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THERPRO The IAEA Database for Thermophysical Properties of Materials in Nuclear Reactors

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THERPRO: The IAEA Database for Thermophysical Properties of Materials in Nuclear Reactors

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1. Background of THERPRO Database Development

- Assurance of accurate materials properties data has become an essential and an important part of all disciplines in science and engineering.
- In the nuclear engineering and industry, fundamental understanding of thermo-physical properties of the materials is crucial for the safety and performance of the current fleet of NPPs and for the development of advanced reactor designs. Thus, along with the necessary data measurements, continuous collection and systematic review/assessment of available data is being urgently demanded.
- IAEA kicked off the first CRP (Coordinated Research Project) on 'Establishment of Thermophysical Properties Data Base for LWRs and HWRs' in late 90's and since then two more CRPs have been organized by IAEA during the last ten years.
- Migration of DOS-based THERSYST DB to web-based data base was carried out during second CRP by ANM Lab. (Advanced Nuclear Materials Lab.) at Hanyang university in Korea and then renamed 'THERPRO' DB.
- At the end of third CRP Agency designated the ANM Lab as the center for THERPRO data base management with the financial support of Korean government. The CNMD (Center for Nuclear materials Database) at Hanyang university currently collects recent data, reviews and assesses the data, and formats them for entry into THERPRO DB.

1. Background of THERPRO Database Development (cont)

□ THERSYST DB: Inactive DOS-based Data Base:

• Developed by IKE (Institut fur Kernenerge und Energiessysteme), Germany

• Developed as a combination of a factual database for thermo-physical properties of solids and a modular program for reactor calculation program RSYST to handle the database contents.

• Designed for mainframe computer (VAX) due to the sensitivity and the complexity of the properties database and later transformed to a stand-alone PC-based database since personal computers became popular and common.

• However, since its operating system was DOS and not upgraded properly, THERSYST DB failed to catch up the contemporary IT development and to meet the users' demand. Thus, it remained inactive and unserviceable even in early 90's.

□ THERPRO Database: Web-based On-line Data Base

• Web-based relational database completely re-designed and re-constructed while keeping the standard data format used in THERSYST DB.

- Operating system : Red Hat Linux release 7.2

- Data base management system : MySQL 3.23.41-1.

2. THERPRO Database: A Web-based Relational DB

- A web-based relational database currently available at
- therpro.iaea.org

• It combines thermo-physical properties database and relational network DB management system using modern information technologies. THERPRO DB currently keeps more than 13,000 thermo-physical properties data tables of more than 1,300 materials.

•THERPRO shows thermo-physical property data as a function of temperature graphically and numerically.

- Three data retrieving ways: Basic, Index, Power search
- Multiple choices of data for comparison
- Each data includes complete information including source of the data
- It offers a user-friendly environment for easy data retrieve.
 - GUI (Graphic User Interface) is utilized.

- Pop-up screen menu and screen buttons are provided to make data selection and plot of the selected data very easy, removing the necessity of memorization of many descriptors.

2. THERPRO Database: A Web-based Relational DB (cont)

Properties Collected in THERPRO

The following properties data are collected and stored in THERPRO, as a function of temperature

	Enthalpy		
Thermal Properties	Specific heat capacity		
	Linear thermal expansion		
	Volumetric thermal expansion		
	Thermal conductivity		
Transport Properties	Thermal diffusivity		
	Electrical resistivity		
Physical Properties	Density		
	Lorenz number		
	Emissivity		
Optical Properties	Absorptivity		
	Reflectivity		
	Transmittance		

