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CORRELATION OF THE THERMOPHYSICAL PROPERTIES OF URANIUM HEXAFLUORIDE OVER A WIDE RANGE OF TEMPERATURE AND PRESSURE

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MANAGED BY
MARTIN MARIETTA ENERGY SYSTEMS, INC.
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Technical Programs and Services

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ABSTRACT

Transient numerical modeling of high-temperature, high-pressure systems requires thermophysical properties correlations that are continuous and well behaved. This report documents the development of such correlations for application to the simulation of uranium hexafluoride (UF_6) cylinders engulfed in fire, and it compares estimated property values to data. With modifications, the Lee-Kesler equation of state and its related methods are recommended for estimating density, enthalpy, and heat capacity of UF_6 vapor and liquid phases. Other liquid and vapor properties correlations evaluated include vapor pressure, surface tension, viscosity, and thermal conductivity. Curve fits to available solid phase data are presented for density, enthalpy, heat capacity, and thermal conductivity. Selected derived properties are also presented. This report covers thermophysical properties of UF_6 up to reduced temperatures of 3.0 and reduced pressures of 3.0.

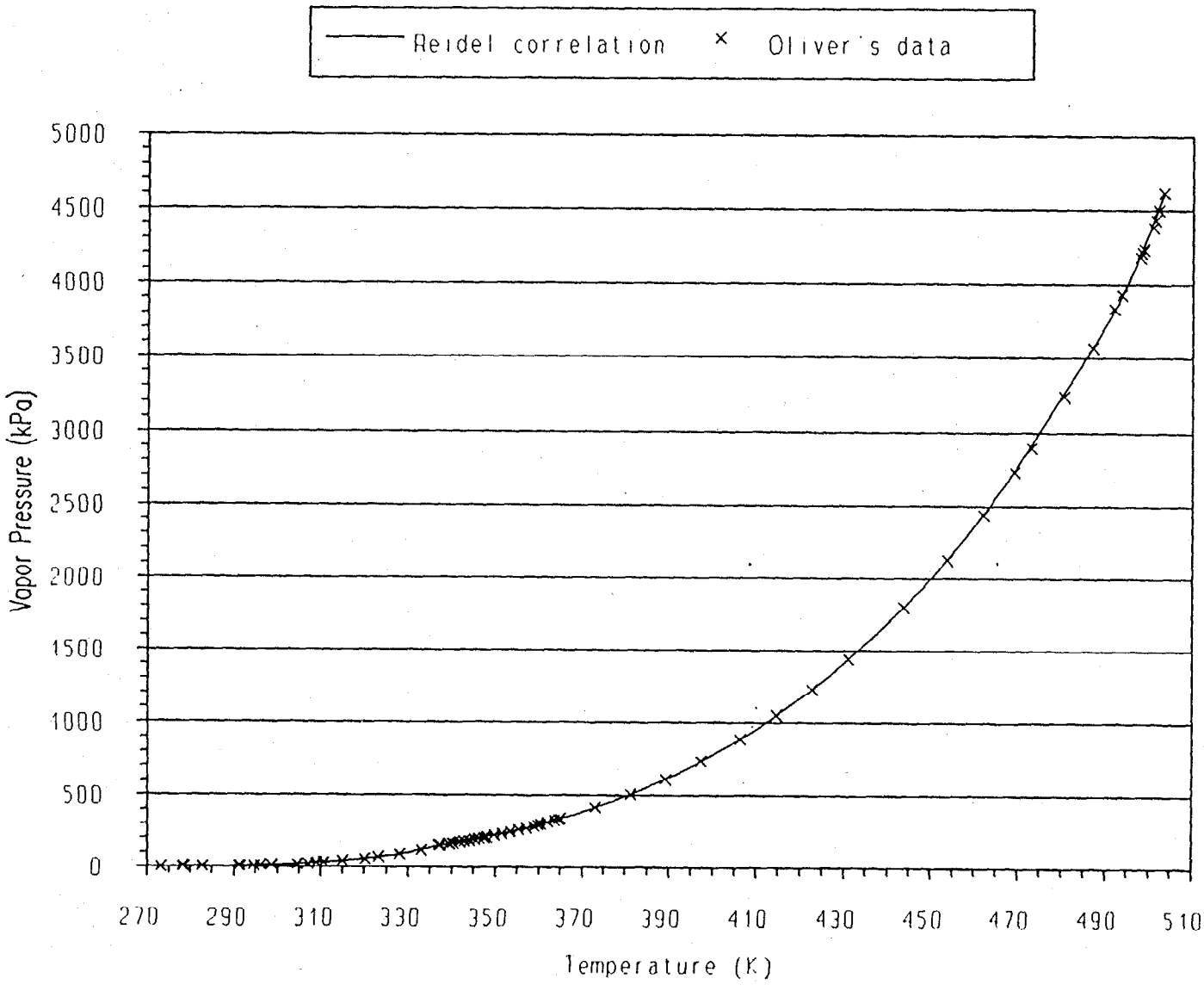

Fig. 3.1. Vapor pressure of UF_6.

1. INTRODUCTION AND SUMMARY

This report is one of several documenting the development of a transient heat transfer/stress analysis model of UF_6 cylinders engulfed in fire. Another report documenting heat transfer correlations for such models is being issued coincident with this report[13]; reports describing and benchmarking the model are future activities. Such modeling requires accurate thermophysical properties of UF_6 over a wide range of temperature and pressure: reduced temperatures ($T_r = T/T_c$) may range from 0.6 to 3.0, while reduced pressures ($P_r = P/P_c$) may range from 0.01 to 3.0. Property data for UF_6 around and beyond the critical point is practically nonexistent; therefore, correlations must be developed to predict the thermophysical properties of UF_6 over these ranges. Since the correlations will be used in numerical models, special care must be taken to ensure that the correlations are continuous over the stated ranges to avoid convergence problems. It is also important to match correlated values with the limited data available.

The primary references utilized in this effort are the prior compilation of UF_6 thermophysical property data and correlations by Dewitt[1] and the Third and Fourth Editions of *The Properties of Gases and Liquids*[8,3] which document numerous correlation methods. The earlier work of Williams[2] was also useful. These references led to the other sources subsequently identified when additional information was required to understand and apply specific correlations and methods. The correlations presented in this report have been converted to metric units; conversion factors to other common units are provided in Appendix A.

Table 1.1 provides a summary of the correlations and methods considered in the course of this modeling effort and highlights the recommended methods. The Lee-Kesler equation of state and its related methods for estimating enthalpy and heat capacity, as modified herein, are the recommended methods for obtaining density, enthalpy, and heat capacity. The primary issues addressed by the modifications were numerical difficulties for $P_R < 1.0$ when $0.95 < T_R < 1.0$ and discrepancies between Lee-Kesler estimates and data. The approaches developed to address these issues could be easily applied to obtain property sets for other substances.

Table 1.1 Summary of Correlations and Methods Considered for Estimating UF_6 Thermophysical Properties
(Recommended methods are **highlighted** by bold type.)

Property	Phase	Correlation or Method	Section	Comments
Critical Properties			2.	
Vapor Pressure		**Riedel**	3.	
Acentric Factor		Pitzer **Lee-Kesler**	4. 4.	
Equation of State/ Density	Vapor	Second Virial Coefficient Redlich-Kwong Malyshev Benedict-Webb-Rubin **Lee-Kesler**	5.1.1 5.1.2 5.1.3 5.1.4 5.1.5	

Property	Phase	Correlation or Method	Section	Comments
Equation of State/ Density	Liquid	Rackett (saturated liquid) Thompson et al. (subcooled liquid) Chueh-Prausnitz (subcooled liquid) Hoge and Wechsler (saturated liquid) Williams (saturated liquid) Lee-Kesler	5.2.1 5.2.2 5.2.2 5.2.3 5.2.3 5.2.3	 Note 1 Note 1 Note 1
	Solid	Williams	5.3	
Enthalpy	Vapor	Williams (low pressure) Yen-Alexander Lee-Kesler	6.1 6.2.1 6.2.2	 Note 2
	Liquid	Yen-Alexander Lu-Hsi-Poon Lee-Kesler	6.3.1 6.3.2 6.3.3	 Notes 2 and 3
	Solid	Kirshenbaum	6.4	
Heat Capacity	Vapor	Williams (low pressure) Lee-Kesler	7.1 7.2	 Note 2
	Liquid	Lee-Kesler	7.3	Notes 2 and 4
	Solid	Kirshenbaum	7.4	
Surface Tension	Liquid	Williams	8.	
Viscosity	Vapor	Chung et al.	9.1	
	Liquid	Orrick and Erbar Chung et al.	9.2 9.2	
Thermal Conductivity	Vapor	Chung et al. Owens and Thodos	10.1 10.3	
	Liquid	Latini Chung et al. Owens and Thodos	10.2 10.2 10.3	
	Solid	Williams	10.4	

1. Use of the Lee-Kesler equation of state for liquid density requires adjustment to match available liquid density data and a supplemental interpolation scheme to obtain reliable results for $P_R < 1.0$ when $0.95 < T_R < 1.0$.

2. Use of the Lee-Kesler method for estimating vapor and liquid enthalpies and heat capacities requires a correction coefficient to the departure function.

3. Use of the Lee-Kesler method for estimating liquid enthalpy requires a supplemental interpolation scheme to obtain reliable results for $P_R < 1.0$ when $0.95 < T_R < 1.0$.

4. Use of the Lee-Kesler method for estimating liquid heat capacity requires that the derivative of the liquid enthalpy be determined numerically for those conditions identified in Note 3.

2. CRITICAL PROPERTIES

The critical properties of uranium hexafluoride are presented in Table 2.1. DeWitt recommends a critical temperature of 503.3 K and a critical pressure of 4.610 MPa (45.5 atm).[1] The value of critical density recommended by DeWitt is 1375 kg/m^3.[1] The value of critical compressibility (0.2821) presented in Table 2.1 is calculated as

$$Z_c = \frac{P_c M_W}{\rho_c R T_c}, \tag{2.1}$$

where P_c = critical pressure,
M_W = molecular weight,
ρ_c = critical density,
R = universal gas constant,
T_c = critical temperature.

The acentric factor, ω, is assumed to have a value of 0.09215 (see Ch. 4). A value of 352.025 kg/kmol is taken as an average molecular weight for UF_6.[2] The triple point temperature and pressure values presented in Table 2.1 were recommended by DeWitt.[1]

Table 2.1. Properties and Critical Constants of Uranium Hexafluoride

Characteristic	Value
Molecular weight	352.025
Acentric factor	0.09215
Triple point temperature	337.2 K
Triple point pressure	152.0 kPa
Critical temperature	503.3 K
Critical pressure	4.610 MPa
Critical compressibility	0.2821
Critical density	1375 kg/m^3

3. VAPOR PRESSURE

The vapor pressure data of Oliver[1] were fit to the Riedel vapor pressure equation. The form of the Riedel equation is[8]

$$\ln P = A + \frac{B}{T} + C\ln T + DT^6 , \tag{3.1}$$

where P is the pressure, T is the temperature, and A, B, and C are constants.

To improve the fit, the data were fit over three ranges of temperature. The first range was from 273.15 to 337.35 K (the triple point); the second range was from 337.35 to 469.17 K; and the third range was from 469.17 K to the critical temperature (503.3 K). The point of demarcation between the second and third ranges was varied to improve the fit. The results of these fits are

Range I: $273.15\ \text{K} \leq T \leq 337.35\ \text{K}$

$$P = 2.3425\exp[28.957 - 29.022\left(\frac{273.15}{T}\right) - 7.1656\ln\left(\frac{T}{273.15}\right)$$

$$+ 6.5400\times10^{-2}\left(\frac{T}{273.15}\right)^6] , \tag{3.2}$$

Range II: $337.35\ \text{K} < T \leq 469.17\ \text{K}$

$$P = 1.5268\times10^2\exp[15.063 - 15.087\left(\frac{337.35}{T}\right) - 4.5612\ln\left(\frac{T}{337.35}\right)$$

$$+ 2.3947\times10^{-2}\left(\frac{T}{337.35}\right)^6] , \tag{3.3}$$

Range III: 469.17 K $< T \leq$ 503.3 K

$$P = 2.7303\times10^3 \exp\left[631.57 - 645.83\left(\frac{469.17}{T}\right) - 722.61\ln\left(\frac{T}{469.17}\right)\right.$$

$$\left. + 14.258\left(\frac{T}{469.17}\right)^6\right], \qquad (3.4)$$

where T = temperature (K),
P = pressure (kPa).

The maximum errors over the three ranges were 0.26, 0.14, and 0.60%, respectively. The vapor pressure of UF_6 is shown graphically in Fig. 3.1.

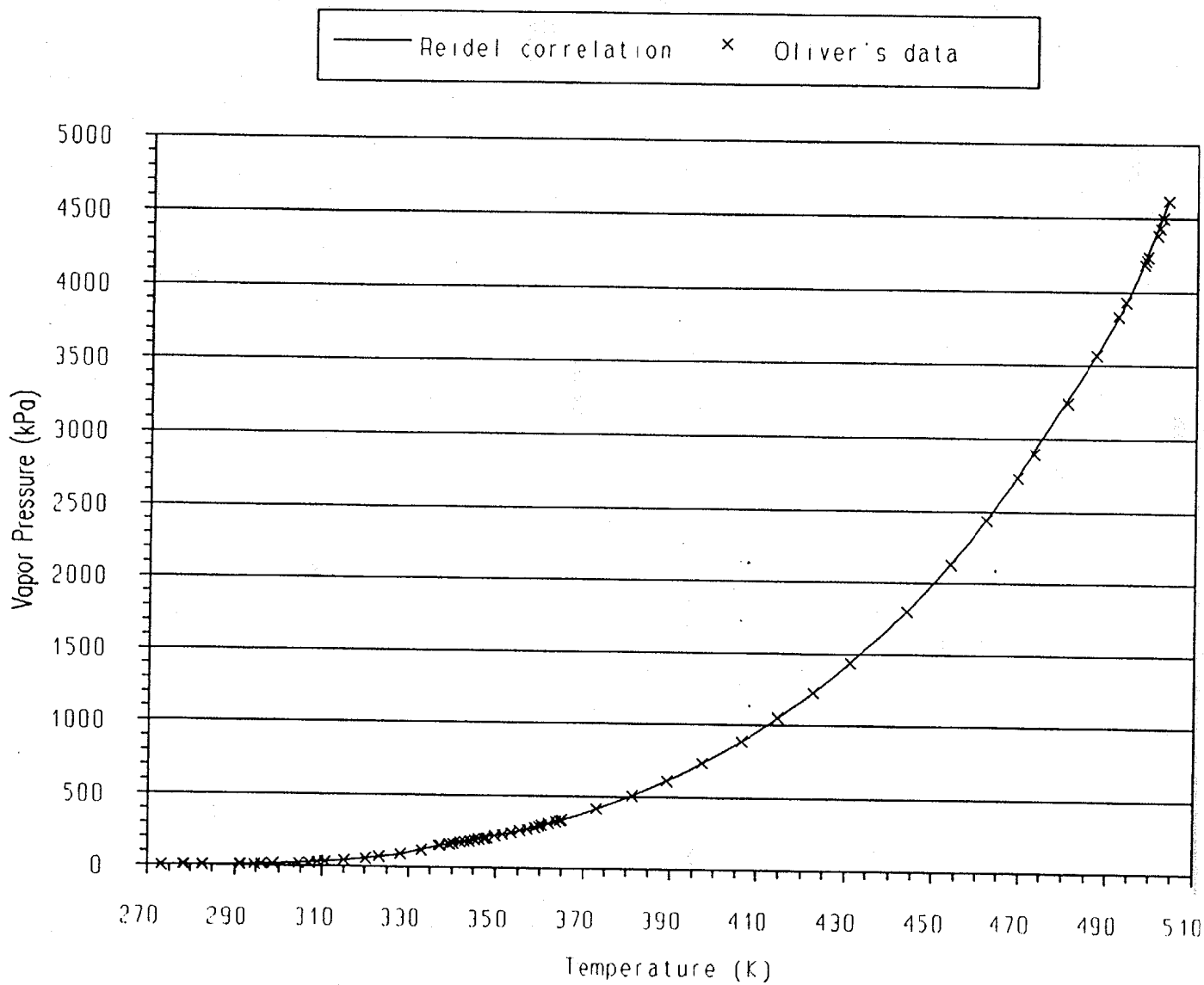

Fig. 3.1. Vapor pressure of UF_6.

4. ACENTRIC FACTOR

The Pitzer acentric factor represents the acentricity or nonsphericity of a molecule and is a pure component constant. The Pitzer acentric factor was developed by comparing the differences in the slopes of the reduced vapor pressure versus reduced temperature plots for monatomic gases versus other substances. From this comparison , the acentric factor (ω) was defined as[3]

$$\omega = -\log P_{vp}(@T_r = 0.7) - 1.0 , \tag{4.1}$$

where P_{vp} = vapor pressure,
T_r = reduced temperature.

Equation 4.1 yields an acentric factor value for UF_6 of 0.2842 . This value seems unusually high since uranium hexafluoride is a symmetrically shaped molecule with no net dipole moment. An alternative computation of the acentric factor has been found to be useful. Lee and Kesler have found that the compressibility at the critical point (Z_c) is related to the acentric factor by[4]

$$Z_c = Z_c^{(0)} + \omega Z_c^{(1)} , \tag{4.2}$$

where $Z_c^{(0)}$ and $Z_c^{(1)}$ are determined from the tables or correlations of Lee and Kesler (see Section 5.1.5).

Inserting the critical compressibility value of 0.2821 and appropriate values of $Z_c^{(0)}$ and $Z_c^{(1)}$ into Eq. 4.2, a value of 0.09215 was obtained for ω. Using this value of ω with the Lee-Kesler method for determining the compressibility of uranium hexafluoride yields values that are close to values of compressibility computed from the virial equation of state truncated to contain only the second virial coefficient, as well as the Redlich-Kwong, Benedict-Webb-Rubin, and Malyshev equations of state (see Table 5.1).

5. EQUATIONS OF STATE AND DENSITY

Several equations of state are examined and their applicability to UF_6 is determined. Correlations are also presented for calculating the density of all phases of UF_6.

5.1 EQUATIONS OF STATE

Many equations of state are available in the literature. Some are generic in nature and others are derived for specific fluids. Among the equations of state considered for UF_6 are the second virial coefficient, Redlich-Kwong, Malyshev, Benedict-Webb-Rubin, and Lee-Kesler.

5.1.1 Second Virial Coefficient Equation of State

The virial equation of state, derivable from statistical mechanics, is explicit with respect to pressure and is a polynomial series in inverse volume . It can be written as[3]

$$P = \frac{RT}{V} + B\frac{RT}{V^2} + C\frac{RT}{V^3} + \dots , \tag{5.1}$$

where P = pressure,
R = gas constant,
T = temperature,
V = specific volume.

The constants B, C, etc. are called second, third, etc. virial coefficients and for pure fluids are functions only of temperature. Aziz and Taylor have retained only the second virial coefficient and have determined B as a function of temperature using intermolecular potential functions.[5] Their results are

$$B = 1\times10^{-3}[T^{1/2}G(\ln T)\exp(1/T)] , \tag{5.2}$$

where B = second virial coefficient (m^3/kmol),
T = temperature (K).

The constant G in Eq. 5.2 is defined as

$$G = -0.101520\times10^6 + 0.613665\times10^5(\ln T) - 0.139355\times10^5(\ln T)^2$$

$$+ 0.140852\times10^4(\ln T)^3 - 0.534487\times10^2(\ln T)^4 \ . \tag{5.3}$$

If T and V are specified, P can be calculated explicitly from Eq. 5.1 and the compressibility (Z) can be computed from

$$Z = \frac{PV}{RT} \ . \tag{5.4}$$

If T and P are specified, then Eq. 5.1 can be rearranged to yield

$$Z^2 - Z - \frac{BP}{RT} = 0 \ . \tag{5.5}$$

This equation can be easily solved for Z using the quadratic formula

$$Z = 0.5 + 0.5\sqrt{1 + \frac{4BP}{RT}} \ . \tag{5.6}$$

However, BP/RT must be greater than -0.25. The equation can also be solved implicitly for Z using root seeking algorithms available on hand calculators or solver packages available on personal computers. If P and V are specified, then T must be iterated upon using Eq. 5.2 to compute B until suitable closure on Eq. 5.1 is obtained.

Table 5.1 shows that the compressibility of uranium hexafluoride calculated from the truncated virial equation agrees well with values calculated by other methods.

5.1.2 Redlich-Kwong Equation Of State

The Redlich-Kwong equation is one of the simplest equations of state. This equation is[6]

$$P = \frac{RT}{V - b} - \frac{a}{T^{1/2}V(V + b)} \ . \tag{5.7}$$

The quantities a and b can be determined by requiring that

$$\left(\frac{\partial P}{\partial V}\right)_{T = T_c} = 0 \quad \textit{and} \quad \left(\frac{\partial^2 P}{\partial V^2}\right)_{T = T_c} = 0 \,, \tag{5.8}$$

at the critical point. This yields the following results for a and b in terms of P_c and T_c:

$$a = \frac{0.4278 R^2 T_c^{2.5}}{P_c} \,, \tag{5.9}$$

$$b = \frac{0.0867 R T_c}{P_c} \,, \tag{5.10}$$

where T_c = critical temperature,
P_c = critical pressure.

If the specific volume, V, is eliminated from Eq. 5.7 using the definition of compressibility , the following equation is obtained that relates the compressibility of uranium hexafluoride with temperature and pressure:

$$Z - \frac{1}{1 - \dfrac{bP}{ZRT}} + \frac{a}{RT^{1.5}\left(\dfrac{ZRT}{P} + b\right)} = 0 \,. \tag{5.11}$$

For specified values of T and P this equation can be solved implicitly for Z.

If P and V are specified and Z is desired, then T can be eliminated using the definition of compressibility. This result is

$$Z - \frac{V}{V - b} + \frac{a Z^{1.5} R^{0.5}}{P^{1.5} V^{1.5} (V + b)} = 0 \,. \tag{5.12}$$

If T and V are specified, P can be solved explicitly from Eq. 5.7, and then Z determined directly from the definition of compressibility.

Values of compressibility of UF_6 calculated by the Redlich-Kwong equation of state are presented in Table 5.1.

