



XA9744601

**INTERNATIONAL NUCLEAR SAFETY
CENTER DATABASE on
MATERIAL PROPERTIES**

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Presentation at

IAEA Consultancy on
Review of Thermophysical Properties of
Materials for Advanced Water Cooled Reactors

Argonne National Laboratory
Argonne, Illinois USA

November 6-8, 1996

INSC PROPERTY NEEDS

- **Properties for Light Water Reactor Safety Analysis & Safety Assessments**
 - Accident Initiation to Severe Accidents
 - Solid Materials
 - Molten Materials & Mixtures
- **Needs Survey of ANL Reactor Safety Staff**
 - Rank Material Properties:
 - High, Medium, Low
 - Rank Determines Order of Assessment
- **Initial Focus**
 - High Priority Properties
 - Russian Reactor Materials
 - Assessments of New Data
- **Future Focus**
 - US Light Water Reactor Property Needs
 - Comparison with US Industry Reference:
 - MATPRO

INSC DATABASE:

REACTOR MATERIALS

Fuel

UO₂

UO₂-PuO₂

UO₂-Gd₂O₃

Cladding

Zr-1% Nb alloy

Zr-2% Nb alloy

Zircaloy 2

Zircaloy 4

Inconel 625

Type 304 Stainless Steel

Absorbers/Moderators

Russian Graphite

Ag-In-Cd Alloy

B₄C

Cadmium in Stainless Steel

Structural Materials

Stainless Steels

Inconel 600

A533B Steel (Vessels)

Coolants

Water

Heavy-water

Concretes

Siliceous

Limestone/Common Sand

Limestone

Russian:Serpentine, Others?

Liquid Mixtures

Zr-Stainless Steel

UO₂-ZrO₂-Stainless Steel

UO₂-ZrO₂

UO₂-ZrO₂-Concrete

UO₂-ZrO₂-Zr

INSC DATABASE:

MATERIAL PROPERTIES

Thermodynamic

Enthalpy
Heat Capacity
Density
Thermal Expansion
Solidus/Liquids (Melting Point)
Enthalpy of Fusion
Vapor Pressure
Boiling Point
Enthalpy of Vaporization
Surface Tension

Transport

Thermal Conductivity
Thermal Diffusivity
Electrical Conductivity
Viscosity
Emissivity

Mechanical

Young's Modulus
Shear Modulus
Poisson's Ratio
Flow Stress
Yield Strength
Tensile Strength
Creep Strength
Biaxial Creep Rupture Strength

STATUS OF INSC

DATA ASSESSMENTS

COMPLETED by ANL

- **Fuel: UO_2 (*Solid & Liquid*)**
Enthalpy, Heat Capacity (298-4500 K)
Melting Point,
Density (298-8000 K)
Thermal Expansion, (298-8000 K)
Thermal Conductivity (298 - 3500 K)
- **Absorbers/Moderators: Graphite**
Enthalpy, Heat Capacity (298-3800 K)
- **Coolant: Water**
Thermodynamic & Transport Properties
- **Cladding/Structural Materials: Zr**
Thermal Conductivity (298 - 2000 K)

STATUS (Continued)

COMPLETED by IBRAE

*(Russian Accademy of Sciences Nuclear
Safety Institute)*

- **Thermodynamic Data (H, C_p)**
Zr, Nb, Ag, In, Cd, B₄C, Fe, Cr, Ni
CaO, MgO, K₂O, Na₂O, SiO₂, Al₂O₃, ZrO₂
- **Absorbers/Moderators: Graphite**
Grades of Russian Graphite, Density,
Thermal Conductivity, Thermal Expansion,
- **Cladding: Zr-1%Nb, Zr-2.5%Nb**
Enthalpy, Heat Capacity (500 - 1600 K),
Enthalpy of Fusion, Solid Phase Diagram,
Density & Thermal Expansion (293-1173 K),
Thermal Conductivity (300-1600 K),
Electrical Resistivity (300-1500 K),
Emissivity (350-700 K),
Estimated: Viscosity, Surface Tension,
Mechanical: Elastic & Shear Modulus, Yield &
Tensile Strength, Elongation, Contraction

