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Development of an Online Nuclear Materials Thermo-physical Property Database (THERPRO)

Seongdeuk Jo and Sama Bilbao y Leon
Division of Nuclear Power, International Atomic Energy Agency (IAEA), Vienna, Austria

Juseong Kim and Yongsoo Kim*
Department of Nuclear Engineering, Hanyang University, Seoul, Korea

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Material properties data are an essential part of major disciplines in many engineering fields. Especially in the nuclear science and engineering, fundamental understanding of the thermo-physical-chemical-mechanical properties of nuclear materials is critical. In fact, accurate and reliable material properties data are required for the evaluation of the performance and safety of current and future nuclear reactors under normal operation or accident conditions.
In this respect, the collection and systematization of openly available thermo-physical properties data as well as necessary new data measurements have been conducted within IAEA's Coordinated Research Project (CRP) on "Establishment of a Thermo-physical Properties Database of LWRs and HWRs". Based on the results of the CRP, an online web-based material properties data base, THERPRO, was developed and it is currently available to registered users in all IAEA Member States. THERPRO is managed by the IAEA designated Center for Nuclear Materials Database (CNMD), located at Hanyang University in Seoul, Korea and it is available through the IAEA public website at http://therpro.iaea.org.

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I. INTRODUCTION

With the explosive expansion of computer applications to design, analysis, simulation and process control, material properties data have become an essential and a crucial part in nuclear engineering and science. The evaluation of reactor performance under normal operation and severe accident conditions is vital for current and future water cooled reactors and requires accurate representations of thermo-physical properties under relevant temperature and neutron fluence conditions. Assuring that the needed thermo-physical properties are sufficiently accurate requires peer review, assessment and evaluation of existing data and selective measurements of new data at conditions for which data are currently lacking or highly inadequate.

The collection and systematization of openly available thermo-physical properties data, as well as the performance of necessary new data measurements have been conducted within the International Atomic Energy Agency's (IAEA) Coordinated Research Project (CRP) on "Establishment of a Thermo-physical Properties Database for LWRs and HWRs". The outcome of this activity is the THERPRO database.

THERPRO is a web-based on-line database (http://therpro.iaea.org), providing thermo-physical material properties data to the registered users in IAEA Member States since 2009 (Fig. 1). So far more than 13,000 property data of about 1,300 materials have been collected and compiled in THERPRO. The latest data published in the related technical reports and journals are being continuously collected and added to the database.

II. DEVELOPMENT OF THERPRO

From 1990 to 1994 the IAEA carried out a CRP on thermo-physical properties of materials for water cooled reactors with the aim to collect and systematize a database of thermo-physical properties for light and heavy water reactor materials. Data already existing at the participating institutes, and new data from some additional measurements carried out within the CRP, were collected. The data were then independently reviewed by Argonne National Laboratory and Atomic Energy of Canada Limited and this database was published in 1997 [1]. The data were stored in electronic format in the THERSYST system, which was maintained by the

*E-mail: yongskim@hanyang.ac.kr

Fig. 1. (Color online) THERPRO database home page.

Institute for Nuclear Technology and Energy Systems, University of Stuttgart in Germany.

Since the results of the work in Ref. 1 showed a large "spread" in some openly available thermo-physical properties data in use at that time, it was decided to establish a new IAEA CRP to critically assess and peer review selected property data and correlations, to extend the database to include properties at severe accident conditions, and to recommend the most appropriate data, if warranted. In particular, this new CRP took critical steps to establish recommended "most appropriate" data with known uncertainties, including peer review of the data, review of the measurement techniques, but also selected new measurements to be performed that were beyond the scope of Ref. 1.

Nine institutes from 7 countries participated in this CRP: Atomic Energy of Canada Ltd (Canada); the Nuclear Power Institute of China (China); the University of West Bohemia (Czech Republic); the Institute of Physics and Power Engineering, and the Institute of High Densities of the Russian Academy of Sciences (Russian Federation); the Bhabha Atomic Research Centre (India); Commissariat à l'Énergie Atomique, Grenoble (France); and Hanyang University and Seoul National University (Rep. Of Korea). Significant contributions were also made by the Argonne National Laboratory (USA).

The objective of this second CRP, which is documented in Ref. 2, was to establish an internationally available, peer reviewed database of properties at normal and severe accident conditions on the Internet. To accomplish that goal, new measurements of thermo-physical properties of Zirconium liquid, Hf, Zr-2.5% Nb and UO_2-Gd_2O_3 were completed. In addition, the CRP carried out the assessment of thermo-physical properties of materials including Zircaloy, Zr-2.5% Nb, Zr-1% Nb, Zr liquid, ThO_2-UO_2, ThO_2, UO_2-Gd_2O_3, UO_2, Russian steels, Hafnium, Corium and Inconel.

Along with the review, assessment and new measurement works, a feasibility study on the conversion of the THERSYST database into a web-based online database was proposed during the 2nd CRP. Given the positive results of this study, the old database was completely redesigned and reconstructed using a powerful relational DBMS (Database Management System) using contemporary information technologies (O/S: Linux, DB: MySQL).

