pressure, for example). Database programs have the ability to search for any record a user needs and manipulate the data in many different ways. This is accomplished by creating a query. Once tables have been established inside of a database, a query can be developed to select a group of fields from those tables, select only those records that adhere to a specific set of criteria, and ready those records for use in a report.

CorrosionDataBase 📀 💉	Composition		CorrosionDa	taBase	Ma	terial	Corro:	ion Performance	Test Cond	ition 🗇	Mechanic
CorrosionDataBase : Table	Alloy	•	Fe •		Ni	-	Cr	- Co	• C	- 1	V -
Characterization	1.1Cr	₹↓	Sort A to Z					<0.05			
Composition	1.9Cr	Z↓	↓ Sort Z to A								
Composition	12Cr	V	Class filter from Allow					0.02	0.01		
Corrosion Performance	12CR-1MO-1WV	~	Test Filters	Trour Anoy					0.11		
Material	13Cr-4Al		Text ritters						0.04	0	
Mechanical Property	14Cr-4Al		201 SS						0.04	0	
Test Condition	16Cr-4Al								0.08	0	
	19Cr		302 55	V 302 55					0.05	0.01	
	19Cr-4Al		✓ 304 55 ✓ 304L SS ☐ 309 SS ☐ 310 SS					0.08	0		
	19Cr-4Al							0.08	0		
	2 1/4Cr-1Mo							0.09			
	2.0Cr		316 SS	✓ 316 SS							
	201 SS		316L SS	~	19.0		0.15	0.25			
	22Cr-4Al		521 55			100			0.1	0	
	302 SS		OK		Can	cel			0.08		
	304 SS	-		010		2012	j.		0.04		
	304 SS	E	Bal	8-0-1	L2.0	18.0	-20.0		0.08		
	304L SS	E	Bal	8.5		18.3	1		0.035	0.06	

Figure 3b: Selecting alloys 302, 304, 304L and 316.

In this project, a layer of query tables to accommodate various queries is being set up. The table relations will reside in the data query module. By doing so, the raw data are isolated from the user and merging with new data is facilitated. New raw data tables can be stored in the data storage module without modification and they can be used simply by extending the relations in the query module. For instance, Figures 4a to 4c provide an illustration of how to query the compositions of one or more given alloys. Figure 4a is a partial view of the Composition Table. To compare the compositions of 302, 304 and 316 alloys, these alloys are simply selected in the drop down table (Figure 4b). Figure 4c shows all the entries that are the related alloys.

CorrosionDataBase 🔍 «	Composition	CorrosionDat	aBase Mater	rial 🔁 Corrosion	Performance	Test Condition	Mechanica
CorrosionDataBase : Table	Alloy 💞	Fe 🔸	Ni 🔹	Cr 🔸	Co 🔹	с -	N -
Characterization	302 SS	Bal	8	18		0.08	
Composition	304 SS	Bal	8.3	18.17		0.04	
	304 SS	Bal	8-0-12.0	18.0-20.0		0.08	
Corrosion Performance	304L SS	Bal	8.5	18.3		0.035	0.06
Material	316 SS	Bal	10.21	17.23		0.05	
Mechanical Property	316 SS	Bal	10- <mark>1</mark> 4	16-18		0.08	
Test Condition	316 SS	Bal	13.6	17.5		0.001	

Figure 3c: A display of the alloy compositions of 302, 304, 304L and 316.

Figure 4a is a partial view of the Corrosion Performance Table. To query entries that have a corrosion weight gain less than (and equal to) 0.005 (mg) for a

specific test duration, this query condition is defined and the database outputs all the entries that satisfy the query condition, as shown in Figure 4b. Such a query is very simple; more complicated queries, such as linear regression and multivariable correlation analyses, can also be performed using Visual Basic programming. Addition of these more complex queries is part of the ongoing work.

All Tables 🔍 🔍	Composition	CorrosionDataBase	Material	Corrosion Perf	ormance 🗇 T
CorrosionDataBase ☆	Alloy 👻	Avg Weight 👻	P (Mpa) 👻	Time (hr) 👻	Temp 🔹
CorrosionDataBase : Table	Ducrolloy SS	0.23	40	160	420
Characterization	Ducrolloy SS	1.079	40	400	420
Composition	Ducrolloy SS	0.3418	40	400	420
	Sanicro28	0.0595	25	168	420
Corrosion Performance	Haynes 188	0.004	24.1	1000	538
Material	Haynes 188	0.003	24.1	5000	538
Mechanical Property	Haynes 188	0.006	24.1	8000	538
Test Condition	Haynes 188	0.0035	24.1	10000	538
Unrelated Objects ¥	Haynes 188	0.0027	24.1	11000	538
	Haynes 25	0.005	24.1	1000	538
	Haynes 25	0.0066	24.1	5000	538
	Haynes 25	0.0078	24.1	8000	538
	Haynes 25	0.0056	24.1	9000	538
	Haynes 25	0.0045	24.1	11000	538
	12CR-1MO-1WVNb	0.02	25	500	290
	12CR-1MO-1WVNk	0.04	25	500	375
	12CR-1MO-1WVNk	0.9	25	500	550
	403 SS		29	312	455