3. OVERVIEW OF THERPRO

□ Standard Data Format in THERPRO

Thermal Conductivity of UO2



3. OVERVIEW OF THERPRO (cont)

Bibliography

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author: Schmidt H.E., Richter J., van den Berg M. institution: Europaeisches Institut fuer Transurane, Karlsruhe, FRG title: Eine neue Methode zur Messung der Waermeleitfaehigkeit. source: BMBW-FB K 70-01(1970),176-200 year of publ.: 1970 language: de 3.1515E+02 6.3000E-02 3.3615E+02 6.6000E-02 3.9415E+02 6.7400E-02 3.9415E+02 6.9100E-02 5.1415E+02 5.5500E-02 5.1415E+02 5.5500E-02 5.9815E+02 4.2500E-02 6.0815E+02 4.3700E-02

• This format is always kept as a standard and, once data or literature is collected, all the relevant information is converted into this form in order to avoid input difficulties and to keep the data base consistency.

• This bibliographical information on each data set is stored and linked to the data set file.



3. OVERVIEW OF THERPRO (cont)

□ Structure of THERPRO DB



□ Three distinct access for data retrieve



Basic search begins by clicking and selecting the major element of the compound in the periodic table of elements



Index search begins by clicking and selecting the major element or material name of the compound in the Symbol of Compound in Index after Index pop-up window is entered



Power search can be easily done by typing the compound name or formula of interest, property of interest, author's name, and/or year of publication in the upper middle area

International Atomic Energy Agency



Fig 2. Data retrieve of THERPRO International Atomic Energy Agency



Index search

Index search begins by clicking and selecting the major element or material name of the compound in the Symbol of Compound in Index after Index pop-up window is entered You can see the element and compund list contained THERPRO DB and you can search the data of THERPRO DB easily using this retrieve if you know material name and chemical formula

Ex: Author's (B.C. AAA) work on thermal conductivity of UO_2

- 1) Type "UO₂" and select "thermal conductivity, Author"
- 2) Select "Author" in Author level
- 3) Select "E5000775" in Report number listed in Report level
- 4) You can be retrieve if authorized about Bibliography data in Bibliography level



Power search

Power search can be easily done by typing the compound name or formula of interest, property of interest, author's name, and/or year of publication in the upper middle area You can search data of THERPRO conveniently if you know author's name by using this retrieve

- Ex: Author's (B.C. AAA) work on thermal conductivity of UO₂
- 1) Click "Index" and select "UO2"
- 2) Select "Author" in Author level
- 3) Select and click "Thermal conductivity" in Property level
- 4) Select "Author" in Author level
- 5) Select "E5000775" in Report number listed in Report level
- 6) You can be retrieve if authorized about Bibliography data in Bibliography level



DEMONSTRATION

Basic search

Index search

Power search





Fig 3. Homepage of THERPRO (Element level for Periodic Table retrieve)

International Atomic Energy Agency



Fig 4. Compound level for Periodic Table retrieve for UO₂

International Atomic Energy Agency

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Fig 5. Compound level for Periodic Table retrieve for UO₂