MATERIAL PROPERTIES

CRITICAL REVIEW PROCEDURE

- **Data Assessment**

 - Collect, Critically Assess All Available Data

 - Recommend Equations

 - Compare with Previous Recommendations

 - Determine Uncertainty in Equations

 - Errors in Data, Theory, Fit

- **Put Recommendations in Database (Rev 0)**

 - Tables, Equations, Graphs

 - Summary of Assessment

 - Detailed Documentation of Assessment

 - Basis for Recommendations

 - Uncertainties

 - Comparison with Other Recommendations

- **Peer Review of Assessment**

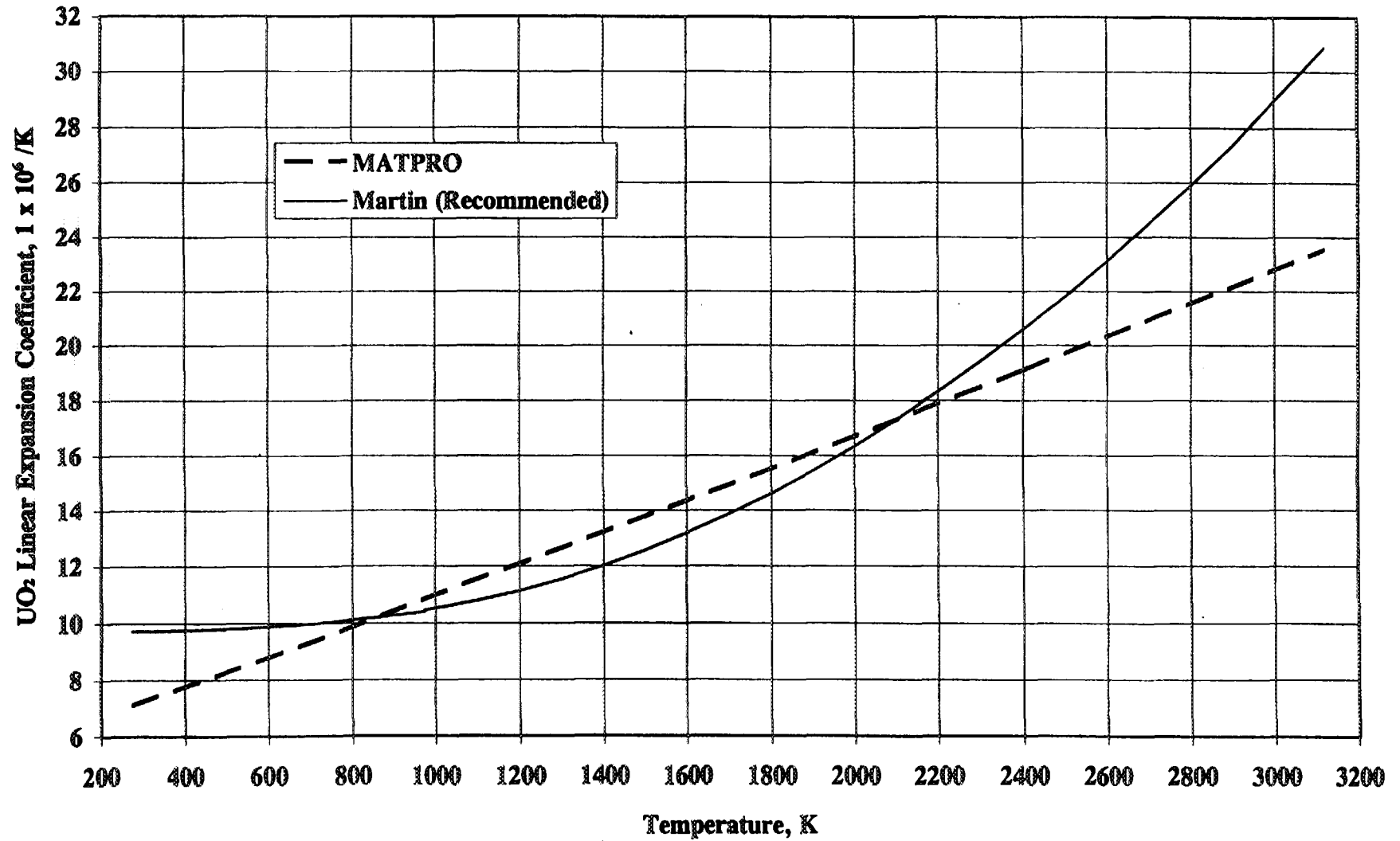
 - Discussions, Reach Consensus

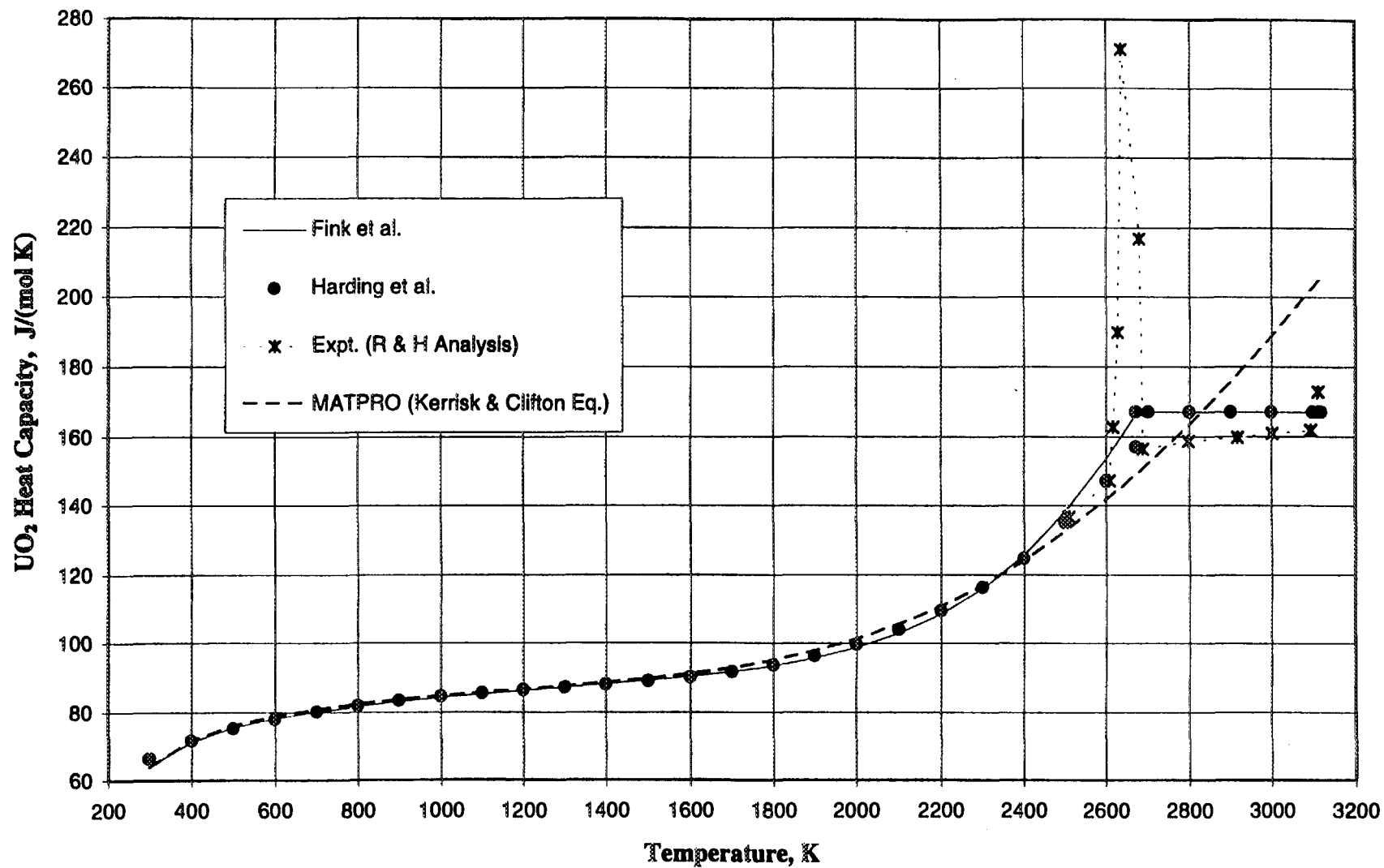
- **Peer Reviewed Recommendation Added to Database (Rev 1)**