Table 5.1. Compressibility of Gaseous Uranium Hexafluoride

T_r	P_r											
	0.01	0.05	0.1	0.2	0.4	0.6	0.8	1.0	1.5	2.0	2.5	3.0
0.70	0.9895	0.9457	Lee-Kesler									
	0.9876	0.9380	Second Virial Coefficient									
	0.9873	0.9397	Magnuson									
	0.9907	0.9521	Redlich-Kwong									
	-	-	Benedict-Webb-Rubin									
	-	-	Malyshev									
0.80	0.9931	0.9648	0.9274									
	0.9921	0.9607	0.9214									
	0.9915	0.9588	0.9208									
	0.9936	0.9672	0.9325									
	0.9926	0.9614	0.9201									
	0.9925	0.9615	0.9194									
0.90	0.9952	0.9759	0.9509	0.8974	0.7697							
	0.9947	0.9734	0.9469	0.8937	0.7875							
	-	-	-	-	-							
	0.9954	0.9766	0.9524	0.9009	0.7799							
	0.9950	0.9738	0.9464	0.8884	0.7524							
	0.9952	0.9758	0.9503	0.8946	0.7534							
0.95	0.9960	0.9797	0.9588	0.9150	0.8152	0.6865						
	0.9955	0.9777	0.9554	0.9109	0.8217	0.7326						
	-	-	-	-	-	-						
	0.9960	0.9800	0.9594	0.9163	0.8193	0.6972						
	0.9958	0.9780	0.9552	0.9076	0.8021	0.6755						
	0.9960	0.9797	0.9587	0.9138	0.8092	0.6668						
1.00	0.9966	0.9829	0.9653	0.9287	0.8483	0.7534	0.6299	0.2820				
	0.9962	0.9811	0.9622	0.9244	0.8587	0.7731	0.6974	0.6218				
	-	-	-	-	-	-	-	-				
	0.9966	0.9828	0.9651	0.9286	0.8489	0.7564	0.6383	0.3085				
	0.9967	0.9829	0.9653	0.9291	0.8520	0.7630	0.6252	0.2794				
	0.9966	0.9828	0.9651	0.9281	0.8459	0.7479	0.6198	0.2765				

1.05	0.9971	0.9854	0.9704	0.9396	0.8735	0.7993	0.7127	0.6046	0.3173	0.3412	0.3969	0.4527
	0.9968	0.9838	0.9676	0.9352	0.8704	0.8056	0.7408	0.6760	0.5140	0.3521	0.1901	0.2810
	-	-	-	-	-	-	-	-	-	-	-	-
	0.9970	0.9851	0.9699	0.9386	0.8720	0.7982	0.7134	0.6097	0.3489	0.3797	0.4320	0.4876
	0.9972	0.9851	0.9698	0.9387	0.8742	0.8048	0.7206	0.6203	0.3114	0.3423	0.3957	0.4523
	0.9971	0.9854	0.9704	0.9396	0.8732	0.7989	0.7137	0.6113	0.3169	0.3422	0.3957	0.4524
1.10	0.9972	0.9860	0.9719	0.9426	0.8801	0.8106	0.7308	0.6339	0.3692	0.3614	0.4105	0.4596
	0.9972	0.9860	0.9720	0.9441	0.8882	0.8322	0.7763	0.7204	0.5806	0.4408	0.3010	0.1611
	-	-	-	-	-	-	-	-	-	-	-	-
	0.9974	0.9870	0.9738	0.9469	0.8905	0.8299	0.7639	0.6908	0.4832	0.4312	0.4636	0.5099
	0.9975	0.9869	0.9736	0.9466	0.8918	0.8355	0.7745	0.7121	0.5078	0.4153	0.4374	0.4812
	0.9976	0.9877	0.9751	0.9495	0.8953	0.8368	0.7732	0.7034	0.5051	0.4125	0.4363	0.4819
1.50	0.9992	0.9957	0.9916	0.9833	0.9666	0.9502	0.9340	0.9183	0.8813	0.8494	0.8303	0.8111
	-	-	-	-	-	-	-	-	-	-	-	-
	-	-	-	-	-	-	-	-	-	-	-	-
	0.9990	0.9951	0.9903	0.9806	0.9616	0.9429	0.9247	0.9072	0.8699	0.8340	0.8106	0.7982
	-	-	-	-	-	-	-	-	-	-	-	-
	-	-	-	-	-	-	-	-	-	-	-	-
2.00	0.9998	0.9990	0.9979	0.9958	0.9921	0.9885	0.9853	0.9825	0.9768	0.9735	0.9738	0.9741
	-	-	-	-	-	-	-	-	-	-	-	-
	-	-	-	-	-	-	-	-	-	-	-	-
	0.9997	0.9984	0.9968	0.9937	0.9878	0.9822	0.9770	0.9722	0.9620	0.9546	0.9501	0.9485
	-	-	-	-	-	-	-	-	-	-	-	-
	-	-	-	-	-	-	-	-	-	-	-	-
2.50	1.0000	1.0000	1.0000	1.0001	1.0005	1.0010	1.0018	1.0027	1.0061	1.0107	1.0172	1.0236
	-	-	-	-	-	-	-	-	-	-	-	-
	-	-	-	-	-	-	-	-	-	-	-	-
	0.9999	0.9996	0.9992	0.9984	0.9970	0.9958	0.9948	0.9941	0.9931	0.9936	0.9954	0.9985
	-	-	-	-	-	-	-	-	-	-	-	-
	-	-	-	-	-	-	-	-	-	-	-	-
3.00	1.0001	1.0005	1.0009	1.0019	1.0039	1.0062	1.0085	1.0109	1 0177	1.0252	1.0339	1.0425
	-	-	-	-	-	-	-	-	-	-	-	-
	-	-	-	-	-	-	-	-	-	-	-	-
	1.0000	1.0001	1.0002	1.0004	1.0008	1.0015	1.0022	1.0031	1.0058	1.0093	1.0136	1.0186
	-	-	-	-	-	-	-	-	-	-	-	-
	-	-	-	-	-	-	-	-	-	-	-	-

5.1.3 Malyshev's Equation Of State

Malyshev formulated an equation of state of the following form[7]

$$Z = 1 + \sum_{m=1}^{5} \sum_{k=0}^{3} b_{mk}/(\tau^k \phi^m) , \tag{5.13}$$

where τ = T/504.5,
ϕ = ρ_c/ρ,
T = temperature (K),
ρ_c = critical density (see Table 2.1),
ρ = density.

Values of the coefficients b_{mk} are given in Table 5.2. It should be noted that a value of 504.5 K is assumed as the critical temperature of UF_6 in Malyshev's equation of state (Eq. 5.13). This value differs from the one used in this report. Values of UF_6 compressibility calculated from Eq. 5.13 are presented in Table 5.1 as a function of reduced temperature and pressure.

Table 5.2. Values of the Coefficients b_{mk} in Malyshev's Equation of State

m	k			
	0	1	2	3
1	18.5047	-53.7362	50.9308	-16.8987
2	-62.5084	180.0905	-169.897	52.5947
3	137.0865	-409.5977	404.1463	-131.0337
4	-104.4291	318.0347	-320.6823	106.5173
5	25.1350	-77.1556	78.6106	-26.4359

Source: Malyshev, V. V., *Experimental Study of Compressibility of Uranium Hexafluoride Over a Broad Range of Parameters of State*, Teplofizicheskie Svoistva Gazov [The Thermophysical Properties of Gases], Moscow, Nauka, 1973, pp. 142-147.

5.1.4 Benedict-Webb Rubin Equation Of State

The Benedict-Webb-Rubin equation of state, written in terms of reduced compressibility (Z_r), is

$$1 - \frac{1}{Z_c Z_r} + \frac{\alpha_1}{Z_r^2} + \frac{\alpha_2}{Z_r^3} - \frac{\alpha_3}{Z_r^6} - \frac{\alpha_4}{Z_r^3}\left[\left(1 + \frac{\alpha_5}{Z_r^2}\right)\exp\left(\frac{-\alpha_5}{Z_r^2}\right)\right] = 0 \,, \tag{5.14}$$

where

$$\alpha_1 = \frac{-D_1 P_r}{T_r} + \frac{D_2 P_r}{T_r^2} + \frac{D_3 P_r}{T_r^4} \,, \tag{5.15}$$

$$\alpha_2 = \frac{-D_4 P_r^2}{T_r^2} + \frac{D_5 P_r^2}{T_r^3} \,, \tag{5.16}$$

$$\alpha_3 = \frac{D_6 P_r^5}{T_r^6} \,, \tag{5.17}$$

$$\alpha_4 = \frac{D_7 P_r^2}{T_r^5} \,, \tag{5.18}$$

$$\alpha_5 = \frac{D_8 P_r^2}{T_r^2} \,, \tag{5.19}$$

where P_r = reduced pressure,
T_r = reduced temperature.

As seen from Eqs. 5.15 - 5.19, use of the Benedict-Webb-Rubin equation of state requires eight constants (D_1 - D_8). To solve for these eight constants, eight sets of values of reduced temperature, pressure, and compressibility are needed to yield eight equations and eight unknowns. The set of eight constants were solved for three distinct temperature-pressure regions. The regions are defined as follows:

Region I: $T_r \leq 1.0$,

Region II: $T_r > 1.0$,
$P_r \geq 1.0$,

Region III: $T_r > 1.0$,
$P_r < 1.0$.

The sets of reduced temperature, pressure, and compressibility that were used for each region are presented in Table 5.3. The compressibilities at each temperature-pressure combination were calculated using Malyshev's equation of state. At the time the Benedict-Webb-Rubin constants were calculated it was thought that Malyshev's equation of state was a correlation of actual data and best represented the compressibility of UF_6. Later, it was determined that the Lee-Kesler method was the best means of calculating the compressibility of UF_6. Table 5.4 contains the sets of constants (D_1 - D_8) for each region defined above.

Once the constants D_1 - D_8 are known, a compressibility can be calculated for any value of temperature and pressure from Eq. 5.14. Values of UF_6 compressibility calculated from the Benedict-Webb-Rubin equation of state are given in Table 5.1 as a function of reduced temperature and pressure.

5.1.5 Lee-Kesler Compressibility Method

The Lee-Kesler method computes the compressibility of the vapor phase as[4]

$$Z = Z^{(0)} + \omega Z^{(1)} . \tag{5.20}$$

The acentric factor, ω, is an indicator of the nonsphericity of a molecule's force field. $Z^{(0)}$ applies to spherical molecules, while the $Z^{(1)}$ term is a deviation function. Values of $Z^{(0)}$ and $Z^{(1)}$ have been tabulated as functions of reduced temperature and pressure.[4]

In addition to tabulated values, the density of UF_6 vapor at any temperature and pressure can be calculated using the following correlation recommended by Lee and Kesler:[4]

$$Z = \frac{P_r V_r}{T_r} = 1 + \frac{B}{V_r} + \frac{C}{V_r^2} + \frac{D}{V_r^5} + \frac{c_4}{T_r^3 V_r^2}\left(\beta + \frac{\gamma}{V_r^2}\right)\exp\left(-\frac{\gamma}{V_r^2}\right) , \tag{5.21}$$

where

$$B = b_1 - b_2/T_r - b_3/T_r^2 - b_4/T_r^3 , \tag{5.22}$$

Table 5.3. Data Used in Benedict-Webb-Rubin Equations

T_r	P_r	Z_r
Range I		
0.7929	0.1089	3.218
0.8325	0.2179	2.965
0.8722	0.3268	2.768
0.9118	0.4357	2.624
0.9514	0.3268	3.018
0.9911	0.2179	3.257
0.9911	0.6536	2.496
1.0	1.0	1.0
Range II		
1.031	1.0893	1.701
1.0704	1.7429	1.262
1.1100	2.3965	1.563
1.1497	3.0501	1.881
1.0109	2.8322	1.483
1.0505	2.3965	1.364
1.0902	1.5251	1.640
1.1298	1.0893	2.537
Range III		
1.0109	0.3268	3.129
1.0307	0.8715	2.280
1.0505	0.4357	3.052
1.0704	0.7625	2.678
1.0902	0.5447	3.005
1.1100	0.6536	2.935
1.1298	0.3268	3.279
1.1497	0.8715	2.835

Table 5.4. Benedict-Webb-Rubin Constants

B-W-R Constants	Range I $T_r < 1.0$ $P_r < 1.0$	Range II $T_r > 1.0$ $P_r > 1.0$	Range III $T_r > 1.0$ $P_r < 1.0$
D_1	1.4148	2.0440	0.9582
D_2	4.1467	3.9863	4.1467
D_3	1.9513	2.3067	1.1221
D_4	2.2682	1.3548	6.8657
D_5	1.0875	1.5783	5.9842
D_6	-0.0174	0.1438	5.7443
D_7	1.8487	1.8649	1.7940
D_8	1.5734	0.4936	17.8076

$$C = c_1 - c_2/T_r + c_3/T_r^3 , \tag{5.23}$$

$$D = d_1 + d_2/T_r . \tag{5.24}$$

Values of the constants b_1, b_2, b_3, b_4, c_1, c_2, c_3, d_1, and d_2 are presented in Table 5.5.

To calculate the density at a given temperature and pressure, the following procedure should be used.

1. Using the simple fluid constants in Table 5.5, solve Eq. 5.21 for $V_r^{(0)}$ at the reduced temperature and pressure of interest. It should be noted that since Eq. 5.21 is implicit with respect to V_r, an iterative solution technique is required (see Appendix B for solution hints).

2. Calculate $Z^{(0)}$, the simple fluid compressibility as

$$Z^{(0)} = \frac{P_r V_r^{(0)}}{T_r} . \tag{5.25}$$

Table 5.5. Values of Constants Used in Lee-Kesler Correlations

Constant	Simple fluids	Reference fluids
b_1	0.1181193	0.2026579
b_2	0.265728	0.331511
b_3	0.154790	0.027655
b_4	0.030323	0.203488
c_1	0.0236744	0.0313385
c_2	0.0186984	0.0503618
c_3	0.0	0.016901
c_4	0.042724	0.041577
$d_1 \times 10^4$	0.155488	0.48736
$d_2 \times 10^4$	0.623689	0.0740336
β	0.65392	1.226
γ	0.060167	0.03754

Source: Lee, B. I., and Kesler, M. G., *A Generalized Thermodynamic Correlation Based on Three-Parameter Corresponding States*, AIChE Journal, Vol. 21, No. 3, May 1975, pp. 510-527.

3. Calculate $V_r^{(l)}$ from Eq. 5.21 using the reference fluid constants in Table 5.5 and the same T_r and P_r values as in Step 1.

4. Calculate $Z^{(r)}$ as

$$Z^{(r)} = \frac{P_r V_r^{(r)}}{T_r} . \tag{5.26}$$

5. Calculate the compressibility at the temperature and pressure of interest as

$$Z = Z^{(0)} + \frac{\omega}{\omega^{(r)}} [Z^{(r)} - Z^{(0)}] , \tag{5.27}$$

where $\omega^{(r)} = 0.3978$.[4]

Tabulated values of $Z^{(l)}$ discussed previously in this section are defined as

$$Z^{(1)} = \frac{Z^{(r)} - Z^{(0)}}{\omega^{(r)}} . \tag{5.28}$$

Values of UF_6 compressibility calculated by the Lee-Kesler method are presented in Table 5.1 as a function of temperature and pressure. Some hints on solving the Lee Kesler compressibility equation (Eq. 5.21) are presented in Appendix B. Amphlett, Mullinger, and Thomas measured the density of UF_6 vapor at 322.4 K and various pressures.[1] This data is presented in Fig. 5.1 along with the values predicted by the Lee-Kesler method.

5.2 LIQUID DENSITY

The density of UF_6 liquid can be determined by several different methods. First, a method is presented for calculating the specific volume (density) of saturated liquid. Next, the Thompson et al. method, which applies a correction factor to the saturated liquid density, and the Chueh and Prausnitz methods are discussed. The Lee-Kesler method, discussed in Section 5.1.5 for the vapor phase, can also be used, with slight modification, to predict liquid densities.

5.2.1 Rackett Equation for the Estimation of Specific Volume of Saturated Liquids

The Rackett equation for the estimation of specific volumes of liquids at saturation is[3]

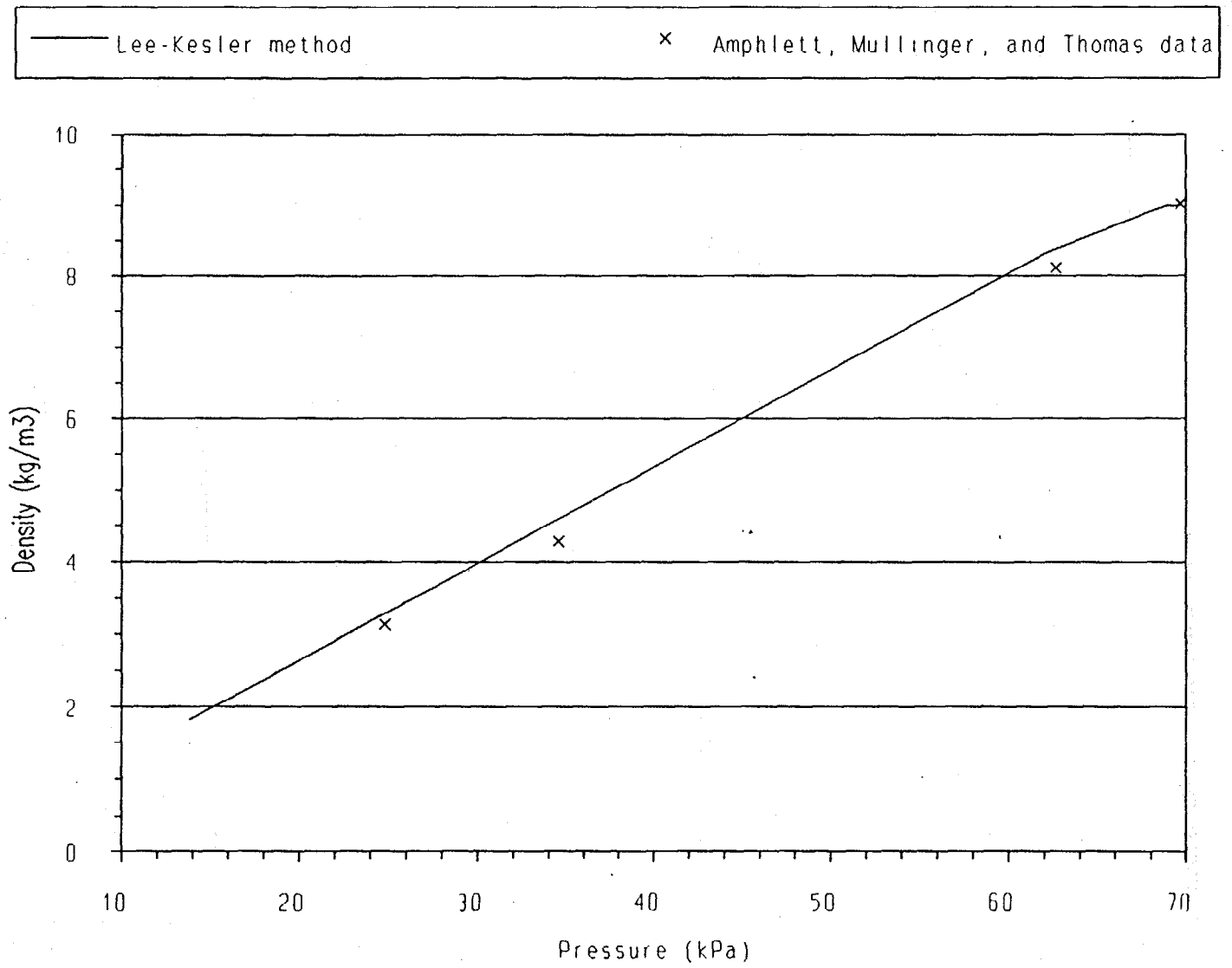

Fig. 5.1. Density of UF_6 vapor predicted by the Lee-Kesler method (T = 322.4 K).

$$V_s = V_s^R Z_c^{\epsilon} , \tag{5.29}$$

where V_s^R = specific volume at saturation at the reference temperature,
Z_c = compressibility at the critical point,

and ϵ is defined as

$$\epsilon = (1 - T_r)^{2/7} - (1 - T_r^R)^{2/7} . \tag{5.30}$$

To ensure a good fit near the critical point, the Rackett equation can be written with the critical point as the reference point. This result is

$$V_s = V_c Z_c^{\epsilon} , \tag{5.31}$$

with

$$\epsilon = (1 - T_r)^{2/7} . \tag{5.32}$$

If good agreement with data is not achieved over the entire range of temperature of interest, the Rackett equation may be written for multiple temperature ranges using reference points other than the critical point.

5.2.2 Estimation of Specific Volume in the Subcooled Region

Thompson et al. have developed a method for estimating the specific volume of subcooled liquids by applying a pressure correction factor to the specific volume of the saturated liquid at the desired temperature.[3] Their pressure correction factor depends upon the acentric factor, the reduced temperature, the critical pressure, and the vapor pressure. Their correlation is

$$V = V_s \left[1 - c \ln\left(\frac{\beta + P}{\beta + P_{vp}} \right) \right] , \tag{5.33}$$

where

$$\beta = P_c [182.4422163(1 - T_r)^{4/3} - 1 - 9.07217(1 - T_r)^{1/3} + 62.45326(1 - T_r)^{2/3}$$

$$- 135.1102(1 - T_r)] , \tag{5.34}$$

and c = a constant,
P = total pressure,
P_{vp} = vapor pressure.

This equation is limited to a maximum value of reduced temperature of approximately 0.95. For values of T_r greater than 0.95 and high pressures and low temperatures, the logarithmic term can become negative.

For reduced temperatures between 0.95 and 1.0, the method of Chueh and Prausnitz may be used.[8] Their equation for estimating the specific volume of subcooled liquids is

$$V = \frac{V_s}{\left[1 + \frac{9Z_c N(P - P_{vp})}{P_c}\right]^{1/9}}, \tag{5.35}$$

where N is a quantity defined by

$$N = (1.0 - 0.89\omega)\exp[6.9547 - 76.2853T_r + 191.3060T_r^2 - 203.5472T_r^3 + 82.7631T_r^4] . \tag{5.36}$$

The value of the constant c in Eq. 5.33 can be determined by setting Eqs. 5.33 and 5.35, evaluated at T_r = 0.95, equal to one another. This results in the following correlation for c:

$$c = \frac{\left[1 + \frac{9Z_c N_{T_r = 0.95}(P - P_{vp,T_r = 0.95})}{P_c}\right]^{1/9} - 1}{\left[1 + \frac{9Z_c N_{T_r = 0.95}(P - P_{vp,T_r = 0.95})}{P_c}\right]^{1/9} \ln\left(\frac{\beta + P}{\beta + P_{vp,T_r = 0.95}}\right)} . \tag{5.37}$$

Defining c in this way forces the two methods to be equal at the switch point resulting in a continuous curve for liquid density. The equations in this section can be used with any consistent set of units.

The density of UF_6 liquid predicted by the Thompson et al. and Chueh-Prausnitz methods is shown graphically in Fig. 5.2 along with the available liquid density data. Since it is unclear at what pressure the density data were taken, values were calculated at both saturation and high pressure (P_r = 3.0) using the Thompson/Chueh-Prausnitz method and are shown in Fig. 5.2. The upper curve represents the high pressure state and the lower curve represents the saturated state.

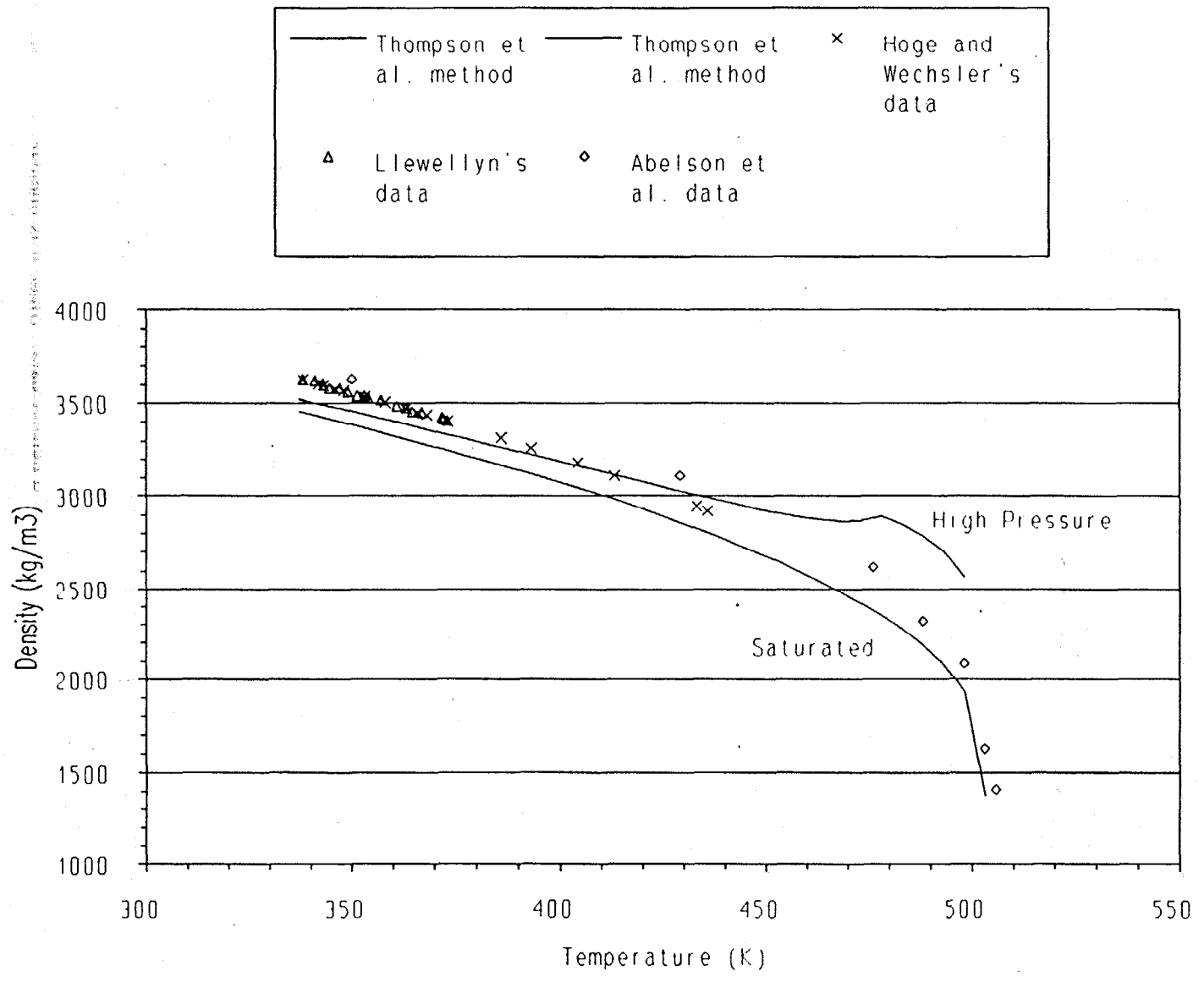

Fig. 5.2. Density of UF_6 liquid predicted by Thompson and Chueh-Prausnitz methods.

5.2.3 Lee-Kesler Compressibility Method

The Lee-Kesler compressibility method described in Section 5.1.5 can also be used to determine the density of UF_6 liquid. If tabulated values are used, care should be taken since the saturated lines in the tables prepared by Lee and Kesler do not necessarily correspond to those of UF_6. If the correlation is used, Appendix B should be referred to for solution hints. Upon close investigation of the Lee-Kesler compressibility correlation, it was discovered that reliable liquid compressibility values could not be obtained for reduced temperatures between 0.95 and 1.0. Therefore, an interpolation scheme was developed to calculate liquid densities at reduced temperatures ranging from 0.95 to 1.0. Basically, the density is determined at five known points (ρ_A, ρ_B, ρ_C, ρ_D, and ρ_E) and the density of interest (ρ_F) is calculated as

$$\rho_F = \rho_A + (\rho_B - \rho_A)\left(\frac{\rho_D - \rho_C}{\rho_E - \rho_C}\right), \tag{5.38}$$

where
ρ_A = saturated liquid density at T_r and $P_{r,sat}$,
ρ_B = liquid density at T_r and P_r = 1.0,
ρ_C = liquid density at T_r = 0.95 and $P_{r,sat}$,
ρ_D = liquid density at T_r = 0.95 and P_r,
ρ_E = liquid density at T_r = 0.95 and P_r = 1.0.

