Preview of DATACHOA Ver. 1.0: Database for Chemical and Physical Properties of Molten Chloride Salts Comprising Actinide and Lanthanide Chloride Salts

Jong-Yun Kim *, Jin-Hong Lee, Tae-Hong Park, Sang-Eun Bae, Young Hwan Cho
Korea Atomic Energy Research Institute
**Corresponding author: kjy@kaeri.re.kr*

1. Introduction

Molten salt is a very attractive medium in many applications [1]. Although, the ionic liquid is a good candidate as a low-temperature molten salt, high-temperature molten chloride salts are of a major interest to the pyroprocess developers in nuclear industries. It is extremely difficult to deal with the highly corrosive hot molten salts comprising highly radioactive actinide and lanthanide elements, and therefore there are a few data for molten salts worldwide [2]. International Atomic Energy Agency (IAEA) provides molten salt database based on a world-wide-web (WWW) server [3]. However, many data useful for the pyroprocess under development in Korea are missing.

We have developed various measurement techniques for obtaining the chemical and physical data of the molten salts over the last four years: absorption spectra, emission spectra, molar absorptivity, Gibbs free energy, apparent potential, activity coefficient, exchange current density, solubility, electrical conductivity, density, surface tension, viscosity, melting point, diffusion coefficient, etc, which have been of our current interests [4]. Those property data are essential in the understanding and the operation of the pyrochemical system. Some properties are intercorrelated, and multi-component molten salt systems can be understood by using a multivariate chemometric data analysis.

Our final goal is to establish the "Expert System", which is defined as a system that emulates the decision-making ability of a human expert [5]. Actually, the expert system is a well-known concept in the artificial intelligence designed to solve complicated problems by knowledge. The first expert systems were developed in the 1970s and then become popular in the 1980s. Although expert systems have been successful in the artificial intelligence, they are not known to chemists or chemical engineers for many years. The DATACHOA is the first step forward to the "Expert System", although the amount of our property data is not currently enough to build up the "Expert System".

2. Methodology of Making DATACHOA

DATACHOA is based on the MVC (Model-View-Controller) model as a widely-adopted architecture for WWW applications and one of the best programming techniques. PHP:Hypertext Preprocessor-based web database program is used for constructing DATACHOA ver. 1.0. PHP is one of the leading web development languages. CakePHP 2.0 is used as the MVC framework for PHP so as to make coding easier. Apache HTTP web server (ver. 2.2.15) was used with MySQL database management program. For the simplicity, AJAX (Asynchronous JavaScript and XML) technique was used in some web pages for getting the data from the server without refreshing the whole page.

Hardware also must be capable of the reliable data storage. Hardware consists of file servers with two dual core AMD Athlon II X2 250 processors connected to a direct attached storage (RAID-5 level) of 1.0 TByte. The Linux CentOS 6.0 was used as an operating system. A permanent external monitoring process watches the condition of the system resources such as RAID status, memory, CPU, network connectivity, system processes, and storage resources.

3. Overview of DATACHOA

In this section some of the characteristic features of DATACHOA are described. DATACHOA includes the data for a single pure component and multi-component molten chloride salts. For searching the property data, the multiple choices are possible for the physical/thermodynamic, chemical/electrochemical, and spectroscopic properties as well as for the elements.

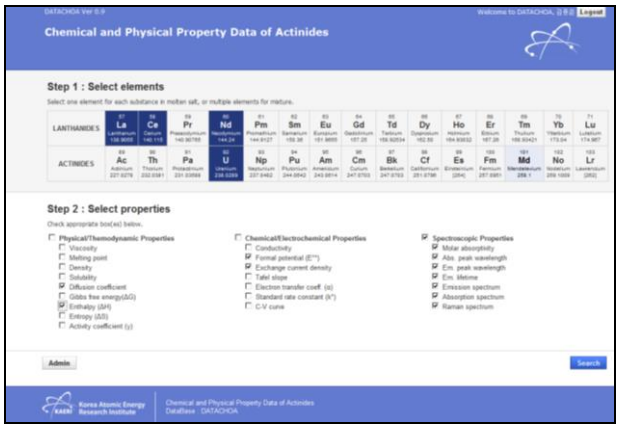

Fig. 1. Main web page of DATACHOA ver. 1.0 with only two-step selection procedure for simplicity.

