

M9705 3026

RECEIVED

MAY 27 1997

OSTI

**International Nuclear Safety Center Database on
Thermophysical Properties of Reactor Materials¹**

J. K. Fink,^{2,4} T. Sofu,³ and H. Ley³

ANL/RE/CP-91778
CONF-970629--

¹ Paper presented at the Thirteenth Symposium on Thermophysical Properties, June 22-27, 1997, Boulder, Colorado, U.S.A.

² Reactor Engineering Division, Argonne National Laboratory, Argonne, Illinois 60439, U.S.A.

³ Reactor Analysis Division, Argonne National Laboratory, Argonne, Illinois 60439, U.S.A.

⁴ To whom correspondence should be addressed.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED *ph*

The submitted manuscript has been authored by a contractor of the U. S. Government under contract No. W-31-109-ENG-38. Accordingly, the U. S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U. S. Government purposes.

MASTER

This work was supported by the U.S. Department of Energy under Contract W-31-109-ENG-38

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, make any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

**Portions of this document may be illegible
in electronic image products. Images are
produced from the best available original
document.**

ABSTRACT

The International Nuclear Safety Center (INSC) database has been established at Argonne National Laboratory to provide easily accessible data and information necessary to perform nuclear safety analyses and to promote international collaboration through the exchange of nuclear safety information. The INSC database, located on the World Wide Web at <http://www.insc.anl.gov>, contains critically assessed recommendations for reactor material properties for normal operating conditions, transients, and severe accidents. The initial focus of the database is on thermodynamic and transport properties of materials for water reactors. Materials that are being included in the database are fuel, absorbers, cladding, structural materials, coolant, and liquid mixtures of combinations of UO_2 , ZrO_2 , Zr, stainless steel, absorber materials, and concrete. For each property, the database includes: (1) a summary of recommended equations with uncertainties; (2) a detailed data assessment giving the basis for the recommendations, comparisons with experimental data and previous recommendations, and uncertainties; (3) graphs showing recommendations, uncertainties, and comparisons with data and other equations; and (4) property values tabulated as a function of temperature.

KEYWORDS: database; fuel; cladding; material properties; reactor materials; thermodynamic properties; transport properties.

1. INTRODUCTION

The International Nuclear Safety Center (INSC) has been established at Argonne National Laboratory to promote continuing improvement of nuclear safety throughout the world through international collaboration in research and development and an open exchange of nuclear safety information. It is to serve as a center for (1) the collection of information important for safety and technical improvements in nuclear power engineering, (2) maintaining core competencies in nuclear reactor design and safety technology, and (3) cooperation in the development of nuclear safety technologies. The INSC Database was created to be a comprehensive resource for safety analysis and risk evaluation of the world's nuclear power plants. The purpose of the database is to provide the data, tools, and information necessary to perform safety analyses that meet accepted international standards. In order to be a readily available information resource to the international community, the database is available on the World Wide Web at <http://www.insc.anl.gov>. The functionality of the database is maintained with the ORACLE Relational Database Management System operating in a UNIX environment. An Internet interface via a Netscape World Wide Web Server provides interactive access to the INSC Database via standard Web browsers.

The INSC Database is divided into 6 main areas: (1) reactor and plant information such as locations on world and country maps and design data, (2) results from safety and risk analyses, (3) safety evaluation methods and computational tools, (4) INSC related activities, (5) links to other information sources and databases such as the U.S. Nuclear Regulatory Commission plant information, and (6) reactor material properties. Critically assessed, peer reviewed material properties are being included in the INSC Database to

meet the needs of analysts using, developing, and validating models and computer codes for reactor safety. Computer codes independently developed that address the same reactor accident conditions frequently disagree not only because of differences in the models of physical phenomena but also because of differences in the material properties used in the models. Disagreement is greatest for severe accidents because the course of the accident can depend strongly on the material's responses which lead to sharp bifurcations in physical behavior and mechanical failure of structures. Accurate material properties are also needed for the design and interpretation of small-scale integral experiments used to validate reactor safety computer codes. Incomplete and/or incorrect property data can produce significant uncertainties in the calculations modeling these experiments and thereby mask deficiencies in the models. Although agreement between code calculations and small-scale experiments can be obtained using inadequate property data, subsequent extrapolations of codes with inadequate property data to full-scale reactor accident conditions can lead to erroneous conclusions.