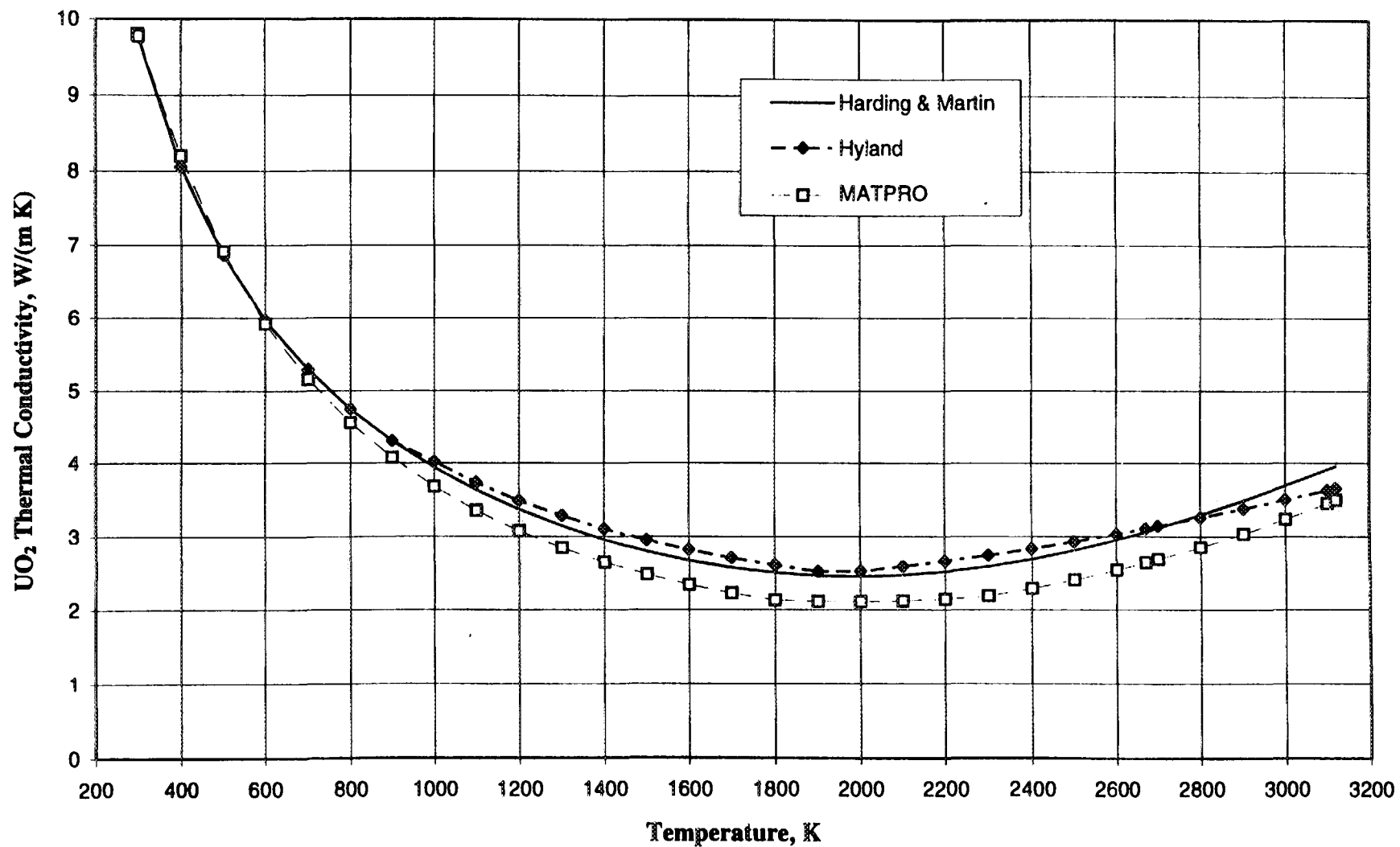
Solid UO₂

- **Solid Thermal Expansion Data -**
 - 293- 2930 K - Hutchings 1987
 - New Recommendation - Martin 1988
 - MATPRO: 1981 Eq. of Olsen Based on 1963 Data of Christensen
- **Solid Phase Transition at 2670 K Confirmed**
 - Neutron Scattering Data - Clausen 1984
 - Cooling Curves - Hiernaut et al. 1993
(New Phase Diagram)
 - Analysis of Heat Capacity Measurements - Ronchi & Hyland 1994
 - Transition not included in MATPRO Eq.
 - MATPRO - 1972 Kerrisk & Clifton Eq.
- **Thermal Conductivity Recommendations -**
 - Based on Physical Models
 - Harding & Martin 1989
 - Hyland 1983
 - MATPRO Eq. has no Physical Basis -
Above 1800 K Deviations -15%

Comparison of Recommended UO_2 Linear Thermal Expansion Coefficient of Martin with MATPRO Recommendation



Comparison of Equations for the Heat Capacity of Solid UO_2 

Comparison of Equations for the Thermal Conductivity of Solid UO_2 

Liquid UO₂ -

- **Liquid Density Measurements**

3120-8000 K -Breitung & Reil 1990
Good Agreement with Drotning 1981
New Recommendation

- **Liquid Thermal Conductivity**

5.6 W/(m K) - 1985 Assessment
2.5 W/(m K) - Tasman et al. 1994
New Heat Capacities Effect Calculation of
Thermal Conductivity from Diffusivity
New Recommendation: 2.5 - 3.6 W/(m K)

- **Liquid Heat Capacity Measurements**

3100 -8000 K Laser Pulse
Ronchi, Hiernaut Selfslag & Hyland 1993
(Dependent on k assumed: 2.5 W/(m K)
New Recommendation -
Combined Fit of H & Cp
(H Data: Leibowitz et al. , Hein & Flagella