## Figure 4a: A portion of the corrosion performance query table.

All Tables	« Composition	CorrosionDataBase	Material	Corrosion Perf	ormance
CorrosionDataBase	Alloy	- Avg Weight 💞	P (Mpa) 🔹	Time (hr) 🛛	Temp 🔹
CorrosionDataBase : Table	Haynes 188	0.004	24.1	1000	538
Characterization	Haynes 188	0.003	24.1	5000	538
	Haynes 188	0.0035	24.1	10000	538
	Haynes 188	0.0027	24.1	11000	538
Corrosion Performance	Haynes 25	0.005	24.1	1000	538
Material	Haynes 25	0.0045	24.1	11000	538
Mechanical Property	410 SS	0.001	34.7	1392	538
Test Condition	410 SS	0.0008	34.7	2592	538
Unrelated Objects	410 SS	0.0028	34.47	3552	538
vinciated objects	410 SS	0.0042	34.47	2592	538
	Hastelloy B	0.0041	24.1	10000	538
	Hastelloy B	0.0038	24.1	11000	538
	Hastelloy C22	0.004	25	500	375
	Hastelloy C22	-0.012	25	500	290
	Hastelloy C22	-0.016	25	500	550
	Hastelloy C276	0.0021	24.1	11000	538
	Hastelloy C276	0.0039	24.1	9000	538
	Hastelloy C276	0.0025	24.1	4000	538

Figure 4b: Display of alloys that have a corrosion weight gain < 0.005 (mg).





## 4.3 Data Display and User Interface

This module contains the user interface that allows the user to manipulate the information stored in the database and to display data in both text and graphic plot formats. The module requires substantial Visual Basic programming. A starting applet allows two login points for general user and administrative support. The general user accesses the database via the user interface to make various queries by selecting conditions. Figure 5 is an example of a graphic plot of "Average Weight Gain Rate - Temperature - Cr content". The Cr content percentage is selected between 15% and 30%, and temperature range is from 290°C to 732°C. From the Figure 5, it is very easy to see how the Cr content or testing temperature affects the corrosion rate. Most of the data collected are at test temperatures (for SCWR) ranging from 450°C to 600°C. We can display the data over a desired range and we also can reveal other elements in the same graphic. Figure 6 is a similar plot that shows the test temperature over the range of interest and it also reveals the Ni content (%). It can be easily seen that a high corrosion rate is normally associated with low Ni content with few exceptions. We can also bring more elements into the same plot. For instance, Figure 7 shows the same plot with Fe content in additional to Cr and Ni. This new graphic reveals that the Fe base alloys have higher corrosion rate than the Ni base alloys. We can also review the corrosion data for a particular group of alloys or individual alloy. In next section, two examples 3xx stainless steels and alloy H800 will be presented.



Figure 6: A query plot of corrosion rate versus temperature and Cr. The associated Ni content (%) is also revealed.



Figure 7: A query plot of corrosion rate versus temperature and Cr, The associated Ni and Fe contents (%) are also revealed.



Figure 8: A graphic comparison of the weight gains of 302, 304, 310 and 316 SS at various testing temperatures at a pressure of 24.5 MPa.

# 5.0 EXAMPLES OF CORROSION PROPERTY ASSESSMENTS USING THE DATABASE

Two examples of corrosion property assessment using the current version of the database are presented here.

- (1) Corrosion rate comparison of 3xx stainless steels in SCW. The database allows users to directly compare the corrosion performance under various test conditions and obtain cross-references. This functionality will be important for material selection. Figure 8 compares the weight gains of 302, 304, 310 and 316 SS at various test temperatures at a pressure of 24.5 MPa. It can be seen that the large corrosion rate is observed at temperature around 538°C. The corrosion rate decreases at a temperature higher than 538°C, which may be attributed to spalling of corrosion products.
- (2) Corrosion rate of Alloy 800H as a function of temperature and test duration. Alloy 800H is widely used as a steam generator tubing alloy. It has good creep properties at high temperatures and is resistant to reducing or oxidising atmospheres. It is known to have microstructure stability in long-term applications at high temperatures. This alloy has been evaluated by several research groups studying the corrosion of materials in hot water under both subcritical and supercritical conditions.



Temp oC 🔻

Figure 9: An example of the database output that shows the weight gain of Alloy 800H at various temperatures (data are from Reference 8).

Figure 9 shows the corrosion weight changes of Alloy 800H at 350°C (subcritical water), 400, 450, 500 and 550°C. The weight change decreases as the temperature is increased from 500 to 550°C, whereas below 500°C the weight change tends to increase with test temperature. This has been attributed to spallation of the oxide from the metal surface [7].

## 6.0 CONCLUSIONS

In this presentation, the basic requirements and design of the corrosion database being developed for the Canadian GEN IV SCWR Program have been described. Illustrations have been provided to demonstrate the functional view of the database, including query tables and user interface applets. The project is still in an early stage and development is underway, including data collection and Visual Basic programming. Even at this preliminary stage, the database is proving to be a valuable tool for the corrosion evaluation of alloys. Examples of corrosion rate assessments of some 3xx stainless steels and of Alloy 800H under various test conditions have been presented.

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