2. MATERIALS AND PROPERTIES INCLUDED IN THE DATABASE

The INSC database is organized so that the user may find material property recommendations from searching on the property or the material. Properties identified for inclusion in the database are thermodynamic, transport, and mechanical properties of solid reactor materials under normal, transient, and severe accident conditions. In addition, thermophysical properties of liquids and liquid mixtures appropriate for severe accident calculations are included. Thermophysical properties being included in the database are:

Thermodynamic Properties:

enthalpy, heat capacity, density, thermal expansion, enthalpy of fusion, solidus/liquidus, melting point, vapor pressure, boiling point, enthalpy of vaporization, and surface tension.

Transport Properties:

thermal conductivity, thermal diffusivity, viscosity, emissivity, and electrical conductivity.

The development of the INSC material property database will be done in cooperation with the proposed IAEA coordinated research program to establish an internationally available, peer reviewed database of thermophysical properties of light-water reactor and heavy-water reactor materials at normal, transient, and severe accident conditions. Therefore the reactor materials identified in the proposed IAEA program, will be included in the INSC database. They are:

- Fuel: UO_2 , $\text{UO}_2\text{-PuO}_2$, irradiated UO_2 , SIMFUEL, $\text{UO}_2\text{-Gd}_2\text{O}_3$, $(\text{UO}_2/\text{PuO}_2)\text{-ThO}_2$, $\text{PuO}_2\text{-ZrO}_2$, Cermet ($\text{UO}_2\text{-Zr}$);
- Cladding: Zircaloy-2, Zircaloy-4, Zr-Nb alloys, and oxidized zirconium alloys;
- Absorbers: Ag-In-Cd, B_4C ;
- Structural Materials: steels, Zr-2.5%Nb, Zircaloy-2, Inconel-800, Inconel-600
- Liquid Mixtures: Combinations of UO_2 , Zr, ZrO_2 , stainless steel constituents, Ag, In, Cd, B_4C , and concrete.

3. CRITICAL ASSESSMENT AND PEER REVIEW PROCESS

The material property recommendations in the INSC Database are based on a critical assessment and peer review process that is summarized in Figure 1 and outlined below:

- (1) collection and critical assessment of all published property data,

- (2) determination of recommended equations to represent the property (which requires assessment of existing recommendations and when appropriate development of new equations by fitting data and checking consistency with recommendations of related properties),
- (3) comparison of recommendation with previous recommendations,
- (4) determination of uncertainties in recommendations from errors in fitting the data, uncertainties in the data, and in the theory used to fit the data, and from comparison of data and other recommendations,
- (5) put recommendation in the database for peer review (version 0),
- (6) independent international peer review of recommendation,
- (7) repeat of steps 2 through 6 until a consensus is reached,
- (8) enter peer reviewed recommendation in the database (version 1), and
- (9) publish recommendations.

As new data or new theories relevant to any material property in the database become available, the critical assessment and peer review process, outlined above, is repeated so that the recommendations in the database remain current. Steps of the critical assessment and peer review process are discussed below using examples from the INSC database.

4. DATA COLLECTION AND SELECTION

A literature search is done to locate thermophysical property data for each material. Data on thermophysical properties of solid reactor materials under normal operating conditions were collected as part of the 1990-1995 IAEA Coordinated Research Program on Thermophysical Properties of Materials for Advanced Water-Cooled Reactors[1] and added to the THERSYST database [2,3] at the University of Stuttgart. After all available data are collected, data are compared for consistency and inconsistent data discarded. When sufficient data are available, inconsistent data are identified by statistical analysis for outliers. If data from different experimenters disagree and insufficient data are available for

a statistical analysis, data are selected based on assessment of the experiment techniques, agreement between two or more independent experiments, and examination of the experimenter's data on reference standards and materials for which more data are available.