The interpolation scheme used for liquid density is illustrated in Fig. 5.3. The saturated liquid density of UF_6 (ρ_A) is determined from the following correlation:

$$\rho_A = 1375 + 244.8(T_c - T)^{1/2} - 9.045(T_c - T), \tag{5.39}$$

where
ρ_A = saturated liquid density (kg/m^3),
T_c = critical temperature (K),
T = temperature (K).

Eq. 5.39 is a curvefit of three saturated UF_6 liquid densities (T_r = 0.948, T_r = 0.95, and T_r = 1.0) predicted by the Lee-Kesler method.

The density of saturated UF_6 liquid predicted by the Lee-Kesler method as described above was compared with the available liquid density data. The liquid densities predicted by the Lee-Kesler method were consistently lower than the data. The saturated liquid density data can be represented by the following correlations:

$337.2 \leq T \leq 423.6$ K :

$$\rho_l = 4042 + 3.373T - 1.360\times10^{-2}T^2, \tag{5.40}$$

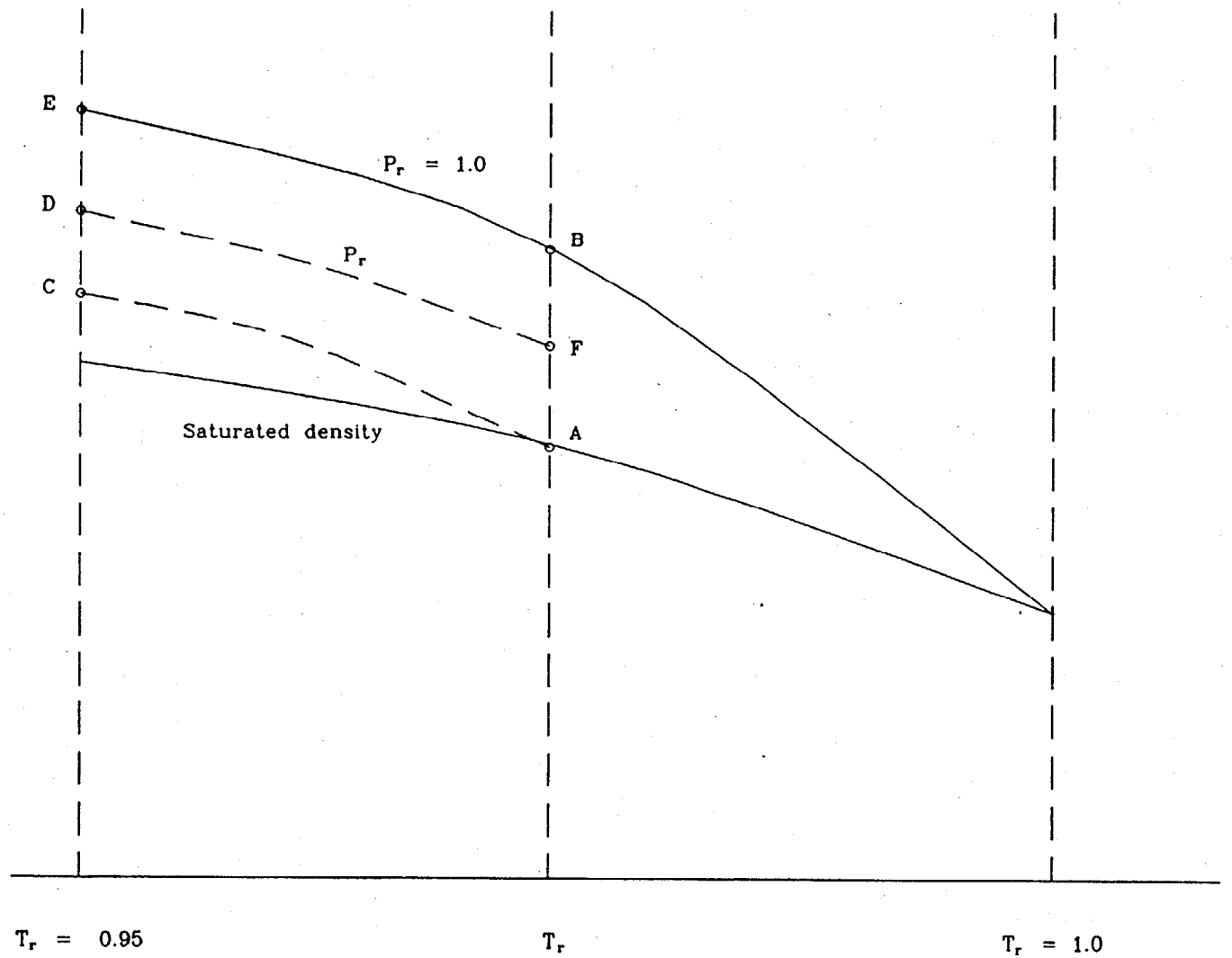

Fig. 5.3. Schematic representation of density interpolation scheme.

T > 423.6 K :

$$\rho_l = 1375 + 224.6(T_c - T)^{1/2} - 4.426(T_c - T) , \tag{5.41}$$

where T = temperature (K),
T_c = critical temperature (K).

Equation 5.40 is modified from the correlation of Hoge and Wechsler[1] and is the result of unit conversion of a similar correlation presented by Williams.[2] Since Eq. 5.40 is not applicable at temperatures approaching the critical temperature, Eq. 5.41 was formulated to calculate liquid densities in this higher temperature range.

In order for the saturated density predicted by Lee-Kesler to match the data, the following density difference is calculated

$$\Delta\rho = \rho_{l,sat} - \rho_{l,L\text{-}K,sat} , \tag{5.42}$$

where $\rho_{l,sat}$ = saturated liquid density predicted by Eqs. 5.40 and 5.41,
$\rho_{l,L\text{-}K,sat}$ = saturated liquid density (i.e., at T and P_{sat}) predicted by the Lee-Kesler correlation.

Therefore, the density at the temperature and pressure of interest is calculated as

$$\rho_{l,L\text{-}K,adj} = \rho_{l,L\text{-}K} + \Delta\rho , \tag{5.43}$$

where $\rho_{l,L\text{-}K}$ = the density at the temperature and pressure of interest calculated by the Lee-Kesler correlation.

The density of saturated liquid UF_6 predicted by the Lee-Kesler method with the suggested modification discussed above is shown in Fig. 5.4 as a function of temperature along with the available liquid density data. It should be noted that Fig. 5.4 is basically a plot of Eqs. 5.40 and 5.41.

5.3 SOLID DENSITY

DeWitt has surveyed the literature and has reported that the relation between density of solid UF_6 and temperature is linear.[1] Three data points corresponding to temperatures of 20.7, 25.0, and 62.5°C were listed. Williams fit these data to a correlation, which after unit conversion becomes[2]

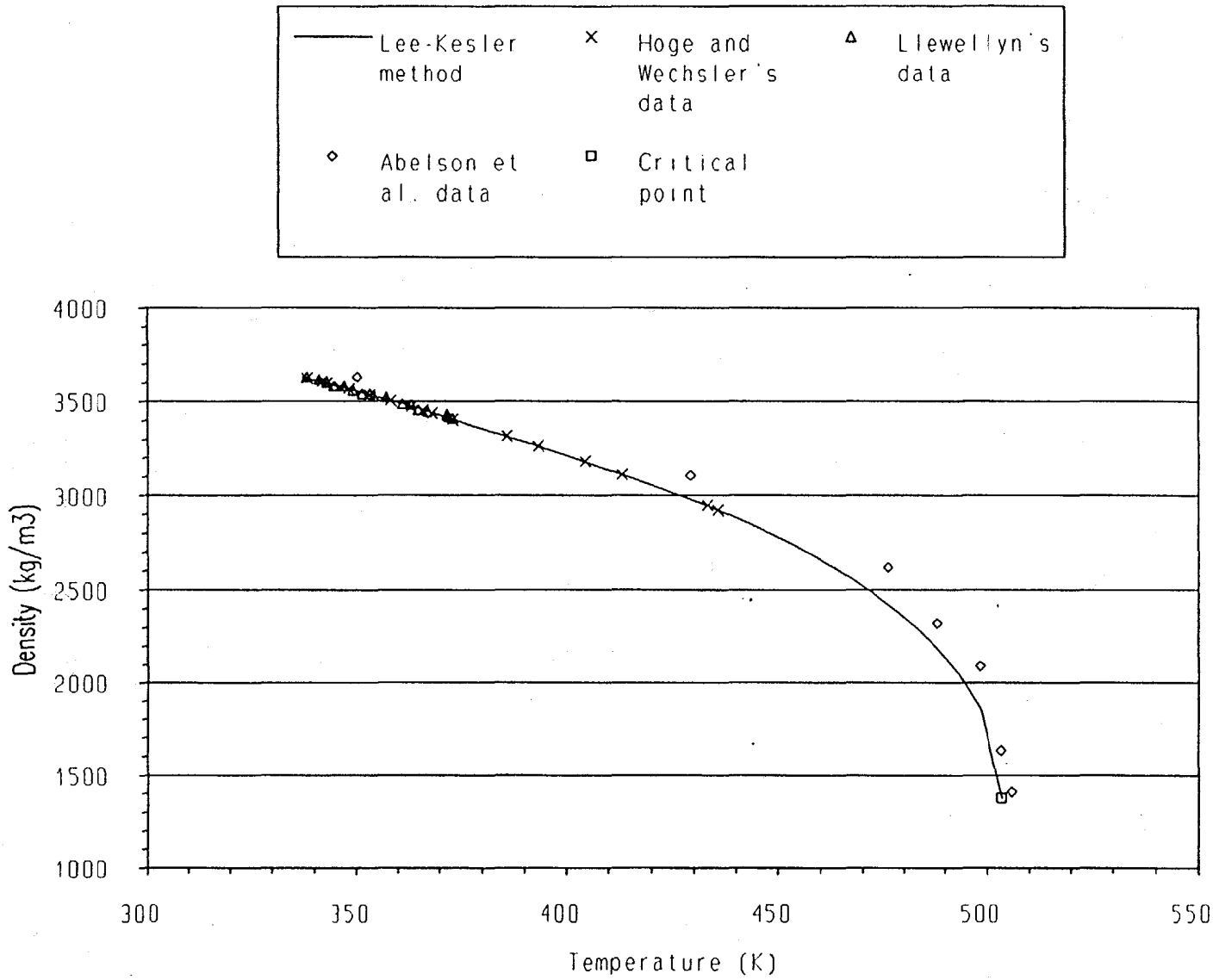

Fig. 5.4. Density of saturated UF_6 liquid.

$$\rho = 6611 - 5.190T, \tag{5.44}$$

where ρ = density (kg/m^3),
T = temperature (K).

The density of solid UF_6 predicted by Eq. 5.44 is shown graphically in Fig. 5.5 along with the available solid density data.

5.4 DENSITY RECOMMENDATIONS

The Lee-Kesler correlation (Eq. 5.21) should be used to calculate the compressibility, and hence density, of both the vapor and liquid phases of UF_6. The calculation of UF_6 liquid density requires the modifications outlined in Section 5.2.3. The density of solid UF_6 can be determined by Eq. 5.44, a curvefit of available solid density data. The density of UF_6 calculated by the recommended methods is shown graphically in Fig. 5.6 as a function of temperature and pressure.

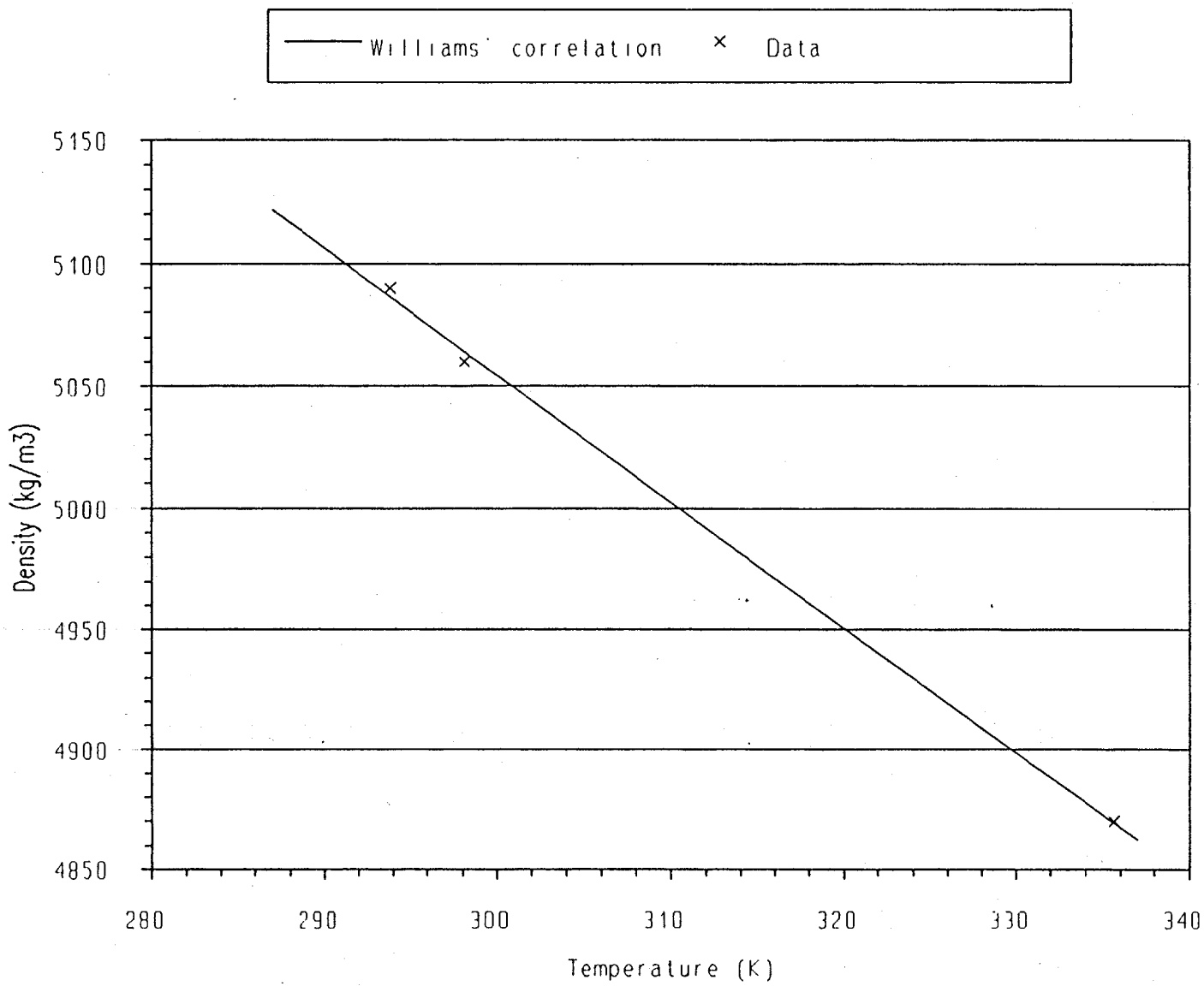

Fig. 5.5. Density of UF_6 solid.

6. ENTHALPY

A comprehensive set of correlations for predicting enthalpies of all phases of UF_6 is presented in this chapter. Where appropriate, multiple methods are discussed and recommendations are made based on the applicability to UF_6.

6.1 LOW PRESSURE ENTHALPY OF VAPOR

The low-pressure enthalpy of UF_6 vapor is determined by

$$H^o = H^o_{ic} + aT + \frac{bT^2}{2} + \frac{cT^3}{3} + \frac{dT^{1.5}}{1.5} + e\ln T + f(T\ln T - T) + g\left[T\arctan\frac{T}{h} - \frac{h}{2}\ln\left(1 + \frac{T^2}{h^2}\right)\right], \tag{6.1}$$

where H^o = low-pressure vapor enthalpy (kJ/kg),
T = temperature (K),
H^o_{ic} = constant of integration (kJ/kg).

Values of the coefficients *a-h* as well as a value of the integration constant are given in Table 6.1. Eq. 6.1 was obtained by integrating the low-pressure heat capacity expression whose derivation is discussed in Chapter 7. The value of the integration constant, H^o_{ic}, is determined by

$$H^o_{ic} = H_{v,ref} - (CF)(H - H^o)_{L\text{-}K,ref} - (H^o - H^o_{ic})_{ref}, \tag{6.2}$$

where $H_{v,ref}$ = saturated enthalpy of UF_6 vapor at the triple point (kJ/kg),
CF = correction factor for Lee-Kesler discussed in Section 6.2.2,
$(H - H^o)_{L\text{-}K,ref}$ = enthalpy departure at the triple point predicted by the Lee-Kesler method (kJ/kg),
$(H^o - H^o_{ic})_{ref}$ = $(H^o - H^o_{ic})$ evaluated at the triple point determined by Eq. 6.1 (kJ/kg).

The value of $H_{v,ref}$ is calculated as

$$H_{v,ref} = 0.5[(\Delta H_{s,ref} + H_{s,ref}) + (\Delta H_{v,ref} + H_{l,ref})], \tag{6.3}$$

where $\Delta H_{s,ref}$ = heat of sublimation at the triple point measured by Masi (135.9 kJ/kg),
$H_{s,ref}$ = enthalpy of UF_6 solid at the triple point calculated by Eq. 6.23 (kJ/kg),
$\Delta H_{v,ref}$ = heat of vaporization at the triple point measured by Masi (81.58 kJ/kg),
$H_{l,ref}$ = enthalpy of UF_6 liquid at the triple point calculated by Lee-Kesler method (kJ/kg).

Table 6.1. Values of the Coefficients in the Low-Pressure Vapor Enthalpy Correlation

Constant	Value
a	1.7043E+06
b	-170.5
c	3.90E-03
d	2.9511E+04
e	-1.6430E+07
f	-4.0663E+05
g	5.736E+05
h	189.1
H_{ic}^{o}	186.2

No experimental data on the low pressure enthalpy of UF_6 vapor could be located in the literature.

6.2 HIGH PRESSURE ENTHALPY OF VAPOR

The enthalpy of high pressure vapor can be determined by several different methods. Among those considered for UF_6 are the Yen-Alexander and Lee-Kesler methods.

6.2.1 Yen-Alexander Method

Yen and Alexander have obtained generalized relations for enthalpy departure of vapors.[8] They recommend the following correlation for enthalpy departure of a superheated vapor

$$\frac{H^o - H}{T_c} = \frac{mP_r\left(1 - \frac{P_r}{X_o}\right)}{\exp[-C_1P_r^2]Y + C_4 + C_5P_r + C_6P_r^2}, \tag{6.4}$$

$$Y = 1 - C_2 - C_4 - C_5P_r + C_2\left[\frac{1}{\pi}\arctan(C_3 - C_3P_r) + 0.5\right]^2, \tag{6.5}$$

where P_r = reduced pressure.

The variables C_1, C_2, C_3, C_4, C_5, C_6, X_o, and m are dependent on the values of reduced temperature and critical compressibility (Z_c). Correlations for calculating these variables are presented in reference 8 for discrete values of Z_c = 0.23, 0.25, 0.27, and 0.29. Interpolation is required if Z_c lies between these values; however extrapolation to Z_c values less than 0.23 or greater than 0.29 is not recommended.[8] Yen and Alexander recommend the following correlation for saturated vapor

$$\frac{H^o - H}{T_c} = \frac{D_1 P_r^{D_2}}{1 + D_3(-\ln P_r)^{D_4}} , \tag{6.6}$$

where D_1, D_2, D_3, and D_4 are dependent on the value of Z_c (see Reference 8). It should be noted that the Yen-Alexander correlations have several discontinuities at various values of reduced temperatures, which could lead to numerical difficulties. For this reason, the Yen-Alexander method will not be considered further.

6.2.2 Lee-Kesler Method

The enthalpy of high-pressure UF_6 vapor can also be determined using the method of Lee-Kesler.[4] The following equation for enthalpy departure is used

$$\frac{H - H^o}{RT_c} = -T_r\left(Z - 1 - \frac{b_2 + 2b_3/T_r + 3b_4/T_r^2}{T_r V_r} - \frac{c_2 - 3c_3/T_r^2}{2T_r V_r^2} + \frac{d_2}{5T_r V_r^5} + 3E\right) , \tag{6.7}$$

where
H = high-pressure enthalpy,
R = gas constant,
T_c = critical temperature,
T_r = reduced temperature,
Z = compressibility,
V_r = reduced volume.

The variable E is calculated as

$$E = \frac{c_4}{2T_r^3\gamma}\left[\beta + 1 - \left(\beta + 1 + \frac{\gamma}{V_r^2}\right)\exp\left(\frac{-\gamma}{V_r^2}\right)\right], \tag{6.8}$$

where values of the constants b_2, b_3, b_4, c_2, c_3, c_4, β, and γ are given in Table 5.5.

To calculate the enthalpy departure at a given temperature and pressure, the following procedure should be followed.

1. Determine $Z^{(0)}$ and $Z^{(1)}$ for the simple fluid as described in Section 5.1.5 at the reduced temperature and pressure of interest. Using Eq. 6.7 and the simple fluid constants in Table 5.5, calculate $[(H - H^o)/RT_c]^{(0)}$. In this calculation, Z is $Z^{(0)}$ and V_r is $V_r^{(0)}$ determined as

$$V_r^{(0)} = \frac{T_r Z^{(0)}}{P_r}. \tag{6.9}$$

2. Repeat step 1, using the same T_r and P_r, but this time using the reference fluid constants from Table 5.5. Using Eq. 6.7, calculate a value of $[(H - H^o)/RT_c]^{(r)}$. In this calculation, Z is $Z^{(r)}$ given by

$$Z^{(r)} = \omega^{(r)}Z^{(1)} + Z^{(0)}, \tag{6.10}$$

where $Z^{(0)}$ and $Z^{(1)}$ are calculated from the Lee-Kesler correlation as described in Section 5.1.5 and $\omega^{(r)} = 0.3978$. V_r in this calculation is $V_r^{(r)}$ given by

$$V_r^{(r)} = \frac{T_r Z^{(r)}}{P_r}. \tag{6.11}$$

3. The enthalpy departure function at the T_r and P_r of interest is determined from

$$\frac{(H - H^o)}{RT_c} = \left[\frac{(H - H^o)}{RT_c}\right]^{(0)} + \frac{\omega}{\omega^{(r)}}\left(\left[\frac{(H - H^o)}{RT_c}\right]^{(r)} - \left[\frac{(H - H^o)}{RT_c}\right]^{(0)}\right). \tag{6.12}$$

Masi has tabulated several values of the heat of vaporization of UF_6.[1] The Lee-Kesler method was used to calculate the heat of vaporization at the same temperatures as Masi's data. These data are presented in Table 6.2. The ratio of Masi's data to values predicted by the Lee-Kesler method were calculated and an average ratio of 1.20650 was obtained. Therefore, the enthalpy of UF_6 vapor can be calculated as

$$H = H^{o} + 1.20650(H - H^{o})_{L\text{-}K} \,. \tag{6.13}$$

Use of the above equation forces the heat of vaporization values calculated by the Lee-Kesler method to agree with Masi's data.

Table 6.2. Heat of Vaporization Values

Temperature (K)	ΔH_v (kJ/kg)		$\Delta H_{v,M}/\Delta H_{v,L\text{-}K}$
	Masi ($\Delta H_{v,M}$)*	Lee-Kesler ($\Delta H_{v,L\text{-}K}$)	
337.21	81.58	67.68	1.205371
340	81.08	67.29	1.204844
350	79.34	65.88	1.204223
360	77.70	64.41	1.206321
370	76.16	62.86	1.211719
			1.20650 (Avg.)

* DeWitt, R., *Uranium Hexafluoride: A Survey of the Physico-Chemical Properties*, GAT-280, Goodyear Atomic Corporation, Portsmouth, OH, 1960.

6.3 ENTHALPY OF LIQUID

Several methods are available for predicting liquid enthalpies. Among those considered for UF_6 are the Yen-Alexander, Lu-Hsi-Poon, and Lee-Kesler methods.