In the reconstruction of the database, the category scheme of THERSYST was preserved while all modular groups of materials were merged into one. For the input entry, the original format of the data set was kept as a standard and all the relevant information was converted into this standardized form to avoid input difficulties and to keep the consistency. New web-based database took the GUI (Graphic User Interface) approach, and thus all descriptors were laid out in the form of buttons in the pop-up windows, which make data selection, manipulation, and representation very user friendly.

This whole task was carried out by Nuclear Materials Laboratory at Hanyang University in Seoul, Korea, with the financial support of the Ministry of Science and Technology of the Korean government (MOST, Now MEST; Ministry of Education, Science and Technology). During the 3rd Research Coordination Meeting (RCM) for this CRP, held in Vienna in 2003, the new name THERPRO was given to this new web-based database.

III. SYNOPSIS OF THERPRO

1. Overall Structure of the Database

THERPRO has a hierarchical structure consisting of several levels: home page, element, compound, property, author, report, and bibliography level. All data sets in each level are interconnected using a network structure and thus every data can be easily retrieved, including the bibliographical information, by an appropriate query action. The internal structure is shown in Fig. 2.

In fact, the THERPRO home page is the top level with the periodic table, which provides easy access to the desired data and supplementary features for a convenient data retrieval.

Element level is the actual first level in the search of the target properties of target materials. When users choose the symbol of the major element of the compound in the periodic table, they will be led to the element level in which they see the list of compounds including the element along with the general properties of the element. When users make a selection of the target compound in the list, THERPRO will guide them to the compound level and there they will find the list of thermo-physical properties of the compound whose data have been collected and stored in the database.

The property level belongs to the database platform in which all the collected data are sorted, classified, and

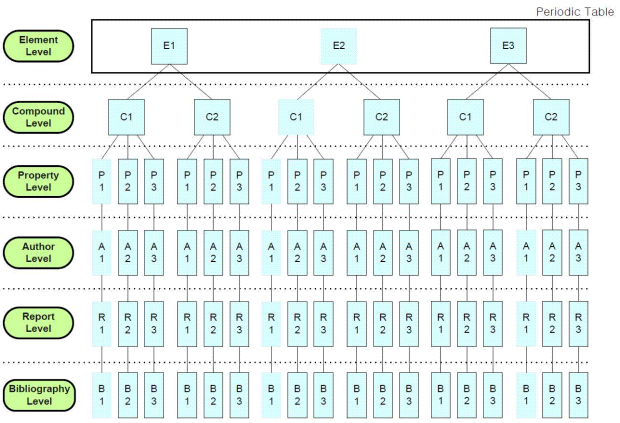

Fig. 2. (Color online) Overall structure of THERPRO database.

stored. All of the properties data and information in this platform are linked to the corresponding compounds in the compound level.

The next three levels, author, report, and bibliography level, constitute the substrate of the database and thus they are constructed in the common layer. When users reach the property level or the substrate, they have to select the author from the authors list as well as the appropriate author's report from the document list. Users can choose multiple authors and multiple reports. Once they select the report and request to plot, they will have the selected property data in graphic form.

The bibliography level is the lowest level in the database structure and accessible only to authorized users. They will see the information including the numeric property data by selecting the report ID number in the screen menu. Since this information has been saved in a text file users can copy and paste it in their own documents.

2. Structure of Standard Data Set

A standard data set has been developed for THERPRO in order to keep the consistency of the collected information and to ease the comparison and the interpretation of the data. The data set consists of five classes: material characterization, data characterization, measurement technique, bibliography, and numerical data (Fig. 3). With this standard category scheme all of the data sets are sorted according to the material's name and/or the chemical formula and then hierarchically ordered in the corresponding level of the database, except the bibliography level. Upon request with appropriate query actions, therefore, any graphic or numeric property data can be reversely extracted from the stored data set in the database. Authorized users can trace back to the information on how the data were generated and with what measurement technique.

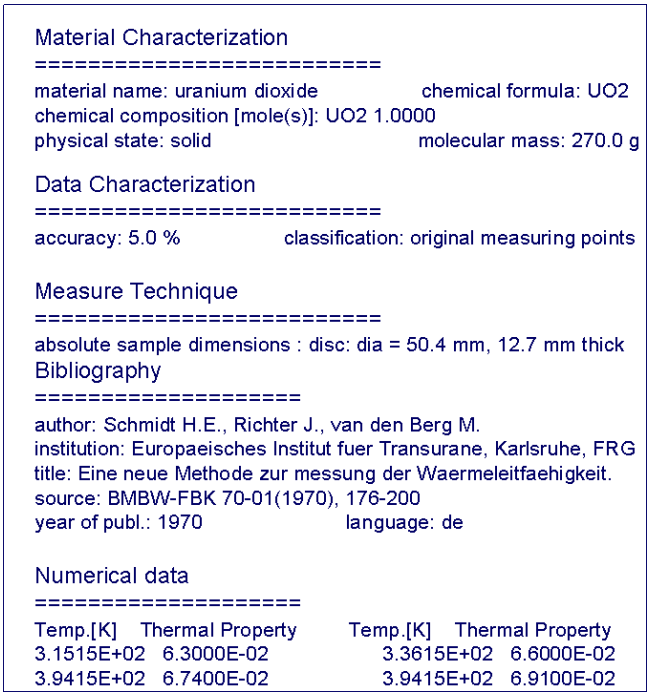

Fig. 3. (Color online) An example of the standard data set.