All available zirconium thermal conductivity data are shown in Figure 2. Data included in the analysis[4] are open circles; inconsistent data are filled symbols. The discarded data include two preliminary data reported by Danielson [5], the data of Mikryukov [6], the data of Vianey [7], and the single datum at 395 K of Peletskii et al.[8]. The data of Mikryukov from two sets of measurements show systematic deviations. One set of data is clearly high relative to the other set and to data from other measurements. The data given by Vianey were discarded because they are high relative to other data and Vianey states that they are inaccurate because of the small size of the sample. The 395 K datum of Peletskii et al. appears to be a misprint because it was not shown in figures in their paper and is clearly high relative to their other data.

5. CRITICAL ASSESSMENTS AND DATA ANALYSIS

If data assessments and critical reviews are available, they are not duplicated but are taken into account in the determination of recommended equations. If no new data are available since the most recent critical assessment and peer review of that assessment confirms the results, then equations from that assessment are recommended. An example is the recommendation of the equation of Breitung and Reil [9] for the vapor pressure over liquid UO_2 [10]. When new measurements are available since the last review, then these new data are compared with the recommendations from that review to determine if the result is consistent with the new data. In the case of thermal expansion of UO_2 , the new

data are sufficiently consistent with the equations recommended by Martin [11] to concur with the recommendations given by Martin. However, data for the thermal conductivity of zirconium obtained since the most recent review by Touloukian et al.[12] showed sufficient disagreement with their equation (labeled CINDAS in Figure 2) that a new assessment of the zirconium thermal conductivity data was made[4].

6. COMPARISON OF RECOMMENDED EQUATIONS

When more than one assessment of the data are available as in the case of the thermal conductivity of solid UO_2 , then the recommendation is based on comparisons of the equations with each other, with the data, and examination of the physical basis for the equations. From examination of recommendations from eight assessments of the thermal conductivity of solid UO_2 [10], the equation of Harding and Martin [13] was selected because it provides a good representation of the data, is physically based with no free parameters to determine from fitting the data, is in good agreement with equations obtained from statistical fits to the data, and is consistent with in-reactor integral measurements. Comparisons of recommended equations with equations available from other assessments are also useful in estimating the uncertainty of the recommended values.

7. CONSISTENCY OF RECOMMENDATIONS

In the assessments of data on thermodynamic and transport properties of each material, checks are made to ensure that the recommendations of related properties are consistent. For example, enthalpy and heat capacity data are fit together so that the equations for these properties are consistent. In the case of heat capacity of liquid UO_2 , the heat capacities reported by Ronchi et al. [14] were obtained from indirect measurements

that required equations for density and thermal conductivity to reduce the data. At temperatures above 4500 K, the densities used in their data reduction differ significantly from recommended densities [10]. To preserve consistency between these related properties, heat capacities above 4500 K reported by Ronchi et al. have not been included in the combined analysis of liquid UO_2 enthalpy and heat capacity data [10].

8. UNCERTAINTIES

One of the principal objectives of these assessments is to provide a reliable estimate of the uncertainty in the recommended equations for each property. Uncertainties are used by reactor safety analysts in determining whether the property values used in an existing code should be modified and in sensitivity calculations. If sensitivity calculations show that the reactor accident scenario deviates significantly by variation of a material property within the uncertainty limits, further measurements of that property are needed to reduce its uncertainty. Thus, sensitivity calculations using reliable uncertainties forms a basis to decide where limited research funds should be directed.