6.3.1 Yen-Alexander Method

Yen and Alexander have obtained generalized relations for enthalpy departure of liquids.[8] They recommend the following correlation for enthalpy departure of a subcooled liquid

$$\frac{H^o - H}{T_c} = F_1(P_r + F_2) + F_3(T_r + F_4) + F_5(T_r + F_6)^2 + F_7(P_r + F_8)(T_r + F_9)$$

$$+ F_{10}\ln P_r + F_{11}(\ln P_r)(\ln T_r) + F_{12}(\ln P_r)(\ln T_r)^2 + F_{13} , \qquad (6.14)$$

where F_1 - F_{13} are dependent on the value of critical compressibility (Z_c). Values of these constants are presented in reference 8 for discrete values of Z_c = 0.23, 0.25, 0.27, and 0.29. Interpolation is required if Z_c lies between these values; however extrapolation to Z_c values less than 0.23 or greater than 0.29 is not recommended.[8] Yen and Alexander recommend the following correlation for saturated liquid

$$\frac{H^o - H}{T_c} = \frac{G_1 + G_2(-\ln P_r)^{G_3}}{1 + G_4(\ln P_r)} , \qquad (6.15)$$

where G_1 - G_4 are dependent on the value of Z_c (see Reference 8). The Yen-Alexander method was not investigated in detail since the correlations contain several discontinuities at various values of reduced temperature, which could lead to numerical difficulties.

6.3.2 Lu-Hsi-Poon Method

The enthalpy of liquid UF_6 can be calculated using the following correlation recommended by Lu, Hsi, and Poon:[9]

$$\frac{H^o - H}{RT_c} = \left[\frac{H^o - H}{RT_c}\right]^{(0)} + \omega\left[\frac{H^o - H}{RT_c}\right]^{(1)} , \qquad (6.16)$$

where

$$\left[\frac{H^o - H}{RT_c}\right]^{(0)} = A_0 + A_1P_r + A_2P_r^2 , \qquad (6.17)$$

and

$$\left[\frac{H^o - H}{RT_c}\right]^{(1)} = B_0 + B_1P_r + B_2P_r^2 . \qquad (6.18)$$

The coefficients A_0, A_1, A_2, B_0, B_1, and B_2 are functions of reduced temperature and are defined as

$$A_i = A_{i0} + A_{i1}T_r + A_{i2}T_r^2 , \tag{6.19}$$

and

$$B_i = B_{i0} + B_{i1}T_r + B_{i2}T_r^2 . \tag{6.20}$$

Values of the coefficients A_{ij} and B_{ij} are given in Table 6.3. The enthalpy of the ideal gas, H^o, is calculated from Eq. 6.1.

Lu, Hsi and Poon recommend that the method described above be used for reduced temperatures less than 0.8.[9] The enthalpy of liquid UF_6 predicted by the Lu-Hsi-Poon method is shown graphically in Fig. 6.1 along with the available liquid enthalpy data. Enthalpies predicted by the Lu-Hsi-Poon method were calculated at the saturated state.

Table 6.3. Lu-Hsi-Poon Coefficients

A_{ij}			
	j = 0	j = 1	j = 2
i = 0	5.742533	0.743206	-3.003445
i = 1	0.075271	-0.500988	0.443336
i = 2	-0.017460	0.054554	-0.045077
B_{ij}			
	j = 0	j = 1	j = 2
i = 0	17.334961	-18.851639	5.325703
i = 1	0.092967	-0.244039	0.158373
i = 2	0.004468	0.001513	-0.002061

Source: Lu, B. C.-Y., Hsi, C., and Poon, D. P. L., *Generalized Correlation of Isothermal Enthalpy Departures for Liquids at Low Reduced Temperatures*, AIChE Symposium Series, No. 140, Vol. 70, pp. 56-62.

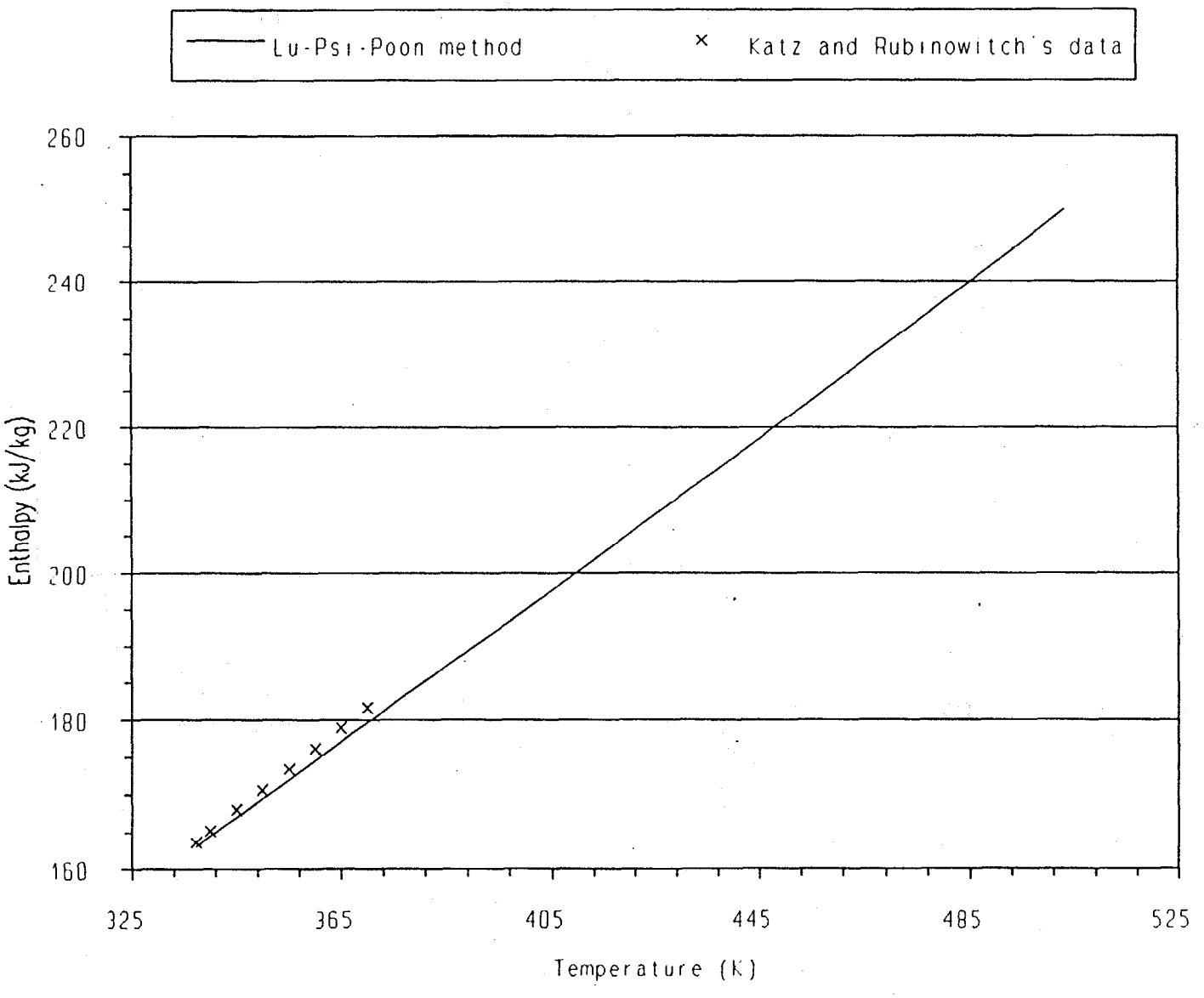

Fig. 6.1. Enthalpy of UF_6 liquid predicted by Lu-Psi-Poon method.

6.3.3 Lee-Kesler Method

The enthalpy of UF_6 liquid may be calculated by the Lee-Kesler method as described in Section 6.2.2 for the vapor. Since the enthalpy correlation contains compressibilities and since accurate values of compressibility are unobtainable from the Lee-Kesler compressibility correlation in the liquid range $0.95 < T_r < 1.0$ (see Section 5.2.3), an interpolation scheme is used for $0.95 < T_r < 1.0$. The enthalpy is calculated in a similar manner as was the liquid density in this range (see Section 5.2.3). Basically, the enthalpy is determined at five known points (H_A, H_B, H_C, H_D, and H_E) and the enthalpy of interest (H_F) is calculated as

$$H_F = H_A + (H_B - H_A)\left(\frac{H_D - H_C}{H_E - H_C}\right), \tag{6.21}$$

where
H_A = saturated liquid enthalpy at T_r and $P_{r,sat}$,
H_B = liquid enthalpy at T_r and $P_r = 1.0$,
H_C = liquid enthalpy at $T_r = 0.95$ and $P_{r,sat}$,
H_D = liquid enthalpy at $T_r = 0.95$ and P_r,
H_E = liquid enthalpy at $T_r = 0.95$ and $P_r = 1.0$.

The saturated UF_6 liquid enthalpy (H_A) is determined from the following correlation:

$$H_A = 2.690\times10^5 - 4.561\times10^3(T_c - T)^{1/2} - 247.8(T_c - T), \tag{6.22}$$

where
H_A = saturated liquid enthalpy (J/kg),
T_c = critical temperature (K),
T = temperature (K).

Eq. 6.22 is a curvefit of three saturated UF_6 liquid enthalpies ($T_r = 0.948$, $T_r = 0.95$, and $T_r = 1.0$) predicted by the Lee-Kesler method.

The enthalpy of liquid UF_6 predicted by the Lee-Kesler method is shown graphically in Fig. 6.2 along with the available liquid enthalpy data. Values predicted by the Lee-Kesler method correspond to the saturated state.

6.4 ENTHALPY OF SOLID

The enthalpy of solid UF_6 may be calculated using the following correlation which is accurate within 0.01% from 265 K to the triple point (337.2 K):

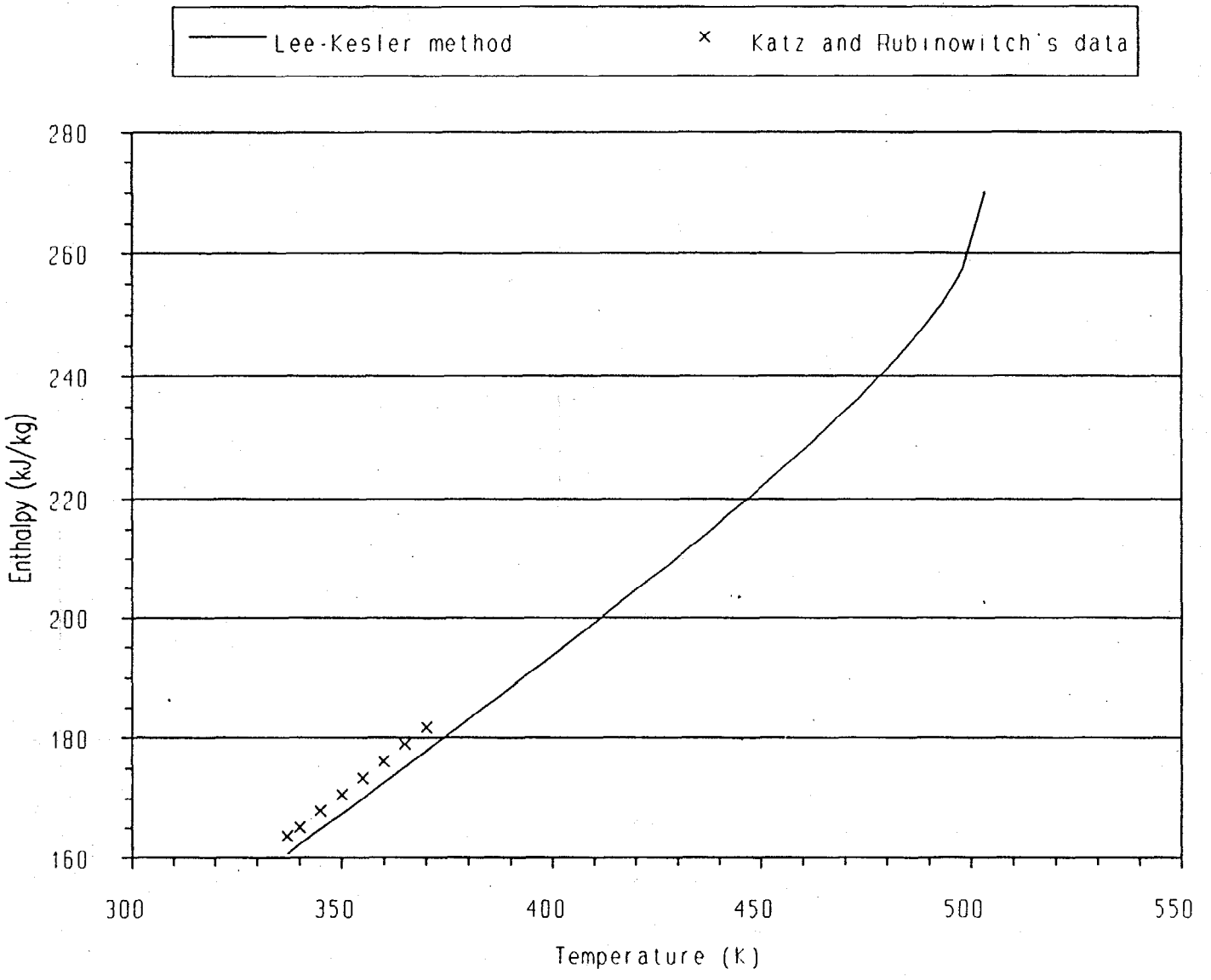

Fig. 6.2. Enthalpy of UF_6 liquid predicted by Lee-Kesler method.

$$H = 1.173\times10^5 - 238.9T + 9.609\times10^{-1}T^2 - \frac{1.246\times10^7}{T}, \qquad (6.23)$$

where H = enthalpy (J/kg),
T = temperature (K).

The form of Eq. 6.23 was suggested by Kirshenbaum who fitted the enthalpy values calculated by Brickwedde, Hoge, and Scott.[1] Williams identified several typographical errors in the solid enthalpy correlation presented in DeWitt.[2] Equation 6.23 incorporates these corrections and has been converted to SI units.

The enthalpy of UF_6 solid predicted by Eq. 6.23 is shown in Fig. 6.3 along with the available solid enthalpy data.

6.5 HEATS OF VAPORIZATION AND HEATS OF SUBLIMATION

Masi has measured five values of the heat of vaporization of uranium hexafluoride from 337.21 to 370 K (see Table 6.2).[1] These data were utilized to adjust the values of enthalpy departure predicted by the Lee-Kesler method as described in Section 6.2.2. The Lee-Kesler method may be used to calculate the heat of vaporization by calculating the vapor and liquid enthalpies and taking the difference between the two values. Alternatively, the Watson correlation may be used to predict heat of vaporization values. The Watson equation relates the heat of vaporization at a reference condition to the reduced temperature. Masi's data at the lower and upper limits were used to determine the exponent in the Watson equation for estimation of the temperature dependence of the heat of vaporization. The Watson equation is[3]

$$\Delta H_v = H_{v,1}[(1 - T_r)/(1 - T_{r,1})]^n, \qquad (6.24)$$

were the subscript 1 denotes the reference conditions. Using the lower limit as the reference temperature, the Watson equation for uranium hexafluoride becomes

$$\Delta H_v = 81.58\left(\frac{1 - T_r}{0.3300}\right)^{0.3123}, \qquad (6.25)$$

where ΔH_v = heat of vaporization (kJ/kg).

Masi also measured the heat of sublimation of uranium hexafluoride over a temperature range of 273.16 to 337.21 K.[1] In a similar fashion these data have been fitted to the Watson equation. The result is

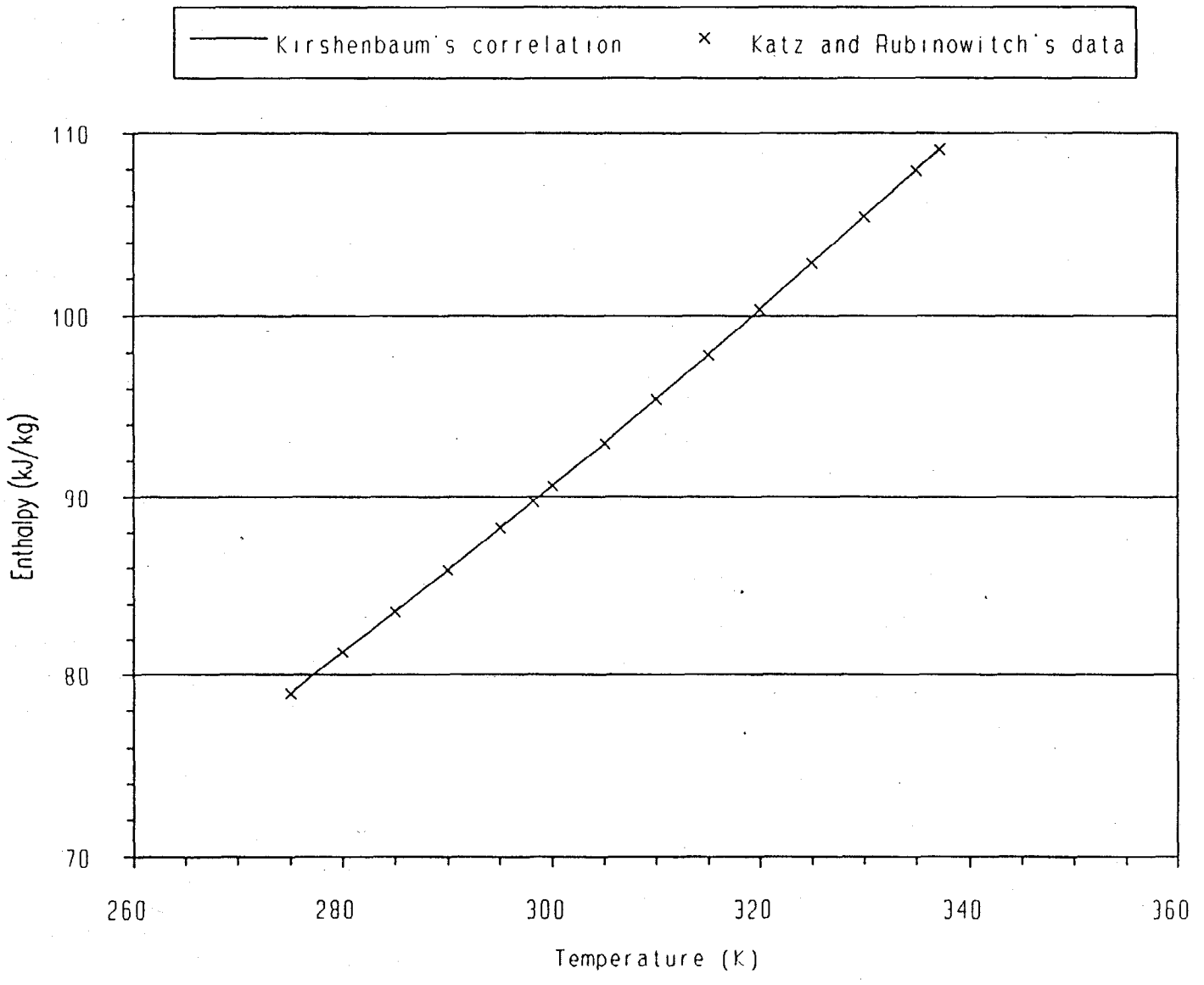

Fig. 6.3. Enthalpy of UF_6 solid.

$$\Delta H_s = 143.0\left(\frac{1 - T_r}{0.4573}\right)^{0.1561}, \tag{6.26}$$

where ΔH_s = heat of sublimation (kJ/kg).

6.6 ENTHALPY RECOMMENDATIONS

The enthalpy of UF_6 vapor should be determined by the Lee-Kesler correlation for enthalpy departure (Eq. 6.7) with the correction factor discussed in Section 6.2.2. The enthalpy of liquid UF_6 should also be determined by the Lee-Kesler correlation for enthalpy departure (an interpolation scheme is recommended for reduced temperatures from 0.95 to 1.0 as discussed in Section 6.3.3). The enthalpy of solid UF_6 can be estimated by Eq. 6.23, which is a curvefit of available data. The enthalpy of UF_6 calculated by the recommended methods is shown graphically in Fig. 6.4 as a function of temperature and pressure. The heats of vaporization and sublimation should be determined by taking the difference between the vapor enthalpy and the liquid or solid enthalpy predicted by the Lee-Kesler method and the curvefit results.

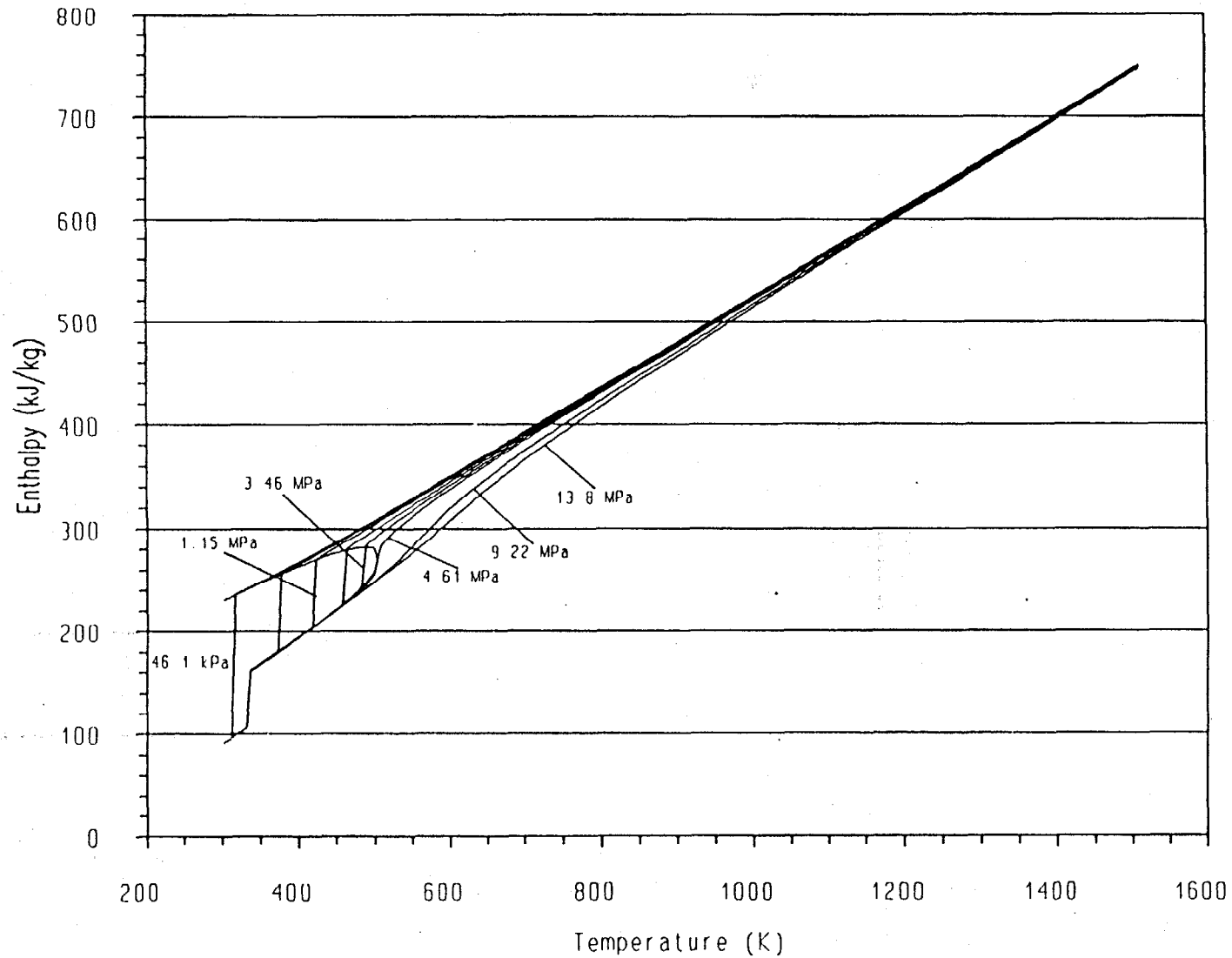

Fig. 6.4. Enthalpy of uranium hexafluoride.

7. HEAT CAPACITY

A comprehensive set of correlations is presented for predicting the heat capacity of all phases of UF_6. Where available, comparisons are made to available data.

7.1 LOW PRESSURE HEAT CAPACITY OF VAPOR

The low-pressure heat capacity of UF_6 vapor is calculated as

$$c_p^o = a + bT + cT^2 + dT^{0.5} + \frac{e}{T} + f\ln T + g\arctan\frac{T}{h} , \tag{7.1}$$

where c_p^o = low-pressure vapor heat capacity (kJ/kg),
T = temperature (K).

The values of the coefficients *a-h* are given in Table 6.1 and were obtained by a curvefit of available heat capacity data.[1,10] Attempts to fit the data to simpler third-order polynomials proved unsuccessful since two temperature ranges were required and a "glitch" was evident at the transition temperature.

The low pressure heat capacity of UF_6 vapor is shown graphically in Fig. 7.1 along with the available low pressure vapor heat capacity data.

7.2 HIGH PRESSURE HEAT CAPACITY OF VAPOR

The heat capacity of high-pressure UF_6 vapor can be determined using the method of Lee and Kesler.[4] The following correlation is used for the heat capacity departure function

$$\frac{c_p - c_p^o}{R} = \frac{c_v - c_v^o}{R} - 1 - T_r \frac{(\partial P_r/\partial T_r)^2_{V_r}}{(\partial P_r/\partial V_r)_{T_r}} , \tag{7.2}$$

where c_p = high-pressure enthalpy,
R = gas constant,
T_r = reduced temperature.