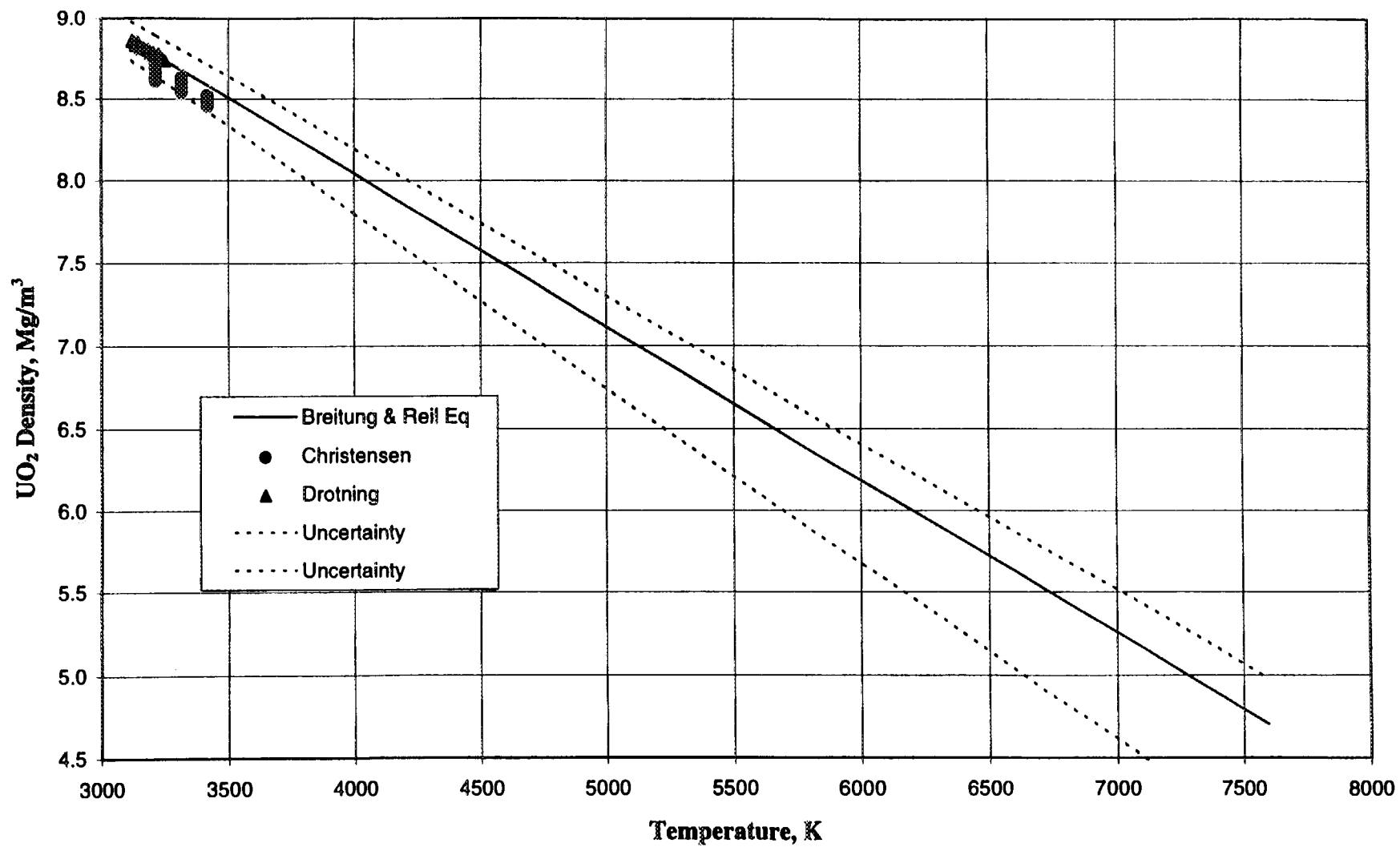
Figure 1 Liquid Density of UO_2 