Uncertainties are determined from errors in the data, the error in the fit to the data, and uncertainties in the theories on which equations are based. When experiment uncertainties are available, they are used to weight the data in the fitting procedure as well as in determining the overall uncertainty of the recommendation. Often, as in the case of the combined fit to the enthalpy and heat capacity of liquid UO_2 , all the data from each experiment are given the same weight. In many cases, rigorous statistical treatment to determine uncertainties is impossible because of lack of information on the experiment

uncertainties. Then deviations of the data and of equations from different assessments are taken into account in determining the uncertainties.

9. RECOMMENDATION PUT IN DATABASE FOR PEER REVIEW

Summaries of the recommendations and assessments are put in the INSC database for peer review. Each summary includes the recommended equations, tabulated values, assessed data, reasons any data were excluded, basis for the recommendations, comparisons with data and with other recommendations, and uncertainties. Graphs of the recommended property values with uncertainties, graphs comparing the recommendations with data and with equations given in other assessments are also included as part of the documentation for peer review. Critical assessments of the thermophysical properties of UO_2 are available in the INSC database and in a report[10] for peer review.

10. PEER REVIEW

The purpose of the peer review is to have an independent examination of the assessments made to verify assumptions, results, and conclusions and to check that the relevant data and literature have been included in the critical assessment. Peer reviews will be made by international experts as part of the proposed IAEA coordinated research program to establish an internationally available, peer reviewed database of thermophysical properties reactor materials. The INSC Database Clipboard will facilitate communication by participants in the peer review by serving as an electronic forum in which reviewers post comments by e-mail and retrieve comments from other reviewers via the World Wide Web. The peer review may lead to reassessments or minor changes which will again be peer reviewed. This process will continue until agreement is reached. The final peer reviewed

recommendations will be included in the INSC database and in a technical document as part of the proposed IAEA coordinated research program.

When new data for a property in the INSC database becomes available, the critical assessment will be repeated so that the INSC database remains current.

ACKNOWLEDGMENTS

The work was supported by the US Department of Energy under Contract W-31-109-ENG-38.

REFERENCES

1. J. Cleveland, ed., *Thermophysical Properties of Materials for Advanced Water-Cooled Reactors*, IAEA Draft Report 1997-1-6 Version (to be published IAEA, Vienna, 1997).
2. *THERSYST: User's Handbook*, IKE-STB-899-87 (Institut für Kernenergetik und Energiesystem, Universität Stuttgart, 1987).
3. G. Jaroma-Weiland, *THERSYST the Database for Thermophysical Properties of Solid Materials*, Proc. of the Thirteenth Symposium on Thermophysical Properties, Boulder, CO (June 22-27, 1997).
4. J. K. Fink and L. Leibowitz, *J. Nucl. Mater.* **226** 44 (1995).
5. G. C. Danielson, *USAEC Report ISC-577* (1954).
6. V. E. Mikryukov, *Astron. Fiz. I. Khim.* **12**, 78 (1957).
7. L. R. Vianey, *Thermal Conductivity of 347 Stainless Steel and Zirconium*, BIM-65 (1951).
8. V. E. Peletskii, A. P. Grishcuk, and Z. A. Musaeva, *Teplofiz Vys. Temp.* **30**, 1090 (1992) [English Translation *High Temp.* **30** 900 (1992)].
9. W. Breitung and K. O. Reil, *Nucl. Sci. Eng.* **101**, 26 (1989).
10. J. K. Fink and M. C. Petri, *Thermophysical Properties of Uranium Dioxide*, ANL/RE-97/2 (Argonne National Laboratory, 1997).
11. D. G. Martin, *J. Nucl. Mater.* **152**, 94 (1888).
12. Y. S. Touloukian, et al., *Thermophysical Properties of Matter, Vol. 12 Thermal Expansion Metallic Elements and Alloys* (Plenum Press, New York, 1975) p. 400.

13. J. H. Harding and D. G. Martin, *J. Nucl. Mater.* **166** 223 (1989).

14. C. Ronchi, J. P. Hiernaut, R. Selfslag, and G. J. Hyland, *Nucl. Sci. Eng.* **113**, 1 (1993).