The partial derivatives in Eq. 7.2 are given by

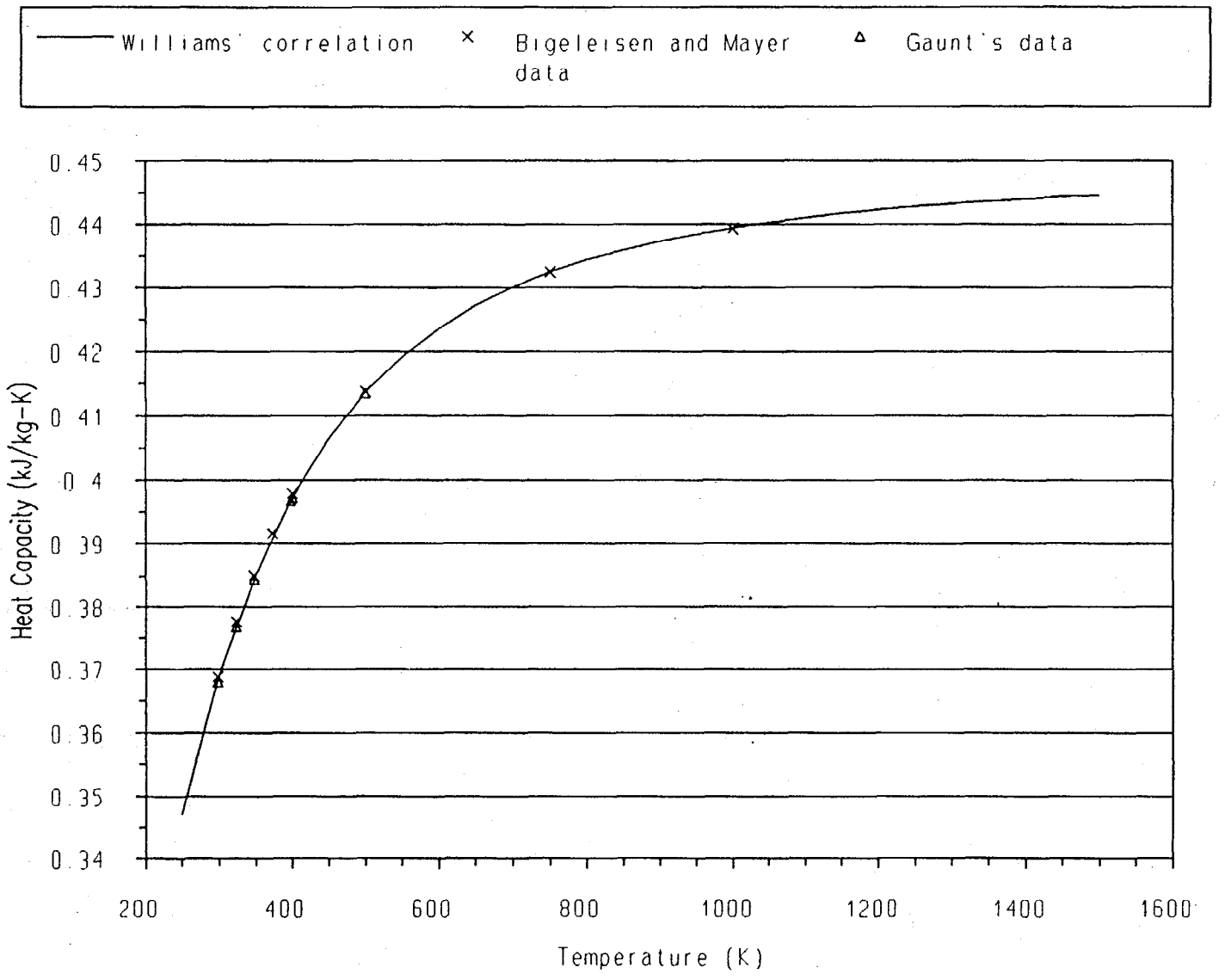

Fig. 7.1. Low pressure heat capacity of UF_6 vapor.

$$\left(\frac{\partial P_r}{\partial T_r}\right)_{V_r} = \frac{1}{V_r} + \frac{b_1 + b_3/T_r^2 + 2b_4/T_r^3}{V_r^2} + \frac{c_1 - 2c_3/T_r^3}{V_r^3}$$

$$+ \frac{d_1}{V_r^6} - \frac{2c_4}{T_r^3 V_r^3}\left[\left(\beta + \frac{\gamma}{V_r^2}\right)\exp\left(-\frac{\gamma}{V_r^2}\right)\right], \tag{7.3}$$

and

$$\left(\frac{\partial P_r}{\partial V_r}\right)_{T_r} = -\frac{T_r}{V_r^2}\left[1 + \frac{2B}{V_r} + \frac{3C}{V_r^2} + \frac{6D}{V_r^5}\right]$$

$$-\frac{c_4 T_r}{T_r^3 V_r^4}\left(3\beta + \left[5 - 2\left(\beta + \frac{\gamma}{V_r^2}\right)\right]\frac{\gamma}{V_r^2}\right)\exp\left(-\frac{\gamma}{V_r^2}\right), \tag{7.4}$$

where V_r = reduced volume.

The constants B, C, and D are given by the following expressions

$$B = b_1 - b_2/T_r - b_3/T_r^2 - b_4/T_r^3 , \tag{7.5}$$

$$C = c_1 - c_2/T_r + c_3/T_r^3 , \tag{7.6}$$

$$D = d_1 + d_2/T_r . \tag{7.7}$$

The isochoric heat capacity departure function appearing in Eq. 7.2 is defined as

$$\frac{c_v - c_v^o}{R} = \frac{2(b_3 + 3b_4/T_r)}{T_r^2 V_r} - \frac{3c_3}{T_r^3 V_r^2} - 6E , \tag{7.8}$$

where the variable E is calculated as

$$E = \frac{c_4}{2T_r^3\gamma}\left[\beta + 1 - \left(\beta + 1 + \frac{\gamma}{V_r^2}\right)\exp\left(\frac{-\gamma}{V_r^2}\right)\right]. \tag{7.9}$$

Values of the constants b_1, b_2, b_3, b_4, c_1, c_2, c_3, c_4, d_1, d_2, β, and γ are given in Table 5.5.

To calculate the heat capacity at a given temperature and pressure, the following procedure should be followed.

1. Determine $Z^{(0)}$ and $Z^{(1)}$ for the simple fluid from the Lee-Kesler correlation as described in Section 5.1.5 at the reduced temperature and pressure of interest. Using Eq. 7.2 and the simple fluid constants in Table 5.5, calculate $[(c_p - c_p^o)/R]^{(0)}$. In this calculation, Z is $Z^{(0)}$ and V_r is $V_r^{(0)}$ determined as

$$V_r^{(0)} = \frac{T_r Z^{(0)}}{P_r}. \tag{7.10}$$

2. Repeat step 1, using the same T_r and P_r, but this time using the reference fluid constants from Table 5.5. Using Eq. 7.2, calculate a value of $[(c_p - c_p^o)/R]^{(r)}$. In this calculation, Z is $Z^{(r)}$ given by

$$Z^{(r)} = \omega^{(r)}Z^{(1)} + Z^{(0)}, \tag{7.11}$$

where $Z^{(0)}$ and $Z^{(1)}$ are obtained from the Lee-Kesler correlation described in Section 5.1.5 and $\omega^{(r)} = 0.3978$. V_r in this calculation is $V_r^{(r)}$ given by

$$V_r^{(r)} = \frac{T_r Z^{(r)}}{P_r}. \tag{7.12}$$

3. The heat capacity departure function at the T_r and P_r of interest is determined from

$$\frac{(c_p - c_p^o)}{R} = \left[\frac{(c_p - c_p^o)}{R}\right]^{(0)} + \frac{\omega}{\omega^{(r)}}\left(\left[\frac{(c_p - c_p^o)}{R}\right]^{(r)} - \left[\frac{(c_p - c_p^o)}{R}\right]^{(0)}\right). \tag{7.13}$$

The heat capacity of UF_6 vapor is calculated as

$$c_p = c_p^o + (c_p - c_p^o)_{L-K}\left(\frac{\Delta H_{v,M}}{\Delta H_{v,L-K}}\right)_{avg} , \tag{7.14}$$

where

$$\left(\frac{\Delta H_{v,M}}{\Delta H_{v,L-K}}\right)_{avg} = 1.20650 . \tag{7.15}$$

For details on how the average heat of vaporization ratio was determined, see Section 6.2.2. No experimental data on high-pressure heat capacity of UF_6 was found in the literature.

7.3 HEAT CAPACITY OF LIQUID

The heat capacity of UF_6 liquid can also be calculated by the Lee-Kesler method as described in Section 7.2. However, since the heat capacity correlations (Eq. 7.2 - 7.9) contain compressibilities (implicitly) and since accurate values of liquid compressibilities are unobtainable from the Lee-Kesler compressibility correlation (Eq. 5.21) in the range $0.95 < T_r < 1.0$ (see Section 5.2.3), an alternate method must be used for $0.95 < T_r < 1.0$. The heat capacity of liquid UF_6 in this range can be approximated as

$$c_p = \left(\frac{\partial H}{\partial T}\right)_p \approx \left(\frac{\Delta H}{\Delta T}\right)_p = \frac{H_T - H_{T-\Delta T}}{T - (T - \Delta T)} = \frac{H_T - H_{T-\Delta T}}{\Delta T} , \tag{7.16}$$

where H = liquid enthalpy,
ΔT = small temperature difference.

The enthalpy of UF_6 liquid is calculated as described in Section 6.3.

The heat capacity of liquid UF_6 predicted by the Lee-Kesler method is shown in Fig. 7.2 along with the available liquid heat capacity data. The lower curve in Fig. 7.2 is the specific heat at constant pressure ($P_r = 3.0$) while the upper curve represents the specific heat evaluated along the saturation curve. It is unclear at what pressure the specific heat data were taken. Fig. 7.2 indicates that the data are bounded by the specific heats calculated by the Lee-Kesler correlation at constant pressure and calculated as $\Delta H/\Delta T$ along the saturation curve.

7.4 HEAT CAPACITY OF SOLID

Kirshenbaum developed a correlation for calculating the heat capacity of solid UF_6 based on experimental data.[1] Williams identified several typographical errors in this correlation presented by DeWitt.[2] After incorporating these corrections and performing unit conversion, this correlation becomes

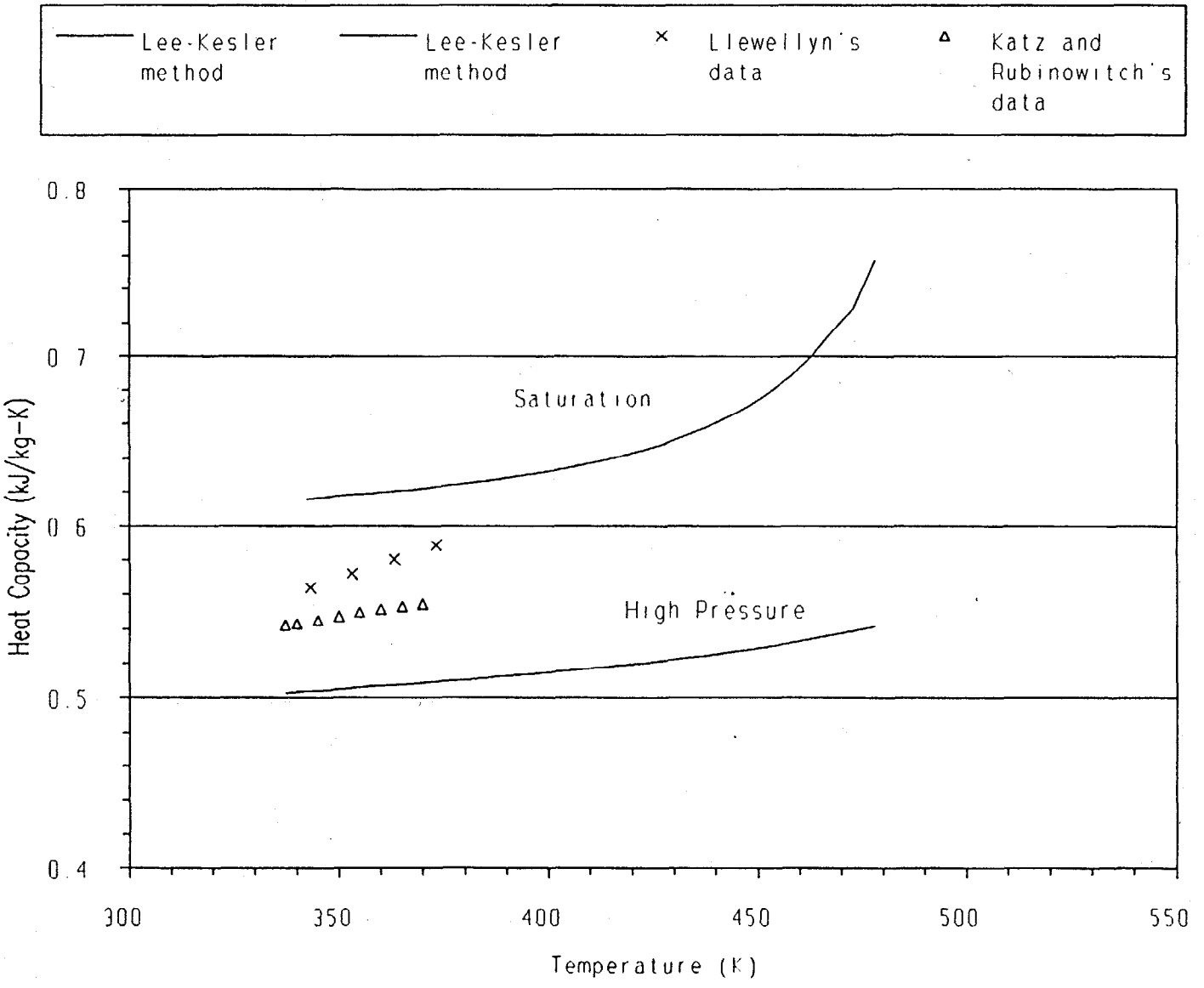

Fig. 7.2. Heat capacity of UF_6 liquid.

$$c_p = -238.9 + 1.922\,T + \frac{1.246\times10^7}{T^2}\,, \tag{7.17}$$

where c_p = heat capacity (J/kg-K),
T = temperature (K).

The above correlation is accurate within 1% between 250 K and the triple point. The heat capacity of UF_6 solid predicted by Eq. 7.17 is shown in Fig. 7.3 along with the available solid heat capacity data.

7.5 HEAT CAPACITY RECOMMENDATIONS

The heat capacity for both the vapor and liquid phases of UF_6 should be calculated from the Lee-Kesler correlation for heat capacity departure (Eq. 7.2) with the modifications discussed in Sections 7.2 and 7.3. The heat capacity of solid UF_6 can be determined from Eq. 7.17, a curvefit of available data. The heat capacity of UF_6 calculated by the recommended methods is shown graphically in Fig. 7.4 as a function of temperature and pressure. It should be noted that the value of heat capacity approaches infinity at the critical point.

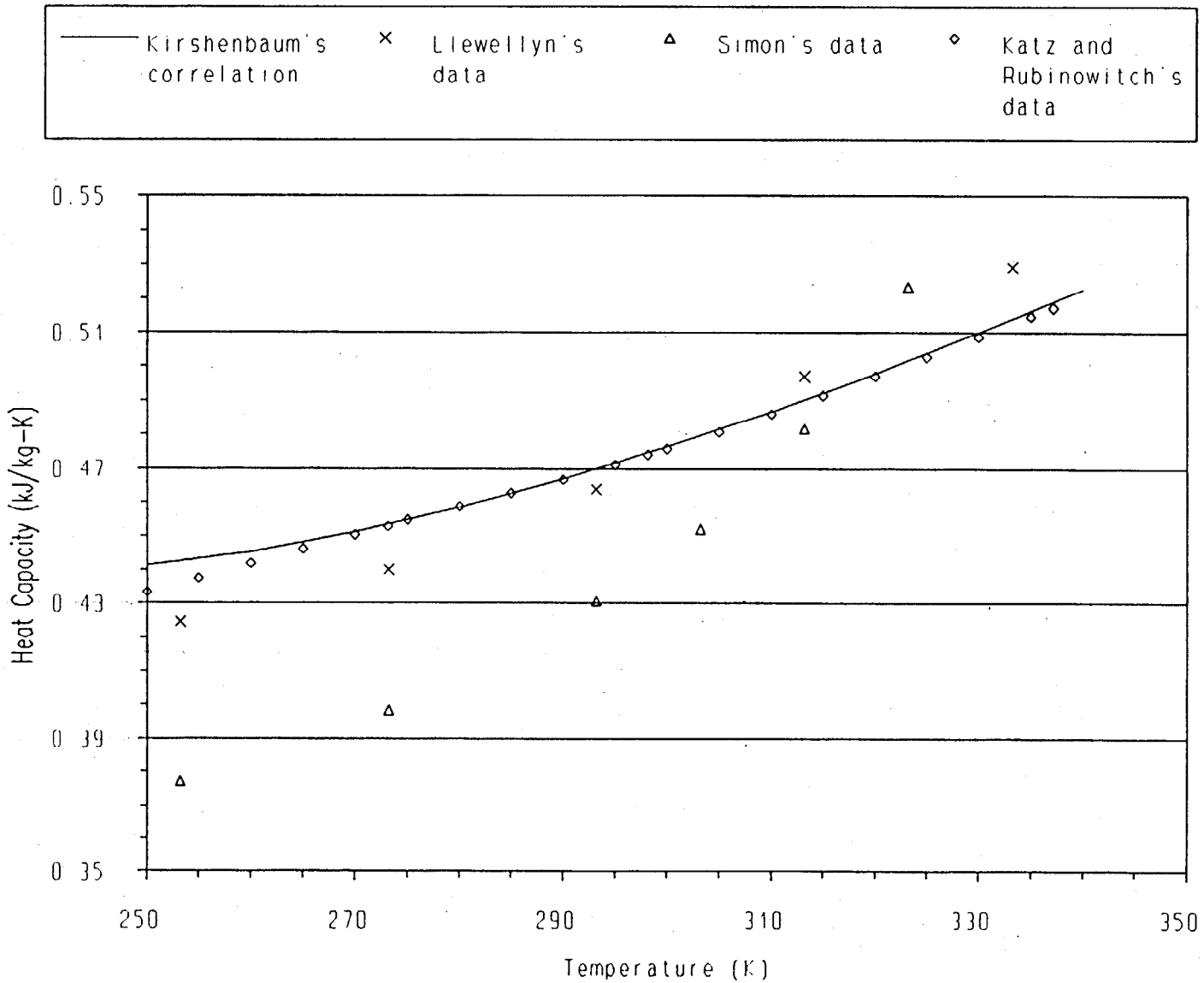

Fig. 7.3. Heat capacity of UF_6 solid.

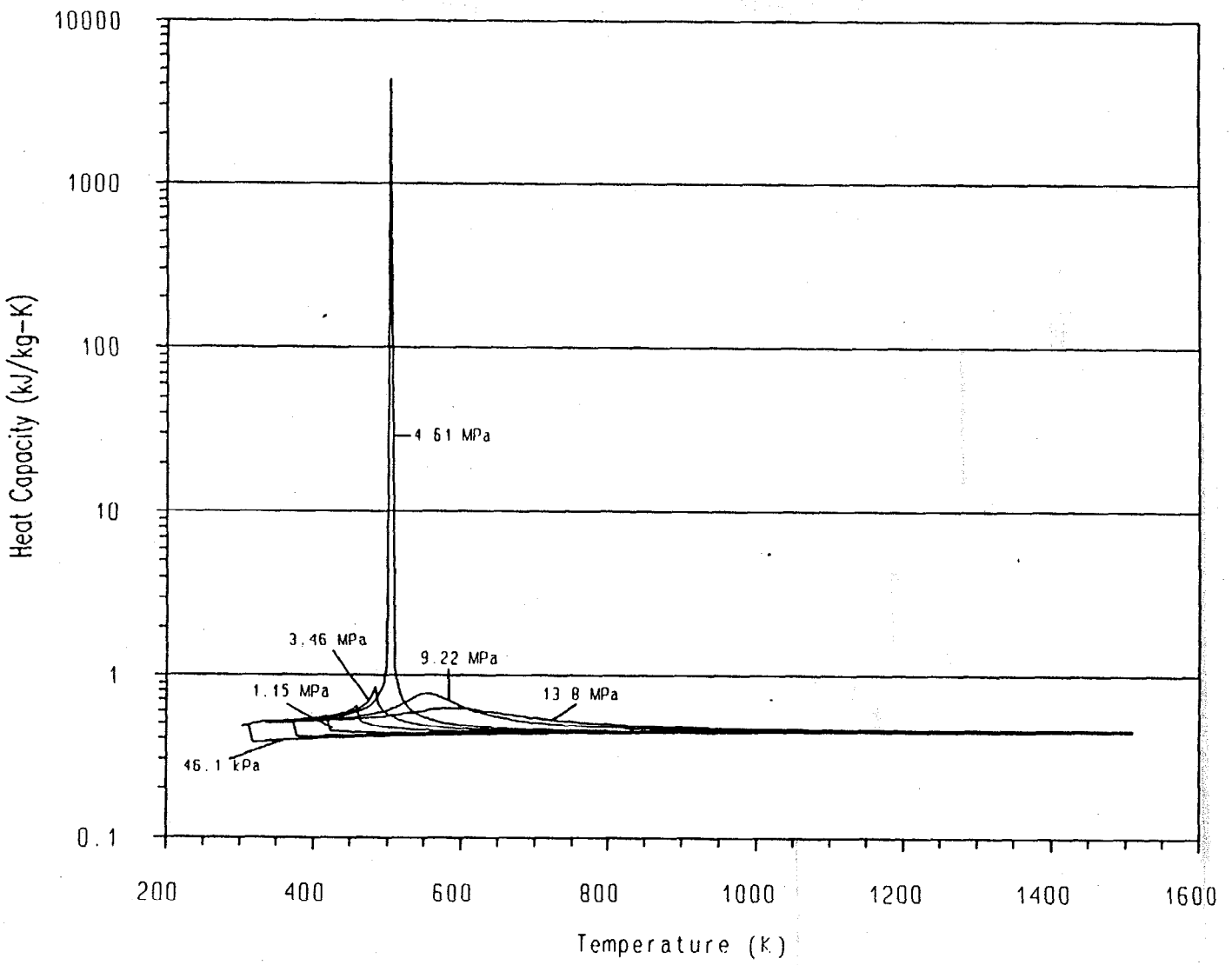

Fig. 7.4. Heat capacity of uranium hexafluoride.

8. SURFACE TENSION OF LIQUID

The surface tension of liquid UF_6 is given by

$$\sigma = 3.246\times10^{-5}\,(T_c - T)^{1.232}\,, \tag{8.1}$$

where σ = surface tension (N/m),
T_c = critical temperature (K),
T = liquid temperature (K).

Eq. 8.1 is a curvefit of data from DeWitt[1] taking into account the fact that the surface tension reduces to zero at the critical point. The surface tension of UF_6 liquid is shown as a function of temperature in Fig. 8.1 along with the available surface tension data.