Fig 6. Property level for Periodic Table retrieve for UO₂



Fig 7. Author, Report, Bibliography level for Periodic Table retrieve for UO₂



Fig 8. UO₂ thermal conductivity plot based on the Fukushima's work



Fig 9. Homepage of THERPRO for Index retrieve

◎ SmAg3	◎ SmSb	● Sn	● Sn,Cd	● Sn,Mg
◎ Sn,Pb	● Sn,Tl	® Sn,Zn	◎ Sn,Zr	● SnO2
● Sr	Sr(NO3)2	SrHfO3	[●] SrMoO4	SrTiO3
SrZrO3	∘ Та	© Ta,Nb	∘Ta,W	∘ Ta,W,Hf
[●] Tb	◎ TbSb	● Тс	∘ Te	● Th
⁰ Th,U	◎ Th3N4	● ThC2	● ThN	⁰ ThO2
◎ ThS	◎ Ti	● Ti,Al	◎ Ti,Al,Fe,Cr,Mo	Ti,Al,Mn
◎ Ti,Al,Mn,X	◎ Ti,Al,Mo,Si	Ti,Al,Mo,X	◎ Ti,Al,Si	● Ti,Al,Sn,X
◎ Ti,Al,Sn,Zr	Ti,Al,Sn,Zr,X	● Ti,Al,V	◎ Ti,Al,V,Sn	• Ti,Al,V,X
◎ Ti,Al,X	◎ Ti,Cr,Al,X	⁰ Ti,Cr,Fe	◎ Ti,Fe,Cr,Mo	◎ Ti,Mn
◎ Ti,Mo	◎ Ti,Sn,Al,Zr	Ti,Sn,Zr,Al,X	● Ti,V	● Ti,V,Al,X
◎ Ti,V,Cr,X	◎ Ti,Zr	● Ti2FeCo	• Ti2O3	⁰ Ti3Ir
Ti4Co3Ni	◎ Ti4Fe3Co	◎ Ti4FeCo3	© TiB2	° TiBe2
◎ TiC	TiC,Ni,NbC	● TiCo	◎ TiFe	◎ TiN
◎ TiO2	© ∏	● Tm	● Tm2O3	• U
● U(C,N)	● U(O,C)	● U,Al	● U,Cr	∘ U,Mg
∘U,Mo	⁰ U,Mo,Ru,X	® U,Mo,X	◎ U,Nb	● U,Si
● U,Ti	• U,V		I,Zr,Mo,Ru,X	• U2C3
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● UAI2	• UAs 🖉 🖌 🖊	ndav ratriava)	IC,C	• UC,U
● UC,UC2	• UC,WC		JCI3	● UCl4
● UCO	● UF4	● UMoC2	• UN	⁰ Un,UO2
⁰ UN,UO3	● UO2	• UO2(OH)2*H2O	• U02,Cr2O3	• UO2,Eu2O3
● UO2,Gd2O3	 UO2,La2O3 	® UO2,Mo	● UO2,Nb2O5	• UO2,Nd2O5
● UO2,PuO2	⁰ UO2,Sc2O3	• UO2,TiO2	● UO2,W	• UO2,X
⁰ UO2.01	● UO3	● UP	• UPt3	• US
● USb	⁰ USe	• USi2	• UTe	• V
● V,Mo	● V,Ti	● V407	• W	• W,Cu
● W,Re	◎ WC,Co	● WO2	• WO3	• Xe
•Y	◎ Y-Si-Al-O-N	• Y2O3	Y2O3,TiO2	• Y3Al5012
⁰ Y4Co3	°Yb	⁰ Yb,Rh,Sn	◎ Yb2O3	• YbZn2
® Zn	Zn(PO3)2	◎ Zn,Al	● Zn,Al,X	• Zn3(PO4)2
◎ ZnF2	◎ ZnO	● Zr	∘ Zr,Al	● Zr,Mo
	® Zr,Sn	◎ Zr,Sn,Fe,Cr	Zr,Sn,O	● Zr,Sn,X
⁰ Zr.Ta	◎ Zr.Ti	◎ Zr.U	Zr.U.Sn	ZrB2