Figure 1 UO₂ Thermal Diffusivity

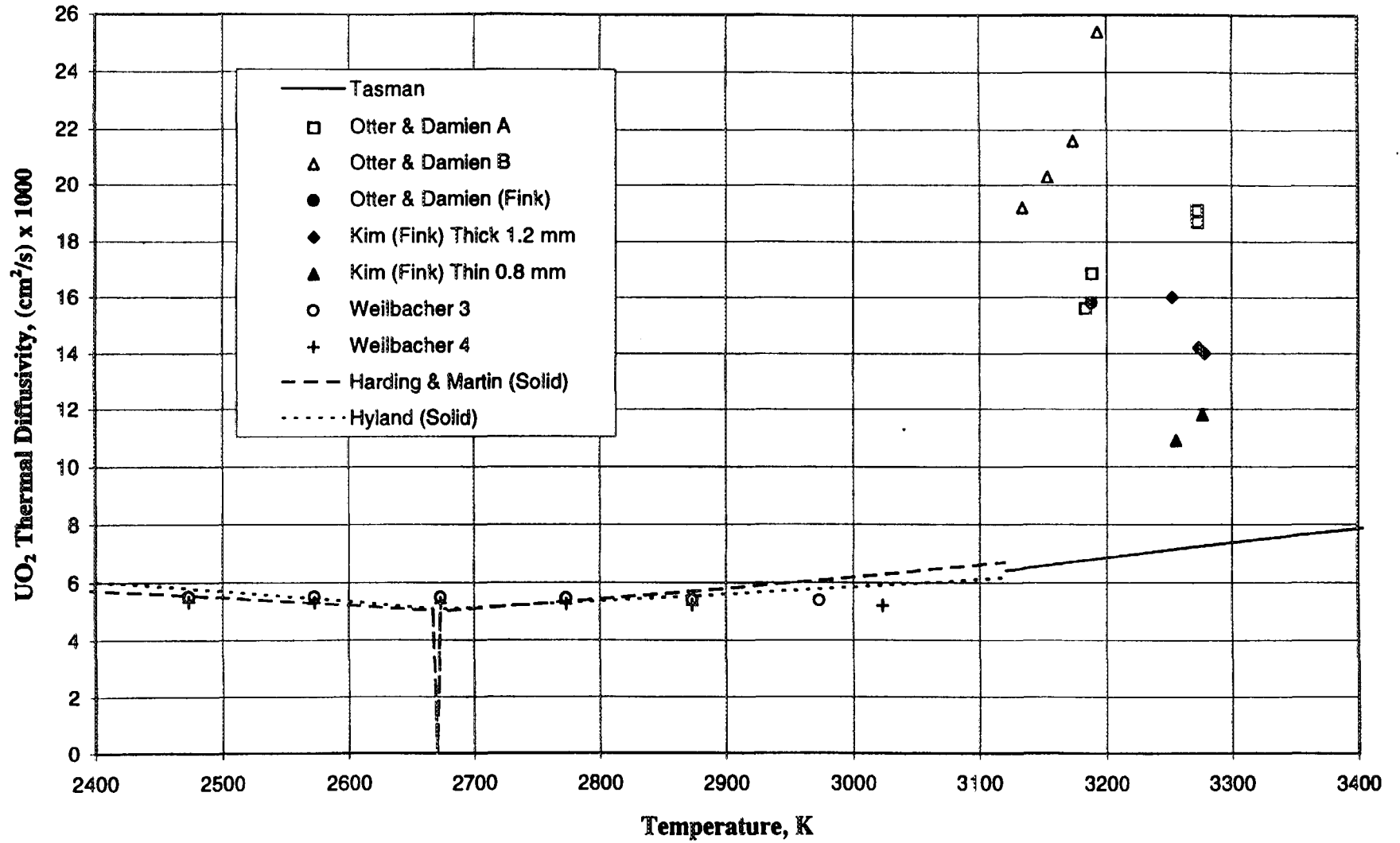