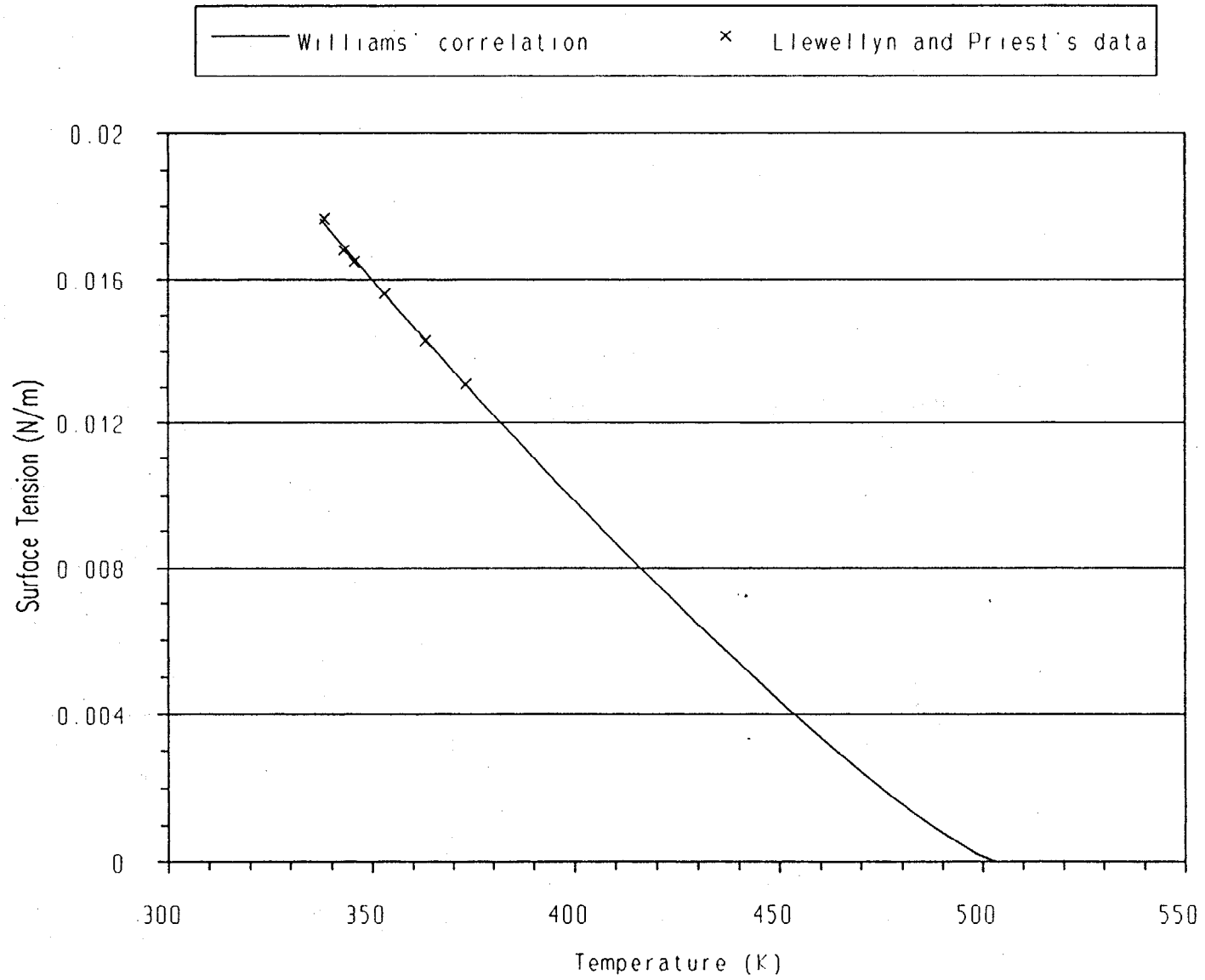

Fig. 8.1. Surface tension of UF_6 liquid.

9. VISCOSITY

Correlations are presented for calculating the dynamic viscosity of both vapor and liquid UF_6. Values predicted by the recommended correlations are compared to available data to ensure accuracy.

9.1 VISCOSITY OF VAPOR

The viscosity of both low and high-pressure vapor may be determined by using the Chung et al. method.[3] Their correlation, in slightly revised form incorporating a temperature dependent leading constant, is

$$\mu = \frac{\mu^*(C_o + C_1 T)[M_W T_c]^{1/2}}{V_c^{2/3}} , \tag{9.1}$$

where
μ = vapor viscosity (micropoise),
T = temperature (K),
M_W = molecular weight (g/gmol),
T_c = critical temperature (K),
V_c = critical volume (cm^3/gmol).

The variable μ^* in Eq. 9.1 is defined as

$$\mu^* = \frac{T^{*1/2}}{\Omega_v}[F_c(G_2^{-1} + E_6 y)] + \mu^{**} , \tag{9.2}$$

where

$$T^* = 1.2593 T_r , \tag{9.3}$$

$$F_c = 1 - 0.2756\omega + 0.059035\mu_r^4 + \kappa , \tag{9.4}$$

$$y = \frac{\rho V_c}{6} , \tag{9.5}$$

$$G_1 = \frac{1 - 0.5y}{(1 - y)^3} , \tag{9.6}$$

$$G_2 = \frac{E_1 \left[[1 - \exp(-E_4 y)]/y\right] + E_2 G_1 \exp(E_5 y) + E_3 G_1}{E_1 E_4 + E_2 + E_3} , \tag{9.7}$$

$$\mu^{**} = E_7 y^2 G_2 \exp[E_8 + E_9 T^{*-1} + E_{10} T^{*-2}] , \tag{9.8}$$

and T_r = reduced temperature,
ω = acentric factor,
μ_r = reduced dipole moment,
κ = association factor,
ρ = vapor molar density (mol/cm^3).

Values of the coefficients E_1-E_{10} are calculated as

$$E_i = a_i + b_i \omega + c_i \mu_r^4 + d_i \kappa . \tag{9.9}$$

Since UF_6 is nonpolar, the reduced dipole moment and the association factor are assumed to have values of zero, and therefore,

$$E_i = a_i + b_i \omega , \tag{9.10}$$

where values of a_i and b_i are given in Table 9.1.

The vapor viscosity collision integral, Ω_v, is defined as

$$\Omega_v = [1.16145 T^{*-0.14874} + 0.52487 [\exp(-0.77320 T^*)] + 2.16178 [\exp(-2.43787 T^*)] . \tag{9.11}$$

The constants C_o and C_1, in Eq. 9.1, were employed in order to curvefit the method of Chung et al. to existing vapor UF_6 viscosity data.[11] Values of C_1 and C_o are

Table 9.1. Values of the Coefficients Used in Chung's Viscosity Correlation

i	a_i	b_i	c_i	d_i
1	6.324	50.412	-51.680	1189.0
2	1.210E-3	-1.154E-3	-6.257E-3	0.03728
3	5.283	254.209	-168.48	3898.0
4	6.623	38.096	-8.464	31.42
5	19.745	7.630	-14.354	31.53
6	-1.900	-12.537	4.985	-18.15
7	24.275	3.450	-11.291	69.35
8	0.7972	1.117	0.01235	-4.117
9	-0.2382	0.06770	-0.8163	4.025
10	0.06863	0.3479	0.5926	-0.727

Source: Reid, R. C., Prausnitz, J. M., and Poling, B. E., *The Properties of Gases and Liquids*, 4th ed., McGraw-Hill Book Company, New York, NY, 1987.

$$C_1 = \frac{\dfrac{V_c^{2/3}}{[M_W T_c]^{1/2}}\left[\dfrac{\mu_L}{\mu^*(T_L, P_{atm})} - \dfrac{\mu_H}{\mu^*(T_H, P_{atm})}\right]}{(T_L - T_H)}, \tag{9.12}$$

and

$$C_0 = \frac{\mu_H V_c^{2/3}}{\mu^*(T_H, P_{atm})[M_W T_c]^{1/2}} - T_H C_1, \tag{9.13}$$

where
T_L = low temperature at which viscosity data is available (K),
T_H = high temperature at which viscosity data is available (K),
μ_L = vapor viscosity at the low temperature (micropoise),
μ_H = vapor viscosity at the high temperature (micropoise),
$\mu^*(T_L, P_{atm})$ = μ^* evaluated at T_L and atmospheric pressure,
$\mu^*(T_H, P_{atm})$ = μ^* evaluated at T_H and atmospheric pressure.

The viscosity of UF_6 vapor is shown graphically in Fig. 9.1 along with the available vapor viscosity data. The viscosities predicted by the Chung et al. method correspond to low pressure ($P_r = 0.01$).

9.2 VISCOSITY OF LIQUID

The viscosity of liquid UF_6 is calculated by one of two methods based on the value of reduced temperature. For low reduced temperatures ($T_r < 0.75$), the method of Orrick and Erbar is used for liquid viscosities.[3] They recommend the following correlation

$$\mu_l = \rho_l M_W \exp[A + B/T] , \tag{9.14}$$

where μ_l = liquid viscosity (centipoise),
ρ_l = liquid density at 20°C (g/cm^3),
M_W = molecular weight,
T = temperature (K).

The constants A and B in Eq. 9.14 are calculated using available liquid viscosity data ($\mu_l = 0.924$ cp @ 67.9°C and $\mu_l = 0.752$ cp @ 99°C).[1]

$$A = \ln\left[\frac{0.752}{\rho_l(M_W)}\right] - \frac{B}{372.15} , \tag{9.15}$$

and

$$B = \ln\left[\frac{0.924}{0.752}\right]\left[\frac{(372.15)(341.05)}{372.15 - 341.05}\right] = 840.60 . \tag{9.16}$$

At reduced temperatures exceeding 0.75, the liquid viscosity should be calculated by the Chung et al. method as recommended by Reid, Prausnitz, and Poling (see Section 9.1).[3] Chung's correlation for the liquid is

$$\mu_l = \mu^* \frac{(C_o + C_1 T)[(MW)T_c]^{1/2}}{V_c^{2/3}} . \tag{9.17}$$

The variable μ^* is calculated by Eq. 9.2 with the exception that the density is taken as the liquid density rather than the vapor density. The constants C_o and C_l in Eq. 9.17 are determined such that 1) the values of viscosity match at the switch point ($T_r = 0.75$), and 2) the liquid viscosity equals the vapor viscosity at the critical temperature.

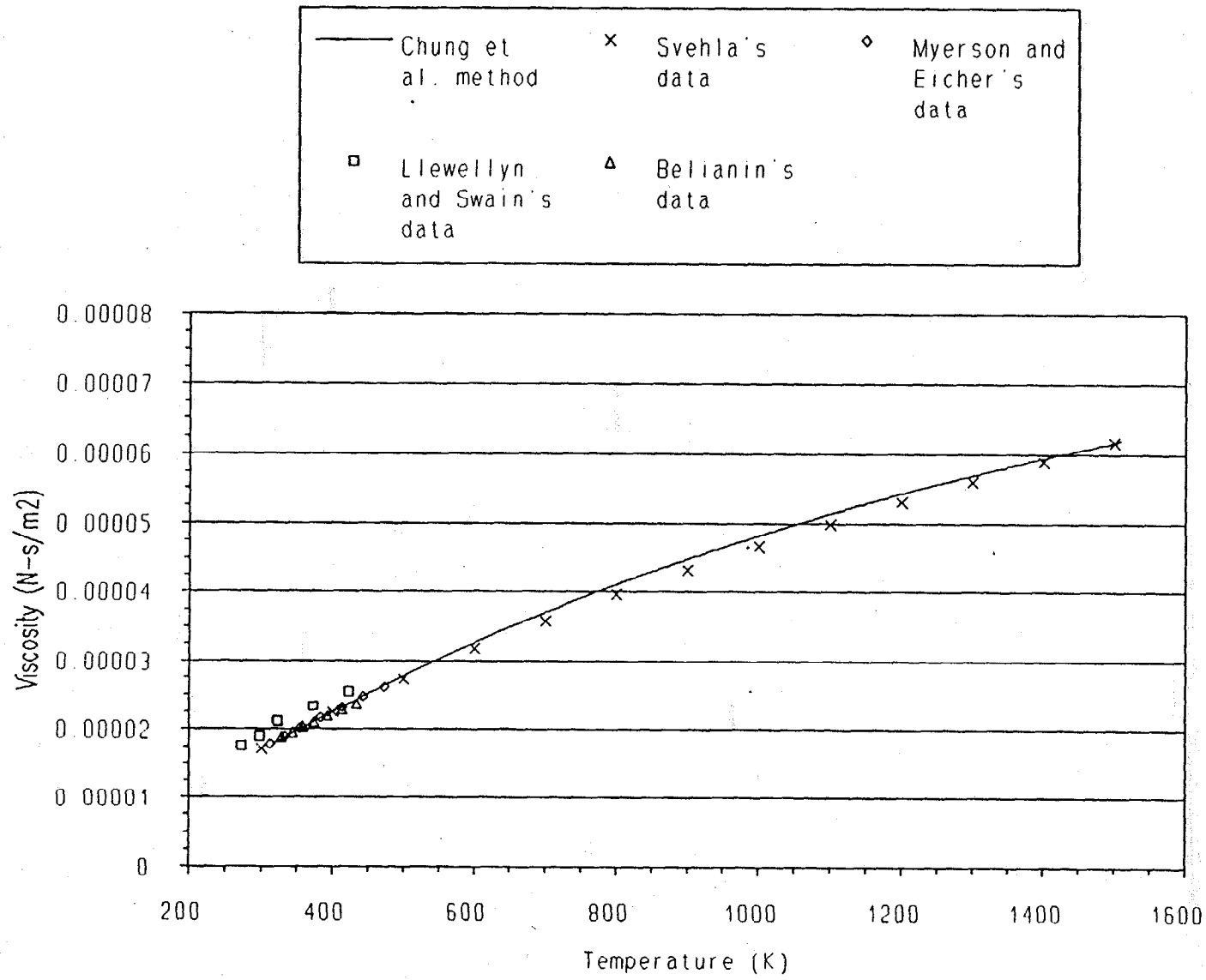

Fig. 9.1. Viscosity of UF_6 vapor.

$$C_1 = \frac{\dfrac{\mu_c V_c^{2/3}}{\mu^*(T_c,P_c)[(MW)T_c]^{1/2}} - \dfrac{\mu_{T_{high}} V_c^{2/3}}{\mu^*(T_{high},P)[(MW)T_c]^{0.5}}}{T_c - T_{high}} , \tag{9.18}$$

$$C_o = \frac{\mu_c V_c^{2/3}}{\mu^*(T_c,P_c)[(MW)T_c]^{1/2}} - C_1 T_c , \tag{9.19}$$

where μ_c = viscosity at the critical temperature (micropoise),
$\mu^*(T_c, P_c)$ = μ^* evaluated at the critical point,
μ_{Thigh} = viscosity of liquid at T_{high} (switch point) calculated by Orrick and Erbar's method (micropoise),
$\mu^*(T_{high}, P)$ = μ^* evaluated at T_{high} (switch point) and pressure of liquid,
T_{high} = temperature at which Orrick and Erbar's method becomes invalid and Chung's method becomes applicable (K).

The viscosity of UF_6 liquid predicted by the Orrick-Erbar and Chung et al. methods is shown graphically in Fig. 9.2 along with the available liquid viscosity data. A slight change in slope is noticeable at the transition temperature (T_r = 0.75) between the two correlations; however, the overall curve is continuous.

9.3 VISCOSITY RECOMMENDATIONS

The viscosity of UF_6 vapor should be calculated using the method of Chung et al. (Eq. 9.1). The viscosity of UF_6 liquid should be calculated by the methods of Orrick-Erbar or Chung et al. depending on the temperature (see Section 9.2). The viscosity of UF_6 vapor and liquid calculated by the recommended methods is shown graphically in Fig 9.3 as a function of temperature and pressure.

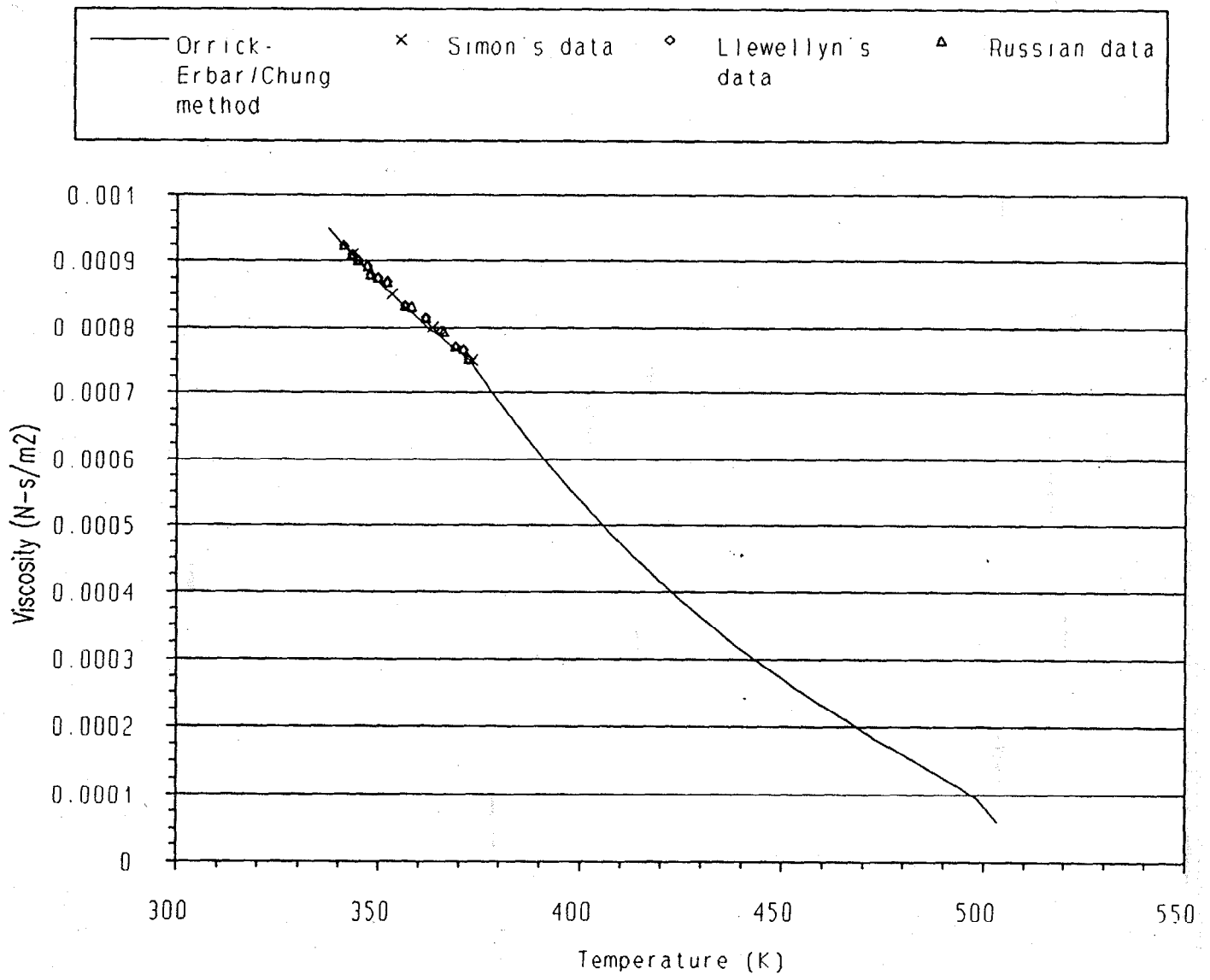

Fig. 9.2. Viscosity of UF_6 liquid.

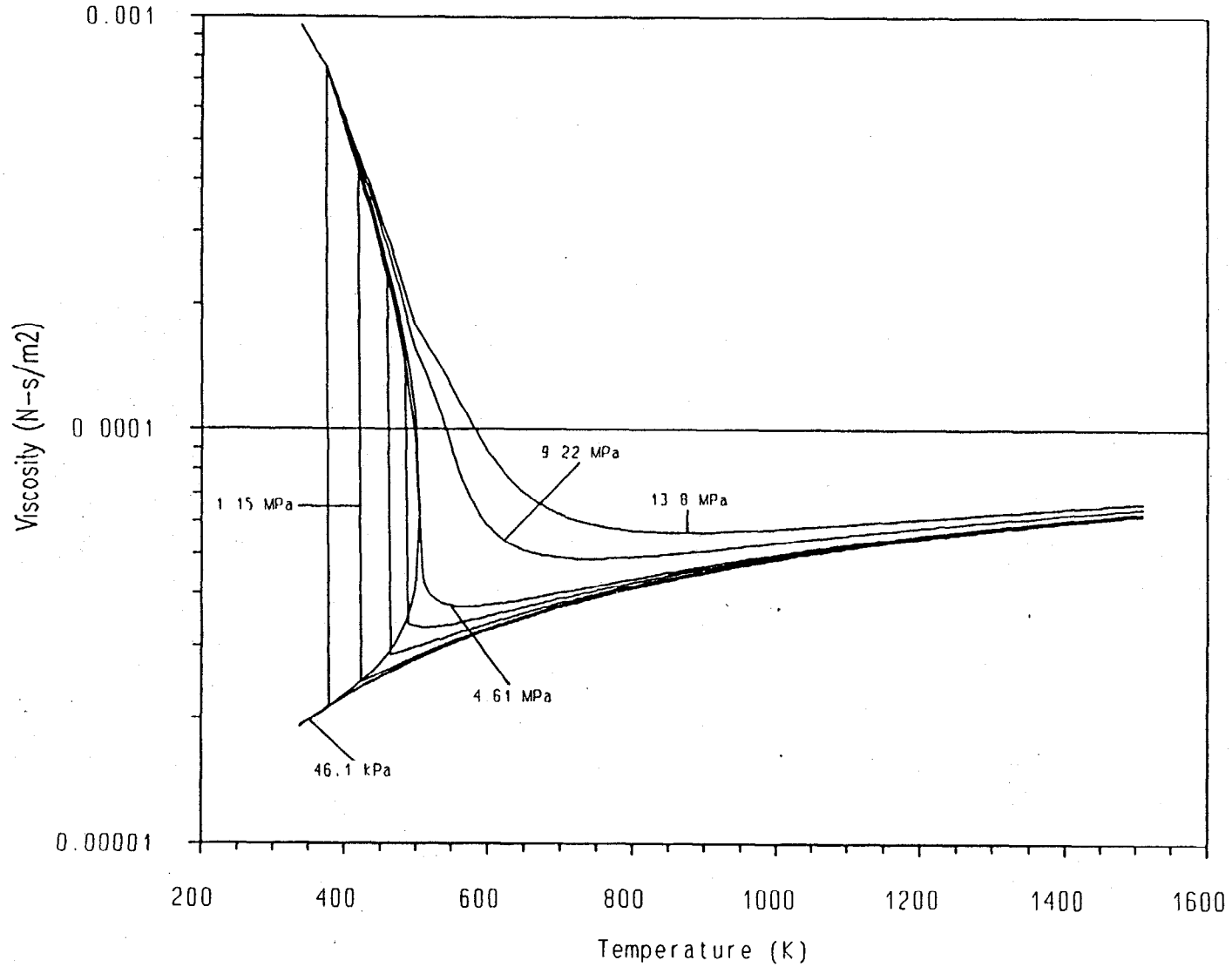

Fig. 9.3. Viscosity of uranium hexafluoride.

10. THERMAL CONDUCTIVITY

Several methods are available for calculating the thermal conductivity of the vapor and liquid phases of a fluid. Among those examined for applicability to UF_6 are the Chung et al., Latini, and residual thermal conductivity methods. In addition, a correlation is presented to calculate the thermal conductivity of solid UF_6. Where available, values predicted by the correlations are compared to the experimental data.

10.1 THERMAL CONDUCTIVITY OF VAPOR

The thermal conductivity of both low and high-pressure vapor can be determined by the method of Chung et al.[3] Their correlation for estimating the thermal conductivity is

$$k_v = \frac{31.2\mu^o\psi}{M_W}(G_2^{-1} + B_6 y) + qB_7 y^2 T_r^{1/2} G_2 , \tag{10.1}$$

where
k_v = vapor thermal conductivity (W/m-K),
μ^o = low pressure gas viscosity (N-s/m^2),
y = $V_c/(6V)$,
T_r = reduced temperature,
V_c = critical volume (cm^3/gmol),
V = vapor molar volume (cm^3/gmol),
M_W = molecular weight (kg/gmol).

The constant ψ in Eq. 10.1 is defined as

$$\psi = 1 + \alpha\left[\frac{0.215 + 0.28288\alpha - 1.061\beta + 0.26665Z}{0.6366 + \beta Z + 1.061\alpha\beta}\right] , \tag{10.2}$$

where
α = c_v/R - 1.5,
β = 0.7862 - 0.7109ω + 1.3168ω^2,
c_v = heat capacity at constant volume (J/gmol-K),
R = gas constant (8.315 J/gmol-K),
ω = acentric factor,
Z = compressibility.

The constant q appearing in Eq. 10.1 is calculated as

$$q = \frac{3.586\times10^{-3}(T_c/M_W)^{1/2}}{V_c^{2/3}} , \tag{10.3}$$

where T_c = critical temperature (K).

The constant G_2 is defined as

$$G_2 = \frac{\frac{B_1}{y}[1 - \exp(-B_4 y)] + B_2 G_1 \exp(B_5 y) + B_3 G_1}{B_1 B_4 + B_2 + B_3} , \tag{10.4}$$

where

$$G_1 = \frac{1 - 0.5y}{(1 - y)^3} . \tag{10.5}$$

The coefficients B_1 - B_7 are functions of the acentric factor (ω), the reduced dipole moment (μ_r), and the association factor (κ).

$$B_i = a_i + b_i\omega + c_i\mu_r^4 + d_i\kappa . \tag{10.6}$$

Since the reduced dipole moment (μ_r) and the association factor (κ) of UF_6 are assumed to have values of zero,

$$B_i = a_i + b_i\omega , \tag{10.7}$$

where values of a_i and b_i given in Table 10.1.

Values predicted by Chung's method (Eq. 10.1) were consistently higher than the data. Therefore, a multiplication factor of 0.8397 was applied to Chung's method in order to obtain good agreement with experimental data. The thermal conductivity of UF_6 vapor predicted by the Chung et al. correlation with the modification discussed above is shown in Fig. 10.1 along with the available vapor thermal conductivity data. The thermal conductivities were calculated in the saturated state. It should be noted that as the temperature approaches the critical temperature, the value of thermal conductivity calculated by the Chung et al. correlation also becomes very large. This is due to the fact that Eq. 10.1 indirectly contains specific heat (which becomes infinite at the critical point).