The philosophy of DATACHOA is to establish a user-friendly web-based database program with a simple structure. At the first step of searching the data of interests, users can select a single or multiple elements as shown in Fig. 1. The section color of the selected

elements turns dark blue. At the second step, the single and multiple selections of the properties are possible in the list of the properties.

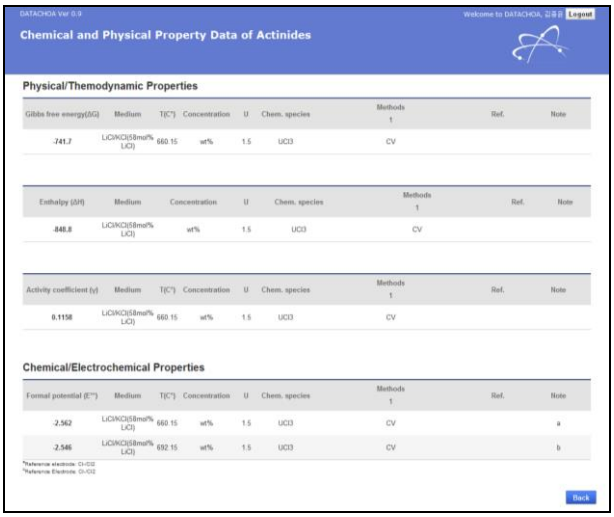

Fig. 2. Search result web page of DATACHOA ver. 1.0 after the multiple choice of the properties at the "Select Properties" step.

All 23 properties are categorized into three classes: physical properties, electrochemical properties, and spectroscopic properties. As an example, when they choose a physical property, all the data belonging to the physical properties provided by DATACHOA, i.e., viscosity, melting point, density, solubility, diffusion coefficient, Gibbs free energy, enthalpy, entropy, and activity coefficient, will be reported after clicking the "search" button as shown in Fig. 2.

Fig. 3. Admininstrator's web page of DATACHOA ver. 1.0, which is designed to be manager-friendly.

But they also can choose each multiple properties belonging to other categories such as density in "Physical/Thermodynamic Properties", exchange current density in "Chemical/Electrical Properties", and molar absorptivity in "Spectroscopic Properties", simultaneously.

DATACHOA is also designed to be manager-friendly. Administrator can generate, delete, and modify user accounts, elements in the periodic table, property data, and property fields very easily as shown in Fig. 3.

4. Conclusions

DATACHOA is our first attempt to collect extensive basic and fundamental properties of molten salts of interest to pyroprocess chemists and engineers in Korea. DATACHOA ver. 1.0 will be released to the pyroprocess engineers within a few months. It will provide useful information on the properties of interest for designing and operating the pyroprocess including the nuclear safeguards.

Acknowledgement

This work was supported by the Nuclear Research and Development Program through National Research Foundation of Korea (No. 2014000288) funded by the Ministry of Science, ICT and Future Planning.

REFERENCES

[1] F. Lantelme and H. Groult, Molten Salts Chemistry: From Lab to Applications, Elsevier, San Diego, 2013.
[2] G. J. Janz, Molten Salts Handbook, Academic Press, New York, 1967.
[3] IAEA Minor Actinide Property Database (MADB) by Integrated Nuclear Fuel Cycle Information Systems (INFCIS)
[4] J.-Y. Kim, Y. S. Choi, S.-E. Bae, D. H. Kim, J.-W. Yeon, and K. Song, Electrical Conductivity Measurement of Molten Salts Using a Two-Electrode Alternative Current Impedance Method, Asian Journal of Chemistry, Vol. 25(12), p. 7028, 2013.
[5] S. J. Russell and P. Norvig, Artificial Intelligence: A Modern Approach, Prentice Hall, New Jersey, 1995.