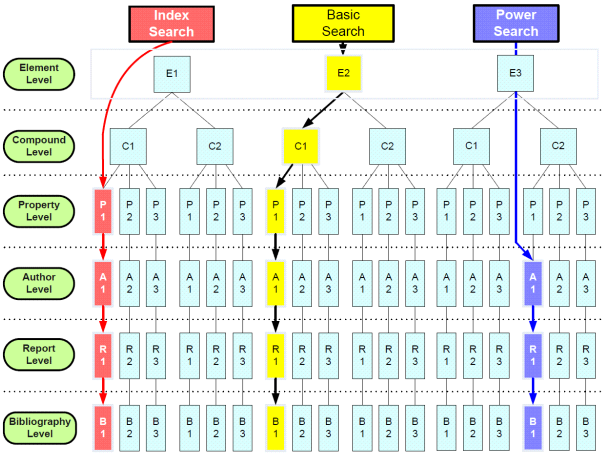

Fig. 4. (Color online) Data retrieval schemes of THERPRO database.

3. Data Retrieval Scheme

THERPRO provides three data retrieving schemes: basic search, index search, and power search. The basic search is the first-step searching method but the other two methods provide a more convenient and powerful data retrieval. Figure 4 shows the sequential flows of the searching ways in the structural diagram.

Once users visit the THERPRO site, they are able to begin the basic search since the periodic table in the home page is actually the entry gate for this search.

Users can also try the index search by selecting the 'index' menu in the right upper part of the home page. All the materials collected in THERPRO have been in-

dexed according to their chemical formula and compound name. Choosing the compound of interest directly takes the user to the compound level.

If users are familiar with THERPRO or know the author who measured the target property of the compound of interest, they can try the power search by typing them in the columns in the upper middle section of the home page. This leads users directly to the property level.

4. User Registration and Authorization

THERPRO has been developed as a common utility for engineers, researchers, and managers working in the nuclear laboratories and industries and is accessible to registered user in all IAEA Member States. Nevertheless, the access to the source data files must be limited for database protection and security. In practice, THERPRO offers three users categories: group 1, group 2, and administrative group. The user group assignment is normally made by the Agency's review committee. All user groups are entitled to make suggestions and comments on the database and propose the modification or correction of data.

Group 1 users can visit any part of the THERPRO database except the detailed bibliography information area. Anyone can be a registered user when they accept the security notice, privacy policy, copyrights, and terms and conditions effectively required by Agency. As stated in the terms and conditions, however, the IAEA has the right to cancel a user registration for the future use if the user provides any fake information during the registration process.

Group 2 users have the right to get any available source file or information including the bibliography information.

Administrators are the users who have rights to modify or correct the data. Only a small number of people such as personnel at the IAEA headquarters and the staff in the THERPRO management center authorized by the Agency fall in this user group.

The security and safety of the database cannot be too much emphasized, especially when it is a nuclear related database such as THERPRO. For this reason, the entire THERPRO system is currently running in the mainframe server of CNMD (Center for Nuclear Materials Database) at Hanyang University under the security protection.

5. Management of THERPRO

Experience tells us that even a database born amid cheers must die out without proper management. The THERSYST database is a good and typical example. Therefore, the CNMD at Hanyang University in Seoul, Korea was designated in May, 2004 as the center for THERPRO management. This was a logical choice, as the laboratory carried out the THERPRO reconstruction task successfully and showed willingness to take the responsibility.

Nowadays the center takes care of the routine maintenance of the THERPRO database and coordinates users and work group support, while collecting new thermophysical properties data of materials publicly published in recent technical journals.

The review and assessment of collected data are coordinated by the center through the online communication tools available in the THERPRO homepage. New data formatted in the standardized form are circulated between the advisory group members and, once final revisions or modifications are prepared, they will be submitted to the Agency for final review and approval. Upon the approval, the new data will be loaded to the THERPRO by the center.

IV. CONCLUSIONS

The IAEA THERPRO database is a peer reviewed database of material properties at normal and severe accident conditions available to all IAEA Member States, and it is readily accessible on the Internet at http://therpro.iaea.org/. As of the end of 2009, THERPRO has more than 289 registered users from about 41 IAEA Member States and about 159 organizations.

The THERPRO database currently contains over 13,000 data files for 1,300 reactor materials, including descriptions of experiments, and bibliographic information. Furthermore, the THERPRO database is continuously updated. For example, in 2009, the THERPRO database was enhanced by including numerous new records related to the thermo-physical properties of Russian nuclear reactors [3].

Registering to use freely the THERPRO database is easy by visiting the THERPRO website. In addition, the managers of THERPRO are very interested in continuously enhancing the database, and as such they welcome organizations interested in contributing new data to be added to the database or in participating in the peer review process for new and existing data.

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