Table 10.1. Values of the Coefficients Used in Chung's Thermal Conductivity Correlation

i	a_i	b_i	c_i	d_i
1	2.4166E+0	7.4824E-1	-9.1858E-1	1.2172E+2
2	-5.0924E-1	-1.5094E+0	-4.9991E+1	6.9983E+1
3	6.6107E+0	5.6207E+0	6.4760E+1	2.7039E+1
4	1.4543E+1	-8.9139E+0	-5.6379E+0	7.4344E+1
5	7.9274E-1	8.2019E-1	-6.9369E-1	6.3173E+0
6	-5.8634E+0	1.2801E+1	9.5893E+0	6.5529E+1
7	9.1089E+1	1.2811E+2	-5.4217E+1	5.2381E+2

Source: Reid, R. C., Prausnitz, J. M., and Poling, B. E., *The Properties of Gases and Liquids*, 4th ed., McGraw-Hill Book Company, New York, NY, 1987.

10.2 THERMAL CONDUCTIVITY OF LIQUID

The thermal conductivity of liquid UF_6 can be determined by Latini's method, which written in slightly revised form is[3]

$$k_l = \frac{(C_o + C_1 T_r)(1 - T_r)^{0.38}}{T_r^{1/6}} . \tag{10.8}$$

DeWitt documents one data point for liquid UF_6 thermal conductivity — at 72°C, the thermal conductivity of liquid UF_6 was found to be 3.83×10^{-4} cal/cm-s-°C.[1] Reid, Prausnitz, and Poling recommend that if the liquid is at a reduced temperature greater than about 0.8, high-pressure vapor correlations (i.e., Chung et al.) should be used to calculate the thermal conductivity of the liquid.[3] Therefore, Latini's correlation can be used to predict the thermal conductivity of liquid UF_6 at reduced temperatures lower than 0.75 and Chung's correlation can be used for reduced temperatures exceeding 0.75.

The constants C_o and C_l in Eq. 10.8 should be calculated in order to match DeWitt's data point as well as produce a continuous function by matching the values predicted by Latini and Chung at the switch point (T_r = 0.75). The constants are therefore defined as

$$C_o = \frac{k_{DeWitt} T_{r,\,DeWitt}^{1/6}}{(1 - T_{r,\,DeWitt})^{0.38}} - T_{r,\,DeWitt} C_1 , \tag{10.9}$$

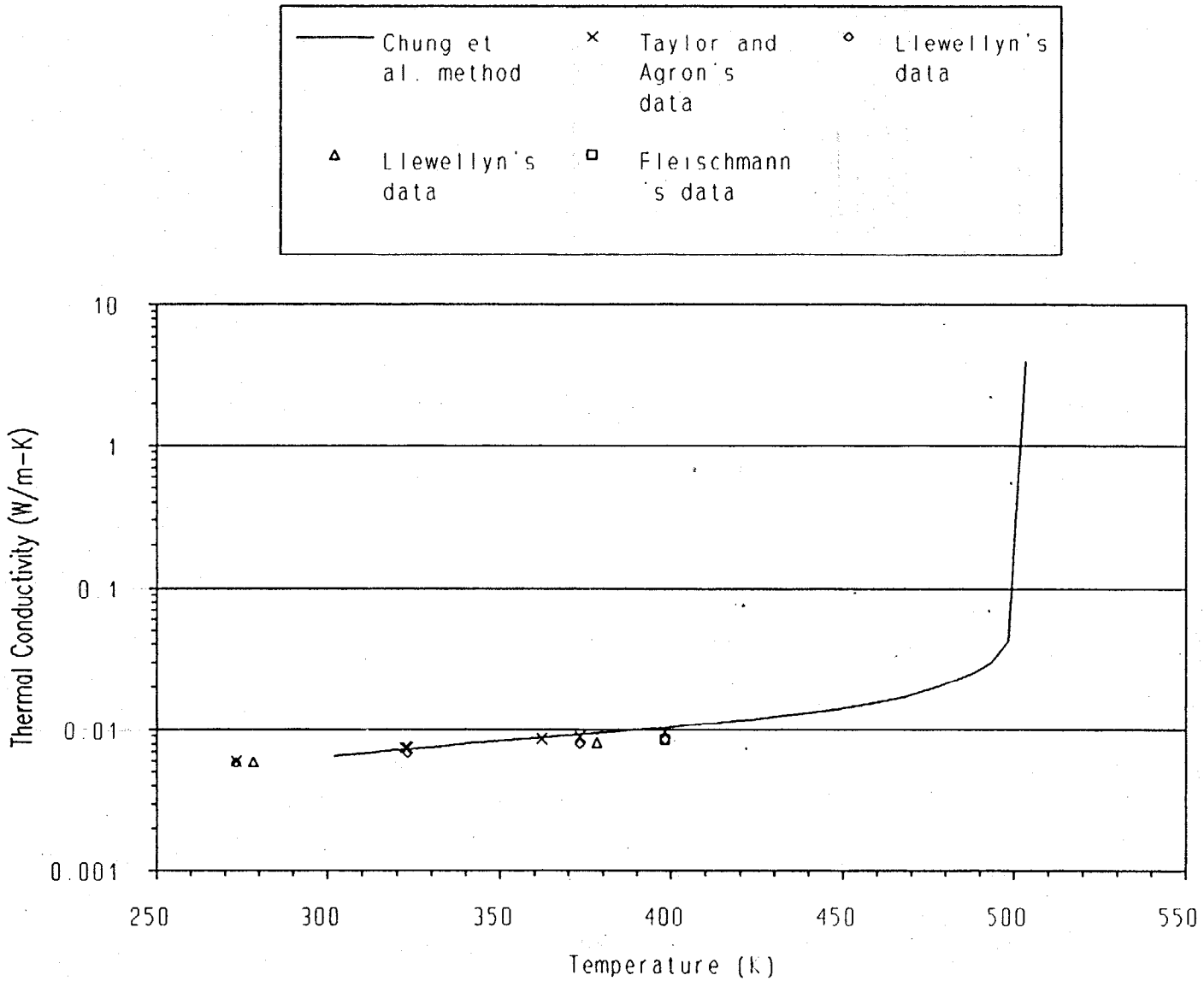

Fig. 10.1. Thermal conductivity of UF_6 vapor predicted by Chung method.

and

$$C_1 = \frac{\dfrac{k_{DeWitt} T_{r,\,DeWitt}^{1/6}}{(1 - T_{r,\,DeWitt})^{0.38}} - \dfrac{k_{Chung} T_{r,\,switch}^{1/6}}{(1 - T_{r,\,switch})^{0.38}}}{(T_{r,\,DeWitt} - T_{r,\,switch})} , \tag{10.10}$$

where k_{DeWitt} = value of liquid UF_6 thermal conductivity provided by DeWitt,
$T_{r,\,DeWitt}$ = reduced temperature corresponding to DeWitt's data point,
k_{Chung} = value of liquid thermal conductivity predicted by Chung at the switch temperature,
$T_{r,\,switch}$ = reduced temperature corresponding to temperature at which Latini's method becomes invalid and Chung's method becomes applicable.

Chung's correlation for liquid thermal conductivity, which will be used for reduced temperatures exceeding 0.75, is

$$k_l = \frac{C\mu^o\psi}{MW}(G_2^{-1} + B_6 y) + qB_7 y^2 T_r^{1/2} G_2 . \tag{10.11}$$

All variables in Eq. 10.11 are as defined as in Section 10.1 with the exception of the molar volume, V, which is taken as the liquid molar volume rather than the vapor molar volume. The leading coefficient, C, is defined as

$$C = (k_c - qB_7 y^2 T_r^{1/2} G_2)\frac{MW}{\mu^o\psi(G_2^{-1} + B_6 y)} , \tag{10.12}$$

where k_c = thermal conductivity at the critical point (W/m-K).

All variables in Eq. 10.12 are evaluated at the critical temperature. By calculating a value of C in this manner, the liquid thermal conductivity is forced to be equivalent to the vapor thermal conductivity at the critical point.

Making the leading coefficient in Latini's correlation a function of temperature allows the liquid thermal conductivity of UF_6 to be represented by a continuous function. It should be noted that the low temperature thermal conductivity is assumed to be independent of pressure, whereas the high temperature thermal conductivity is a function of pressure.

The thermal conductivity of liquid UF_6 predicted by the Latini and Chung et al. methods is shown in Fig. 10.2 along with Priest's data point. The thermal conductivities were calculated in the saturated state. The transition between the two correlations (T_r = 0.75) is evident in Fig. 10.2. It should also be noted that the thermal conductivity becomes very large at the critical temperature.

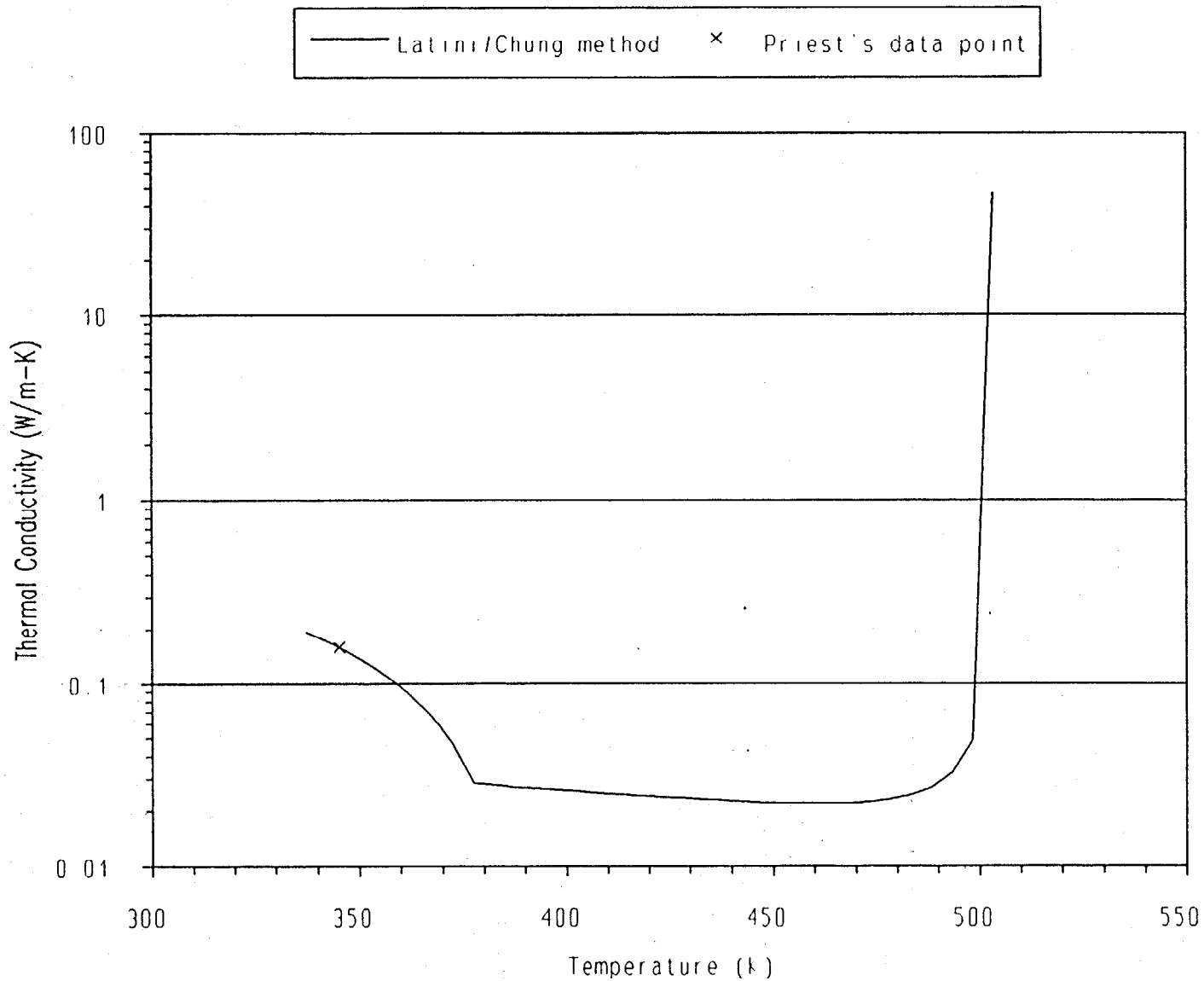

Fig. 10.2. Thermal conductivity of UF_6 liquid predicted by Latini/Chung method.

10.3 METHOD OF RESIDUAL THERMAL CONDUCTIVITIES

Since most correlations for thermal conductivity include specific heat as a variable (i. e., Chung's method discussed in the two preceding sections), any spikes or discontinuities in the specific heat curves are also present in the thermal conductivity curves. In order to avoid any numerical problems or difficulties that might arise from non-smooth thermal conductivity curves, a method based on a residual thermal conductivity vs density relationship will be investigated. Such a method which produces smooth, continuous thermal conductivity curves is proposed by Owens and Thodos for inert gases.[12]

Low pressure vapor thermal conductivities of UF_6 vapor are presented in DeWitt over a limited temperature range (0 - 125°C).[1] Low pressure (P_r = 0.001) vapor thermal conductivities were calculated using Chung's method discussed previously (see Section 10.1). Values of low pressure thermal conductivity calculated by Chung's method over the range of interest ($0.6 \geq T_r \geq 3.0$) were used to obtain the following correlation for low pressure UF_6 vapor thermal conductivity in W/m-K:

$$k^o = -3.316\times10^{-3} + 1.791\times10^{-2}\,T_r - 2.085\times10^{-3}\,T_r^2 \,. \tag{10.13}$$

The next step in the method of Owens and Thodos is the formulation of a correlation between the residual thermal conductivity and the density. Chung's method with the appropriate correction factor (see Section 10.1) was used to calculate values of saturated vapor thermal conductivities at reduced temperatures of 0.6 to 0.9. With both the saturated and low pressure thermal conductivities known, residual thermal conductivities ($k - k^o$) can be calculated. A residual thermal conductivity can also be calculated for the single liquid data point presented in DeWitt.[1] Using the Lee-Kesler method, saturated densities were calculated which correspond to each of the residual thermal conductivity data points. These data are represented by the following correlation for residual thermal conductivity in W/m-K as a function of density:

$$k - k^o = -9.007\times10^{-6} + 9.945\times10^{-6}\rho + 9.089\times10^{-9}\rho^2 \,, \tag{10.14}$$

where ρ = density (kg/m^3).

If the temperature and pressure are known, the low pressure thermal conductivity can be calculated from Eq. 10.13 and the density can be obtained by a method such as Lee-Kesler. The residual thermal conductivity can then be obtained from Eq. 10.14. Finally, the thermal conductivity at the temperature and pressure of interest can be determined from the values of residual and low pressure thermal conductivities.

$$k = (k - k^o) + k^o \,. \tag{10.15}$$

The method described above applies to both liquids and vapors.

The thermal conductivities of UF_6 vapor and liquid predicted by the residual thermal conductivity method are shown in Figs. 10.3 and 10.4 along with the available data. The thermal conductivities were calculated in the saturated state. As seen in Figs. 10.3 and 10.4, the curves are smooth and continuous and have finite values near the critical point.

10.4 THERMAL CONDUCTIVITY OF SOLID

The thermal conductivity of solid UF_6 is given by the following correlation derived by Williams[2]

$$k_s = -3.645\times10^{-2} + 1.895\times10^{-3}T\,, \tag{10.16}$$

where k_s = thermal conductivity of solid (W/m-K),
T = temperature (K).

Equation 10.16 is a linear fit of two solid thermal conductivity data points documented by Williams.[2]

10.5 THERMAL CONDUCTIVITY RECOMMENDATIONS

The method of residual thermal conductivities (see Section 10.3) is recommended for calculating the thermal conductivities of both vapor and liquid UF_6. The thermal conductivity of solid UF_6 can be estimated by Eq. 10.16. The thermal conductivity of UF_6 calculated by the recommended methods is shown graphically in Fig. 10.5 as a function of temperature and pressure.

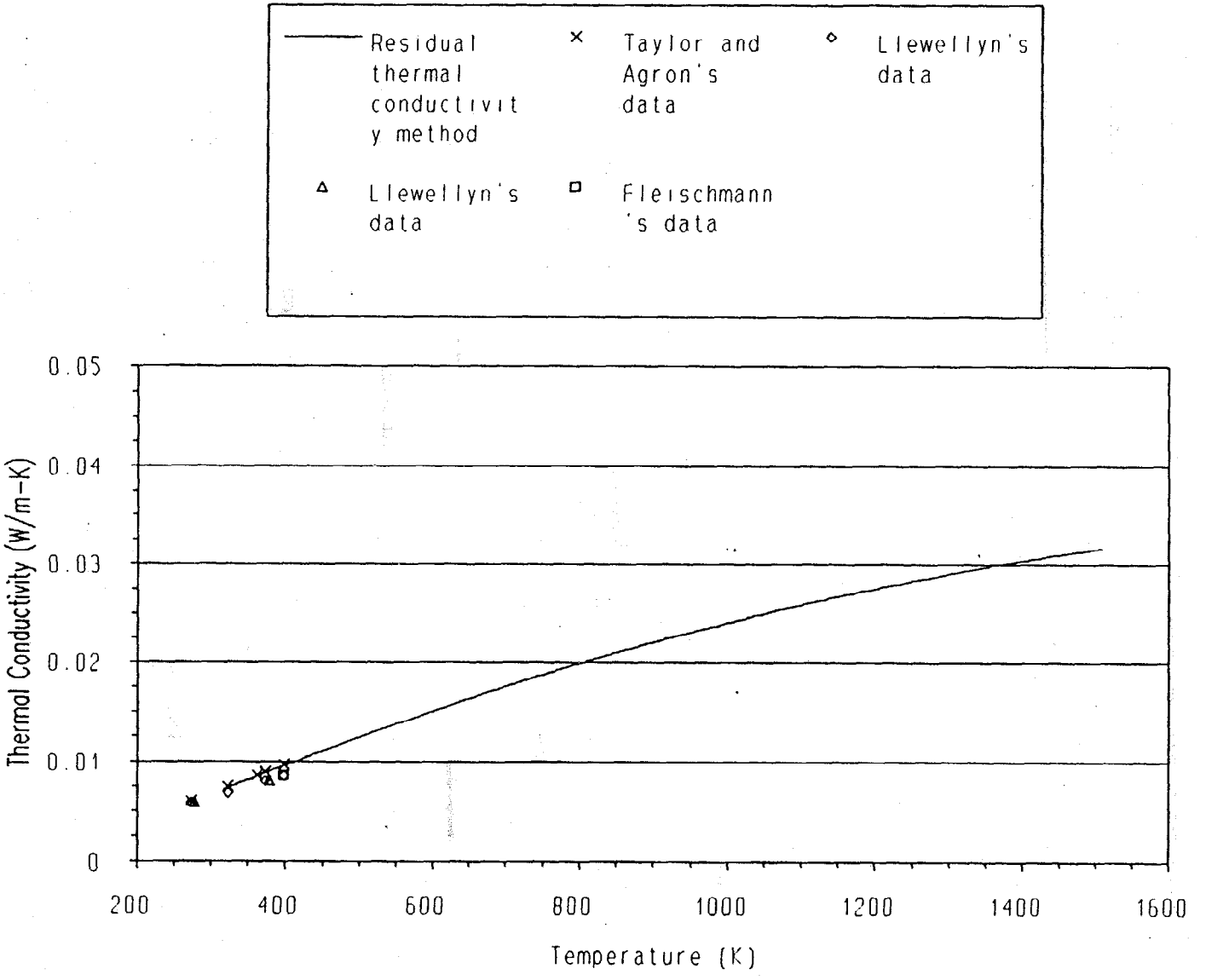

Fig. 10.3. Thermal conductivity of UF_6 vapor predicted by residual thermal conductivity method.

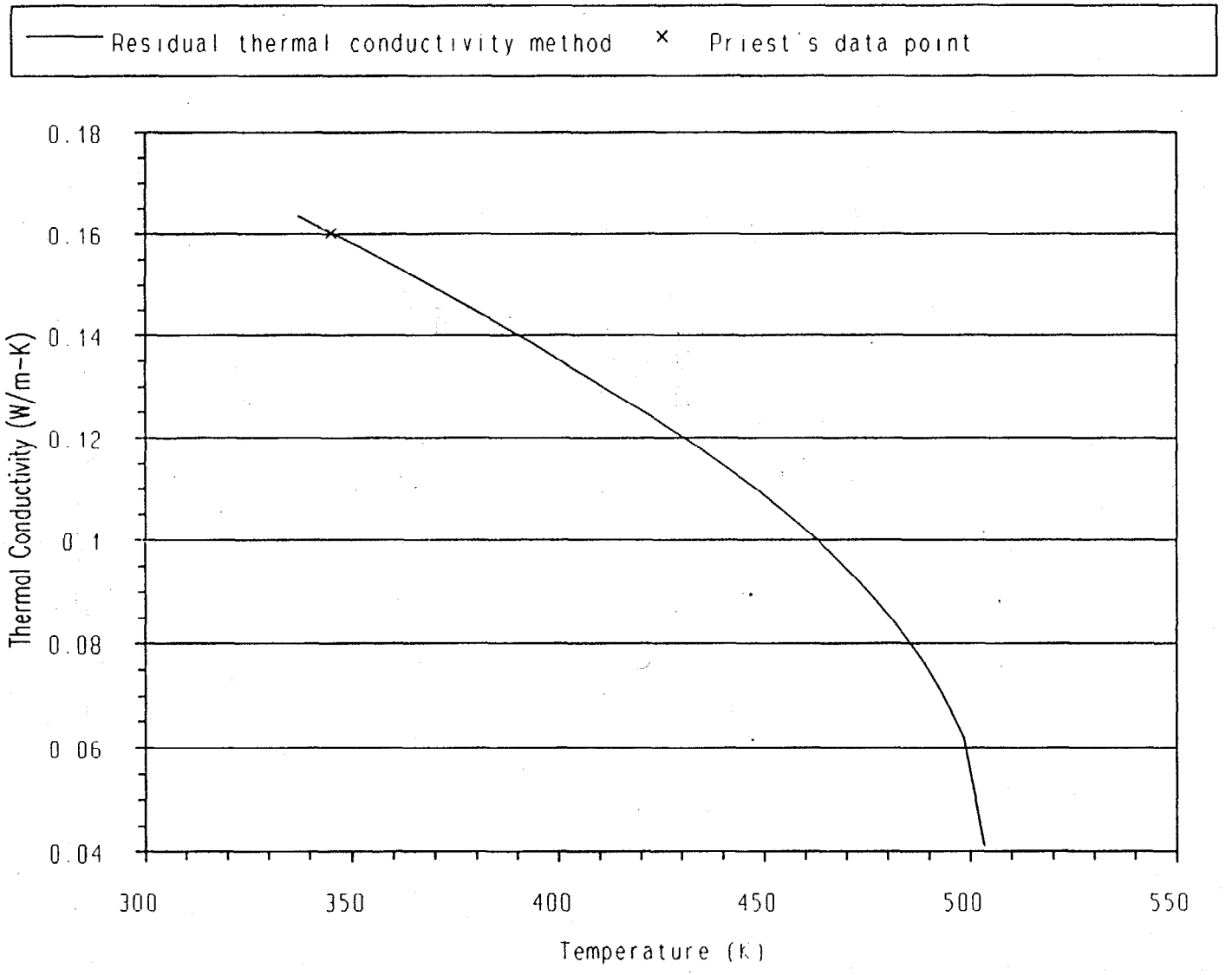

Fig. 10.4. Thermal conductivity of UF_6 liquid predicted by residual thermal conductivity method.