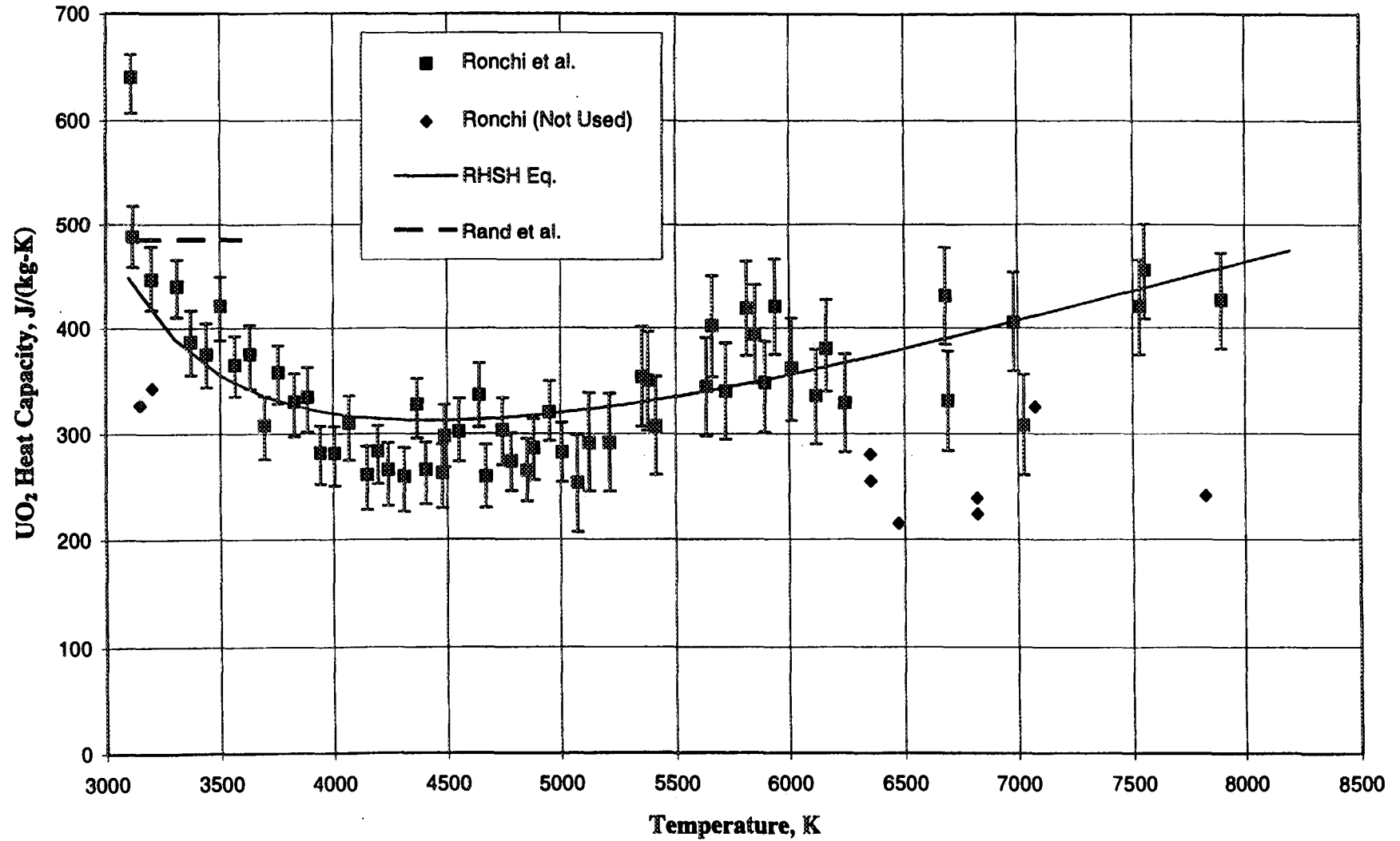