Fig 10. Symbol list in Index retrieve for UO₂



Fig 11. Compound list in Index retrieve for UO₂



Fig 12. Compound list in Index retrieve for UO₂



Fig 13. Author, Report, Bibliography level for Compound list retrieve for UO₂



Fig 14. UO₂ thermal conductivity plot based on the Fukushima's work

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		Bibliography	Abdusalvamova M N	• Abeles B	Aheles B	
	 Adler P. 	 Affortit C. 	 Aivazov M.I. 	Alexander C.A.	 Alexas A. 	
	Amasovich E.S.	Amato I.	Amitin E.B.	Ammar M.M.	Andon R.J.L.	
	• Andrew J.F.	• Andrianova V.G.	ANL	• Arai Y.	 Arais S. 	
	 Arbeitskreis 	• Arbeitskreis Thermophysik	 Arendts F.J. 	 Argent B.B. 	 Arityumov A.V. 	
	• Arkhipov V.A.	Arthur J.S.	 Arutyunov A.V. 	Asamoto R.R.	 Asano K. 	
	 Ashley T.S. 	• Atroshenko E.S.	Babbitt J.D.	Backlund N.G.	 Bailey L.C. 	
	Bairamashvili I.A.	 Baker D.E. 	 Baker R.D. 	 Balankin S.A. 	 Baleva M.I. 	
	Ball J.G.	Banchila S.N.	 Barabanova L.G. 	Barnard B.R.	 Barnes B.T. 	
	 Basak U. 	• Batalin G.I.	 Batalis A.P. 	 Bates J.C. 	 Bates J.L. 	
	Bauhofer W.	Baxter W.G.	 Beauvy M. 	• Beile J.	Bel skaya E.A.	
	Belenkii G.L.	• Bell I.P.	 Belyaev R.A. 	Benbachir K.	Bendick W.	
	Benedict U.	Bentsen L.D.	 Berlincourt T.G. 	 Berton A. 	 Bethoux O. 	
	Bhatt H.	Bhide V.G.	 Bidwell C.C 	Bing G.	 Binkele L. 	
	Biran de A.	 Bird B.L. 	 Bischof J. 	• BMI	◎ Bober M.	
	Bocker S.	Bode K.H.	• Boehm R.	Bogaard R.	 Bogaard R.H. 	
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	Brandon J.R.	 Brandt N.B. 	 Brandt R. 	 Brandt van der B. 	 Brauner J. 	
	 Brennan J.J. 	 Brett N.H. 	 Brooks C.R. 	 Brophy J.H. 	 Brown W.B. 	
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	 Buravoi S.E. 	 Buravoy S.E. 	 Butera R.A. 	 Butler C.P. 	 Byron Brown W. 	
	Cabannes F.	 Calaway W.F. 	 Calza-Bini A. 	 Cappelletti R.L. 	 Carniglia S.C. 	
	 Casey D.N. 	 Cate J.T. 	 Cezairliyan A. 	 Challis L.J. 	 Chang Y.A. 	
	 Charles J. 	 Chasanov M.G. 	 Chekhovskii V. Ya. 	 Chekhovskoi V.Ya. 	• Chelkowski A.	
	• Chen Y.	 Chereau P. 	 Chevrier J. 	 Chiotti P. 	 Chirigos J.N. 	
	• Cho H.K.	 Chubb W.F. 	 Chupina L.I. 	Chyung K.	 Clifton D.G 	
	Colins J.G.	 Collocott S.J. 	Colvin R.V.	 Connelly D.L. 	 Conway J.B. 	
	 Cook M. 	Cordaro J.F.	Cordfunke E.H.P.	• Cote P.J.	Counsell J.F.	
	 Crane J. Crane build J. 	• Crangle J.	 Craynest van J.C. 	• Culbert H	Culbert H.V.	
	 Czochralski J. 	D.L.Martin	D.M.Bailey	• Danan J.	 Daniel J.L. Daniel J.L. 	
	• Danna J.	• Dao J.N.	 Dauchier M. de Paraeda D.C. 	 Dauchier M.N. Da Copieda R 	 Daudin B. Da Navian C.U. 	·
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Fig 15. Author list in Index retrieve for UO₂



Fig 16. Author list in Index retrieve for UO₂

3) Power Search

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4. THERPRO UPCOMING ACTIVITIES

□ System Upgrade

- Supported by Korean government
- Includes:
 - Hardware and software
 - DB management and operating system
 - Index Search system: Author index search system
 - DB system protection and user support system
 - Materials re-categorization
 - Advisory work group forum modification

Creation of an Advisory Group to supervise the quality of the data included

- Data Update & Addition of WCR new data
- Expanding the THERPRO DB to include materials from other reactor types
 - Fast Reactors, Gas Cooled Reactors, etc
 - The THERPRO infrastructure would be made available to other groups interested in creating DBs for their data