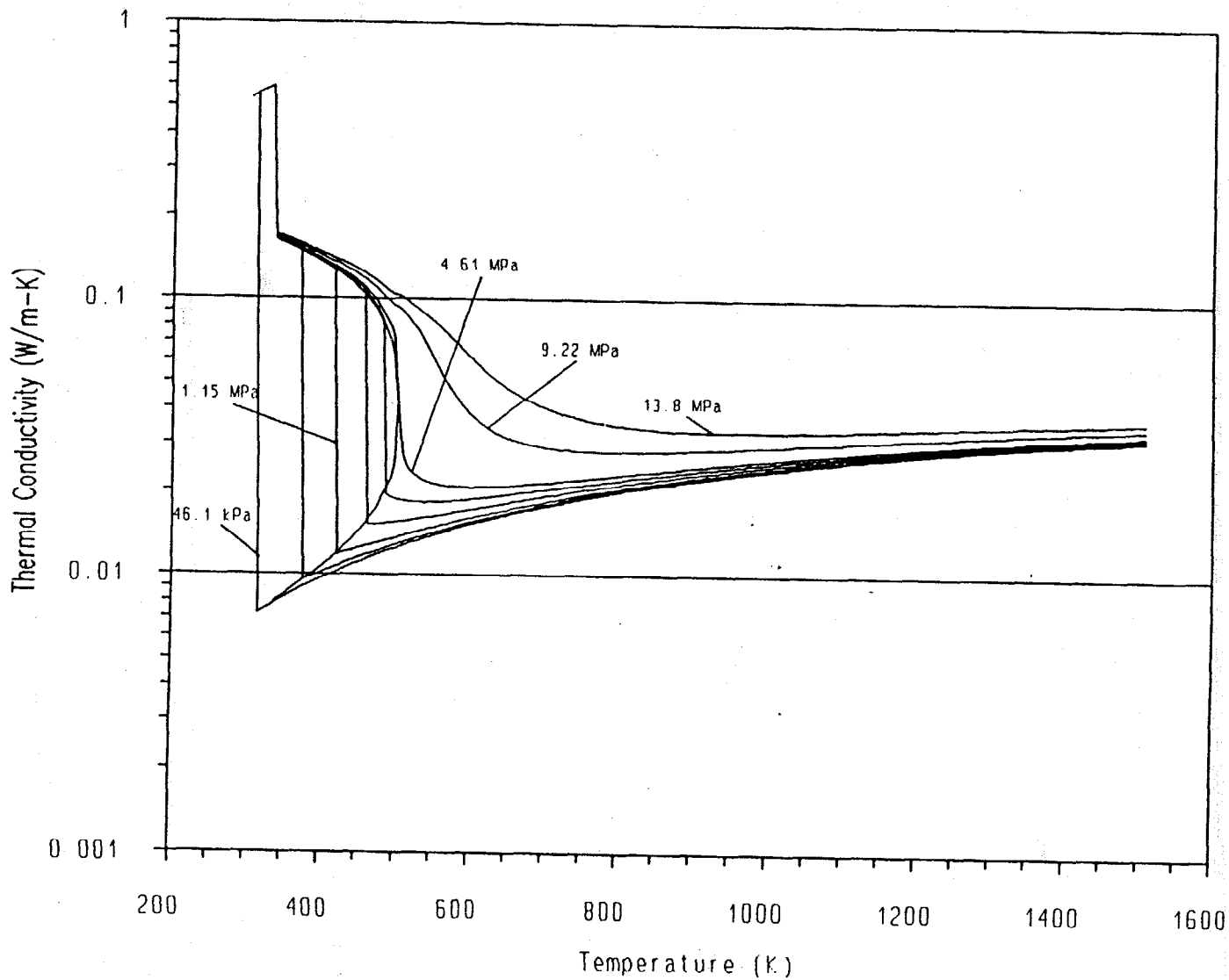

Fig. 10.5. Thermal conductivity of uranium hexafluoride.

11. ADDITIONAL THERMODYNAMIC PROPERTIES

Several additional thermodynamic properties of UF_6 can be derived from properties discussed in earlier chapters. These derived properties include the kinematic viscosity, Prandtl number, thermal diffusivity, and the coefficient of expansion.

11.1 KINEMATIC VISCOSITY

The kinematic viscosity (ν) is defined as

$$\nu = \frac{\mu}{\rho}, \tag{11.1}$$

where μ = dynamic viscosity,
ρ = density.

The kinematic viscosity of UF_6 vapor and liquid is shown graphically as a function of temperature and pressure in Fig. 11.1. The viscosity and density were calculated by the methods recommended in Sections 9.3 and 5.4, respectively.

11.2 PRANDTL NUMBER

The Prandtl number (Pr) is defined as

$$Pr = \frac{c_p \mu}{k}, \tag{11.2}$$

where c_p = specific heat,
k = thermal conductivity.

The Prandtl number of UF_6 vapor and liquid is shown graphically as a function of temperature and pressure in Fig. 11.2. The specific heat, viscosity, and thermal conductivity were calculated by the methods recommended in Sections 7.5, 9.3, and 10.5, respectively.

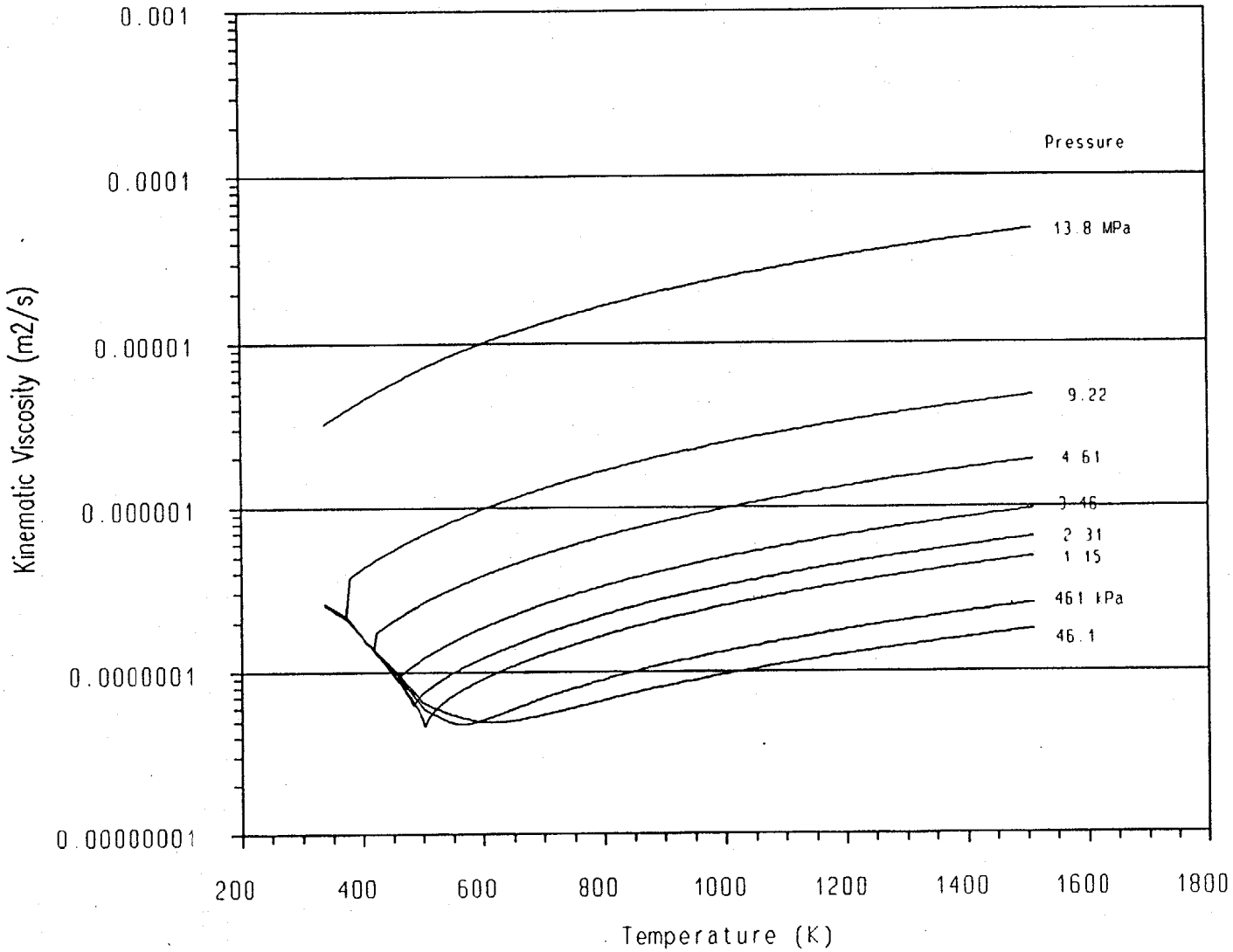

Fig. 11.1. Kinematic viscosity of uranium hexafluoride.

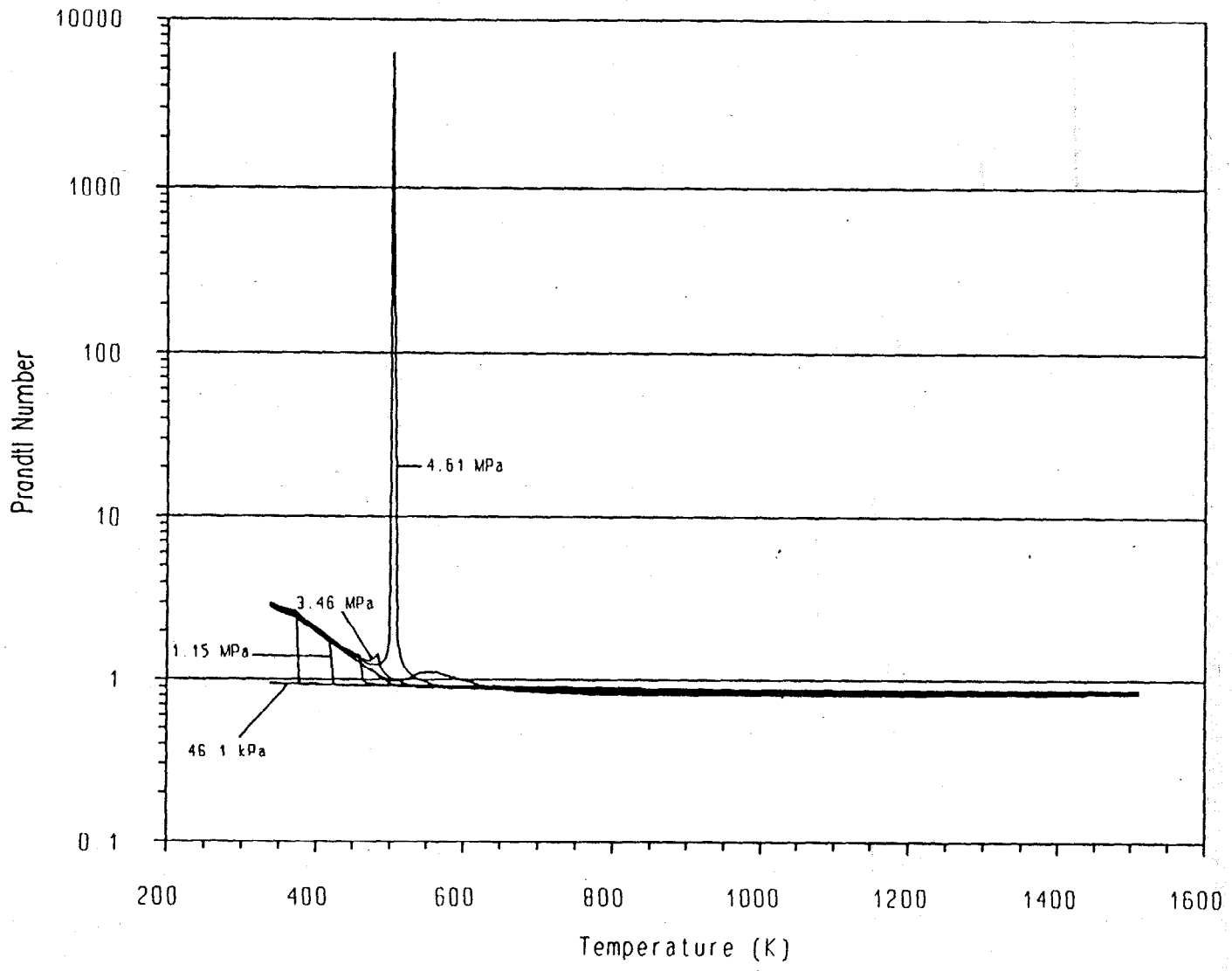

Fig. 11.2. Prandtl number of uranium hexafluoride.

11.3 THERMAL DIFFUSIVITY

The thermal diffusivity (α) is defined as

$$\alpha = \frac{k}{\rho c_p} . \tag{11.3}$$

The thermal diffusivity of UF_6 vapor and liquid is shown graphically as a function of temperature and pressure in Fig. 11.3. The thermal conductivity, density, and specific heat were calculated by the methods recommended in Sections 10.5, 5.4, and 7.5, respectively.

11.4 COEFFICIENT OF EXPANSION

The coefficient of expansion (β) is defined as

$$\beta = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_P , \tag{11.4}$$

where ρ = density,
T = temperature,
P = pressure.

11.4.1 Vapor Coefficient Of Expansion

The coefficient of expansion of UF_6 vapor (β_v) can be estimated as

$$\beta_v = -\frac{1}{\rho_{T,P}}\left[\frac{\rho_{T,P} - \rho_{T+\Delta T,P}}{T - (T+\Delta T)}\right] , \tag{11.5}$$

where $\rho_{T,P}$ = density evaluated at T,
T = absolute temperature,
$\rho_{T+\Delta T,P}$ = density evaluated at $T+\Delta T$,
ΔT = small temperature increment.

In determining the vapor coefficient of expansion, a small temperature increment is added to the reference temperature to ensure that the fluid is still in the vapor state. The coefficient of expansion of UF_6 vapor is shown in Fig. 11.4 as a function of temperature and pressure.

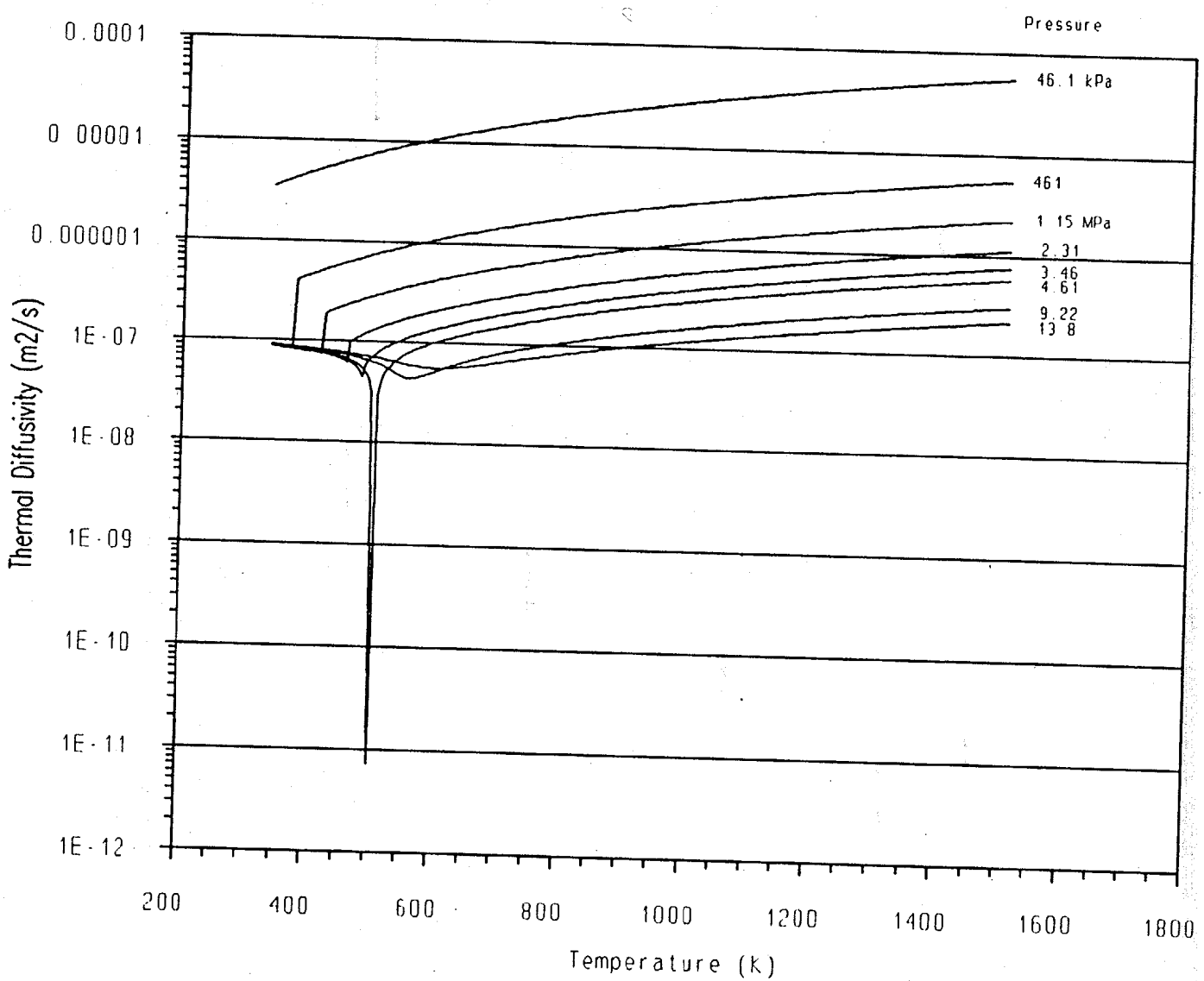

Fig. 11.3. Thermal diffusivity of uranium hexafluoride.

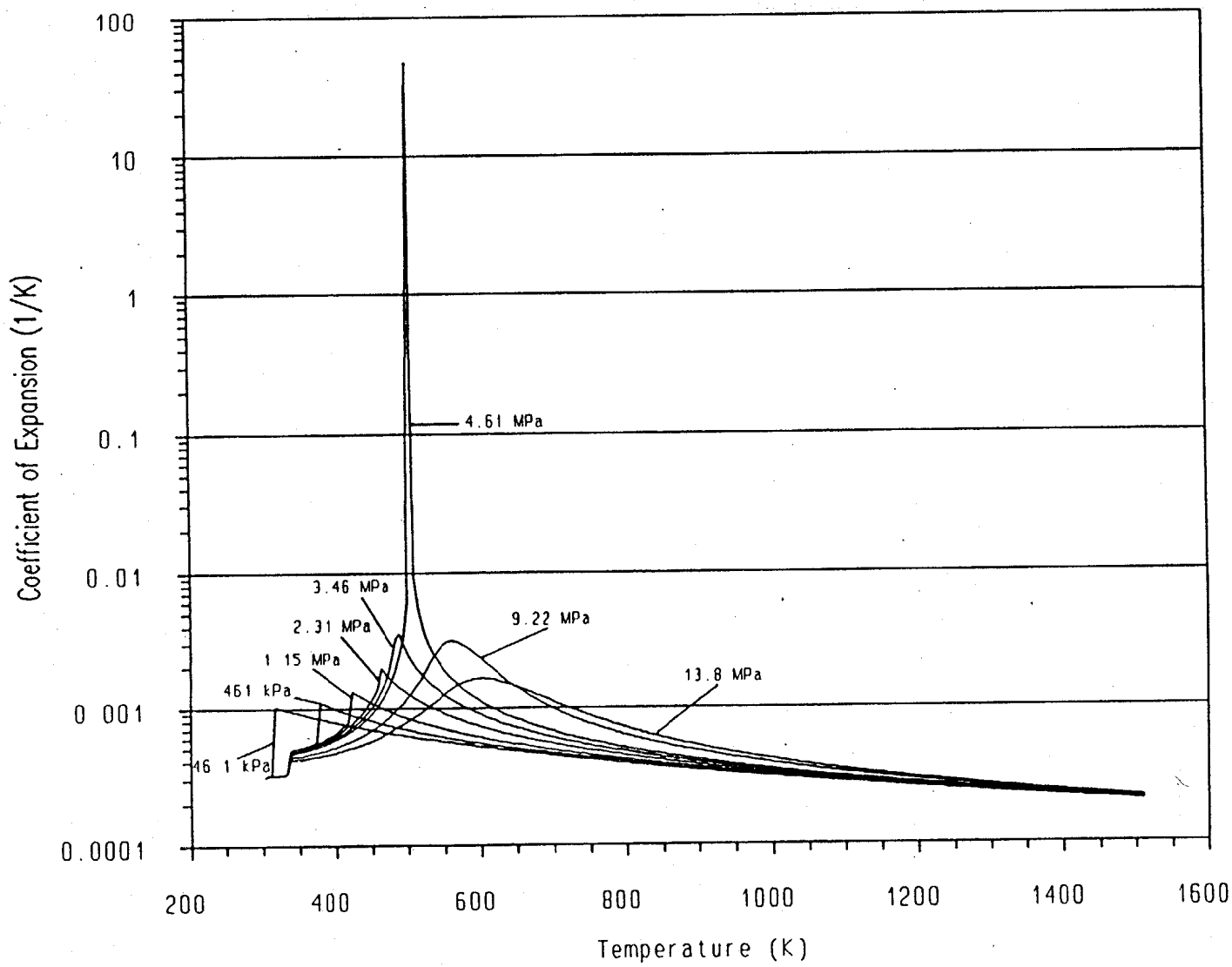

Fig. 11.4. Coefficient of expansion of uranium hexafluoride.

11.4.2 Liquid Coefficient Of Expansion

The coefficient of expansion of UF_6 liquid (β_l) can be estimated as

$$\beta_l = -\frac{1}{\rho_{T,P}}\left[\frac{\rho_{T,P} - \rho_{T-\Delta T,P}}{T - (T-\Delta T)}\right], \tag{11.6}$$

where $\rho_{T-\Delta T,P}$ = density evaluated at T-ΔT (kg/m^3).

In determining the liquid coefficient of expansion, a small temperature increment is subtracted from the reference temperature to ensure that the fluid is still in the liquid state. The coefficient of expansion of liquid UF_6 is shown in Fig. 11.4 as a function of temperature and pressure.

11.4.3 Solid Coefficient Of Expansion

The coefficient of expansion of UF_6 solid can be estimated as

$$\beta_s = \frac{5.190}{\rho_s}, \tag{11.7}$$

where β_s = solid coefficient of expansion (1/K),
ρ_s = solid density (kg/m^3).

Equation 11.7 was obtained by differentiating Eq. 5.44 and substituting the result into Eq. 11.4. The density of solid UF_6 can be determined using Eq. 5.44. The coefficient of expansion of solid UF_6 is shown in Fig. 11.4 as a function of temperature.

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APPENDIX A

Conversion Factors

Table A.1. Conversion Factors for Thermophysical Properties

Property	To convert from	to	multiply by	to	multiply by
Coefficient of Expansion	1/K	1/K	1.0	1/°R	1.8
Density	kg/m^3	g/cm^3	1.0E-03	lb_m/ft^3	6.2428E-02
Dynamic Viscosity	$N\text{-}s/m^2$ or kg/m-s	g/cm-s	1.0E+01	lb_m/ft-hr	2.4191E+03
Enthalpy	J/kg	cal/g	2.3885E-04	Btu/lb_m	4.2992E-04
Pressure	Pa or N/m^2	atm	9.8692E-06	psia	1.4504E-04
Heat Capacity	J/kg-K	cal/g-°C	2.3885E-04	Btu/lb_m-°F	2.3885E-04
Kinematic Viscosity	m^2/s	cm^2/s	1.0E+04	ft^2/hr	3.8750E+04
Specific Volume	m^3/kg	cm^3/g	1.0E+03	ft^3/lb_m	1.6018E+01
Surface Tension	N/m	g/s^2	1.0E+03	lb_f/ft	6.8522E-02
Thermal Conductivity	W/m-K or J/s-m-K	cal/s-cm-K	2.3901E-03	Btu/hr-ft-°F	5.7779E-01
Thermal Diffusivity	m^2/s	cm^2/s	1.0E+04	ft^2/hr	3.875E+04

Source : *ASTM Standard for Metric Practice*, E380-79, American Society for Testing and Materials, Philadelphia, PA, 1980.

APPENDIX B

Lee-Kesler Compressibility Correlation Solution Hints

Lee-Kesler Compressibility Correlation Solution Hints

As mentioned in Chapter 5, the Lee-Kesler compressibility correlation is implicit with respect to reduced volume. Therefore, in order to solve Eq. 5.21 for reduced volume, an iterative solution technique is required. One such technique which proved successful was the Reguli-Falsi method. This method requires solution of the following equation:

$$f(V_r) = 0 = \frac{-P_r V_r}{T_r} + 1 + \frac{B}{V_r} + \frac{C}{V_r^2} + \frac{D}{V_r^5} + \frac{c_4}{T_r^3 V_r^2}\left(\beta + \frac{\gamma}{V_r^2}\right)\exp\left(-\frac{\gamma}{V_r^2}\right). \tag{B.1}$$

The first step in solving Eq. B.1 is to obtain a fixed value of V_r, which we will call $V_{r,f}$. A first guess of reduced volume, $V_{r,g}$, is also required. Equation B.1 should be evaluated at both $V_{r,f}$ and $V_{r,g}$ to obtain the two values $f(V_{r,f})$ and $f(V_{r,g})$. A new guess for reduced volume is calculated as

$$V_r = V_{r,f} - f(V_{r,f})\left[\frac{V_{r,g} - V_{r,f}}{f(V_{r,g}) - f(V_{r,f})}\right]. \tag{B.2}$$

The new value of V_r calculated from Eq. B.2 is then substituted for $V_{r,g}$ in Eq. B.1 to obtain $f(V_{r,g})$. This procedure is repeated until convergence is obtained.

After thoroughly investigating the Lee-Kesler compressibility equation, it was discovered that the correlation has multiple roots (as many as three) for some combinations of temperature and pressure. Therefore, care must be taken in selecting values of the fixed point and first guess for the solution of accurate and reliable compressibilities. The following values which are in some cases functions of temperature were determined by a trial and error procedure and seem to produce reliable compressibility values.

If $P_r \leq 1.0$ and $T_r \leq T_{r,sat}$ (i.e., liquid),
$V_{r,f} = 0.185T_r - 0.035$,
$V_{r,g} = 0.1429T_r + 0.05714$.

If $P_r \leq 1.0$ and $T_r > T_{r,sat}$ (i.e., vapor),
$V_{r,f} = 55.0$,
$V_{r,g} = 54.0$.

If $P_r > 1.0$,
$V_{r,f} = 0.185T_r - 0.035$,
$V_{r,g} = 0.1429T_r + 0.05714$.

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