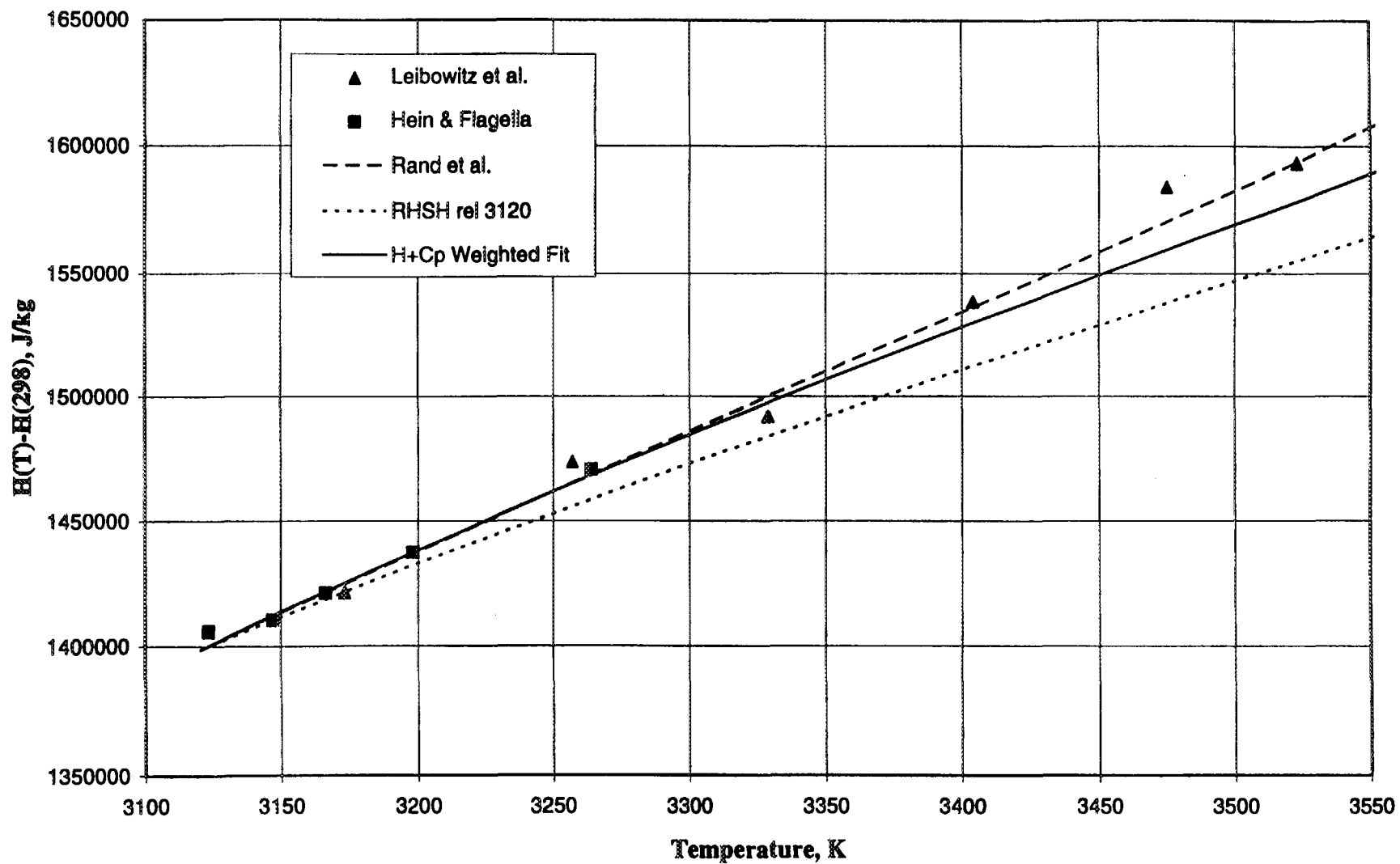
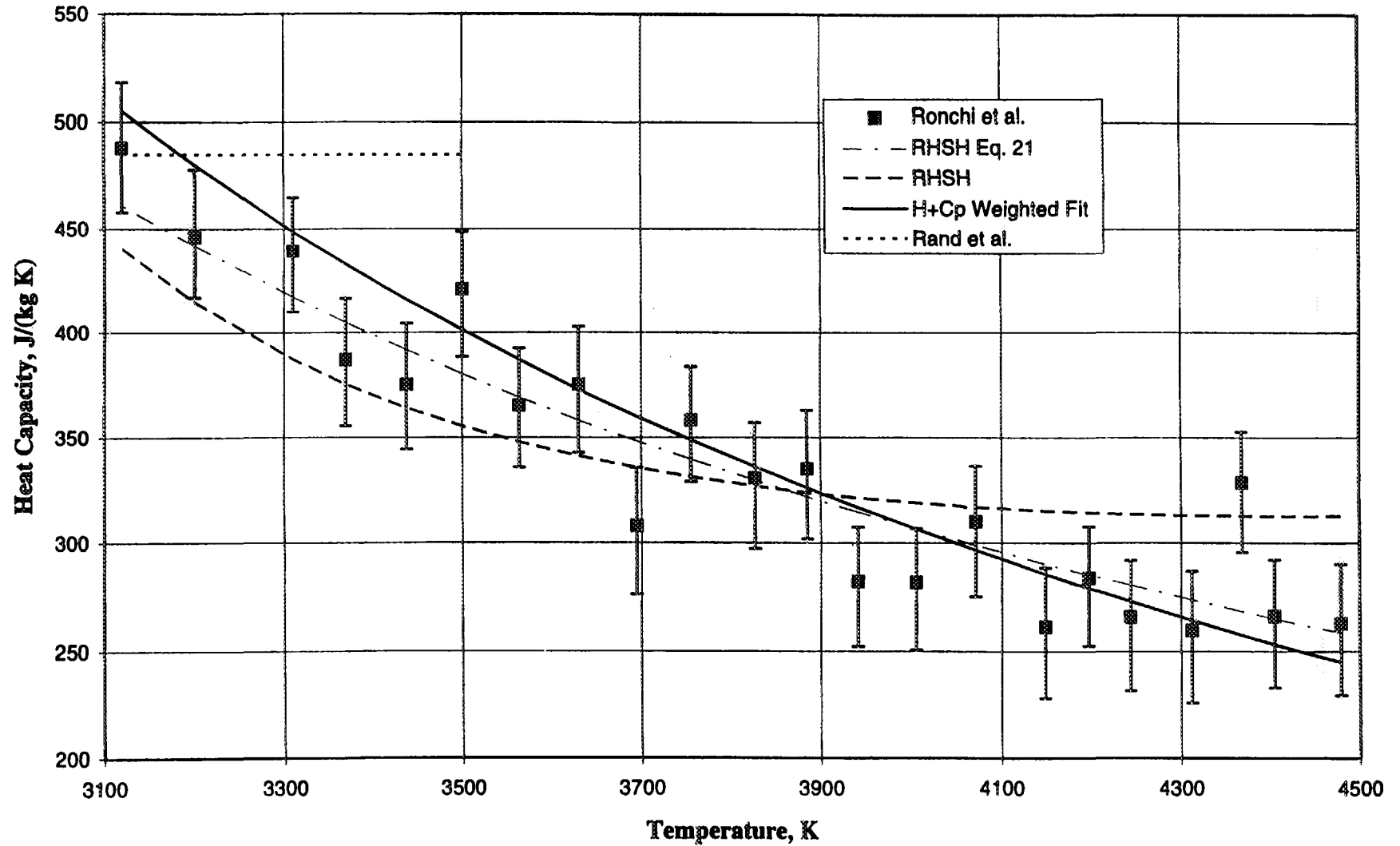


Figure 4 Liquid UO_2 Heat Capacity Measurements of Ronchi et al.

Comparison of Equations for the Enthalpy of Liquid UO_2



Liquid UO_2 Heat Capacity

Suggested Goals for IAEA CRP

- **Collect & Systematize All Data**
(Put in THERSYST Database at Stuttgart)
Solid Data Not in First CRP
e.g.: UO_2 + Fission Products
Liquid Data
- **Data Assessment**
- **Recommend Equations**
Best Equation; More than One Equation if
Fit Data Equally
- **Determine Uncertainties**
- **Peer Review of Recommendations**
- **Reach International Agreement**
Important for Conflicting Data
- **Put in INSC Database (Rev 1)**
- **Issue IAEA Technical Report**

INSC POSSIBLE CONTRIBUTIONS

- **DEPENDENT ON FUNDING & NEEDS**
- **DATA ASSESSMENTS -**
 - High Priority Properties
 - Medium Priority Properties
 - Irradiated Fuel (?)
- **PEER REVIEW OF ASSESSMENTS**
- **PUT ASSESSMENTS ON INSC DATABASE FOR WORLD ACCESS**
 - ANL Assessments
 - Link to IBRAE Assessments
 - Assessments of Others (?)
- **MEASUREMENTS/ANALYSES (???)**
 - Irradiated Fuel (?)
 - Liquid UO_2 - C_p , k (?)
 - Liquid Mixtures (UO_2 - Zr O_2 - Zr) (?)

Properties to Include in IAEA CRP

- Thermodynamic Properties (Solids & Liquids)
- Transport Properties of Solids & Liquids
(Except Electrical Conductivity)
- Irradiation Effects on Thermophysical Properties
(When Data Available)
- Mechanical Properties of Solids (???)
First CRP Limited to Thermophysical Properties
Program Limited to \approx 3 Years

Materials to Include in IAEA CRP

Fuel

UO₂ UO₂-PuO₂ UO₂-Gd₂O₃

UO₂ + Fission Product Oxides Irradiated UO₂ (where available)

Cladding

Zr Alloys: *Zr-1% Nb*, Zr-2.5% Nb, Zircaloy 2, Zircaloy 4

Oxidation of Zr Alloys

Ni-Cr Alloys: Inconel 600, Inconel X-750, Hastelloy, *Inconel 625*

Absorbers/Moderators (Same as First CRP)

Ag-In-Cd Alloy

B₄C

Structural Materials (Same as First CRP)

Austenitic Stainless Steels:

Martensitic Stainless Steels

Liquid Mixtures

Zr-Stainless Steel

UO₂-ZrO₂-Stainless Steel, UO₂-ZrO₂-Zr

UO₂-ZrO₂ UO₂-ZrO₂-Concrete

Properties of Components of Mixtures

*Methods to Determine Mixture Properties as a Function of
Composition, Solid Fraction, Temperature*